ACTIVITY-COMPOSITION RELATIONS IN $MnCr_2O_4$-$CoCr_2O_4$ SOLID SOLUTIONS AND STABILITIES OF $MnCr_2O_4$ AND $CoCr_2O_4$

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ABSTRACT

ACTIVITY-COMPOSITION RELATIONS IN $MnCr_2O_4$-$CoCr_2O_4$ SOLID SOLUTIONS AND STABILITIES OF $MnCr_2O_4$ AND $CoCr_2O_4$

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Activities of CoO were measured in the oxide and spinel solutions of the system MnO-CoO-Cr_2O_3 at 1300 °C with the aim of deriving information on the thermodynamic properties of spinel phases. Synthetic samples in selected phase assemblages of the system were equilibrated with a gas phase of known oxygen partial pressures at a total pressure of one atm. Activities of cobalt oxide along the MnO-CoO binary were also measured by emf the method.

The data on CoO activities and the directions of conjugation lines between coexisting oxide and spinel phases were used to establish the activity-composition relations in spinel solid solutions at 1300 °C. The $MnCr_2O_4$ - $CoCr_2O_4$ solid solutions exhibit positive deviation from ideality at this temperature.

The standard free energy of formation of $CoCr_2O_4$ from its components (CoO + Cr_2O_3) at 1300 °C was measured as -37,636 J/mole, and that

of $MnCr_2O_4$ was calculated as -42,278 J/mole. The activities determined in the stoichiometric spinel solid solutions were compared with those predicted from cation distribution models. The cation distribution in $CoCr_2O_4$ and $MnCr_2O_4$ were calculated by x-ray diffraction methods.

Keywords: Thermodynamics, Solid Solutions, Manganese, Cobalt, Chromites.

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ÖZ

$MnCr_2O_4$-$CoCr_2O_4$ KATI ÇÖZELTİLERİNDE AKTİVİTE-KOMPOZİSYON İLİŞKİLERİ , $MnCr_2O_4$ ve $CoCr_2O_4$'TIN KARARLILIKLARI

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MnO-CoO-Cr_2O_3 sistemindeki oksit ve spinel eriyiklerinde CoO aktiviteler 1300 °C de spinel fazlarının termodinamik özellikleri hakkında bilgi üretmek amacıyla ölçüldü. Sistemdeki faz bölgelerinden seçilen sentetik numuneler, 1 atmosferdeki oksijen kısmi basıncı bilinen gaz fazı ile dengeye getirildi. Aynı zamanda MnO-CoO çiftli sisteminde kobalt oksit aktiviteleri emf metodu ile ölçüldü.

Kobalt oksit aktiviteleri ile ilgili bilgiler, oksit ve spinel eriyikleri arasındaki denk faz bağ çizgilerinin yönleri, 1300 °C'de spinel katı çözeltisindeki aktivite-kompozisyon ilişkilerinin belirlenmesinde kullanıldı. $MnCr_2O_4$-$CoCr_2O_4$ katı çözeltileri bu sıcaklıkta pozitif sapma gösterir.

$CoCr_2O_4$ 'tin standard serbest oluşum enerjisi -37636 J/mol olarak ölçüldü ve $MnCr_2O_4$'tınki -42278 J/mol olarak hesaplandı. Stokiometrik spinel katı çözeltilerinden elde edilen aktiviteler katyon dağılım modellerinden belirlenenlerle

karşılaştırıldı. $CoCr_2O_4$ ve $MnCr_2O_4$' taki katyon dağılımı x-ışınları difraksiyon metodları ile hesaplandı.

Anahtar Kelimeler: Termodinamik, Katı Çözeltiler, Mangan, Kobalt, Kromit.

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LIST OF SYMBOLS

ΔG^o	Standard free energy change, J/mole
ΔG^m	Standard free energy of mixing, J/mole
a	Activity
γ	Activity coefficient
α	α - function
K	Equilibrium constant
N	Mole fraction
n	Number of moles
F	Faraday constant
E	Electromotive force, volt
log	Common logarithm
ln	Natural logarithm
P	Pressure, atm
T	Absolute temperature, K
θ	Diffraction angle, degree
u	Oxygen parameter
x	Degree of disorder

CHAPTER I

INTRODUCTION

Oxide phases having spinel structure attracted considerable research interest during the past fourty years owing to their importance in a variety of technological applications, particularly in the area of fine ceramics. The name spinel was assigned originally to the mineral $MgO.Al_2O_3$. This compound occurs in nature and it can be formed synthetically by reacting the individual oxides MgO and Al_2O_3 at elevated temperatures. The crystal structure of $MgO.Al_2O_3$ is determined to consist of a face centered cubic array of large oxygen ions having 64 tetrahedral and 32 octahedral interstitial sites which can be occupied by the smaller magnesium and aluminum cations in its unit cell. This spinel unit cell structure is shown schematically in Figure 1.

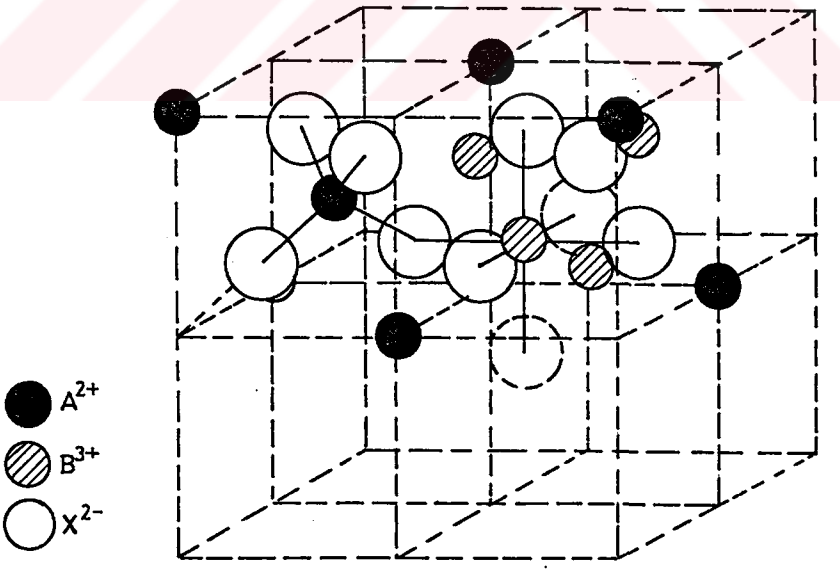


Figure 1. The Structure of Spinel Unit Cell with Alternating Tetrahedral (AO_4) and Octahedral [BO_6] Coordinated Units.

Studies on complex oxide systems revealed the existence of numerous oxide compounds and their solid solutions having the same crystal structure as the spinel mineral $MgO.Al_2O_3$. The general molecular formula for this large group of compounds can be written as $AO.B_2O_3$ or AB_2O_4 where A stands to designate the divalent cations like Mg^{++}, Ca^{++}, Fe^{++}, Ni^{++}, Mn^{++}, Zn^{++}, Co^{++}, and Cu^{++}. The B type cations in the structure are trivalent ; common examples are Al^{+++}, Fe^{+++}, Cr^{+++}, Mn^{+++}, and Ge^{+++}. Spinel compounds are generally named after their trivalent cation; hence, for example, if the B cation is aluminum the compound is called "aluminate", if B is iron the compound is called "ferrite", and when B is chromium the compound is called "chromite".

There are two extreme cases for the formation of the spinel structure. If all the divalent cations occupy the tetrahedral positions and all trivalent cations the octahedral positions of the spinel lattice the compound is termed "normal spinel". An "inverse spinel" is formed when the tetrahedral sites are occupied by half of the B ions while the A ions and the remaining half of the B ions go to occupy the octahedral sites. In order to show the site occupancies the molecular formula for a normal spinel is written as $(A)[B]_2O_4$ and the molecular formula for an inverse spinel is written as $(B)[AB]O_4$. The brackets (..) and [..] designate, respectively, the tetrahedral and octahedral positions.

Many of the actual spinels are between normal and inverse types, hence they are called "mixed" spinels. The molecular formula for a mixed spinel in which the A and B type cations occupy the tetrahedral and octahedral sites randomly is written as follows :

$$(A_{1-x}B_x)[A_xB_{2-x}]O_4$$

In this formula, the parameter "x" defines the distribution of cations in the spinel structure in terms of the fraction of tetrahedral sites that are occupied by B ions. This parameter is commonly called "the disorder parameter" or "the degree of inversion". The value for x is 0 for a normal spinel and 1 for an inverse spinel. A spinel with x=2/3 is known as a "random" one. The degree of inversion in a mixed spinel depends on the temperature and the partial pressure of oxygen of the gas phase at which the spinel is processed. The variations in "x" cause marked changes in thermochemical, electronic, and magnetic properties of the spinel ceramics.

Various kinds of spinels have found wide technological applications. For example, spinel aluminates are important in the production of high-temperature cements. Spinel ferrites occupy a central position in electronic and magnetic ceramics; ferrites of Zn, Mn, Mg, and Ni are used extensively as soft magnets in the production of computer memory chips, indicator cores, recording heads, and millimetric wave control devices. The spinel chromites are receiving increased interest due to their use in making ceramic sensors for gas and moisture detection and monitoring; typical examples are porous $MgCr_2O_4$ ceramics for toxic gas detection and $MgCr_2O_4$-TiO_2 ceramics for moisture [1,2]. The spinel type solid solutions that are formed from Ni, Mn, Co, and Cu oxides have excellent thermal and electrical stability, hence these are used for making a variety of ceramics like NTC type thermistors, heat flow monitors, vacuum and pressure gages, dc-ac converters, and voltage regulators [3].

As mentioned above, the actual spinels encountered in technological ceramics are of mixed type in which the cations distribution parameter "x" controls many of physical and thermal properties. Hence, tailoring the properties of spinel ceramics is, in essence, tailoring the cation distribution. In this regard, studies

directed towards the understanding of spinel formation and cation distribution contribute a great deal to the basic science and technology for production of such ceramics. High temperature thermochemical studies on oxide systems containing spinel phases serve to generate basic information which can be used quite effectively for process design and control during the manufacture of spinel ceramics.

The intelligent processings of spinel ceramics require a thorough knowledge of equilibrium relations at subsolidus temperatures between all possible phases in the oxide system of the spinel under consideration. The present study was undertaken in order to establish these relations in the system MnO-CoO-Cr_2O_3 at 1300°C. The temperature selected is typical for firing spinel ceramics. At this temperature the system is characterized by two distinct series of solid solutions as illustrated in Figure 2. MnO and CoO are each with the simple cubic structure; they form an unbroken series of solid solutions at the base of the MnO-CoO-Cr_2O_3 composition triangle. Along the binaries MnO-Cr_2O_3 and CoO-Cr_2O_3 the spinel compounds $MnO.Cr_2O_3$ - $CoO.Cr_2O_3$ form, respectively. These spinels are miscible in all proportions, hence the second continuous solid solution series in the main ternary is formed among the spinels. The dashed curves drawn above and below the $CoO.Cr_2O_3$ and $MnO.Cr_2O_3$ join represent possible deviations from stoichiometry in the spinel solutions.

The specific objectives of the present work were set as follows:

1) Measurement of the thermodynamic activities of CoO in selected phases and phase assemblages in the ternary system.

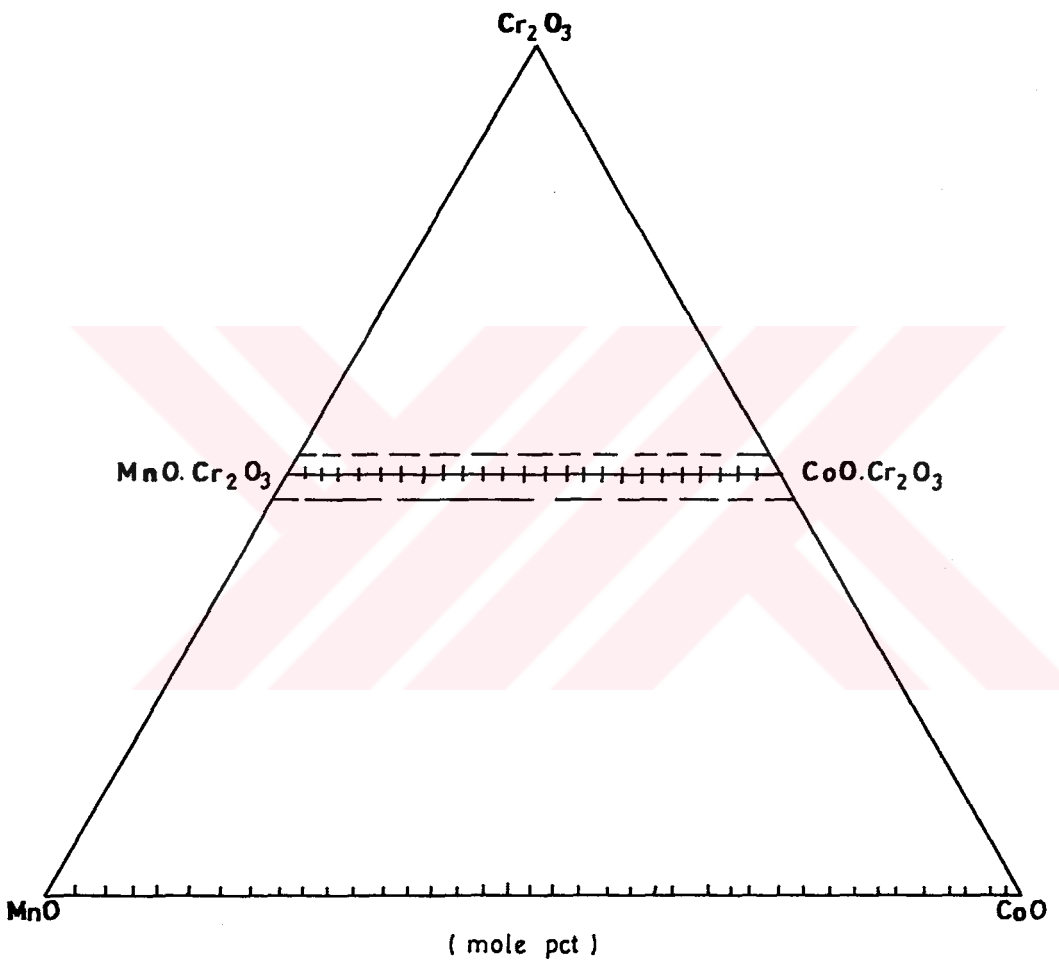


Figure 2. The Solid Solution Series MnO - CoO and $MnCr_2O_4$ - $CoCr_2O_4$ in the MnO-CoO-Cr_2O_3 System.

2) Determination of compositions of conjugate oxide and spinel solid solutions by establishing the directions of conjugation lines between these two phases.

3) Determination of the stability of the compound $CoO.Cr_2O_3$.

4) Derivation of the activity-composition relations in spinel solutions and information on the stability of the compound $MnO.Cr_2O_3$.

5) Determination of the degree of disorder in the stoichiometric end member spinels and use this for the development of thermochemical model for spinel solutions.

The thermochemical studies to meet objectives were based upon the methods of gas equilibrations, emf measurements using solid oxide cells, and XRD work.

CHAPTER II

PREVIOUS WORK

Prior to this work, a complete thermodynamic study on the MnO-CoO-Cr_2O_3 system was not conducted at 1300 °C. However, parts of the system have been the subject of numerous studies. The information hitherto gathered in these earlier investigations are presented in the following.

2.1. The Manganese - Oxygen System

Phase relations in the manganese-oxygen system were determined by Phillips and Muan [4] as a function of temperature and the partial pressure of oxygen in the coexisting gas phase. The phase diagram resulting from their work is shown in Figure 3, enlarged within the composition interval Mn-Mn_2O_3. The solid lines in the diagram are phase boundaries and the dashed lines represent the oxygen partial pressures in equilibrium with condensed phases.

The compound MnO, which carries importance for this work, is completely stoichiometric under reducing conditions. The partial pressure of oxygen for Mn-MnO equilibrium at 1300 °C is $1.45*10^{-18}$ atm [5]; when the oxygen partial pressure is lower than this value MnO will turn completely into metallic Mn. On the higher side of the Mn-MnO equilibrium partial pressure, MnO appears to be

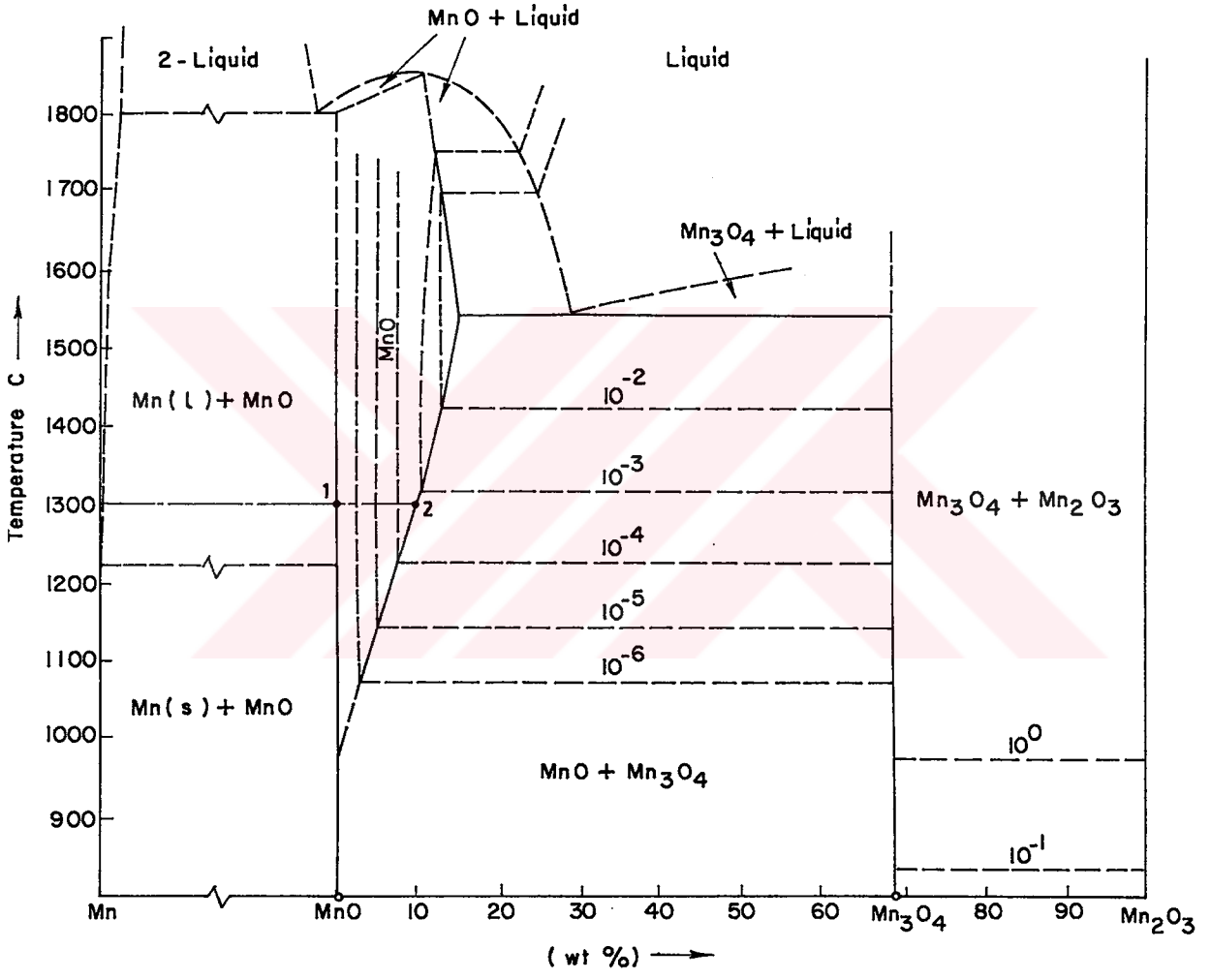


Figure 3. The Phase Diagram for the System Mn-O between Mn and Mn_2O_3 compositions. After Phillips and Muan [4].

nonstoichiometric with considerable excess of oxygen over the stoichiometric composition particularly at temperatures above 1000 °C. At a given temperature, the amount of excess oxygen that can be accommodated in the cubic MnO lattice increases with increasing oxygen partial pressure. Thus, at 1300 °C, it is possible to prepare MnO of variable compositions ranging from point "1" to point "2" by manipulating the oxygen potential of the gas phase.

2.2 Cobalt - Oxygen System

Phase relations in the cobalt-oxygen system are not known in any detail. However, the oxides Co_3O_4 and CoO are known to exist [6] . From these two oxides Co_3O_4 is stable in air only up to 950 °C; when heated above this temperature it is converted into CoO. Thus, for the purposes of this study the only stable oxide of cobalt can be considered as CoO.

The conditions for thermodynamic equilibrium between metallic cobalt and CoO has been studied by several investigators [7-10] using either gas equilibration or emf techniques. The equilibrium is represented by the following reaction:

$$Co + \frac{1}{2}O_2 \Leftrightarrow CoO \qquad (1)$$

Aukrust and Muan [7] used well-metered mixtures of CO and CO_2 gases in order to establish the equilibrium partial pressures of oxygen for the

coexistence of Co and CoO in the temperature interval 1006 to 1655 °C. Their data could be expressed by the following analytical equation :

$$\log P_{O_2}\,(\text{atm}) = 7.600 - 25000 * \frac{1}{T} \qquad (2)$$

where T is in K. Jacob and Pandit [8] used the same gas equilibration technique and obtained the following relationship:

$$\log P_{O_2}\,(\text{atm}) = 7.427 - 24500 * \frac{1}{T} \qquad (3)$$

There are two separate investigations of Co - CoO equilibrium based on emf measurements using calcia stabilized zirconia (CSZ) solid electrolytes. The first of these belongs to Tretjakow and Schmalzried [9] with the following cell configuration:

$$\text{Pt, Co+CoO} \mid \text{CSZ} \mid \text{Air, Pt} \qquad (4)$$

This was essentially a concentration cell with air(P_{O_2} = 0.21 atm) serving as the reference electrode. The cell was operated in the temperature range of 727 °C to 1227 °C. When the emf data obtained from the cell were converted into oxygen partial pressures the temperature dependence would be as follows:

$$\log P_{O_2}\,(\text{atm}) = 8.136 - 25180 * \frac{1}{T} \qquad (5)$$

The experimental data obtained in gas equilibration measurements by Aukrust and Muan [7] and by Jacob and Pandit [8] are shown in the form of $\log P_{O_2}$ versus 1/T plots in Figure 4. The emf data of Tretjakow and Schmalzried are also shown in the same figure by open circles. It can be observed that while the data from the two separate gas equilibration experiments are in reasonable agreement the emf work of Tretjakow and Schmalzried [9] gives considerably higher oxygen partial pressures. It should be pointed out that the emf cell configuration described by Eqn.(4) is amenable to polarization due to the large differences in the concentrations at the reference and the unknown compartments of the cell. Hence the data expressed by Eqn.(5) may be quite unreliable.

Recently, Hugh and O'Neill [10] made careful emf measurements on the Co-CoO equilibrium by using the following cell configurations:

$$\text{Pt, Co+CoO} \mid \text{CSZ} \mid \text{Ni+NiO, Pt} \qquad (6)$$

$$\text{Pt, Co+CoO} \mid \text{CSZ} \mid \text{Fe+FeO, Pt} \qquad (7)$$

The emf data obtained from these two types of cells would yield the following relationship in the temperature interval 527 °C to 1124 °C:

$$\log P_{O_2} = -\frac{25683}{T} + 26.565 - 6.40916 \log T + 1.31536 * 10^{-3} T \qquad (8)$$

The data of Hugh and O'Neill [10] are shown with bold triangles in Figure 4. The agreement with gas equilibration data is remarkable due to the fact that the effects of concentration polarization were eliminated.

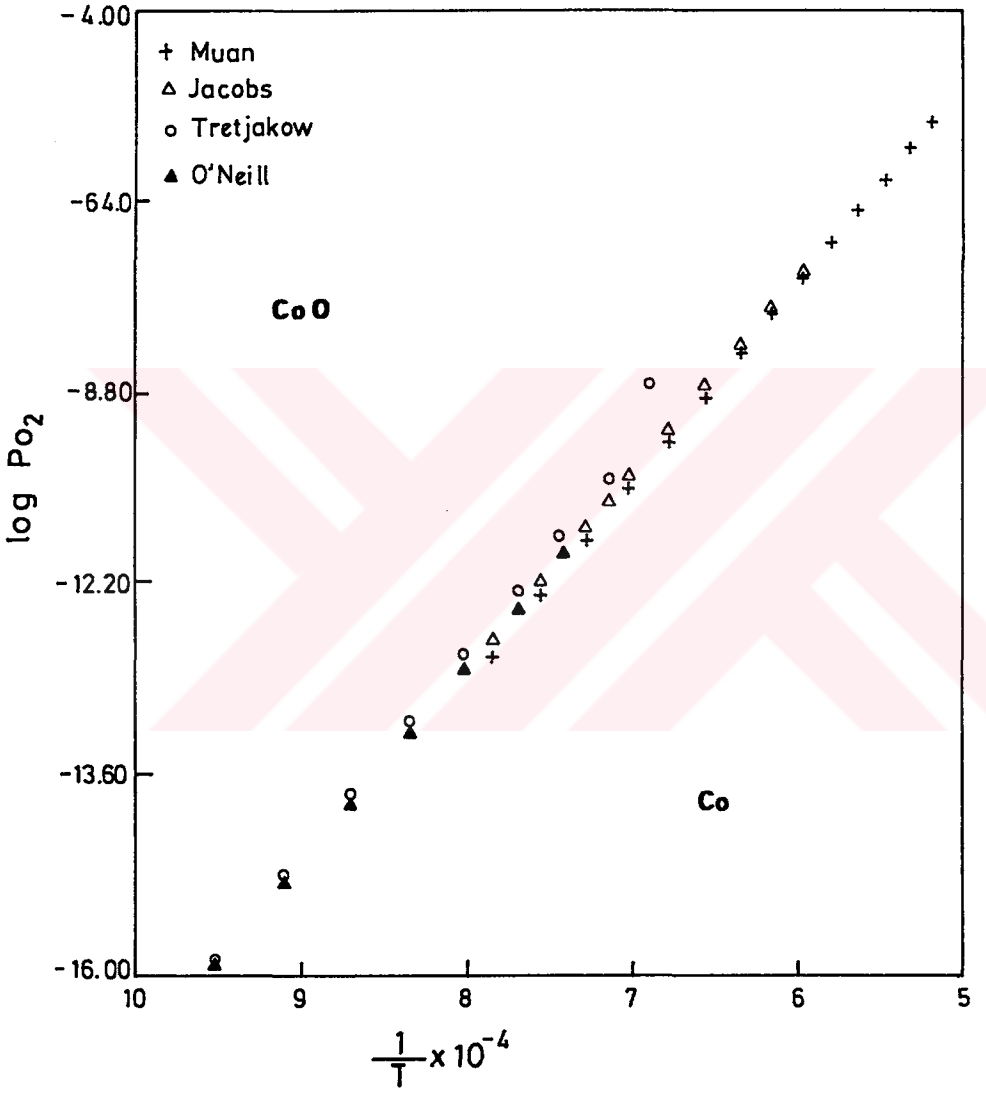


Figure 4. Stabilities of the Phases Co and CoO as a Function of Oxygen Partial Pressure and Temperature. (inverse K scale).

At the temperature of present investigation (1300 °C) the partial pressure of oxygen for the coexistence of Co and CoO in accordance with Eqn.(1) is $10^{-8.2932}$ from Aukrust and Muan [7], $10^{-8.1567}$ from Jacob and Pandit [8] and $10^{-8.1814}$ from Hugh and O'Neill [10]. These values correspond to the situation when both Co and CoO are in their pure states. When, for example, CoO occurs in a solid solution phase then the equilibrium between metallic cobalt and CoO in the oxide solution will be established at lower oxygen partial pressures, in accordance with the equilibrium constant of Eqn.(1).

2.3. The System MnO - CoO

The system MnO-CoO is part of the main Mn-Co-O ternary under reducing conditions. The phase relations in the Mn-Co-O ternary were studied by Aukrust and Muan [11] in the presence of an oxidizing atmosphere and a diagram in the form of Co_3O_4 - Mn_3O_4 is available. In contrast, since no experimental work has hitherto been carried under reducing conditions the phase relations in the MnO-CoO system still remain to be determined.

Bergman and Augren [12] carried a critical assessment on the thermochemical data available in literature on members of the MnO-CoO binary. Their work permitted them to calculate the phase diagram by means of a computer program developed by Jansson [13] and plot the model as shown in Figure 5. The simulated diagram predicts a miscibility gap in the solid state at very low temperatures but complete mutual solubility of MnO and CoO in each other at

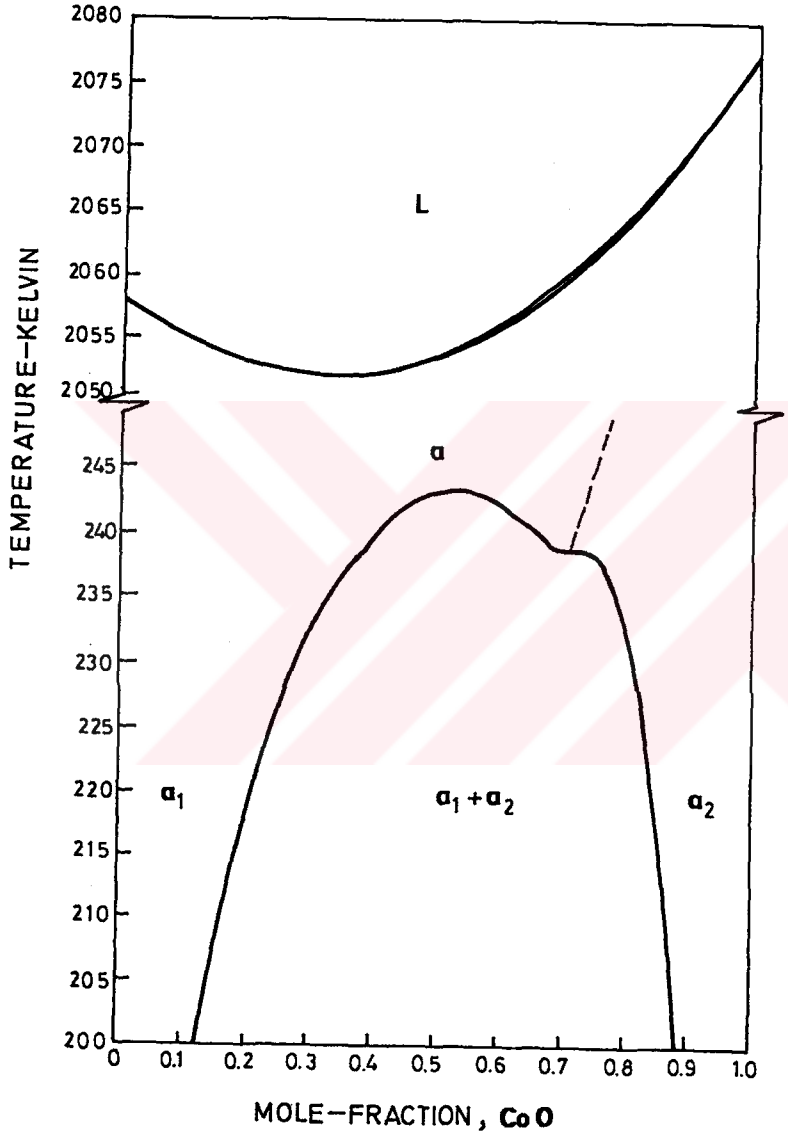


Figure 5. Phase Diagram Model for the System MnO-CoO, after Bergman and Agren [12].

room temperature. The MnO-CoO solid solutions have sodium chloride structure and remain stable at temperatures up to 1780 °C.

Thermodynamics of the MnO-CoO solid solutions were tackled first by Aukrust and Muan [7] in 1963. Their preliminary work conducted at 1200 °C, by using thermogravimetric methods were quite inconclusive. Evans and Muan [14] repeated the work in a more careful manner by equilibrating members of the solution series with CO + CO_2 gas mixtures. This study, conducted at 1250 °C, revealed that MnO-CoO solid solutions exhibit slight positive deviations from ideality as shown open by circle in the activity-composition plot of Figure 6.

Catlow et al. [15], and later, Paulson [16] determined the activities in MnO- CoO solid solutions by emf methods using solid electrolytes. The cell configuration of Catlow et al. [15] was:

$$\text{Pt, Fe+"FeO"} \mid \text{CSZ} \mid \text{Co} + (\text{Mn,Co})\text{O}_{ss}, \text{Pt} \qquad (9)$$

where "FeO" is wustite in equilibrium with metallic iron, and $(Mn,Ni)O_{ss}$ is the MnO - NiO solid solution of known composition in the cell. With this cell, Catlow et al [15] could perform emf measurements in the temperature interval 650 to 1250 °C. Above 1250 °C, irreducibly falling emf's were obtained due to a reaction between cell components. The emf results of Catlow et al. [15], converted into CoO activities at 1250 °C are shown with bold circles in Figure 6.

Most recent study on the thermodynamics of MnO - CoO solid solutions is that due to Paulsson [16]. His cell emf set-up was:

Pt, Co+CoO | CSZ | Co+(Mn,Co)Oss, Pt (10)

The emf data of Paulsson [16] were taken in the temperature range 627 to 1177 °C. His results, converted to CoO activities by extrapolation to 1250 °C are shown in Figure 6 by open squares.

When Figure 6 is examined, the activities of CoO measured in MnO-CoO solid solutions by both of the emf methods mentioned above also show slight positive deviations from ideality. The deviation is less pronounced as compared to the data given by Evans and Muan [14].

2.4. The Systems $MnO-Cr_2O_3$ and $CoO-Cr_2O_3$

Phase diagrams for the systems $MnO-Cr_2O_3$ and $CoO-Cr_2O_3$ are not known. Previous studies on these systems were confined mainly to the determination of the stabilities of the spinel compounds $MnCr_2O_4$ and $CoCr_2O_4$. Various such studies revealed that the terminal solubilities of MnO and CoO in Cr_2O_3 were negligible. Similarly, both MnO and CoO would dissolve negligible amounts of Cr_2O_3 at temperatures up to 1500 °C.

The standard free energy of formation of $CoCr_2O_4$ were determined in several separate investigations using either the emf methods or the gas equilibration techniques. The reaction for the formation of $CoCr_2O_4$ from CoO and Cr_2O_3 can be described as follows:

$$CoO + Cr_2O_3 = CoCr_2O_4 \quad (11)$$

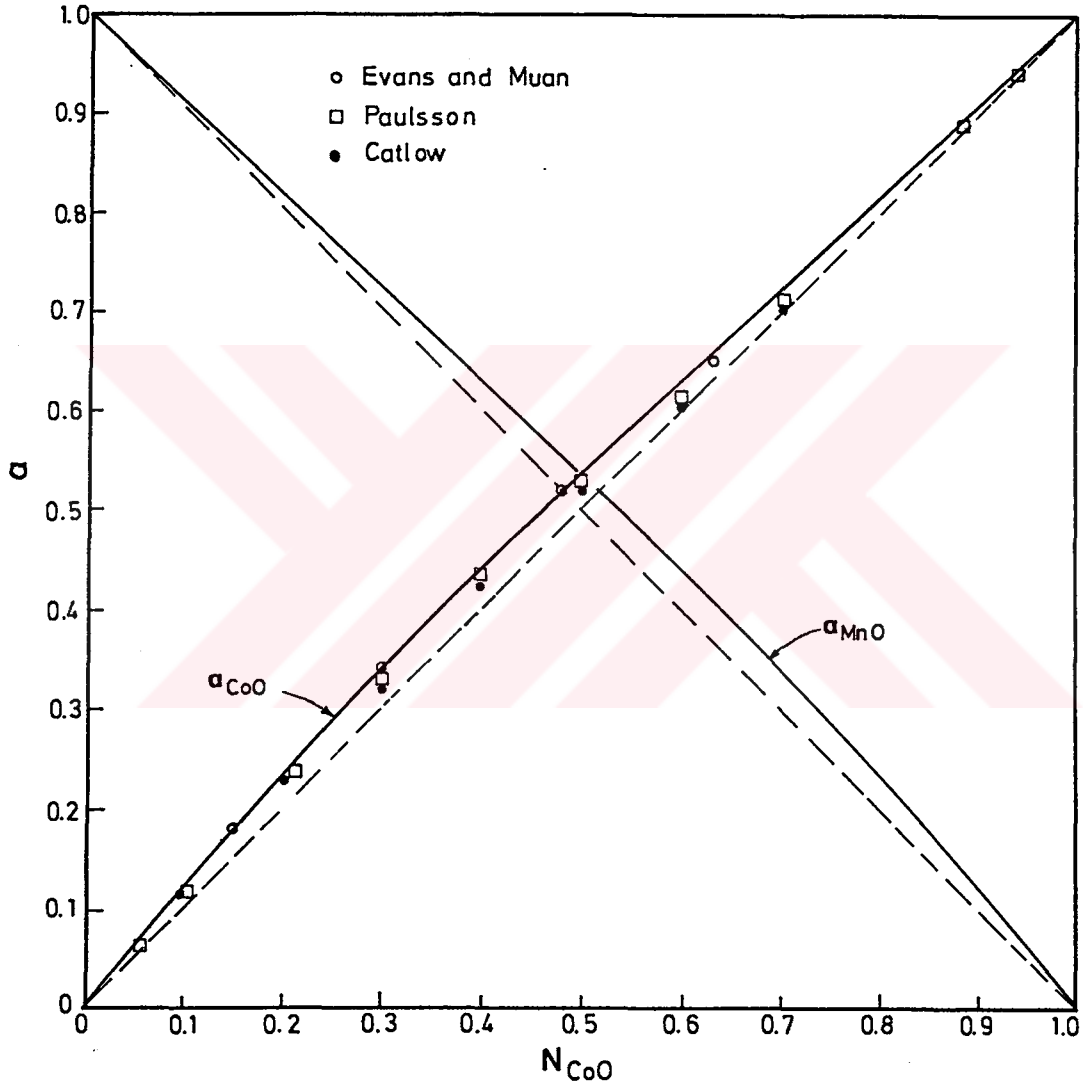


Figure 6. Activity-Composition Relations in the System MnO-CoO at 1250 °C, as Determined by the Present Investigations.

Kunnmann, Rogers, and Wold [17] were the starters to measure the standard free energy change associated with the above reaction in the temperature interval 800 to 1100 °C. Their work was based upon equilibrating mixtures of $CoCr_2O_4$ and Cr_2O_3 with CO_2 + CO gas atmospheres and determining the critical CO_2/CO ratio at which metallic cobalt would start to form in the solid phase assemblage. The results of this preliminary work could be expressed by the following equation :

$$\Delta G^{o}_{CoCr_2O_4} = -121.743 + 0.0625 \cdot T \quad kJ / mole \tag{12}$$

where $\Delta G^{o}_{CoCr_2O_4}$ stands to designate the standard free energy of formation of $CoCr_2O_4$ from its oxide components, CoO and Cr_2O_3.

Aukrust and Muan [18] made a spot determination of $\Delta G^{o}_{CoCr_2O_4}$, again by gas equilibration, and obtained a value of -46.82 ± 2.51 kJ/mole at 1350 °C. The same was done by Jacob and Fitzner [19] , their value for $\Delta G^{o}_{CoCr_2O_4}$ was - 49.79 kJ/mole at 1100 °C.

The reaction given in Eqn.(11) was studied by Tretjakow and Schmalzried [9] in temperature range 727 to 1227 °C, using the following emf cells:

$$Pt,\ Co+Cr_2O_3+CoCr_2O_4 \mid CSZ \mid Air(P_{O_2}=0.21\ atm.),\ Pt \tag{13}$$

$$Pt,\ Cr+CoO+CoCr_2O_4 \mid CSZ \mid Air(P_{O_2}=0.21\ atm.),\ Pt \tag{14}$$

Their emf results yielded the following expression for $\Delta G^{o}_{CoCr_2O_4}$ as a function of temperature:

$$\Delta G^{o}_{CoCr_2O_4} = -80.925 + 2.412*10^{-2}\,T \ \text{kJ / mole} \qquad (15)$$

Kubaschewski [20] made a thorough survey of data on $\Delta G^{o}_{CoCr_2O_4}$ and suggested the following equation as the best fit for the temperature range 727 to 1376 °C.

$$\Delta G^{o}_{CoCr_2O_4} = -59.356 + 8.36T \ \text{kJ / mole} \qquad (16)$$

The data available on the standard free energy of formation of $CoCr_2O_4$ from the sources mentioned above are shown graphically in Figure 7. Spot determination made by Aukrust and Muan [18] looks to lie close to the line drawn from Kubaschewski's suggestion. Tretjakow and Schmalzried's [9] emf measurements might have suffered from the polarization effects mentioned earlier, hence their results are quite different from those of others. The earliest data provided by Kunmann, Rogers, and Wold [17] seem to be in gross conflict with later determinations owing, probably, to the data then available to them on the free energy of formation of CoO which has seen several modifications later on. The discrepancies on $\Delta G^{o}_{CoCr_2O_4}$ values shown in Figure 7 is evidence for the need of better determinations on this quantity.

In contrast to the abundance of data on $\Delta G^{o}_{CoCr_2O_4}$, the stability of $MnCr_2O_4$ remained virtually unknown until Jacob and Fitzner [19] made an estimate for $\Delta G^{o}_{MnCr_2O_4}$ from their work on the spinel-oxide equilibria in the MnO-CoO-Cr_2O_3 system at 1100 °C. The value for $\Delta G^{o}_{MnCr_2O_4}$ suggested by Jacob and Fitzner [19] at this temperature is -59.065 kJ/mole which represents the

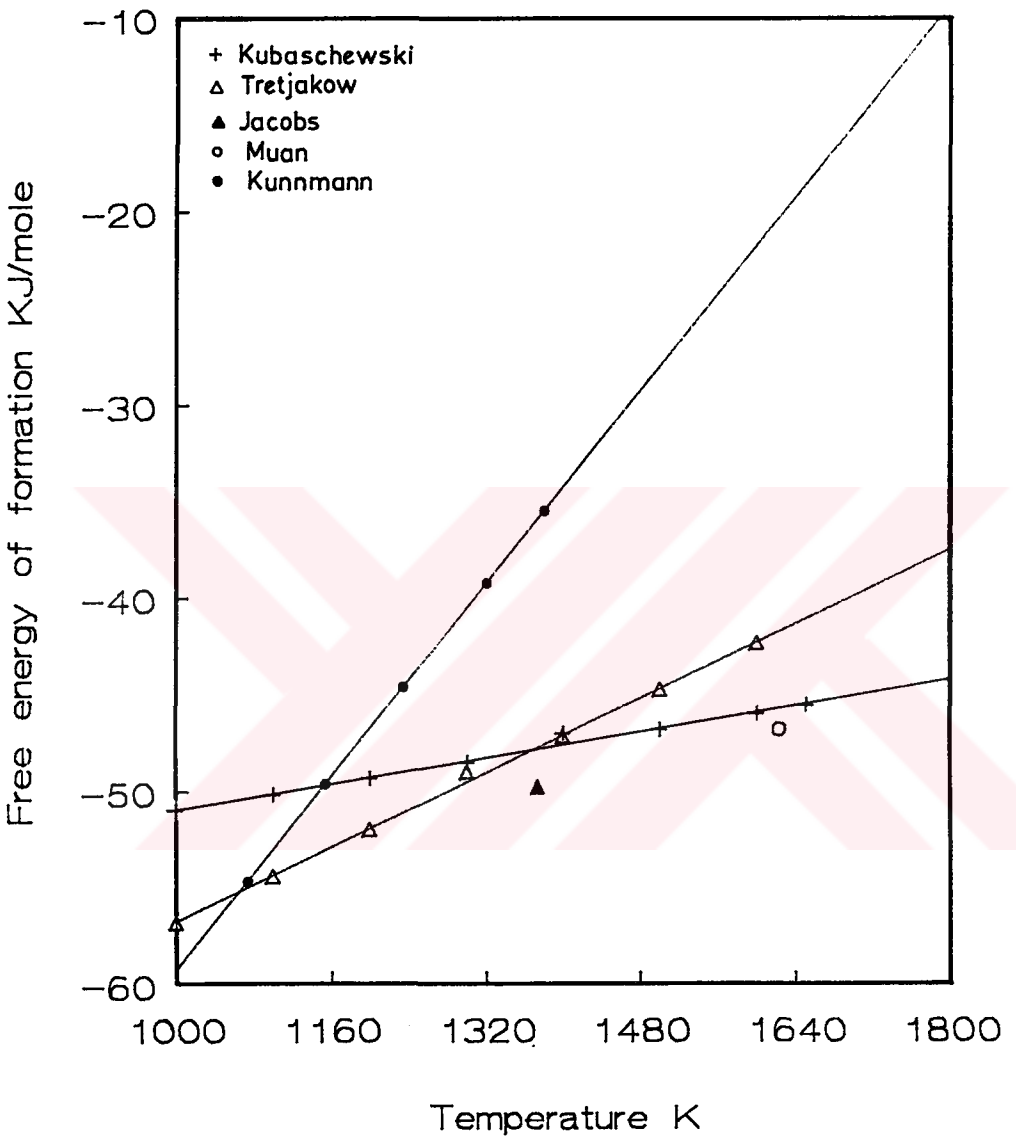


Figure 7. The Standard Free Energy of Formation of $CoO.Cr_2O_3$ from CoO and Cr_2O_3. (See text for the equations.)

standard free energy of formation of $MnCr_2O_4$ spinel from its oxide components, MnO and Cr_2O_3.

The directions of conjugation lines between coexisting spinel and oxide solid solutions of the MnO-CoO-Cr_2O_3 system, determined by Jacob and Fitzner [19] at 1100 °C are shown in Figure 8. This diagram precludes the existence of non-stoichiometry in the spinel solution series towards the MnO- CoO join. Therefore, the thermodynamic treatment of the conjugation data, performed by these authors, and hence the value estimated for $\Delta G^{o}_{MnCr_2O_4}$ should be invalid.

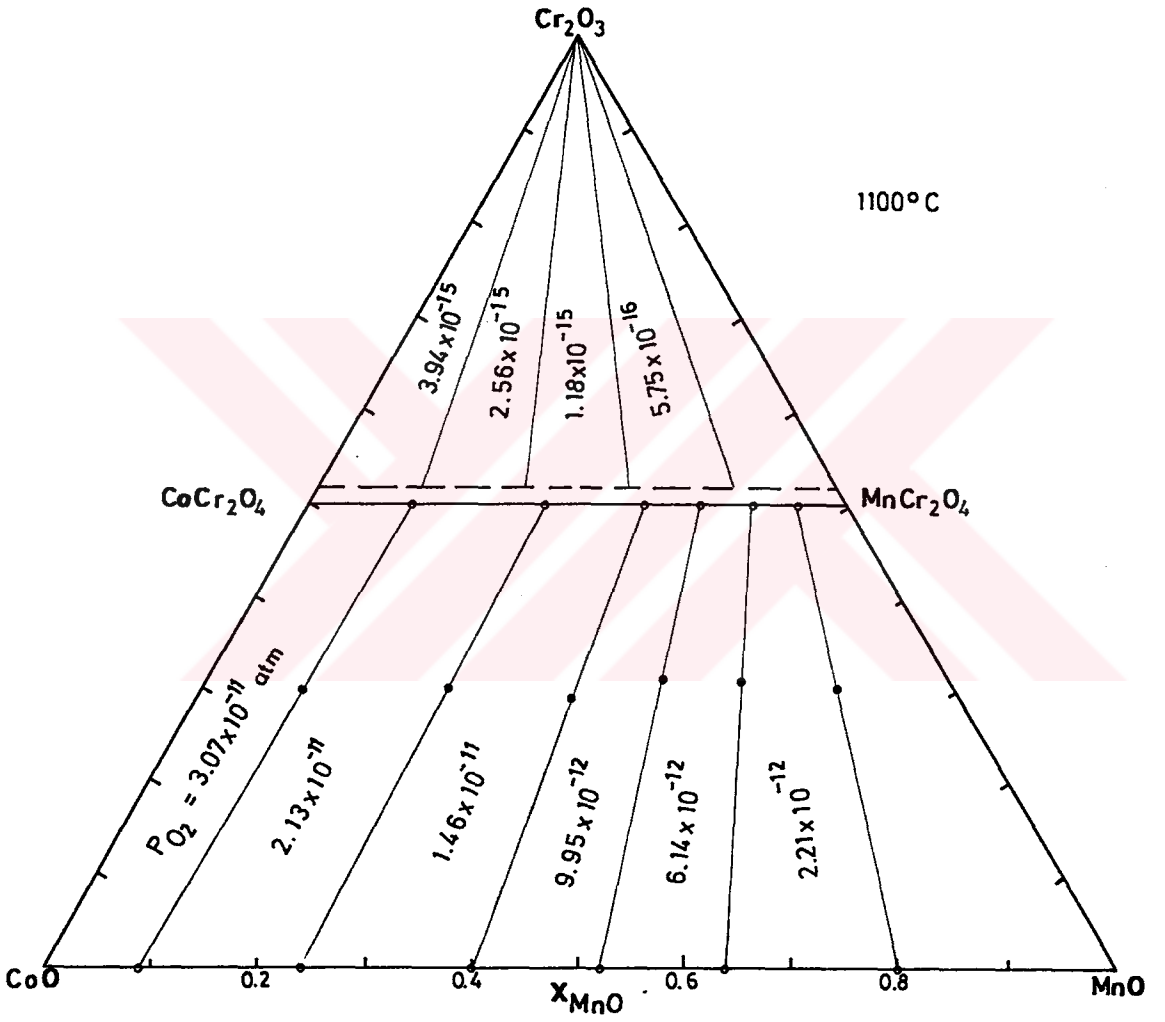


Figure 8. Composition of Conjugate Phases in the System MnO-CoO-Cr_2O_3 at 1100 °C, After Jacob and Fitzner [19].

CHAPTER III

EXPERIMENTAL PROCEDURE

3.1 General Approach

The samples belonging to the system MnO-CoO-Cr_2O_3 were prepared by mixing the powders Mn_3O_4, CoO, and Cr_2O_3, in desired proportions. These mixtures were milled intimately in order to obtain homogeneous distribution of components and then were compacted in the form of cylindrical pellets. The pellets were sintered at high temperatures and under controlled oxygen partial pressures in order to form the desired phases or phase assemblages of oxide and spinel solid solutions in the MnO-CoO-Cr_2O_3 ternary.

Experiments were conducted at 1300 °C for determining the thermodynamic activities of CoO in selected phase assemblages of the system. The major experimental tool for this purpose was the method of gas equilibrations using well-metered mixtures of CO_2 and H_2 gases. These determinations were also aided by electromotive force measurements in some selected cells using a calcia stabilized zirconia solid electrolyte.

The boundaries between various phases of the system at 1300 °C were determined by examining the quenched samples under metallographic microscope or by x-ray diffraction. The conjugation lines between coexisting (Mn,Co)O and

$(Mn,Co)Cr_2O_4$ solid solutions were established by thermodynamic methods. The same procedure was applied for checking the directions of conjugation lines in the spinel + chromia part of the system.

The cation distribution in stoichiometric spinel phases was studied by structural analysis based on x-ray diffraction methods and multiple iterative calculations using models available in literature for examining the spinel structure.

3.2. Details

The details applying to various aspects of the experimental procedure are presented in the following.

3.2.1. Starting Materials:

The materials that were used in preparation of samples were as follows.

a : Manganese Oxide:

The source of MnO was high purity MnO_2 powder obtained from Aldrich Chemical Company, Inc. The Aldrich 24,344 MnO_2 powder had a starting purity over 99 %. MnO_2 powder was placed in a platinum crucible and calcined at 1100 °C for 48 hours. The calcination step expelled the volatiles and converted manganese dioxide into Mn_3O_4, in the form of a sintered mass. This mass was crushed and ground to -35 μm. after cooling the sinter to room temperature. MnO required in a sample pellet was introduced in the form of fine Mn_3O_4

powder; the Mn_3O_4 reduced easily to MnO during curing of the sample pellets under reducing conditions, permitting to form the desired phases or phase assemblages having all manganese in divalent state of oxidation, i.e. as MnO.

b) Cobalt Oxide:

CoO was obtained by heating Merck 2543 Co_3O_4 powder in an alumina crucible at 1100 ^oC for 24 hours in air. This calcination converted all cobalt into the CoO form, as determined by x-ray diffraction. The calcined mass was crushed and ground to -35 μm. prior to its use.

c) Chromium Oxide:

Analytical reagent grade powder Merck 2483 chromium oxide powder was the source of Cr_2O_3. The as-received powder was heated in a platinum crucible at 700 ^oC for 24 hours in order to drive off any moisture and volatiles. The purity of Cr_2O_3 so obtained was better than 99.5 wt % .

3.2.2. Preparation of Samples

The samples that were used in the experiments were prepared by either the "mixed oxide route" or by the "liquid mix process". The processing steps involved in these two different methods are given in the following.

3.2.2.1. The Mixed Oxide Route

In the mixed oxide route, the samples in the MnO-CoO-Cr_2O_3 system

were prepared from the powders of Mn_3O_4, CoO, and Cr_2O_3. In order to prepare a sample of selected composition, the individual oxide powders were weighed in calculated proportions; the mixture was placed in an agate mortar and blended by continuous grinding with the pestle for 45 minutes. Acetone was used as the blending-milling medium in order to obtain better homogenization.

When the acetone evaporated completely, the dry powder mixture was pressed into dense cylindrical pellets 1 cm in diameter, using a hardened steel die and a uniaxial load of 1500 kg/cm2. The pellets were placed in a platinum crucible and heated in a muffle furnace at 1100 °C for 48 hours. At the end of this preliminary heat treatment the pellets were cooled to room temperature, crushed and ground to -35 μm. and then repelletized. These pellets were then heated in a vertical tube furnace at 1300 °C for 72 hours under a controlled gas atmosphere having a partial pressure of oxygen $P_{O_2}=10^{-8}$ atm. This atmosphere was reducing enough to convert all Mn_3O_4 into MnO but sufficiently oxidizing not to cause any metal formation.

The lengthy blending-milling of powder mixtures under acetone and the two thermal treatments described above allowed MnO, CoO, and Cr_2O_3 to react completely and yield fully homogenized samples. The thermal treatments were effective in developing the desired oxide phases or phase assemblages prior to final equilibration experiments and the procedure adopted shortened the duration of the subsequent equilibration runs considerably.

3.2.2.2. The Liquid Mix Process

The liquid mix process was developed first by Pechini [21] in the

1960's in order to prepare very fine titanate and niobate powders suitable for ceramic capacitor manufacture. The process was later modified and popularized by Prof. Harlan Anderson of Ceramic Engineering Department of University of Missouri at Rolla for commercial production of variety of fine electronic ceramic powders; Eror and Anderson [22] reported that powders of over 100 different oxide compounds could be prepared by this technique.

The liquid mix process utilizes weak acidic solutions of the cations involved in the oxide powder to be synthesized. These solutions are mixed in desired final stoichiometry, the aqueous mixture is then polymerized in the presence of an organic reagent, typically ethylene glycol. The organic polymer is then burned and the mass is calcined; the resulting material is very fine powders of the sought oxide compound or oxide solid solution. The powders are highly sinterable due to enhanced diffusion derived from their increased surface area.

This particular process was used in the present thesis work in order to prepare the MnO-CoO solid solution samples required for activity determinations through electromotive force measurements. The starting chemicals were water soluble salts mangan-II-tetrahydrate (Merck 5940 powder with 0.069 % impurities) and cobalt-II-tetrahydrate (Merck 2436 powder with 0.227 % impurities), Merck grade anhydrous citric acid to obtain the weak acidic medium, and Merck 949 liquid ethylene glycol to serve as the polymerizing agent.

In order to prepare a MnO-CoO solid solution of known composition with the liquid mix process, the nitrate powders were weighed according to the required stoichiometry and they were dissolved in distilled water by stirring in a pyrex beaker. The amounts of citric acid and ethylene glycol added to the aqueous

solution were, respectively, 1.4 times and 1.2 times the total weight of the oxide mixture to be produced. The solution, usually 50 milliliter in volume, was heated to 90 °C in order to dissolve the salts completely and ensure homogenization. The resulting clear solution was evaporated over a steam bath until an amorphous organic polymer was formed. The solid polymer was heated in the beaker to 400 °C to burn off as much of the polymer as possible. The sample at this stage was black and brittle. It was ground, screened and transferred into a platinum crucible and heated in a vertical tube furnace stepwise, at 800 °C for 8 hours and then at 1300 °C for 24 hours. The furnace atmosphere during heating was maintained at a constant oxygen partial pressure of $P_{O_2}=10^{-8}$ atm.

The typical x-ray diffraction patterns for a (Mn,Co)O solid solution prepared by the Pechini process is given in Figure 9. The diffractogram at 400 °C shows the serrated pattern after the polymer burning stage, whereas the pattern of the fully developed solid solution after firing at 1300 °C is quite smooth. The exact final compositions of the (Mn,Co)O solid solutions produced by the liquid mix process were determined by comparing the spacing of their (200) planes with a standard d_{200}-versus composition plot for MnO-CoO solid solutions as will be described in later sections of the thesis.

3.2.3 Gas Equilibration Experiments

The gas equilibration experiments were performed in order to identify the stability areas of various phases present in the system MnO-CoO-Cr_2O_3 at 1300 °C and also to determine the activities of cobalt oxide in solid solution or in two-phase mixture areas of the system. The major pieces of equipment involved in these experiments were a vertical tube high- temperature furnace operating at 1300 °C

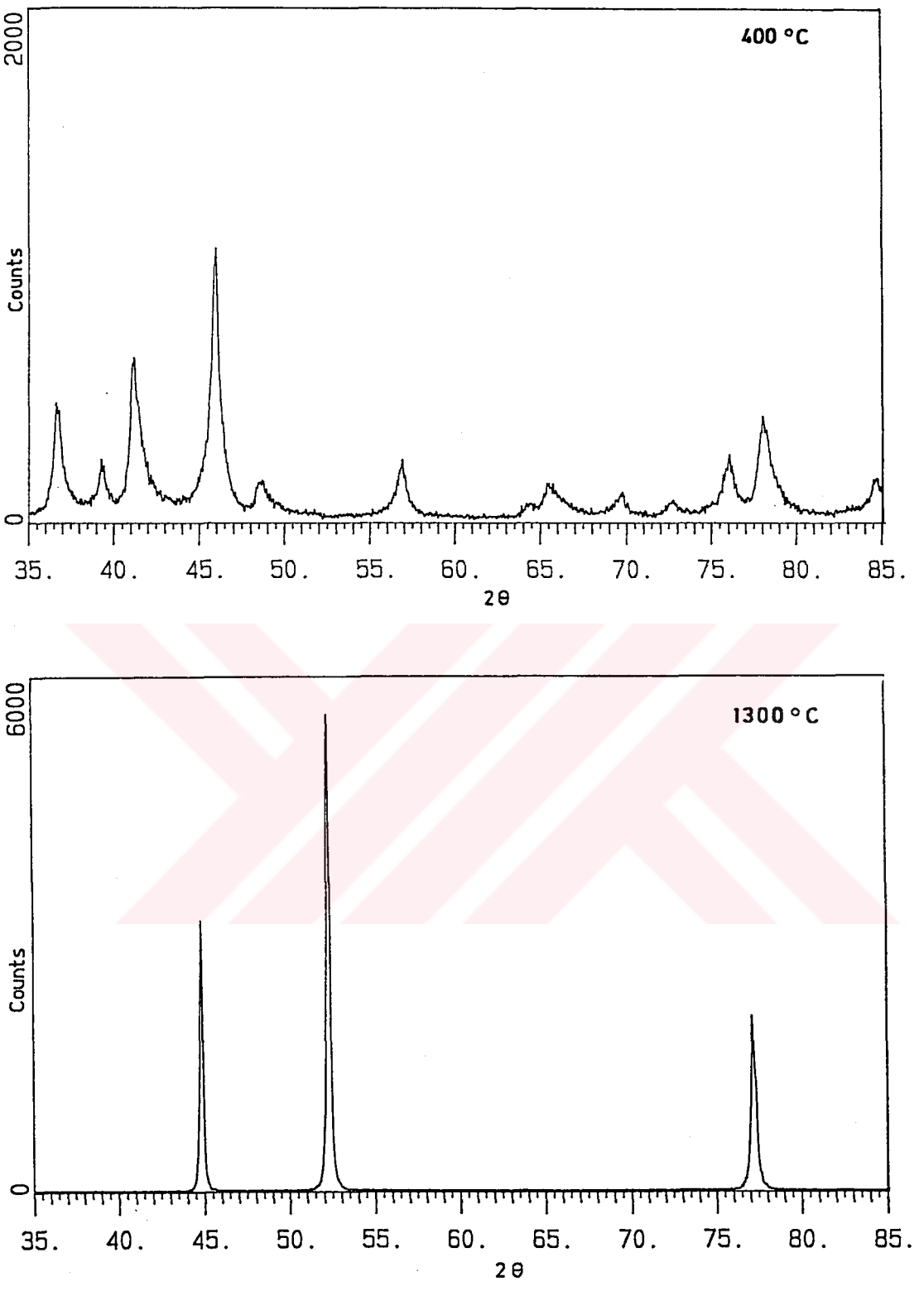


Figure 9. X-ray Diffraction Patterns for a (Mn,Co)O Solid Solution Prepared by the Pechini Process.

and a gas proportioning system which served to prepare mixtures of CO_2 and H_2 gases with well-controlled volumetric ratios. These gas mixtures provided the means for generating gas atmospheres of controlled oxygen partial pressures inside the furnace tube. A schematic drawing of the gas equilibration set-up is shown in Figure 10.

In an equilibration run, the sample of known composition was suspended into the hot zone of the furnace where it was brought into contact with the CO_2+H_2 gas mixture. The sample was reacted with the gas for a predetermined length of time until the phase or phases corresponding to the imposed P_{O_2} developed. Upon termination of this equilibration stage the sample was cooled rapidly by quenching it in water. Because the rapid quench does not allow time for transformation, the phases that would be determined in the quenched samples would represent those which were present at the equilibration temperature.

The details involved in determining the cobalt oxide activities or in establishing the stability areas of condensed phases in the system by the gas equilibration technique will be given in sections pertaining to presentation of experimental data. At this stage, it is appropriate to describe the equilibrium furnace and the gas mixing system and also the manner by which the temperatures and oxygen partial pressures were controlled during equilibration experiments.

3.2.3.1 The Equilibration Furnace

A home-made vertical tube furnace was used for conducting the equilibration experiments at 1300 °C. The furnace, capable of reaching 1500 °C, was heated by four silicon carbide hot rod elements. An alumina tube, 40 mm ID

with 3 mm wall thickness, was inserted vertically into the space heated by the four elements. This tube served as the chamber in which equilibration reactions between samples and the gas phase took place.

The male part of a pyrex ground glass joint, carrying a side arm for gas admission, was cemented to the bottom opening of the furnace tube. The female part of the joint was shaped into the form of a quench cup fitted with a U-tube attachment for admission of quench water. The narrow meniscus of the U-tube was filled with a small quantity of water in order to prevent air intake into the furnace tube from bottom. During the equilibration runs the reservoir of the quench cup was kept dry so that the furnace atmosphere remained unaffected by water vapor. Likewise, the top of the furnace tube was also closed by the sample holder so that no air would diffuse into the tube from top.

The furnace was powered from an external electrical circuit the basic units of which were a variac and a Pye-Ether Digi temperature controller. The controller, coupled to a thyristor, was actuated with Pt - Pt13 % Rh thermocouple. This power and control circuit allowed to maintain the temperature in the furnace tube constant at 1300 °C within ± 2 °C. A standardized thermocouple of same composition was used to measure the actual sample temperatures at the start and the end of each equilibration run. The length of the hot zone, where the sample was situated, was about 4 cm; over that length the temperature variation was within ±2 °C.

3.2.3.2 The Gas Mixing System

The gas mixtures having definite CO_2 to H_2 volumetric mixing ratios

were prepared by using a gas mixer similar to the one described by Darken and Gurry [23]. This device, shown in Figure 10, contains two differential manometers for metering the individual gases and each manometer has a leveling bottle of its own for adjusting the height of the manometer fluid. The open U-arms of each manometer are connected with a capillary tube. The leveling bottles and their extensions are filled with copper sulfate. The manometer fluid is n-butyl pythalate.

The volumetric flow-rate of a gas passing from a manometer is a function of both the height of the manometer and the diameter of the capillary linking its arms. The flow rate of the gas can be kept constant at a desired set value by clamping the leveling bottle to a vertical bar and letting the excess of the gas escape through the bleeder tube.

The individual capillaries for CO_2 and H_2 gases were calibrated against the height of their manometer fluids by the soap-bubble coloumn method. A vertical 50 cc capacity burette with a soap solution reservoir at the bottom was used for this purpose. Measuring the time necessary for the gas to pick up a bubble and travel through 40 cc volume of the burette permitted calculation of the flow rate in cc/sec. Figure 11 to 13 display the flow rate calibrations made for different capillaries at hand.

The gas train for preparing the gas mixtures for equilibration runs included individual cylinders of CO_2 and H_2, a purification system, the metering manometers, and a mixing chamber. Before entering the metering manometers the CO_2 and H_2 gases were purified from their oxygen by passing them through a coloumn of copper chips heated at 500 ^oC. The moisture in the gases were absorbed by the silica gel. The gas mixing chamber was a bottle filled with glass

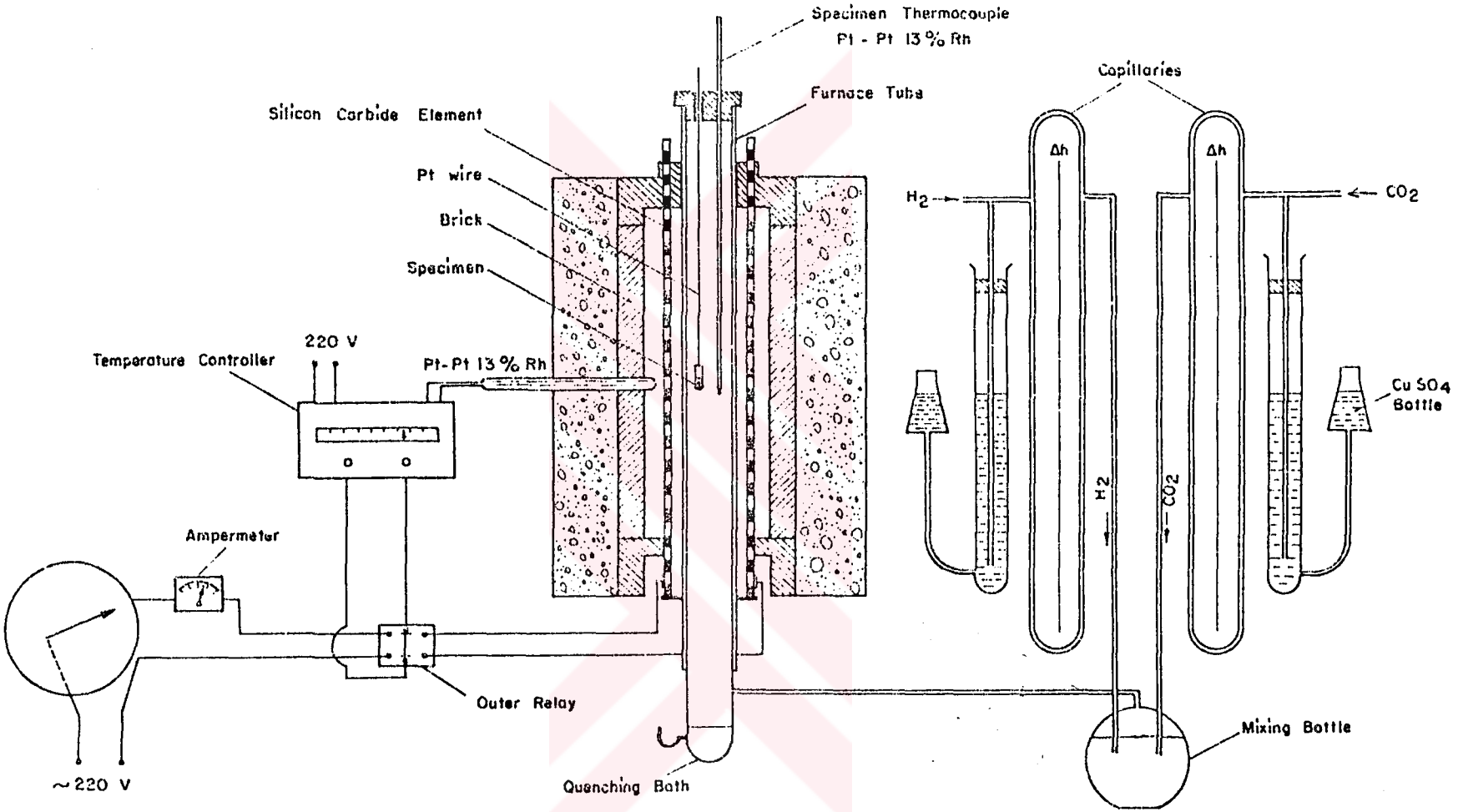


Figure 10: Position of Furnace, Specimen and Gas Mixing System.

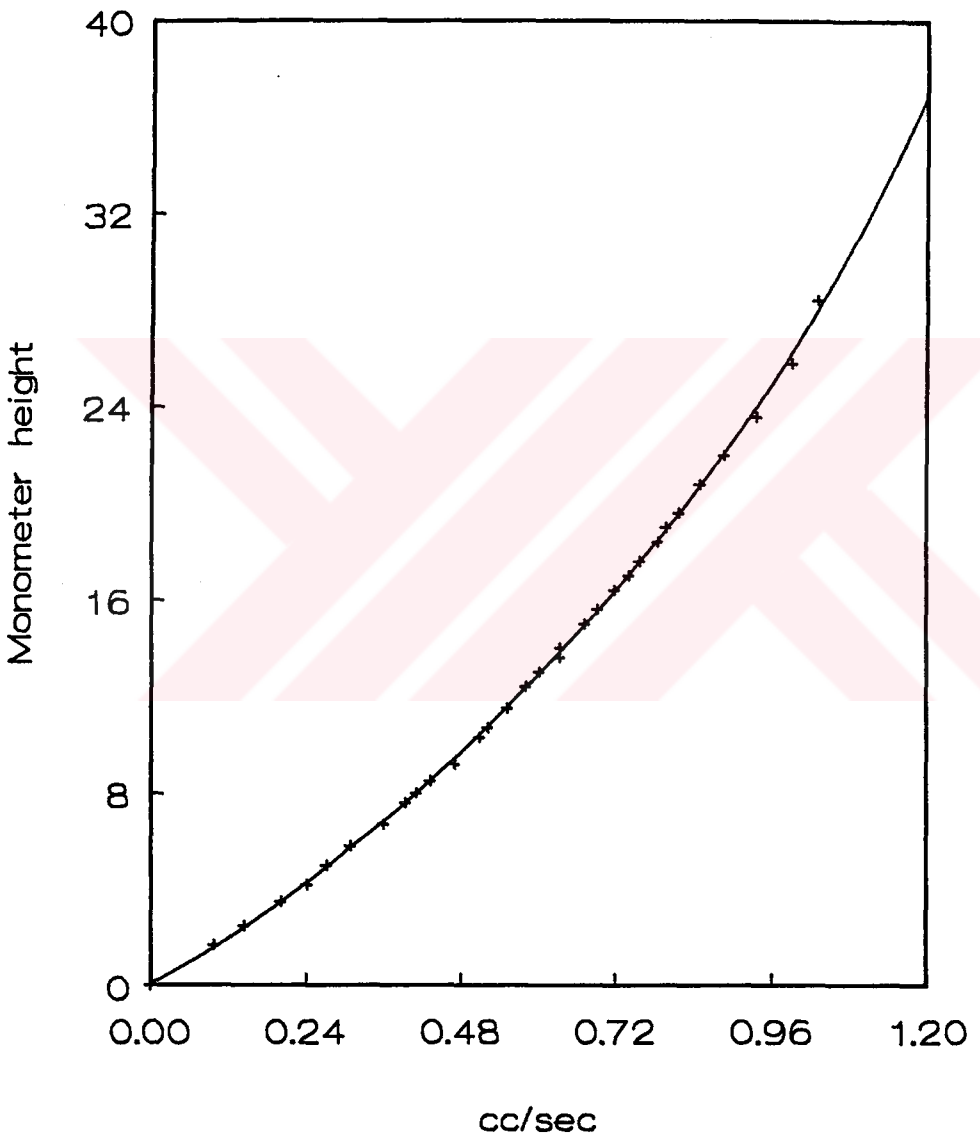


Figure 11. The Flow Rate Calibration Curve of CO_2 Capillary.

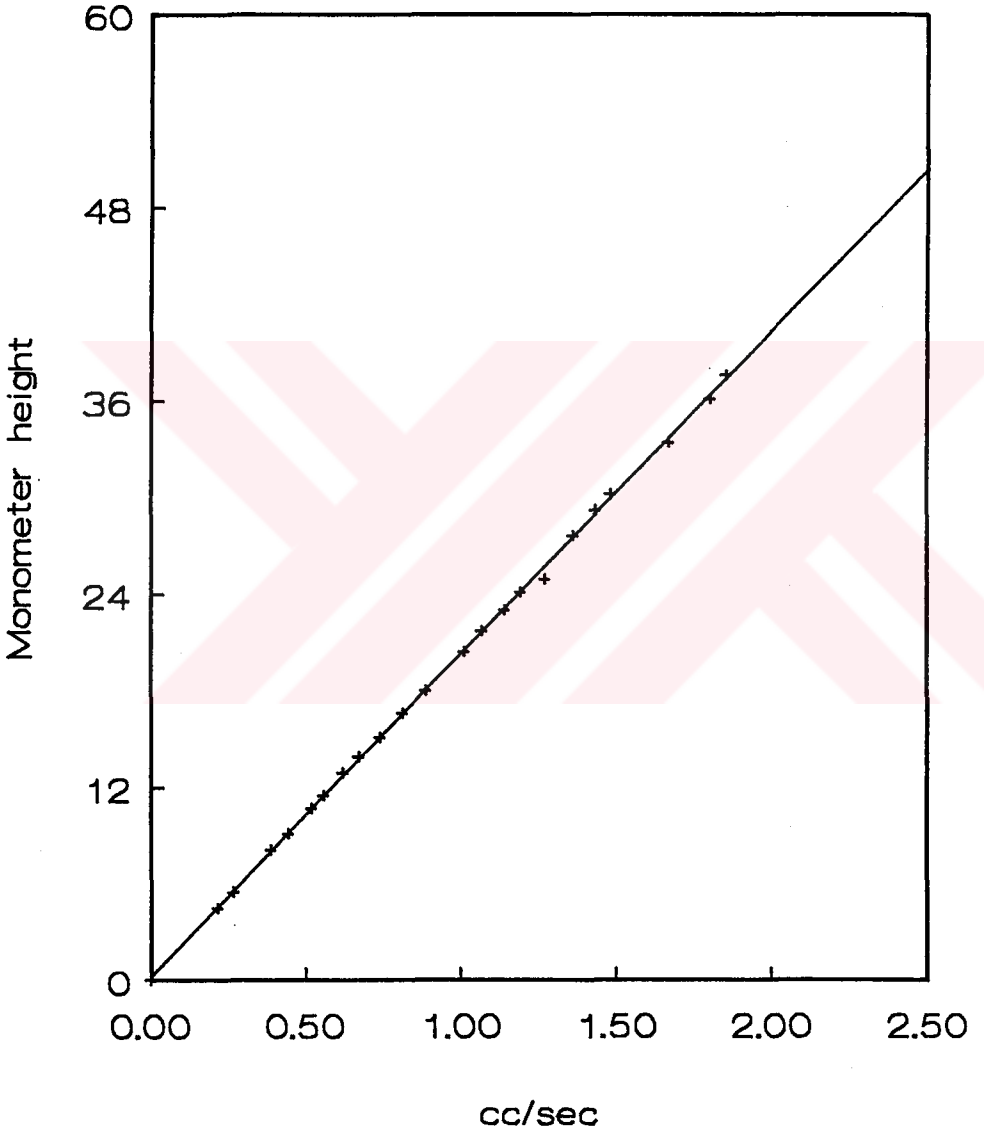


Figure 12. The Flow Rate Calibration Curve of H_2 Capillary.

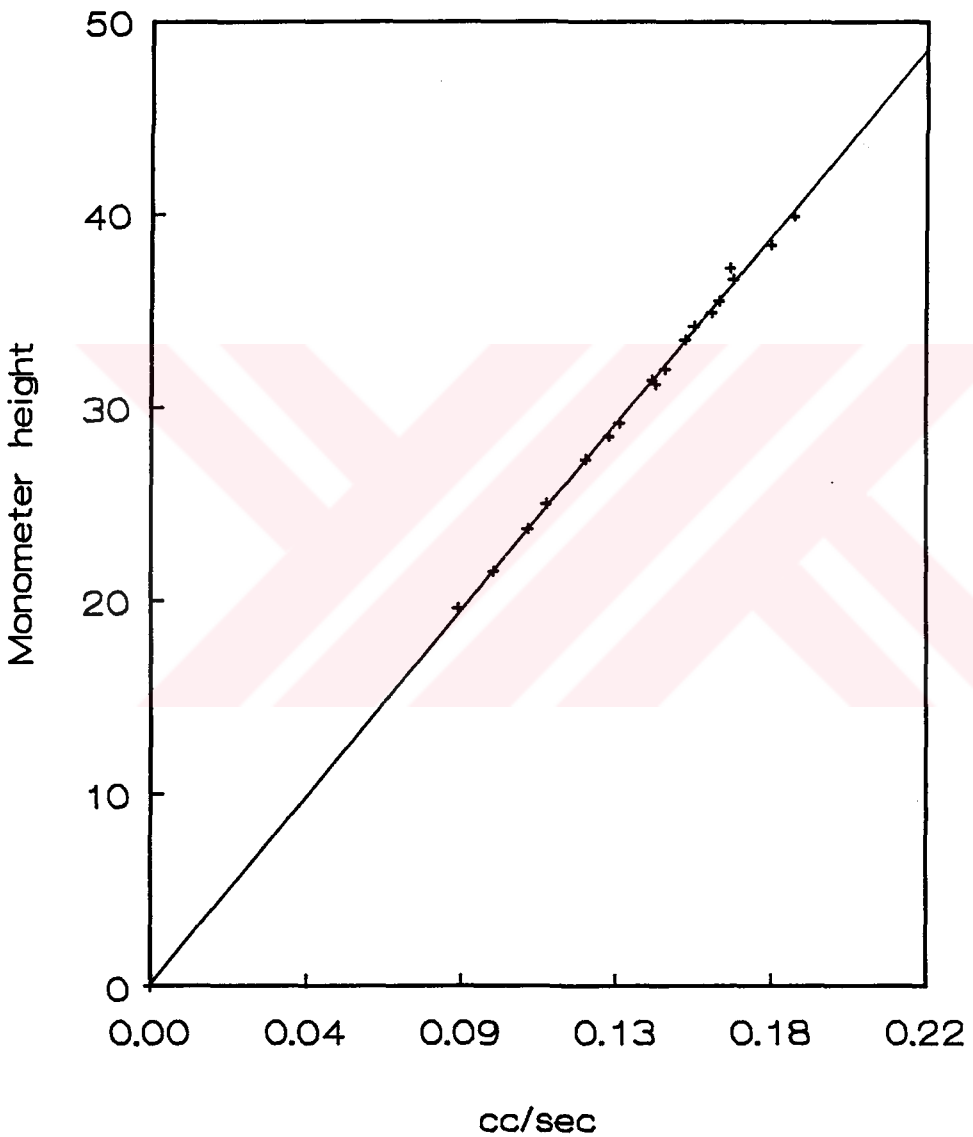


Figure 13. The Flow Rate Calibration Curve of H_2 Capillary.

wool. The metered gas mixture was fed into the furnace tube from bottom by connecting the outlet of the gas mixing chamber to the pyrex joint glass fixture.

The partial pressure of oxygen generated by a $CO_2 + H_2$ gas mixture of known volumetric ratio inside the furnace tube at the sample temperature could be calculated by considering the following equilibria in the gas phase :

$$CO + \frac{1}{2}O_2 = CO_2 \quad (17)$$

$$CO_2 + H_2 = CO + H_2O \quad (18)$$

The equilibrium constants for Reactions 17 and 18 are:

$$K_{17} = \frac{P_{CO_2}}{P_{CO} * (P_{O_2})^{1/2}} \quad (19)$$

$$K_{18} = \frac{P_{CO} * P_{H_2O}}{P_{CO_2} * P_{H_2}} \quad (20)$$

The values of K_{17} and K_{18} at 1300 °C are $10^{4.8624}$ and $10^{0.4587}$, respectively [24]. Assume that (r) moles of CO_2 and 1 mole of H_2 are mixed initially, so that the initial mixing ratio is denoted by:

$$r = \frac{CO_2}{H_2}$$

At equilibrium, if (x) mole of CO forms from this mixture, (x) mole of H_2O also forms according to the stoichiometry of Reaction (18). Thus, in the equilibrium mixture, the number of moles of each gas and the corresponding partial pressures at 1 atm total pressure will be:

n_{CO_2} = r–x mole, $P_{CO_2} = \frac{r-x}{r+1}$ atm,

n_{H_2} =1-x mole, $P_{H_2} = \frac{1-x}{r+1}$ atm,

n_{H_2O} =x mole, $P_{H_2O} = \frac{x}{r+1}$ atm,

n_{CO} =x mole. $P_{CO} = \frac{x}{r+1}$ atm.

When the expressions for partial pressures are inserted into Eqns.(19), and (20), and upon rearrangement, we obtain the following set:

$$r = (1+10^{4.8624} * \sqrt{P_{O_2}}) * x \quad (21)$$

$$\sqrt{P_{O_2}} = \frac{x}{10^{5.3211} * (1-x)} \quad (22)$$

In order to calculate the gas mixing ratio CO_2/H_2 for a desired P_{O_2} ,first x is solved from Eqn.(22) and then r is obtained from Eqn.(21) by using the (P_{O_2} ,x) combination of the previous step.

3.2.3.2. The Gas Equilibration Run

For an equilibration run, small pellets of the homogenized oxide mixtures were placed in thin Pt crucibles and equilibrated in the hot zone of the furnace with CO_2/H_2 gas mixtures of predetermined oxygen partial pressures. These Pt crucibles were impregnated previously with Mn and Co in order to avoid losses of manganese and cobalt into platinum from the samples. The crucibles were

suspended into the hot zone of the equilibration furnace by a thin Pt-wire. The top of the furnace tube was covered by a refractory lid with a hole for sample suspension. The temperatures within the furnace tube were measured by the standardized Pt-Pt 13% Rh thermocouple. The flow rates of gas mixtures were adjusted within 1 to 1.5 cc/sec, so that the effects of thermal segregation would be eliminated.

The duration of an equilibration run was about 24 hours. Because of the thermal treatments applied in sample preparation, preliminary experiments indicated that equilibrium was attained in about 10 hours from the start of an equilibration run. After equilibration, the samples were quenched to room temperature by dropping them into water. The quenching water was admitted to the quench cup just before dropping the sample. Phase identifications in quenched samples were done by examining their polished sections under microscope. The quenched samples were mounted in epoxy resin and the sections were prepared by conventional metallographic techniques. When necessary, phase identifications were aided by x-ray diffraction studies on powdered samples.

3.2.4. X-Ray Analysis

In the present study XRD was used as the tool for checking sample compositions in the MnO-CoO solution series, in the identification of spinel phase boundaries, and for determining the degree of inversion in spinel samples.

The x-ray powder diffraction patterns of samples were obtained with a computer-controlled Rigaku-diffractometer. Fe Kα was used as the x-ray beam. The background and the Fe Kα_2 peaks in each x-ray powder diffraction pattern

were eliminated by a computer program. A calibration check was made with a silicon standard before each x-ray study.

3.2.5. Electromotive Force Measurements.

The activities of CoO in MnO-CoO solid solutions were measured by using an emf technique with oxygen concentration cells containing calcia stabilized zirconia as solid electrolyte. The cell used in this investigation was;

$$Pt\,|\,Co,CoO\,|\,CSZ\,|\,Co,CoO_{ss}\,|\,Pt\,| \qquad (23)$$

where CoOss represents cobalt oxide in solid solution with manganese oxide. The over-all cell reaction for the above configuration can be written as :

$$CoO = CoO_{ss} \qquad (24)$$

The standard Gibbs free energy change for Reaction (24), ΔG^{o}_{24} is given by the equation :

$$\Delta G^{o}_{24} = -2*F*E \qquad (25)$$

where E is the cell emf and F is the Faraday constant.

The application of Eqn.(25) would imply that the conduction in solid electrolyte was predominantly ionic in the range of temperatures and oxygen partial pressures used in the present investigation and also that any reaction between the electrode materials and the electrolyte was negligible.

The cell arrangement is schematically shown in Figure 14. The cell assembly was enclosed in a 1.5 cm diameter quartz tube. The inner tube was the solid CSZ electrolyte, containing the reference half cell. The tip of the CSZ tube was platinized inside and outside by decomposition of chloroplatinic acid ($PtCl_4.2HCl.6H_2O$) to obtain a good contact. The bottom support tube was made from quartz and held the solid solution in an alumina crucible.

The emf cell assembly was heated to desired temperatures in a vertical tube furnace. This furnace was non-inductively wound with Kanthal resistance wire. In order to eliminate induction effects on cell emf, a cylindrical Kanthal shield was wrapped around the alumina tube which housed the entire cell assembly. The shield was grounded during emf measurements. The temperature in the hot zone was measured with a standardized Pt-Pt10% Rh thermocouple. The combined length of the cell compartments was 2 cm. The length of the hot zone was 5 cm; the presence of the Kanthal shield aided in establishing this uniform hot zone with ± 1 °C variations in the set temperature.

3.2.5.1. Cell Operation

In a typical run, about 2 gm. of the sample + cobalt mixture was packed into the alumina crucible. Similarly, the reference mixture was packed to the inner tip of the CSZ tube. The Pt lead wire was placed firmly in these mixtures by coiling them and packing the powders over the coils. The CSZ tube was placed upon the sample mixture in the alumina crucible. The rubber corks holding the CSZ tube and the quartz support tube exerted sufficient pressure to ensure good contact between the electrolyte and the sample electrode.

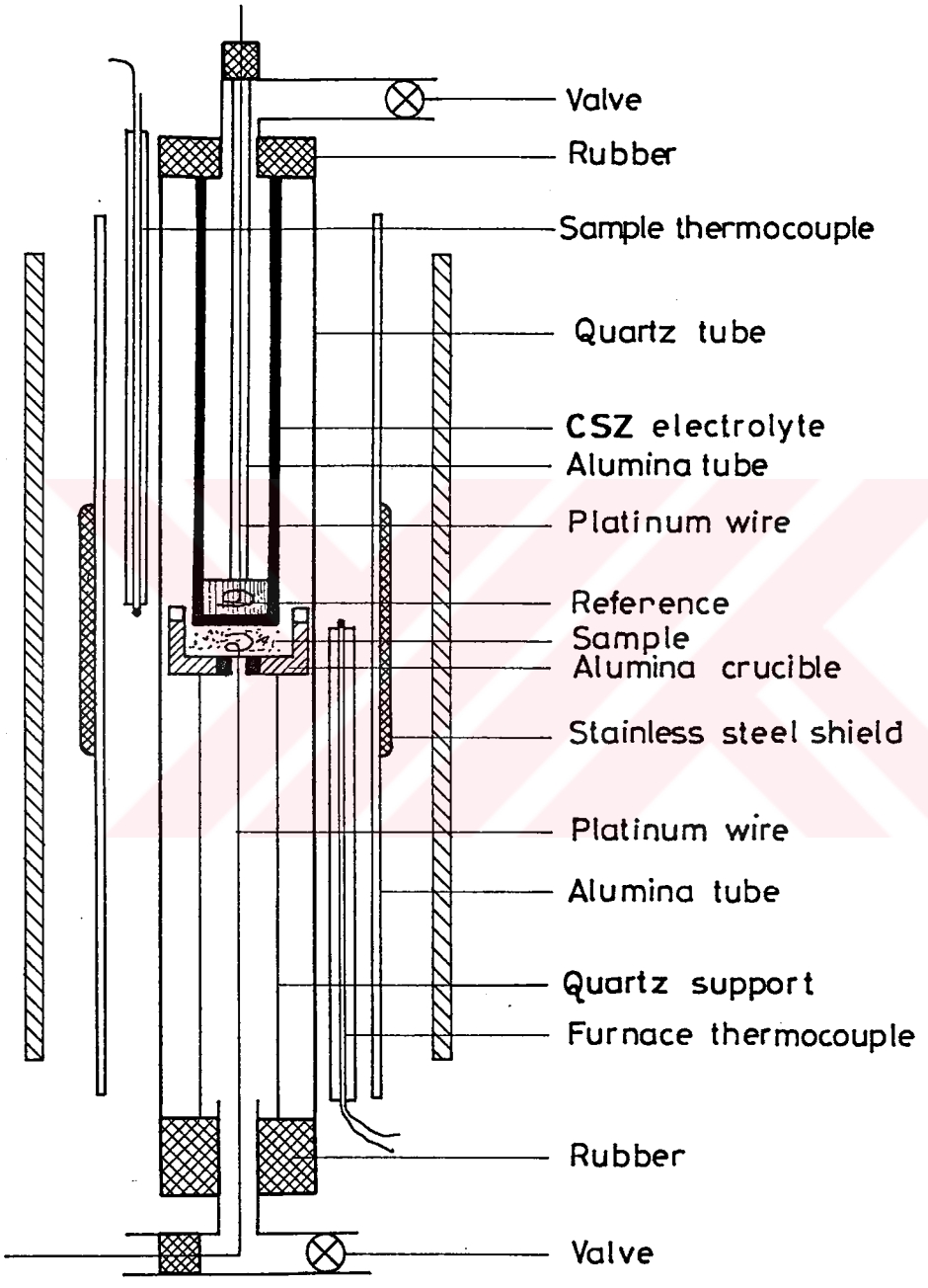


Figure 14. EMF Set up.

After assembling the cell as described above, the quartz tube housing the cell was flushed with purified argon gas for about 20 minutes. At the end of this period the gas inlet and outlet valves were closed and emf experiment were performed in the presence of a static argon atmosphere.

In order to start an emf experiment, the furnace was heated to 930 °C and the cell was kept at this temperature for 24 hours to allow setting of the equilibrium. After this period, emf data were taken at temperatures raised by 10 to 30 °C increments. At each constant temperature the stable emf data was taken after allowing the cell to remain at the temperature for at least 1 hour. This duration would be about 10 hours at lower temperature (≈730 °C) and would be less than 15 min. when the cell temperature was raised above 1200 °C. Standard precautions were taken to ensure reversible cell operation.

CHAPTER IV

RESULTS and DISCUSSION

In order to establish the phase relations and activities of CoO in the $MnO\text{-}CoO\text{-}Cr_2O_3$ system, series of samples were prepared and then equilibrated at 1300 °C with a gas phase of known oxygen partial pressure for 24 hr. The data obtained in the equilibration experiments, EMF measurements and x-ray studies and the thermodynamic calculations performed through their use are presented in the following sections.

4.1 The Co-CoO Equilibrium

The equilibrium between metallic cobalt, cobalt oxide, and the oxygen in the gas phase was expressed in Section 2.2 by the reaction:

$$Co + \frac{1}{2}O_2 = CoO \qquad (1)$$

In view of the discrepancies existing in previous data on partial pressures of oxygen for the coexistence of cobalt and cobalt oxide [7,10], an independent determination for this quantity had to be made during the course of the present study at 1300 °C.

The determination of P_{O_2} for the equilibrium represented by Reaction (1) at 1300 °C, in the present study, was based upon equilibrating pieces of pure CoO or pure Co with CO_2-H_2 gas mixtures of known volumetric ratios. When the starting material was CoO, the equilibrium was approached from the reducing side in which CoO was subjected to the action of CO_2/H_2 atmospheres; the CO_2/H_2 ratio of the gas mixture was lowered progressively until metallic Co would form. When metallic cobalt was taken as the starting material, equilibrium was approached from the oxidizing side by subjecting Co to gas mixtures with progressively higher CO_2/H_2 ratios until Co would convert into CoO.

Each equilibration run lasted 24 hours. At the end of every run the equilibrated sample was quenched into water and then examined for the stable phase. The presence of CoO or Co could be established from differences in their luster either by observing directly with naked eye or by looking into polished sections of quenched samples in an optical microscope. When necessary, phase identification was aided by x-ray diffraction as well.

The results of equilibration runs are given in Table 1. The column labeled $r = \frac{CO_2}{H_2}$ shows the volumetric ratios of mixing of CO_2 and H_2 gases. The column -log P_{O_2} shows the oxygen partial pressures calculated from these "r" values by using Eqns.(21) and (22). The last column of the table indicates the stable phases observed after quenching.

Table 1. Critical Runs for the Determination of the Equilibrium Partial Pressure of Oxygen for the Reaction $Co + 1/2\,O_2 = CoO$ at 1300°C.

Starting Sample Composition	Imposed Gas Ratio $r = \frac{CO_2}{H_2}$	Calculated $-\log P_{O_2}$	Phases Present
CoO	7.620	8.0332	CoO
	7.000	8.1152	CoO
	6.762	8.1475	CoO
	6.663	8.1616	CoO
	6.604	8.1644	CoO
	6.525	8.1819	CoO + Trace Co
	6.455	8.1915	Co
Co	6.450	8.1923	Co
	6.500	8.1854	Co
	6.550	8.1780	CoO

The data in Table 1 shows that the CO_2+H_2 gas mixture with $r = \frac{CO_2}{H_2} = 6.525$ resulted in the development of the Co + CoO phase assemblage; hence this mixing ratio represents the equilibrium gas. The partial pressure of oxygen corresponding to this specific r value was $P_{O_2}=10^{-8.1819}$ atm, as calculated from Eqns.(21) and (22).

The value $P_{O_2}=10^{-8.1819}$ atm determined in the present study for Co-CoO equilibrium at 1300 °C is in very good agreement with that obtained from recent data of O'Neill [10]. From his emf equation a value of $P_{O_2}=10^{-8.1814}$ atm can be calculated at 1300 °C for Reaction (1). The excellent concordance of these P_{O_2} values was taken as an indication of the fact that the gas-equilibration set-up and procedures used in the present study would produce reliable data in phase equilibria and thermodynamic investigations on the oxide system at hand.

4.2. Variation of d_{200} with Composition in MnO-CoO Solid Solutions

MnO and CoO have similar crystal structures. Both are NaCl-type and most intense refractions occur from their (200) planes. The interplanar spacing between (200) planes are shown by d_{200}; the ASTM card file values being 2.130 for CoO and 2.223 for MnO. This spread in the d_{200} values of CoO and MnO is not so large as compared to that known for NiO-MnO series, yet it could be used advantageously to determine the unknown compositions in CoO - MnO solutions if an accurate calibration chart would be made available. The chart would describe

the variation of d_{200} in CoO-MnO solid solution as a function of solution composition.

In order to prepare the d_{200}-composition chart, selected members of MnO-CoO solid solutions were equilibrated at 1300 °C with a CO_2/H_2 gas mixture that would yield a partial pressure of oxygen $P_{O_2}=10^{-8}$ atm in the furnace tube. This oxygen pressure is reducing enough to keep all manganese in divalent state but oxidizing enough not to cause precipitation of metallic cobalt.

The MnO-CoO solid solution samples were equilibrated with the gas phase described above each for 48 hours and then quenched to room temperature. The d_{200} values of these samples were determined by running their x-ray diffraction at a scanning speed of 1/8 °/min.; silicon was used as the internal standard and Fe $K\alpha_1$ was used as Radiation.

The 2θ values for d_{200} peaks and the corresponding d_{200} values determined in MnO-CoO solid solutions are given in Table 2. Figure 15 shows the variation of d_{200} values with composition. The behavior shows negative deviation from Vegard's law. The experimental data obtained by Biggers and Muan [25] are tabulated in the last column of Table 2. It can be observed that d_{200} values determined in the present study are in good agreement with the results reported earlier by Biggers and Muan [25].

Table 2. Variation of d_{200}-spacing with Composition Along the MnO - CoO Binary. ($\lambda_{K\alpha_1}$ =1.93597)

Sample Composition (mole fraction)		2θ	d_{200}-spacing	d_{200}-spacing
N_{CoO}	N_{MnO}			[25]
1.0	0.0	54.065	2.1298	2.130
0.9	0.1	53.882	2.1365	2.137
0.8	0.2	53.662	2.1446	2.144
0.7	0.3	53.390	2.1547	2.155
0.6	0.4	53.185	2.1624	2.165
0.5	0.5	52.895	2.1734	2.174
0.4	0.6	52.647	2.1829	2.183
0.3	0.7	52.369	2.1939	2.194
0.2	0.8	52.148	2.2023	2.202
0.1	0.9	51.935	2.2107	2.214
0.0	1.0	51.654	2.2219	2.222

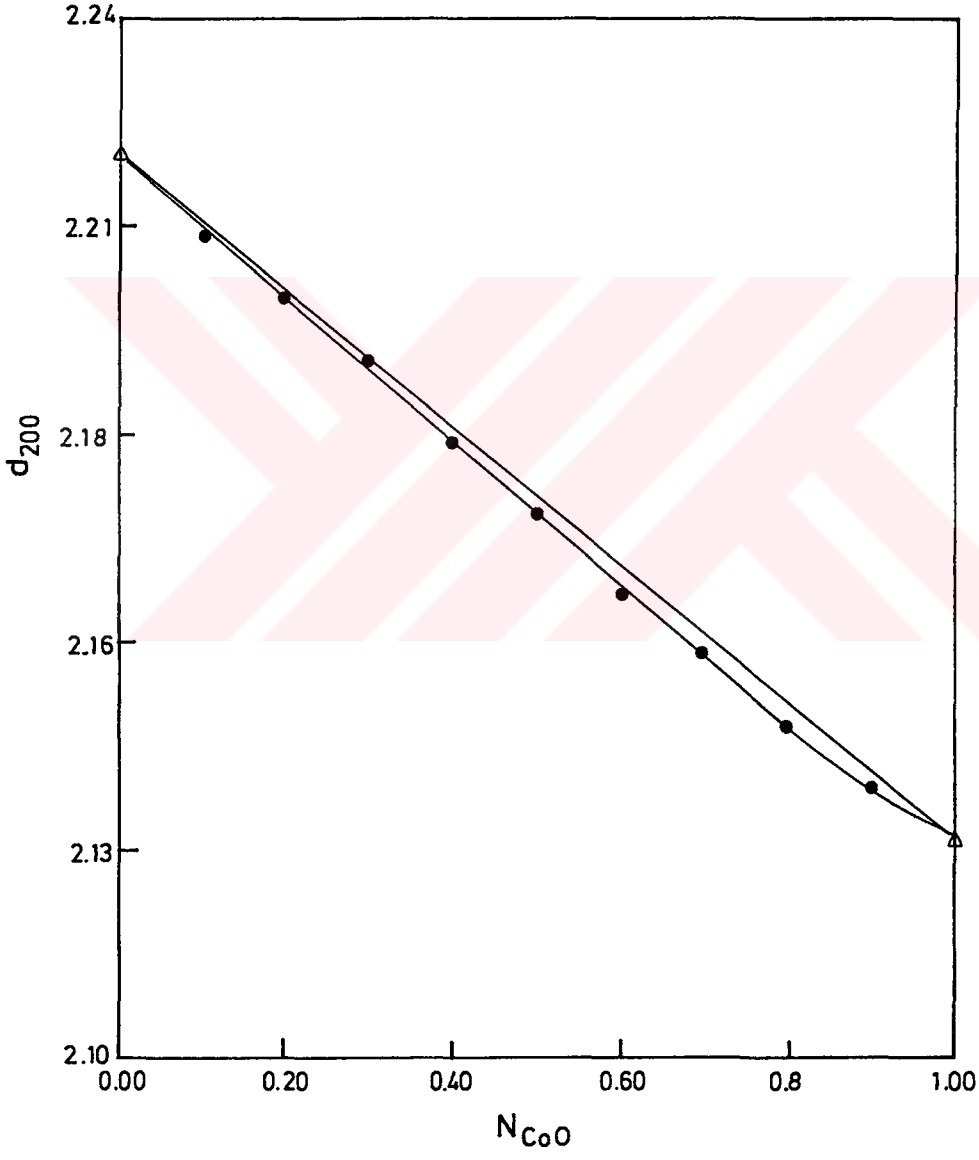


Figure 15. Variations of d_{200}-Spacing along the MnO-CoO Binary.

4.3 Activities of CoO in MnO-CoO Solid Solutions

In the present study, activities of CoO in MnO-CoO solid solutions were determined at 1300 °C using two different experimental techniques: (1). Metal precipitation through gas equilibrations, and (2) EMF measurements in solid oxide electrolyte cells. The details of these techniques and the data obtained from them are presented in the following sections.

4.3.1 The Gas Equilibration Technique

In the gas equilibration technique, selected samples in the MnO-CoO solid solution system were equilibrated with CO_2 + H_2 gas mixtures of variable CO_2/H_2 ratio. The ratio CO_2/H_2 was made progressively lower until precipitation of metallic phase was observed in each sample. In mixture of MnO-CoO, the stability of MnO is much higher than that of CoO; in other words, CoO represents the easily reducible component. Therefore, when MnO-CoO solid solutions are reduced, the first metal phase to appear will be essentially pure cobalt in all samples except probably those very high in MnO content.

For a MnO-CoO solid solution of given composition the equilibrium between metallic cobalt, oxygen and oxide solution can be represented by the equation:

$$Co_{(s)} + \frac{1}{2}O_{2(g)} = CoO_{(ss)} \qquad (26)$$

where the subscripts (s), (g), and (ss) denote, the solid metal phase, gas, and oxide solid solution, respectively. The activity of cobalt in the metallic phases coexisting with MnO-CoO solution series may be set equal to unity, and equilibrium constant for Reaction (26) can be expressed as ;

$$K_{26} = \frac{a_{CoO_{ss}}}{P_{O_2}^{1/2} * a_{Co}} \tag{27}$$

where P_{O_2} is the partial pressure of oxygen in equilibrium with the oxide solid solution and metallic cobalt. In the pure Co-O system the activities of CoO and Co are taken as unity, then the equilibrium constant K_{26} becomes:

$$K_{26} = \frac{1}{\left(P_{O_2}^{*}\right)^{1/2}} \tag{28}$$

where $P_{O_2}^{*}$ represents the partial pressure of oxygen in equilibrium with pure CoO and Co.($P_{O_2}^{*} = 10^{-8.1819}$ atm at 1300°C). Combining Eqns.(27) and (28), the activity of CoO may be written as,

$$a_{CoO} = \left(\frac{P_{O_2}}{P_{O_2}^{*}}\right)^{1/2} \tag{29}$$

In the present work values of P_{O_2} for the equilibrium Reaction (26) were determined for nine selected samples of MnO–CoO solid solutions. This was done

by subjecting the solid solution selected to gas mixtures of descending CO_2/H_2 ratios until the metallic cobalt was precipitated.

Table 3 shows the compositions of the MnO-CoO solid solutions subjected to gas equilibration measurements and the range of variations in CO_2/H_2 ratios for each sample until the appearance of metallic cobalt. The oxygen partial pressures in -log P_{O_2} column of table were calculated from Eqns.(21) and (22). The phases present in quenched samples were identified by metallographic examination of their polished sections. The fact that the metallic phase was essentially pure cobalt which was established by SEM analysis of the metallic precipitates.

For a MnO-CoO sample of known composition the value of P_{O_2} that would be used in the calculation of the CoO activity from Eqn.(29) was taken as that P_{O_2} where a trace amount of Co precipitate was observed first. When it was impossible to catch this trace precipitation, P_{O_2} for Eqn.(29) was taken as the average of the two P_{O_2} values at which the MnO-CoO was stable last upon reduction and the cobalt precipitation was observed first under reducing conditions.

The partial pressures of oxygen, determined as described above, for the equilibrium Reaction (1) and the activities of CoO calculated by the use of these in Eqn.(29) are summarized in Table 4. The CoO activities determined in MnO-CoO solid solution at 1300 °C are shown graphically in the activity-composition plot of Figure 17.

Table 3. The Phases Observed in CoO - MnO Solid Solutions at 1300 °C as a Function of the CO_2/H_2 Ratio of the Coexisting Gas Phases.

Sample No	Sample Composition (mole fraction)		Gas Mixing Ratio	$-\log P_{O_2}$	Phases Present
	N_{CoO}	N_{MnO}	$r = \frac{CO_2}{H_2}$		
2	0.90	0.10	6.416	8.1977	SS
			6.326	8.2110	SS
			6.148	8.2384	SS
			6.043	8.2553	SS
			5.956	8.2686	SS + Trace Co
3	0.80	0.20	5.558	8.3364	SS
			5.507	8.3448	SS
			5.417	8.3606	SS
			5.371	8.3692	SS + Co
			5.250	8.3910	SS + Co
			5.122	8.4168	SS + Co
			5.042	8.4306	SS + Co
4	0.70	0.30	4.587	8.5233	SS + Co
			4.647	8.5105	SS + Co
			4.791	8.4806	SS + Co
			4.851	8.4684	SS
5	0.60	0.40	4.444	8.5547	SS
			4.384	8.5682	SS
			4.265	8.5976	SS
			4.216	8.6070	SS + Co

Table 3. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	N_{MnO}	Gas Mixing Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
			4.163	8.6198	SS + Co
6	0.50	0.50	3.300	8.8545	SS + Co
			3.368	8.8340	SS + Co
			3.519	8.7892	SS + Co
			3.556	8.7787	SS + Co
			3.664	8.7482	SS + Co
			3.700	8.7303	SS
			3.874	8.6917	SS
7	0.40	0.60	3.916	8.6809	SS
			3.410	8.8212	SS
			3.405	8.8230	SS
			3.308	8.8526	SS
			3.144	8.9049	SS
			3.096	8.9210	SS + Co
8	0.30	0.70	2.828	9.0155	SS
			2.657	9.0814	SS
			2.601	9.1037	SS
			2.589	9.1088	SS
			2.583	9.1113	SS
			2.534	9.1318	SS

Table 3. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	N_{MnO}	Gas Mixing Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
8	0.30	0.70	2.522	9.1370	SS + Co
			2.466	9.1608	SS + Co
			2.435	9.1743	SS + Co
			2.404	9.1880	SS + Co
			2.373	9.2019	SS + Co
			2.342	9.2161	SS + Co
			2.287	9.2423	SS + Co
			2.187	9.2606	SS + Co
9	0.20	0.8	2.112	9.3289	SS
			1.992	9.3930	SS
			1.910	9.4398	SS
			1.885	9.4547	SS + Co
!0	0.10	0.90	1.247	9.9277	SS
			1.217	9.9540	SS
			1.118	10.0530	SS + Co
			1.082	10.0912	SS + Co
			1.075	10.0991	SS + Co

SS : (MnO-CoO) Solid Solution.

Co : Metallic Cobalt Precipitate

Table 4. Activities of CoO in CoO-MnO Solid Solution at 1300 °C.

Sample Composition (mole fraction)		Equilibrium	Cobalt Oxide Activity
N_{CoO}	N_{MnO}	$-\log P_{O_2}$	a_{CoO}
0.90	0.10	8.2686	0.9050
0.80	0.20	8.3649	0.8100
0.70	0.30	8.4745	0.7140
0.60	0.40	8.6013	0.6170
0.50	0.50	8.7432	0.5240
0.40	0.60	8.9129	0.4310
0.30	0.70	9.1344	0.3340
0.20	0.80	9.4472	0.2330
0.10	0.90	10.0021	0.1230

4.3.1 The EMF Technique

The cell,

$$Pt,\ Co+CoO\ |CSZ|\ Co+CoO_{ss},Pt \qquad (30)$$

was operated in the temperature interval 434 °C to 1207 °C. Higher temperatures were avoided in order to escape from anomalous emf's that would be caused by reactions between cell components. At the lower temperatures, up to 600 °C, the time to bring the cell into equilibrium would take several days. Hence, the above cell configuration was effective in the temperature range 600 °C to 1210 ° C.

The individual electrode reactions could be written as ;

$$\text{Sample half cell ; } Co_{(s)} + 1/2\ O_2 \Leftrightarrow (CoO)ss \qquad (31)$$

$$\text{Reference Half cell ; } Co_{(s)} + 1/2O_2 \Leftrightarrow CoO \qquad (32)$$

The emf measured by the cell would be related to the half-cell oxygen partial pressures by the well-known equation :

$$E(\text{volt}) = -\frac{RT}{2F}\ln\left(\frac{P_{O_2}}{P^{*}_{O_2}}\right)^{\frac{1}{2}} \qquad (33)$$

where R is the gas constant, F is the Faraday's constant (96487 coulomb/mole), and T is the absolute temperature. The term $\left(\frac{P_{O_2}}{P^{*}_{O_2}}\right)^{\frac{1}{2}}$ is the same as that given in Eqn.(29) so that it can be set equal to a_{CoO} in the MnO-CoO solid solutions. Thus,

$$E(\text{volt}) = -\frac{RT}{2F}\ln a_{CoO} \tag{34}$$

Hence, making the reference electrode to consist of the Co+CoO mixture simplified the data processing because cobalt oxide activity in the MnO-CoO solid solution could be obtained easily from Eqn.(33) simply by using the measured EMF and the cell temperature.

The MnO-CoO solid solution samples used in EMF experiments were prepared by the Pechini method [21], in accordance with the procedure described in Section 3.2.2.2 The compositions of these samples were checked by comparing their d_{200} spacing with the standard curve established in Figure 15. The starting compositions before EMF experiments were, in mole fractions of CoO, 0.134, 0.326, 0.400, 0.544, 0.648.

The EMF data obtained in these samples at various cell temperatures are given in Tables 5 through 9. For a given sample, the EMF data were taken both at ascending and descending temperatures in order to ensure reproducibility. Depending upon the sample composition, the reproducibility at rising and falling temperatures varied within 0.1 to 0.5 mV for the same sample temperature. Also,

Table 5. Emf Data in MnO-CoO Solid Solution with N_{CoO}= 0.134

Temperature K	E (millivolt)	Temperature K	E (millivolt)	Temperature K	E (millivolt)
1034	70.94	1187	85.33	1333	100.73
1071	74.39	1212	89.55	1353	102.24
1088	76.96	1240	90.33	1389	105.60
1110	79.54	1255	92.33	1393	105.74
1112	79.73	1261	93.87	1404	106.25
1146	81.42	1266	94.90	1414	106.93
1175	82.43	1266	94.84	1455	110.72
1176	82.45	1299	97.83	1480	113.32
1186	85.32	1321	99.02		

Table 6. Emf Data in MnO-CoO Solid Solution with N_{CoO}=0.326

Temperature K	E (millivolt)	Temperature K	E (millivolt)	Temperature K	E (millivolt)
974	33.67	1235	50.18	1357	55.86
070	39.16	1235	50.34	1357	56.00
1080	39.58	1238	50.40	1374	56.92
1081	39.85	1255	50.90	1376	57.07
1085	41.43	1261	51.78	1396	58.67
1121	42.31	1264	52.24	1398	58.81
1144	43.74	1264	52.31	1407	59.51
1174	45.85	1318	53.42	1428	60.24
1176	45.91	1336	54.45	1450	60.58
1178	46.28	1356	55.78		

Table 7. Emf Data in MnO-CoO Solid Solution with N_{CoO}=0.400

Temperature K	E (millivolt)	Temperature K	E (millivolt)	Temperature K	E (millivolt)
870	25.20	1152	39.36	1341	48.64
921	27.85	1168	39.57	1364	48.84
951	29.54	1175	39.92	1382	49.72
981	30.83	1216	40.81	1402	50.69
1035	33.52	1248	44.20	1428	51.97
1085	36.37	1254	44.91	1438	52.46
1095	37.04	1256	45.01	1447	52.90
1148	38.99	1318	46.75		

Table 8. Emf Data in MnO-CoO Solid Solution with N_{CoO}=0.544.

Temperature K	E (millivolt)	Temperature K	E (millivolt)	Temperature K	E (millivolt)
997	22.89	1254	29.82	1346	31.51
1056	24.29	1257	29.84	1351	31.42
1077	24.83	1261	29.87	1359	31.57
1085	25.02	1267	29.93	1365	31.72
1095	25.24	1275	30.05	1373	31.90
1101	25.54	1280	30.14	1380	32.06
1112	25.92	1291	30.28	1382	32.21
1141	26.49	1298	30.46	1389	32.34
1153	26.79	1305	30.31	1399	32.62
1168	26.92	1311	30.58	1409	33.12
1185	27.67	1317	30.68	1415	33.26
1193	27.92	1321	31.00	1424	33.55
1200	28.02	1326	31.02	1430	33.72
1209	28.18	1328	30.91	1442	34.00
1215	28.27	1332	31.11	1447	34.18
1232	28.50	1334	31.24	1452	34.33
1240	28.72	1338	31.26	1459	34.50
1247	29.69	1344	31.40	1463	34.61

Table 9. Emf Data in MnO-CoO Solid Solution with N_{CoO}=0.648

Temperature K	E (millivolt)	Temperature K	E (millivolt)	Temperature K	E (millivolt)
907	14.71	1183	20.16	1342	22.84
920	15.11	1199	20.58	1357	22.91
949	15.34	1222	20.61	1363	23.07
993	15.60	1241	20.81	1374	23.21
1042	16.79	1260	21.18	1384	23.68
1051	16.88	1276	21.31	1400	24.20
1084	17.66	1286	21.39	1418	24.47
1090	18.02	1315	22.43	1427	24.68
1142	18.82	1335	22.54	1438	24.91
1165	18.92	1338	22.60	1449	25.21

during EMF measurements at a constant temperature, the cell was polarized occasionally for 2 second durations, by short circuiting the lead wires; after polarization the EMF would resume its equilibrium value in less than 5 minutes.

The typical durations for operating the EMF cell with a MnO-CoO solid solution sample of selected composition was about 2 weeks. At the end of this period the EMF furnace was cooled to room temperature, the cell was dismantled, and the composition of the sample was checked by the d_{200}-spacing measurements. In general, the samples retained their initial composition within ±0.001 mole fraction of CoO.

The EMF data given in Tables 5 to 9 are displayed graphically in Figure 16 in the form of EMF (millivolt) versus Temperature (K) plots. For all the samples studied, the data could be fitted into the following relationship:

$$E = A + BT + CT \ln T \qquad (35)$$

This equation assumes constant but non-zero values of the heat capacities Δc_p of cell reaction. The values of the parameter A, B, and C for each of the MnO-CoO solid solutions considered were determined by regression analysis and the temperature dependence of their EMF were obtained as summarized in Table 10.

The EMF equations given in table can be used to deduce the activities of CoO in MnO-CoO solid solutions at 1300 °C. This extrapolation is justified since no phase transformations occur in Co, CoO, and (Mn,Co)O solid solutions up to and

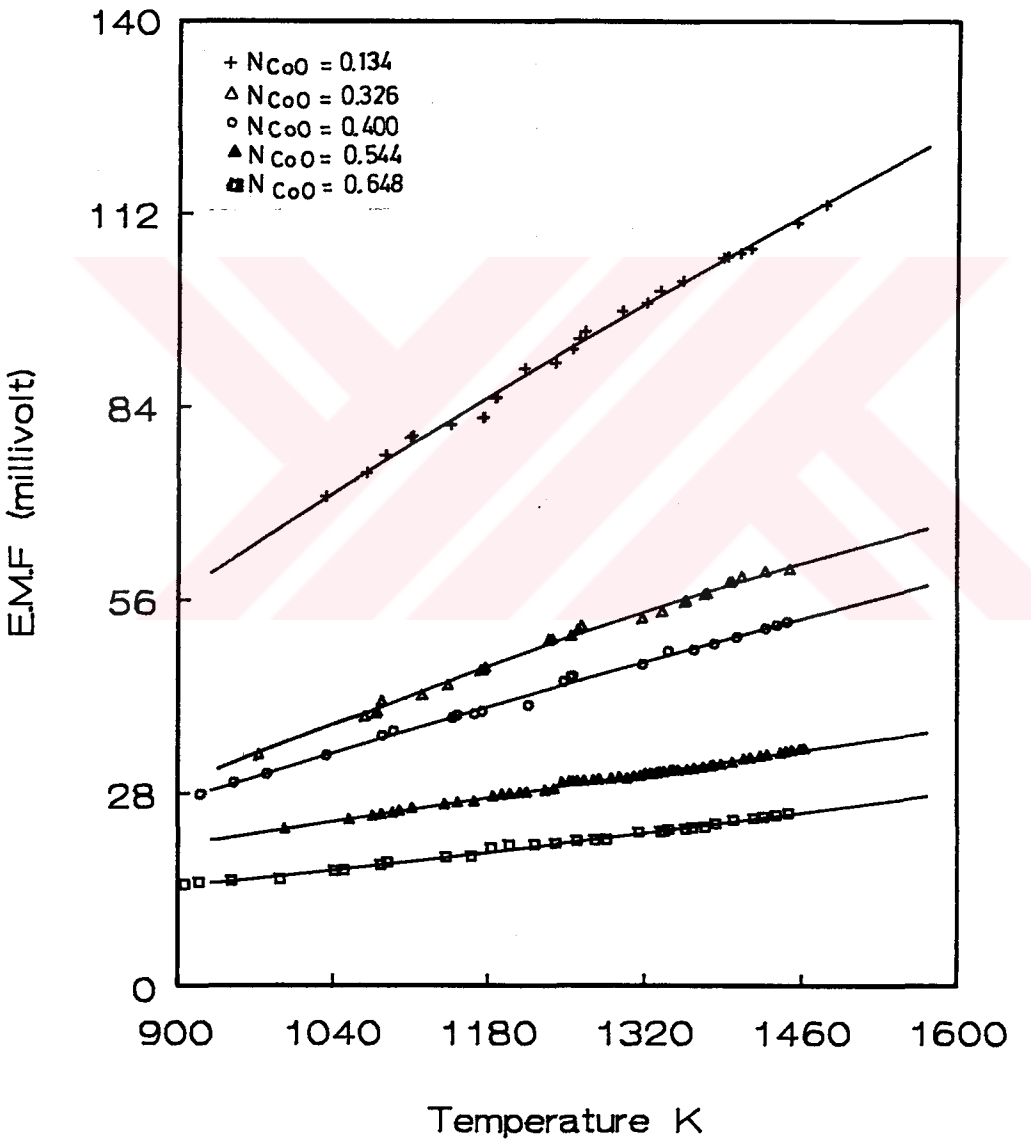


Figure 16. Variation of EMF (millivolt) with Temperature (K) .

Table 10. A Summary of E Values Obtained for the Solid Solutions Studied. The Values, A,B, and C Correspond to General Equation ;

$E(mV) = A + BT + CT\ln T$

Sample Composition (mole fraction)					1300 °C	
					E (millivolt)	a_{CoO}
N_{CoO}	N_{MnO}	A	B	C		
0.134	0.866	-72.739778	0.388490	$-3.598*10^{-2}$	121.7619	0.166
0.326	0.674	-92.748225	0.529336	$-5.8154*10^{-2}$	66.5625	0.374
0.400	0.600	-33.245029	0.170303	$1.5228*10^{-2}$	58.328	0.422
0.544	0.456	-5.884366	$5.29612*10^{-2}$	$-3.4941*10^{-3}$	37.010	0.579
0.648	0.352	9.007942	$-6.5486*10^{-2}$	$1.05216*10^{-2}$	27.822	0.663

beyond this temperature. The last column in Table 10 shows the cobalt oxide activities in the MnO-CoO solid solutions studied in EMF measurements. The activities of CoO so obtained are also shown in Figure 17 by bold circles. The activity-composition curve displayed for CoO in Figure 17 is constructed by joining the data from gas equilibration runs and emf measurements.

4.4. Activities of MnO in MnO-CoO Solid Solutions

The activities of CoO measured in MnO-CoO solid solutions at 1300 °C were joined by the smooth activity-composition curve in Figure 17. This curve was used to obtaine the MnO activities in the same solutions, first by solving for the activity coefficients, γ_{MnO} from the following relationship:

$$\ln \gamma_{MnO} = -N_{CoO} * N_{MnO} * \alpha_{CoO} - \int_{N_{MnO}=1}^{N_{MnO}=N_{MnO}} \alpha_{CoO} * dN_{MnO} \qquad (36)$$

Eqn.(36) is quite well-known in solution thermodynamics ; it is a result of the Gibbs-Duhem treatment using α-function method developed by Darken and Gurry [23]. The parameter α_{CoO} is defined as :

$$\alpha_{CoO} = \frac{\ln \gamma_{CoO}}{(1 - N_{CoO})^2} \qquad (37)$$

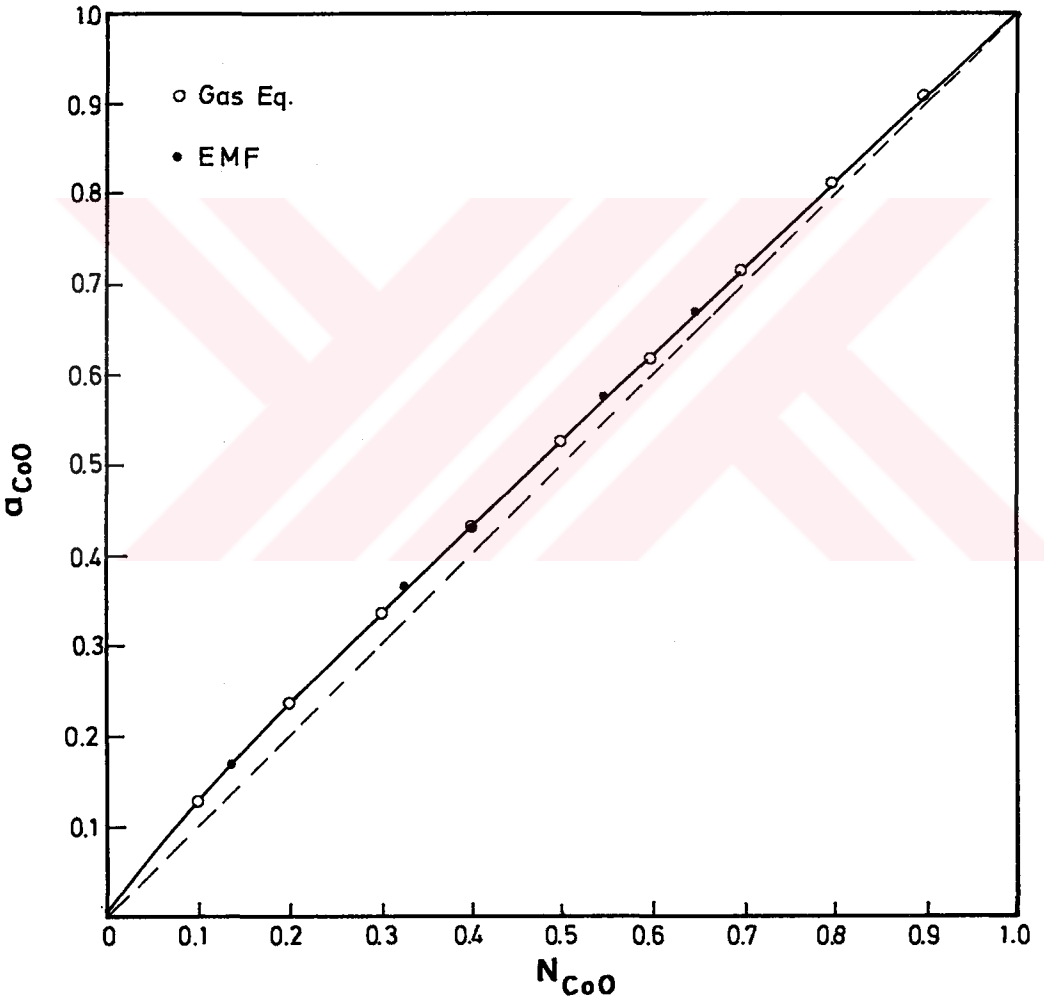


Figure 17. Activity of CoO as a Function of Composition in the MnO - CoO System at 1300°C.

where $\gamma_{CoO} = \frac{a_{CoO}}{N_{CoO}}$.

The values for α_{CoO} were obtained from the activity-composition plot given in Figure 17; these are listed in Table 11. Then, the integral in Eqn.(36) was evaluated graphically in order to solve for γ_{MnO} values given in table. The activities of MnO in MnO-CoO solid solutions were calculated from $a_{MnO} = \gamma_{MnO} * N_{MnO}$; these are listed in Table 11 and displayed in graphical form in Figure 18.

The CoO activities determined in the present study at 1300 °C in selected samples of MnO-CoO solid solutions are in very good agreement with the results reported earlier by Catlow et al.[15] and Paulsson [16]. The emf data of these investigators [15,16] could be extrapolated to 1300 °C, because no phase transformations occur either in Co or in (Mn,Co)O solid solutions [12] up to this temperature. The emf results of Catlow et al [15] and Paulsson [16] converted into CoO activities at 1300 °C are shown with bold circles and open squares in Figure 18, respectively.

4.5. The Stability Field of Manganese Chromite at 1300 °C

In order to establish the stability field of manganese chromite, along the $MnO-Cr_2O_3$ join, six samples were prepared and were equilibrated with a gas phase of $P_{O_2}=10^{-10}$ atm. for 48 hours at 1300 °C. This atmosphere was reducing

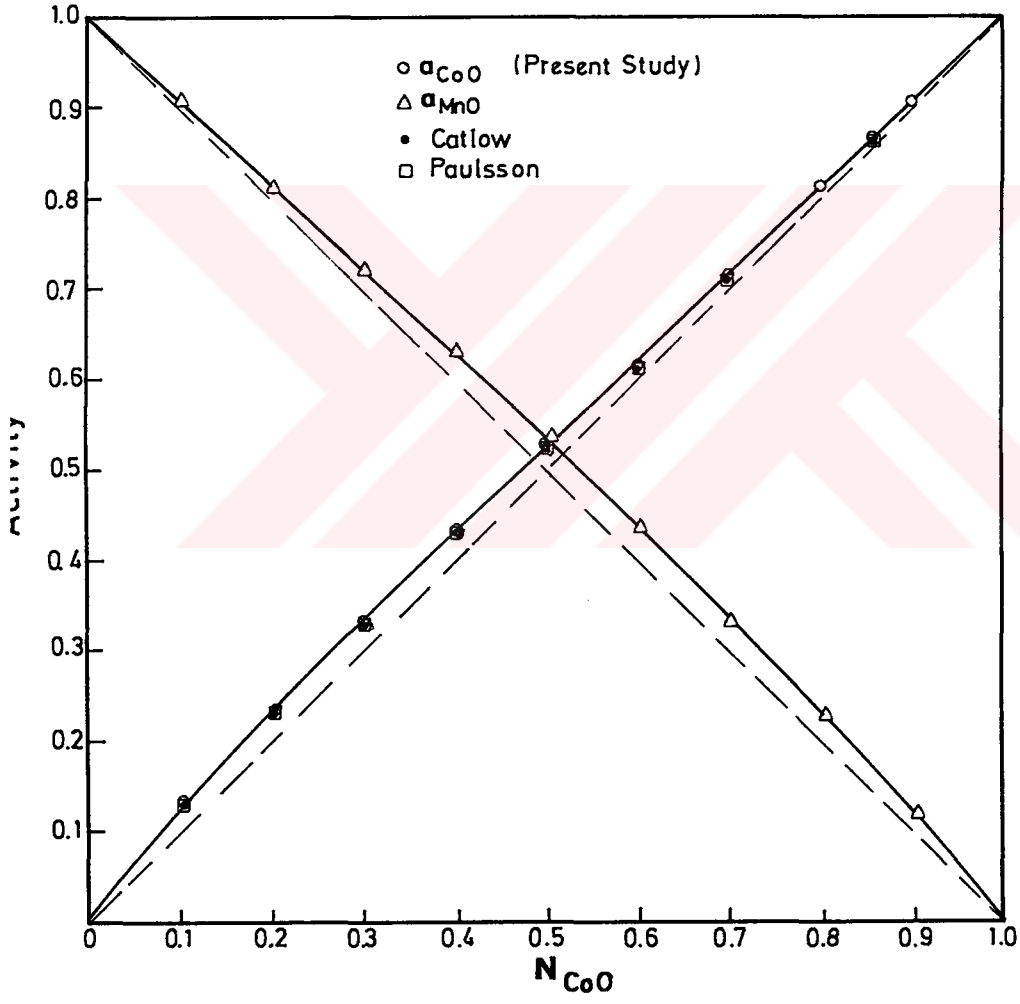


Figure 18. Activity of CoO and MnO as a Function of Composition in the MnO - CoO System at 1300°C.

Table 11. Activities of MnO in the MnO-CoO solid Solutions.

Sample Composition N_{CoO}	N_{MnO}	a_{CoO}	$\alpha_{CoO} = \frac{\ln\gamma_{CoO}}{(1-N_{CoO})^2}$	γ_{MnO}	a_{MnO}
0.10	0.90	0.123	0.2556	1.0026	0.9023
0.20	0.80	0.233	0.2386	1.0122	0.8097
0.30	0.70	0.334	0.2191	1.0275	0.7193
0.40	0.60	0.431	0.2073	1.0457	0.6274
0.50	0.50	0.524	0.1875	1.0696	0.5343
0.60	0.40	0.617	0.1746	1.0946	0.4378
0.70	0.30	0.714	0.2200	1.0006	0.3335
0.80	0.20	0.810	0.3106	1.1375	0.2275
0.90	0.10	0.905	0.5540	1.1875	0.1187

enough to keep all the manganese in divalent state without reduction to metallic form. [4]

The equilibrated samples were quenched to room temperature and the phases present in them were determined by X-ray diffraction. The compositions of the samples studied and the results of phase identification are given in Table 12. The relevant x-ray diffraction diagrams are shown in Figure 19. In accordance with these results, manganese chromite appears as a solid solution phase extending from N_{MnO}=0.500 to N_{MnO}=0.550 at 1300 °C. Thus, $MnCr_2O_4$ in equilibrium with Cr_2O_3 is stoichiometric, whereas the compound dissolves considerable excess of MnO when in contact with manganese oxide under reducing conditions.

4.6. The Stability Field of Cobalt Chromite

As mentioned earlier in Section 2.4. the terminal solid solubilities of CoO in Cr_2O_3 and Cr_2O_3 in CoO in solid state are negligible. In the CoO-Cr_2O_3 system the spinel compound $CoCr_2O_4$ exists with unknown limits of non-stoichiometry with respect to both CoO and Cr_2O_3. Jacob and Fitzner [19], in their studies on the MnO-CoO-Cr_2O_3 system at 1100 °C, noted that $CoCr_2O_4$ might dissolve excess Cr_2O_3 but the compound would be perfectly stoichiometric with respect to CoO, i.e, it would not contain any excess or deficit of CoO.

In the present study, experiments were done along the CoO-Cr_2O_3 join of the system in order to generate information regarding any possible deviation

Table 12 . Phases Present in the Samples Along the MnO-Cr_2O_3 Join, at 1300 °C under $P_{O_2}=10^{-10}$ atm.

Sample No	Sample Composition (mole fraction)		Phases Present After Equilibration
	N_{MnO}	$N_{Cr_2O_3}$	
30	0.46	0.54	Manganese Chromite + Cr_2O_3
29	0.48	0.52	Manganese Chromite + Cr_2O_3
25	0.50	0.50	Manganese Chromite
26	0.54	0.46	Manganese Chromite
27	0.56	0.44	Manganese Chromite + MnO
28	0.58	0.42	Manganese Chromite + MnO

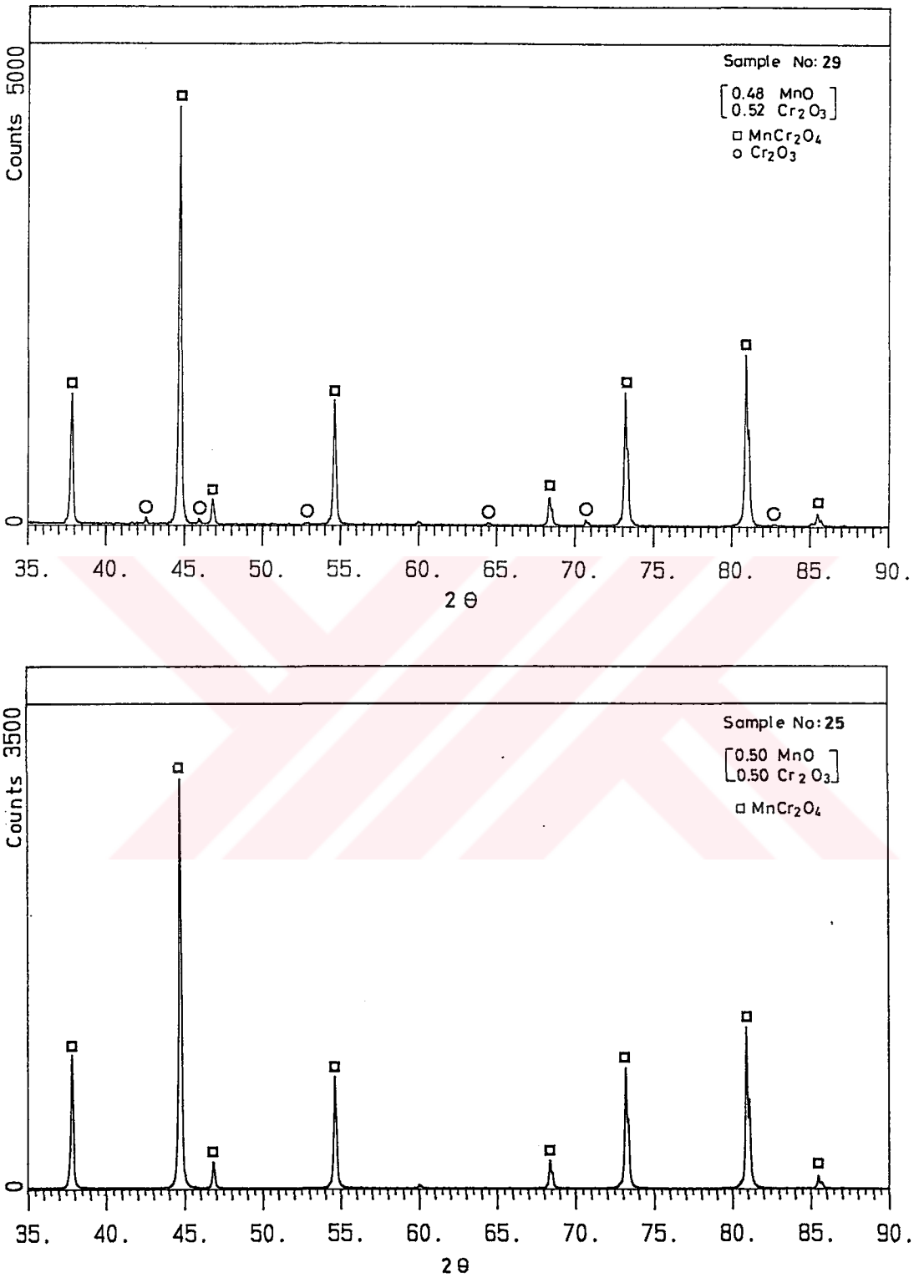


Figure 19. X-ray Diffraction Pattern of the Samples along the MnO-Cr_2O_3.

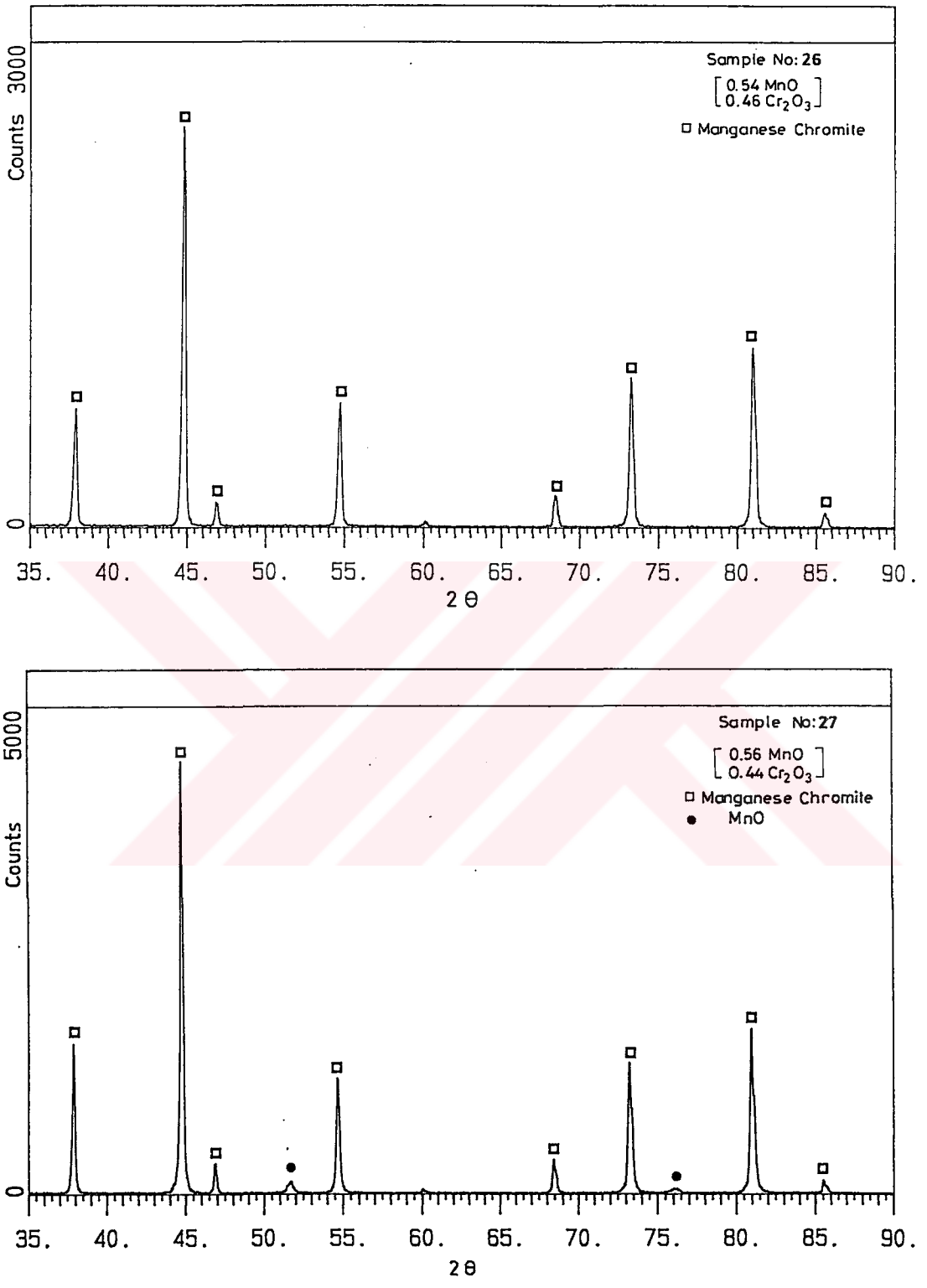


Figure 19. (continued)

from stoichiometry in the $CoCr_2O_4$ compound at 1300 °C. For this purpose, a series of CoO-Cr_2O_3 samples were prepared along the join with compositions as indicated in Table 13. These samples were equilibrated with a gas phase having $P_{O_2}=10^{-8}$ atm, each for 72 hours, at 1300 °C. The samples were then quenched to room temperature and the phases present were examined by optical microscopy and by x-ray diffraction.

$CoCr_2O_4$ has poor sinterability, furthermore because of similar reflectivities and fine grained structure, it was impossible to identify different phases under microscope. On the other hand, x-ray diffraction on powders of quenched samples gave some evidence on the extended stability region of $CoCr_2O_4$ towards the CoO corner at 1300 °C; Table 13 shows the results of these x-ray diffraction determinations. According to the results of XRD work, shown in Figure 20, the spinel compound $CoCr_2O_4$ was perfectly stoichiometric with respect to Cr_2O_3 but it would dissolve a small excess of CoO towards the CoO corner. Thus, the stability field for $CoCr_2O_4$ would extend from $N_{CoO}=0.50$ to $N_{CoO}=0.515$ at 1300 °C, meaning that $CoCr_2O_4$ would exist as a solid solution field in this region.

In order to verify the results of XRD studies, limits of non-stoichiometry in $CoCr_2O_4$ were also determined thermodynamically by measuring the activities of CoO in the same samples sited in Table 13. The reaction considered was:

$$Co + 1/2\ O_2 = (CoO)_{sp} \qquad (38)$$

Table 13. Phases Determined by XRD work in the Samples along the CoO-Cr_2O_3 Join. (T=1300°C ,P_{O_2} = 10^{-8} atm.)

Sample No	Sample Composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	Present Phases After Equilibration
35	0.400	0.600	Cobalt Chromite + Cr_2O_3
36	0.480	0.520	Cobalt Chromite + Cr_2O_3
19	0.500	0.500	Cobalt Chromite
59	0.505	0.495	Cobalt Chromite
60	0.510	0.490	Cobalt Chromite
37	0.520	0.480	Cobalt Chromite + CoO
38	0.54	0.46	Cobalt Chromite + CoO

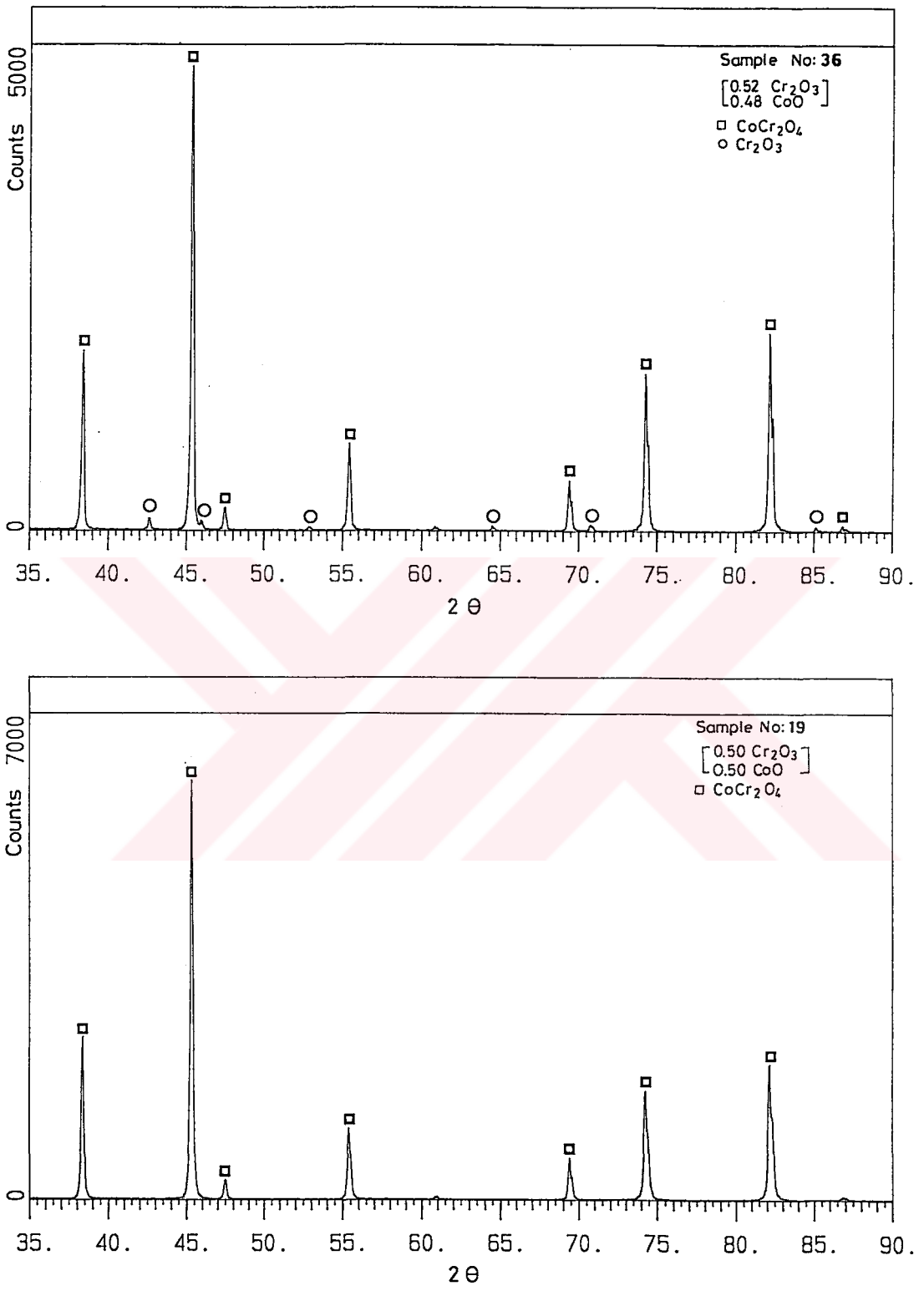


Figure 20. X-ray Diffraction Pattern of the Samples along the CoO-Cr_2O_3.

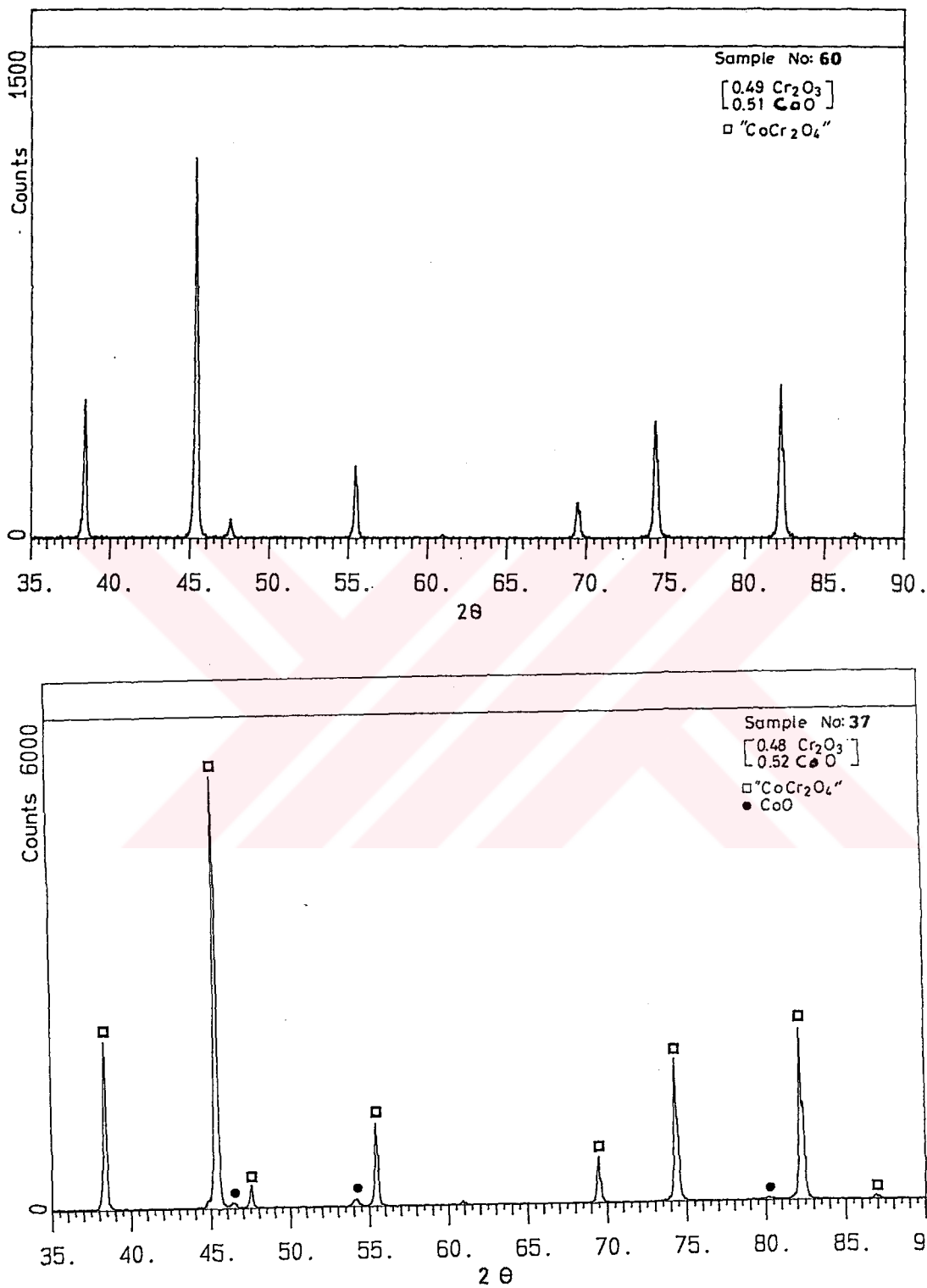


Figure 20. (continued)

where sp denotes CoO in the CoO-$CoCr_2O_4$ solid solutions. The partial pressures of oxygen for the start of metallic cobalt precipitation in samples of Table 13 were determined by equilibrations with CO_2-H_2 gas atmospheres at 1300 °C. The procedure was similar to that described in Section 4.3.1. for MnO-CoO solid solutions. The experimental data concerning these equilibration runs are given in Table 14.

Data on the partial pressures of oxygen in equilibrium with metallic cobalt and CoO-Cr_2O_3 samples in Table 14 were used to calculate the activities of CoO, from Eqn.(29), in the phase assemblages of these samples. The results on CoO activities are summarized in Table 15 and displayed graphically by the bold curve in Fig. 21. In this figure, the region where the CoO activity remains constant at 0.056 corresponds to the presence of this phases Cr_2O_3 + $CoCr_2O_4$. while passing the composition N_{CoO}=0.5 which represents the stoichiometric $CoCr_2O_4$, the activity curve exhibits a sharp inflection.

In the narrow composition range N_{CoO}=0.50 to N_{CoO}=0.51, the CoO activity exhibits a rather fast rise with composition from a_{CoO}=0.056 to a_{CoO} = 1.0. Within this region the cobalt spinel "$CoCr_2O_4$" with increasing amounts of CoO in its structure is the stable phase . At N_{CoO} = 0.51 the spinel becomes saturated with CoO, the formula for the saturated compound can be written as $Co_{1.030}Cr_{1.919}O_4$.

The activities of Cr_2O_3 in the cobalt chromite solid solution were calculated by a Gibbs-Duhem integration according to the equation;

Table 14. Data Obtained in Gas Equilibration Runs in the System CoO-Cr_2O_3 at 1300°C.

Sample No	Sample composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	Imposed Gas Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
35	0.40	0.60	0.376	11.2876	SS + Co
			0.387	11.2571	SS + Co
			0.397	11.2277	SS + Co
			0.408	11.1992	SS + Co
			0.440	11.1189	SS + Co
			0.622	10.7333	SS + Co
			0.637	10.7160	SS + Co
			0.663	10.6555	SS
36	0.48	0.52	0.840	10.3866	SS
			0.743	10.5298	SS
			0.666	10.6550	SS
			0.631	10.7171	SS + Co
19	0.50	0.50	0.386	11.2571	SS + Co
			0.395	11.2277	SS + Co
			0.404	11.1991	SS + Co
			0.415	11.1716	SS + Co
			0.424	11.1448	SS + Co
			0.637	10.7160	SS + Co

Table 14. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	Imposed Gas Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
19	0.50	0.50	0.663	10.6565	SS
			0.675	10.6402	SS
			0.735	10.5428	SS
37	0.52	0.48	7.000	8.1152	SS
			6.663	8.1616	SS
			6.604	8.1644	SS
			6.446	8.1932	SS + Co
38	0.54	0.46	6.762	8.1475	SS
			6.604	8.1712	SS
			6.441	8.1941	SS + Co
58	0.75	0.25	6.604	8.1712	SS
			6.446	8.1933	SS + Co
			6.058	8.2534	SS + Co
59	0.505	0.495	6.604	8.1712	SS
			1.706	9.5669	SS
			1.522	9.7008	SS + Co
			1.381	9.8096	SS + Co
			1.290	9.8896	SS + Co
			1.225	9.9474	SS + Co

Table 14. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	Imposed Gas Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
60	0.51	0.49	6.604	8.1712	SS
			6.444	8.1933	SS + Co
			6.058	8.2534	SS + Co

SS : Spinel Solid Solution or Spinel Solid Solution + Oxide Solution

Co : Metallic Cobalt Precipitate.

Table 15. Activities of CoO as a Function of Composition along the CoO - Cr_2O_3 Join at 1300°C.

Sample No	Sample Composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	Equilibrium $-\log P_{O_2}$	Cobalt Oxide Activity a_{CoO}
35	0.400	0.600	10.6850	0.056
36	0.480	0.520	10.6850	0.056
19	0.500	0.500	10.6850	0.056
59	0.505	0.495	9.6290	0.189
60	0.510	0.490	8.1819	1.000
37	0.520	0.480	8.1819	1.000
38	0.540	0.460	8.1819	1.000
58	0.750	0.250	8.1819	1.000

$$\log a^{II}_{Cr_2O_3} = \log a^{I}_{Cr_2O_3} - \int_{a^{I}_{CoO}}^{a^{II}_{CoO}} \frac{n_{CoO}}{n_{Cr_2O_3}} d\log a_{CoO} \qquad (39)$$

where $\log a^{I}_{Cr_2O_3}$ was set to equal zero at the boundary where spinel phase is in equilibrium with Cr_2O_3. The results of the integration of Eqn.(39) are listed in Table 16 and the variation of chromium oxide activities with respect to composition is shown in Figure 21.

The result of XRD work and thermodynamic determination of the stability region for cobalt-chromium spinel refute clearly the earlier assumptions made by Jacob and Fitzner [19] regarding the stability field of this compound.

4.7. The Standard Free Energy of Formation of $CoCr_2O_4$

The results given in Table 16 and Figure 21 could be used to calculate the standard free energy of formation of the stoichiometric spinel compound $CoCr_2O_4$ from its component oxides, CoO and Cr_2O_3. Considering the following formation reaction :

$$CoO + Cr_2O_3 = CoCr_2O_4 \qquad (11)$$

The standard free energy change of the above reaction can be written as :

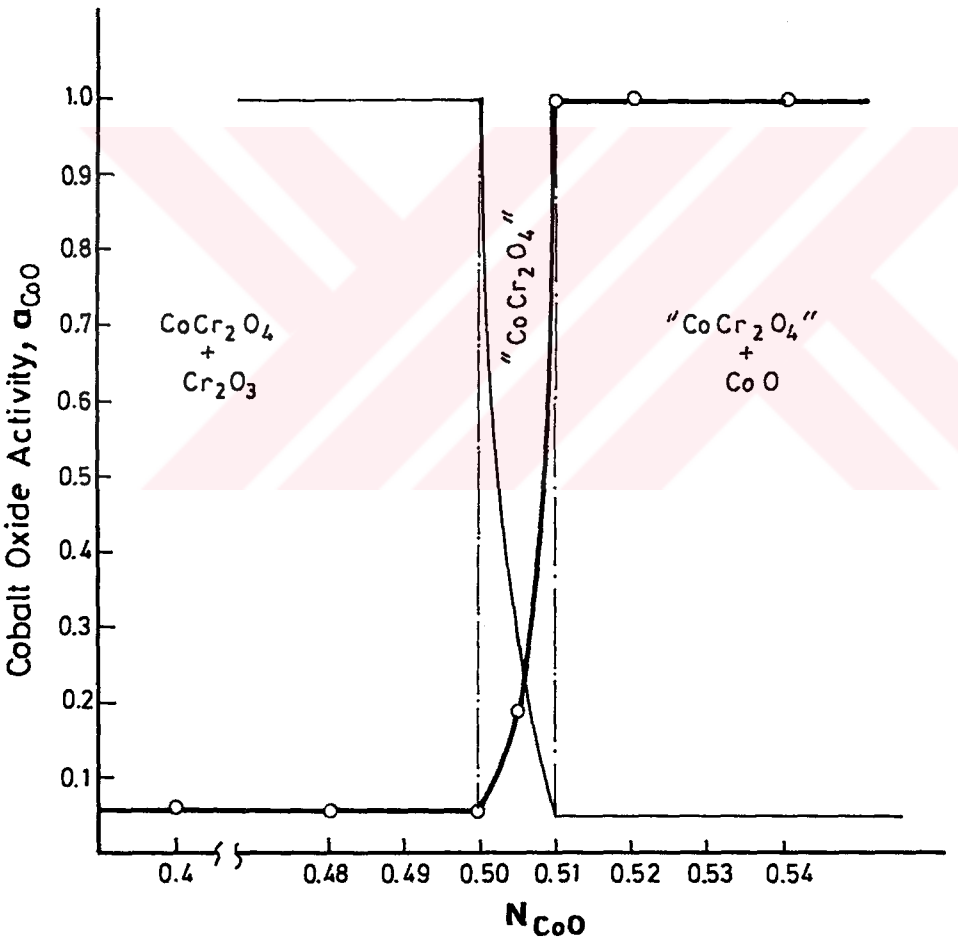


Figure 21. Activities of CoO and Cr_2O_3 along the Join Cr_2O_3 - CoO at 1300 °C.

$$\Delta G_{11} = -RT\ln \frac{a_{CoCr_2O_4}}{a_{CoO} \cdot a_{Cr_2O_3}} \qquad (40)$$

Referring to Figure 21 ; at the stoichiometric spinel composition we have :

$$a_{CoO} = 0.056,\ a_{Cr_2O_3} = 1,\ \text{and}\ a_{CoCr_2O_4} = 1.$$

$a_{Cr_2O_3}$ could be taken as unity because Cr_2O_3 in equilibrium with the spinel is essentially pure. By inserting these value into Eqn.(40), following value was obtained for $\Delta G^o_{CoCr_2O_4}$ at 1300 °C.

$$\Delta G^o_{CoCr_2O_4} = RT\ln a_{CoO} = 8.314*1573*\ln 0.056 = -37636\ \text{J/mole}.$$

The accuracies of measured CoO activities, and hence the activities of other components derived by Gibbs-Duhem treatment of a_{CoO} data are effected mainly by the errors involved in P_{O_2} values. The log P_{O_2} values reported in various tables of this thesis are estimated to be correct to less than ±0.010; this estimate is based on the possible errors of reading the heights of the manometer liquids of the gas mixer. As explained in Section 4.3 cobalt oxide activities were calculated from the expression:

$$a_{CoO} = \left(\frac{P_{O_2}}{P^*_{O_2}} \right)^{\frac{1}{2}} \qquad (29)$$

Thus the error expression for a_{CoO} would be:

$$\Delta a_{CoO} = \frac{1}{2} a_{CoO} (\Delta \log P_{O_2}) \qquad (41)$$

Eqn.(41) can be used to calculate errors involved in various values of a CoO. A critical cobalt oxide activity, for example, is 0.056, this value affects the standard free energy of formation of $CoCr_2O_4$, and it also affects the activity- composition relations in $MnCr_2O_4$-$CoCr_2O_4$ solid solutions. From Eqn.(41), the error in a_{CoO}=0.056 can be calculated as follows:

$$\Delta a_{CoO} = 1/2 * (0.056) * (0.010) = 0.00028$$

Hence, the gas mixing system permits to measure low CoO activities with high accuracy. The error reflected upon ΔG^o of $CoCr_2O_4$ at 1300 °C would be :

$$\Delta G^o = \Delta(RT \log a_{CoO})$$
$$= RT\, \Delta(\log a_{CoO})$$
$$= RT\, \Delta a_{CoO}/a_{CoO}$$
$$= 150 \text{ J/ mole.}$$

When the error in temperature is also taken into consideration, the error equation becomes:

$$\Delta(\Delta G^o) = R\left(\Delta T \cdot \log a_{CoO} + T \frac{\Delta a_{CoO}}{a_{CoO}} \right) \qquad (42)$$

In the present study, the temperatures were measured and controlled with an estimated accuracy of ±2 °C. At 1300 °C based on a maximum error of 2 °C in temperature, the overall error in ΔG^o of $CoCr_2O_4$ will be:

$\Delta(\Delta G^o) = \pm 197$ J/mole

Thus, according to the present results, the standard free energy of formation of the cobalt chromite compound from its pure component oxides is -37636 ± 197 J/mole.

Apart from quantitative errors involved in the measurement of CoO activities mentioned above, an additional source of error is involved in the interpretation of metallographic specimens. If the starting pellets are inhomogeneous, the cobalt precipitates appear as localized clusters. In homogeneous samples, on the other hand, cobalt precipitation occurs uniformly throughout the specimen section. In this work, the samples showing clusters of cobalt precipitates were discarded and new pellets were prepared in order to eliminate the uncertainties originating from inhomogeneous samples.

The free energy of formation of "$CoCr_2O_4$" from CoO and Cr_2O_3 was evaluated by using the values of a_{CoO} and $a_{Cr_2O_3}$ from Table 16 in the following equation ;

$$\Delta G_{"CoCr_2O_4"} = RT\ln(a_{CoO} \cdot a_{Cr_2O_3})$$

The calculated values are given in the last coloumn of Table 16.

Table 16. Activities of Cr_2O_3 as a Function of Composition along the CoO -Cr_2O_3 Join at 1300°C and Free Energy of Formation of $CoCr_2O_4$ from Its Oxide Component.

Sample Composition (mole fraction)					-log		-ΔG
$N_{Cr_2O_3}$	N_{CoO}	a_{CoO}	-log a_{CoO}	$\frac{n_{CoO}}{n_{Cr_2O_3}}$	$a_{Cr_2O_3}$	$a_{Cr_2O_3}$	kJ/mole
0.500	0.500	0.056	1.252	1.0000	0.0000	1.000	37.636
0.499	0.501	0.080	1.097	1.0040	0.1553	0.699	37.714
0.498	0.502	0.100	1.000	1.0080	0.2529	0.559	37.719
0.497	0.503	0.120	0.921	1.0120	0.3327	0.465	37.748
0.496	0.504	0.150	0.824	1.0161	0.4310	0.371	37.792
0.495	0.505	0.189	0.724	1.0202	0.4328	0.293	37.833
0.494	0.506	0.240	0.620	1.0243	0.4391	0.230	37.912
0.493	0.507	0.300	0.523	1.0284	0.7387	0.183	37.991
0.492	0.508	0.500	0.301	1.0325	0.9675	0.108	38.195
0.491	0.509	0.600	0.221	1.0366	1.0503	0.089	38.317
0.490	0.510	1.000	0.00	1.0408	1.2798	0.053	38.416

The information available in the literature on $\Delta G^{o}_{CoCr_2O_4}$ is scattered. For example, at the temperature of present investigation the free energy of formation for cobalt chromite in accordance with Eqn.11 is -23.430 kJ/mole from Kunnmann, Rogers, and Wold [17], -42.984 kJ/mole from Tretjakow and Schmalzried [9], and -46.206 kJ/mole from Kubaschewski's suggestion [20]. The earliest data provided by Kunnmann, Rogers, and Wold [17] seem to be in gross conflict with later determinations owing, probably, to the data then available on the free energy of formation of CoO which has seen several modifications later on. Tretjakow and Schmalzried [9] measured the free energy of formation of "$CoCr_2O_4$" in equilibrium with CoO, their emf measurements might have suffered from the polarization effects [26,27].

4.8. The Stability Field of Ternary Spinel Solutions

From the results presented in Sections 4.5 and 4.6 on the stability regions of $MnCr_2O_4$ and $CoCr_2O_4$, the existence of a solid solution field for ternary spinels was anticipated in the MnO-CoO-Cr_2O_3 system. This ternary solution region with approximate phase boundaries is shown in Figure 22. with the hatched area. The upper boundary represents the compositions of ternary spinel solutions that are saturated with essentially pure Cr_2O_3. The lower boundary is the locus of points at which spinel solutions are in equilibrium with MnO-CoO solid solutions of variable composition ; this boundary starts from N_{MnO}=0.55 along, the MnO-Cr_2O_3 join and terminates at N_{CoO}= 0.51 at the CoO-Cr_2O_3 binary.

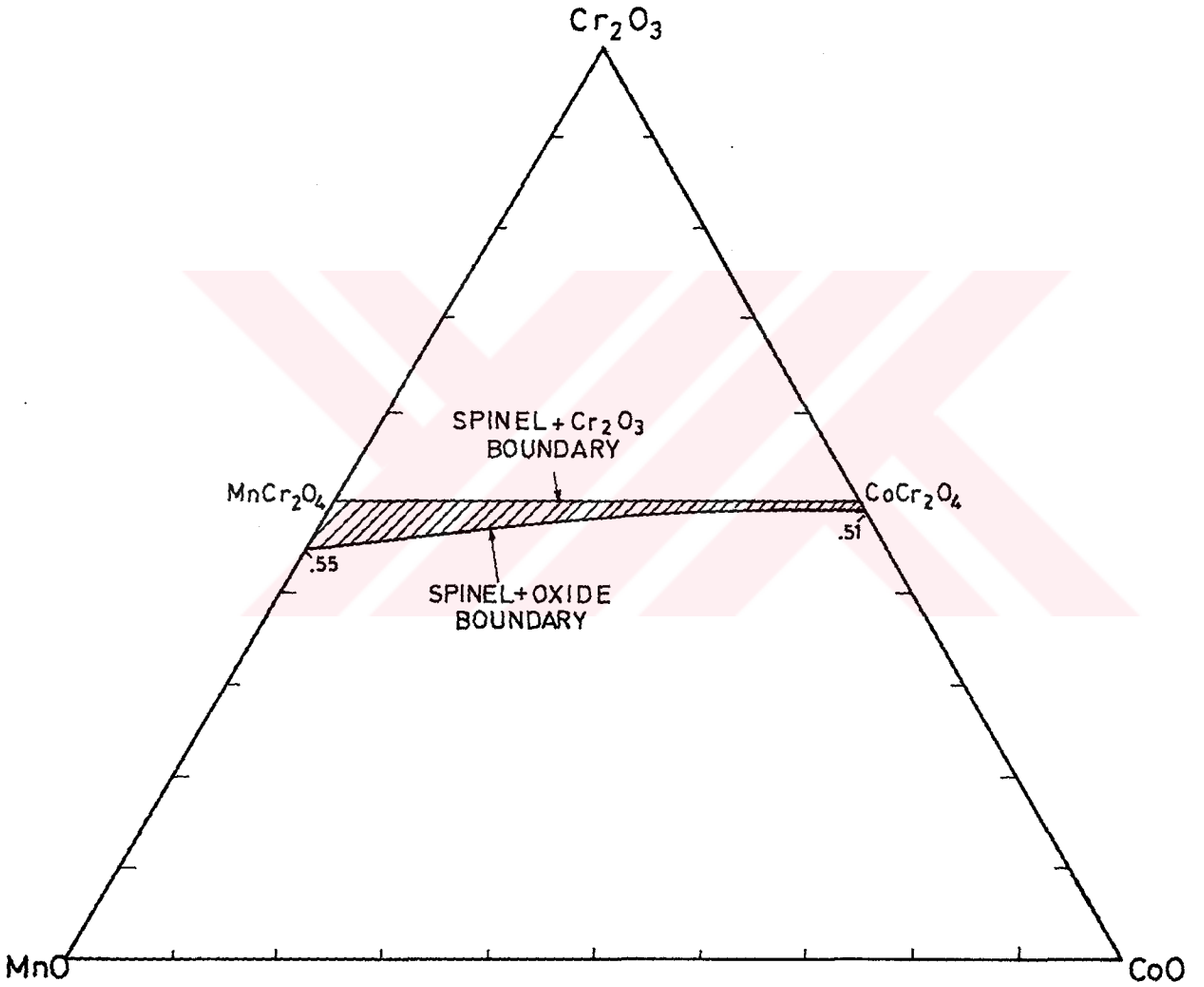


Figure 22. The Approximate Location of the Ternary Spinel Field in the MnO -CoO - Cr_2O_3 system at 1300 °C.

In order to determine the exact locations of the spinel field boundaries 25 samples were prepared in the MnO-CoO-Cr_2O_3 ternary with compositions given in Table 17. The compositions selected are shown also in Figure 23 to help visualize their location. Each one of these samples were equilibrated with a gas phase of $P_{O_2}=10^{-8}$ atm, for 48 hours at 1300 °C. After equilibration, the samples were quenched to room temperature and the phases present in them were determined by x-ray diffraction. As will be discussed, in a later section, identification of the phase boundaries were also supplemented by thermodynamic activity measurements.

The phases determined by XRD in the 25 quenched samples of Table 17 are shown in the last column of the table. The XRD patterns of these are given in Figure 24.

The samples numbered from 39 to 43 in Table 17 were located in composition slightly above the $MnCr_2O_4$-$CoCr_2O_4$ join. The quenched phases in all these samples were Spinel + Cr_2O_3. The samples numbered from 20 to 24 were located exactly on the line connecting $MnCr_2O_4$ and $CoCr_2O_4$ compositions ; all these contained single spinel phase. Since no evidence for excess Cr_2O_3 dissolution was found, the upper boundary of the spinel field was affirmed as the $MnCr_2O_4$-$CoCr_2O_4$ join.

Sample pairs (49,54), (50,56), (61,46), (21,45), and (20,44) served to delineate the lower boundary. XRD patterns of the first members of these pairs contained spinel only, and trace amount of MnO-CoO solid solution appeared as the additional phase in the patterns of the second members. Samples marked 51, 52,53,55, and 57 contained more of (Mn,Co)O as the second phase. Thus,Spinel +

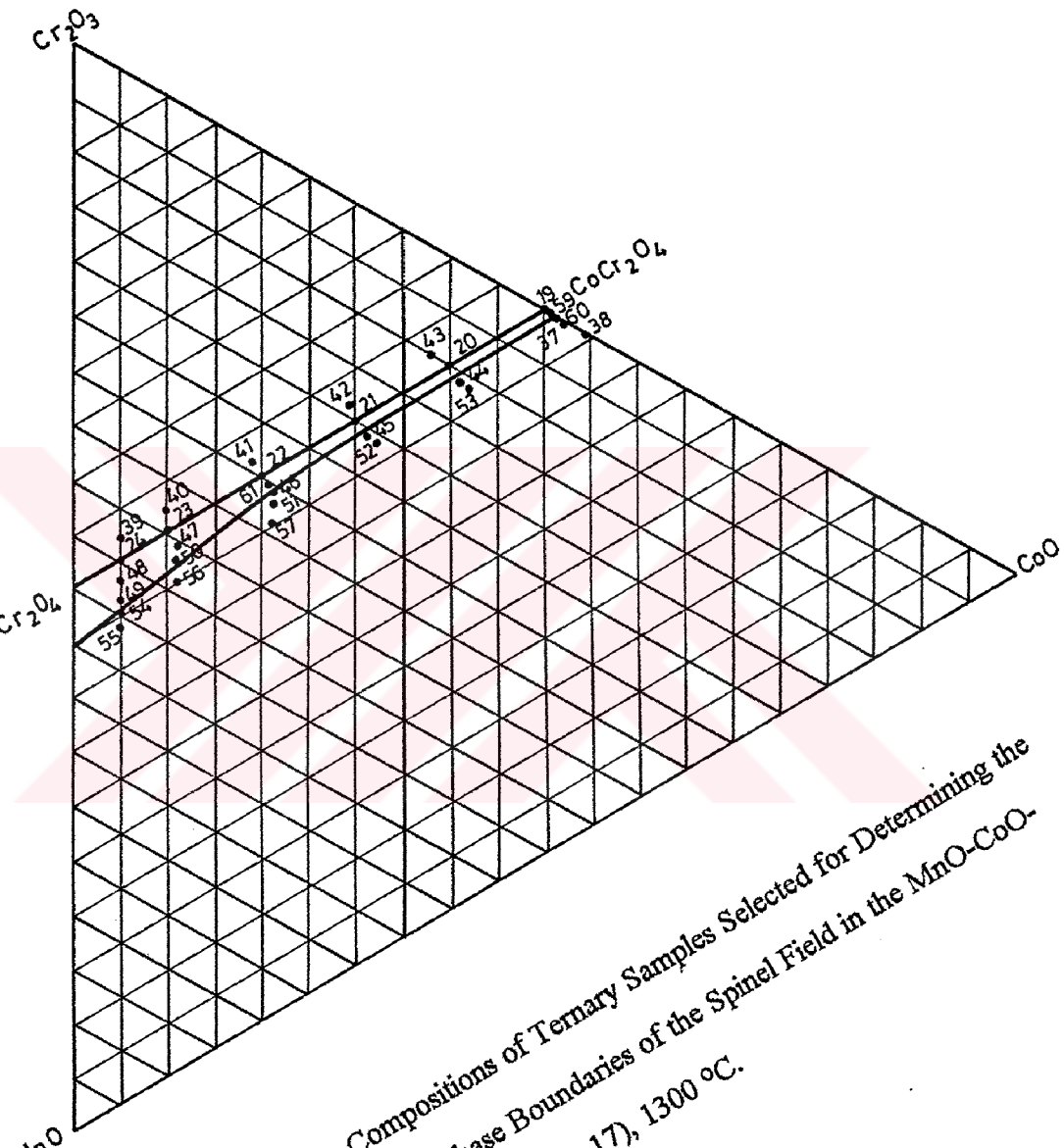


Figure 23. The Compositions of Ternary Samples Selected for Determining the Location of Phase Boundaries of the Spinel Field in the MnO-CoO-Cr_2O_3.(Compare Table 17), 1300 °C.

Table 17. Phases Present in the Samples in the MnO-CoO-Cr_2O_3 Ternary.

(T=1300°C, $P_{O_2}=10^{-8}$atm.)

Sample No	Sample Composition (mole fraction)			Phases Present After Equilibration
	N_{MnO}	N_{CoO}	$N_{Cr_2O_3}$	
39	0.43	0.05	0.52	Spinel Solution + Chromium Oxide
24	0.45	0.05	0.50	Spinel Solution
48	0.47	0.05	0.48	Spinel Solution
49	0.49	0.05	0.46	Spinel Solution
54	0.50	0.05	0.45	Spinel Solution + Oxide Solution
55	0.51	0.05	0.44	Spinel Solution + Oxide Solution
40	0.38	0.10	0.52	Spinel Solution + Cr_2O_3
23	0.40	0.10	0.50	Spinel Solution
47	0.41	0.11	0.48	Spinel Solution
50	0.42	0.11	0.47	Spinel Solution
56	0.44	0.11	0.45	Spinel Solution + Oxide Solution
41	0.29	0.19	0.52	Spinel Solution + Cr_2O_3
22	0.30	0.20	0.50	Spinel Solution
61	0.30	0.21	0.49	Spinel Solution
46	0.31	0.21	0.48	Spinel Solution + Oxide Solution
51	0.32	0.21	0.47	Spinel Solution + Oxide Solution
57	0.33	0.22	0.45	Spinel Solution + Oxide Solution
42	0.19	0.29	0.52	Spinel Solution + Cr_2O_3
21	0.20	0.30	0.50	Spinel Solution
45	0.21	0.31	0.48	Spinel Solution + Oxide Solution
52	0.21	0.32	0.47	Spinel Solution + Oxide Solution
43	0.10	0.38	0.52	Spinel Solution + Cr_2O_3
20	0.10	0.40	0.50	Spinel Solution
44	0.11	0.41	0.48	Spinel Solution + Oxide Solution
53	0.11	0.42	0.47	Spinel Solution + Oxide Solution

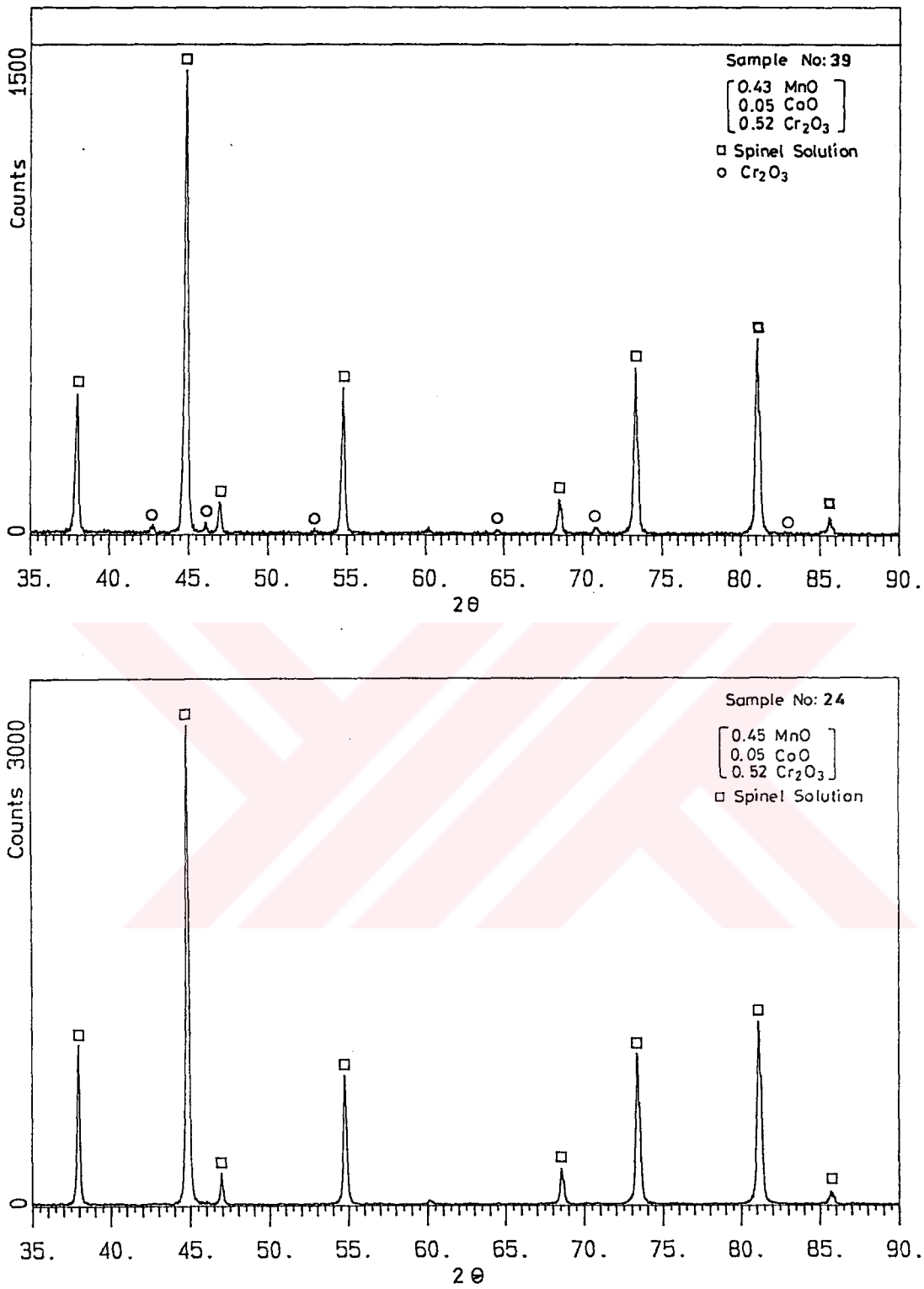
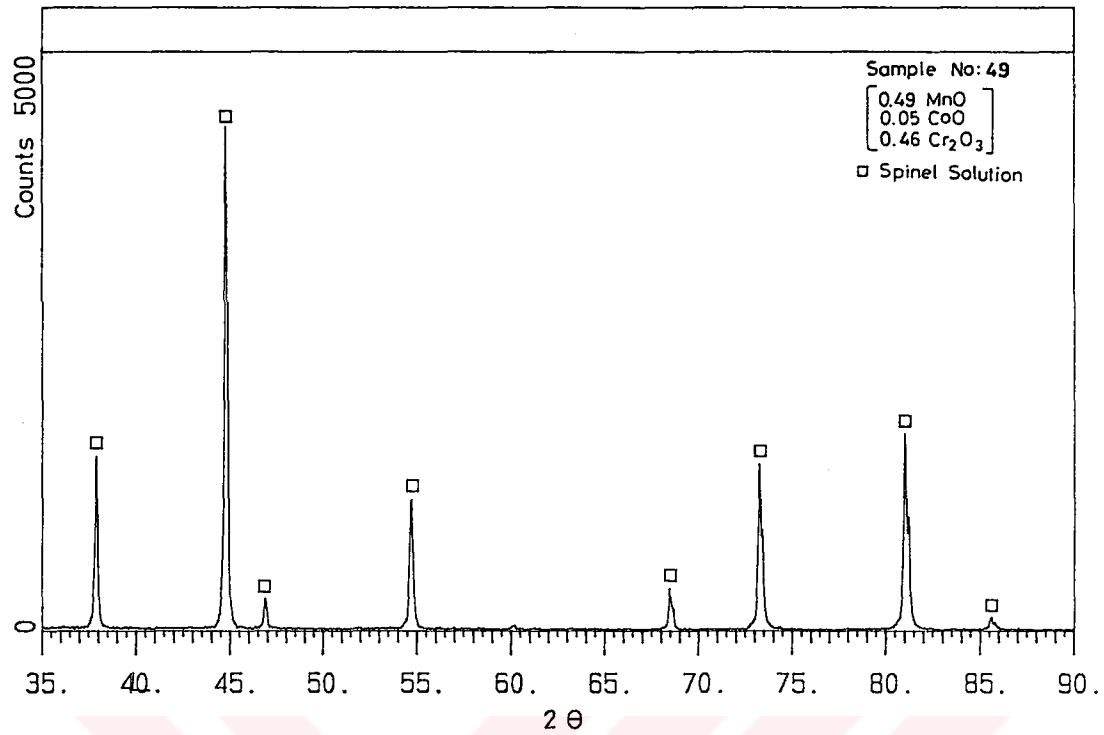


Figure 24 . X-ray Diffraction Patterns of the Quenched Samples of Table 17.



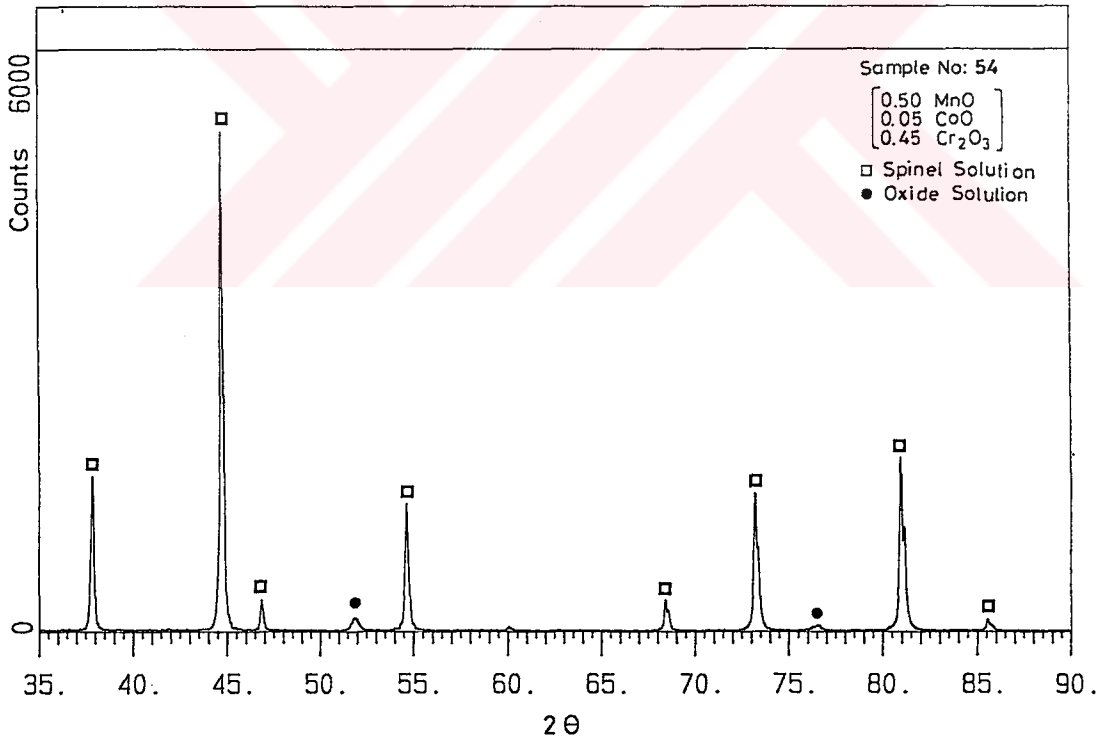
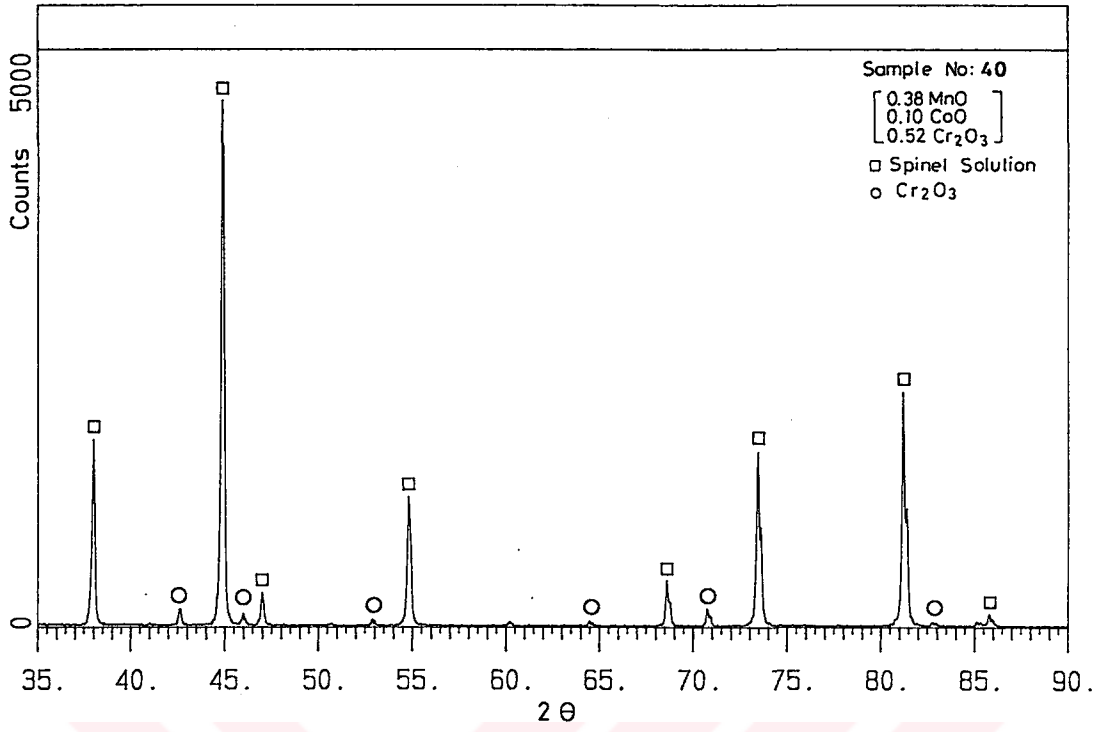
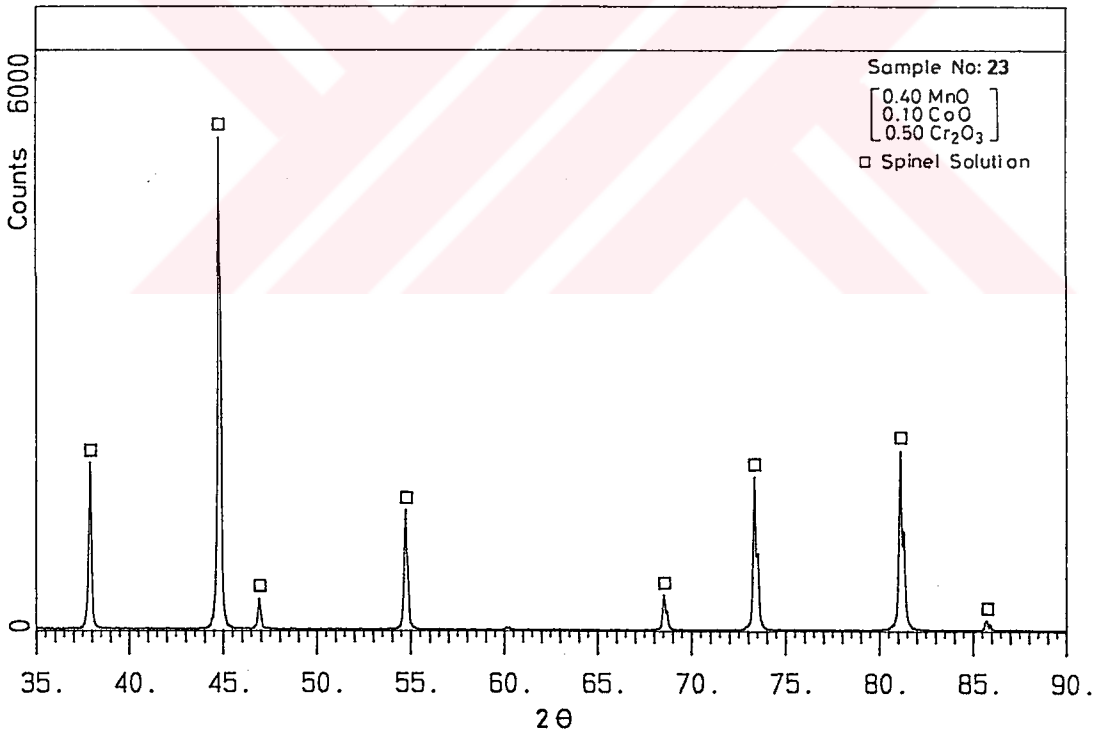


Figure 24 . (continued)





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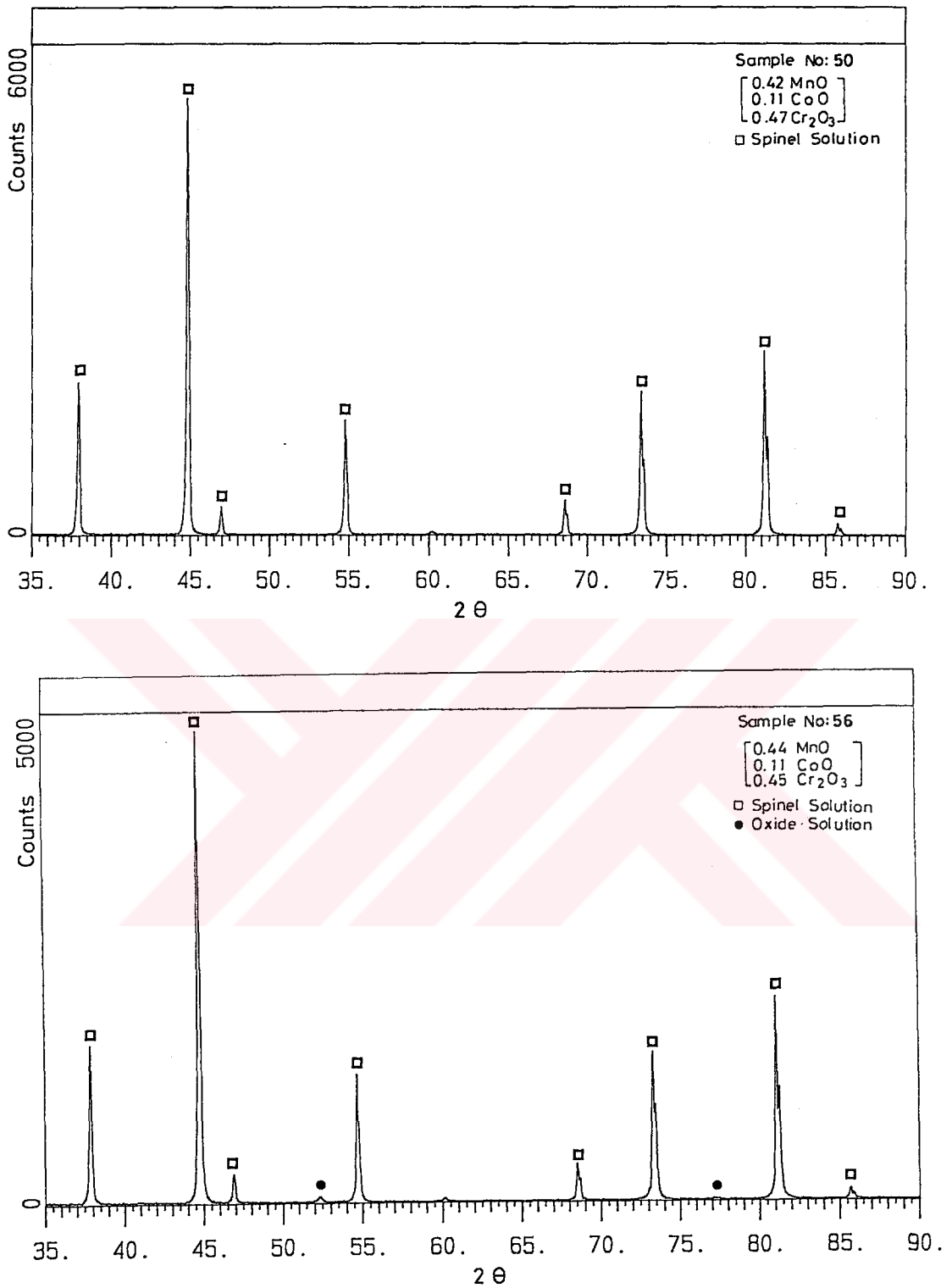

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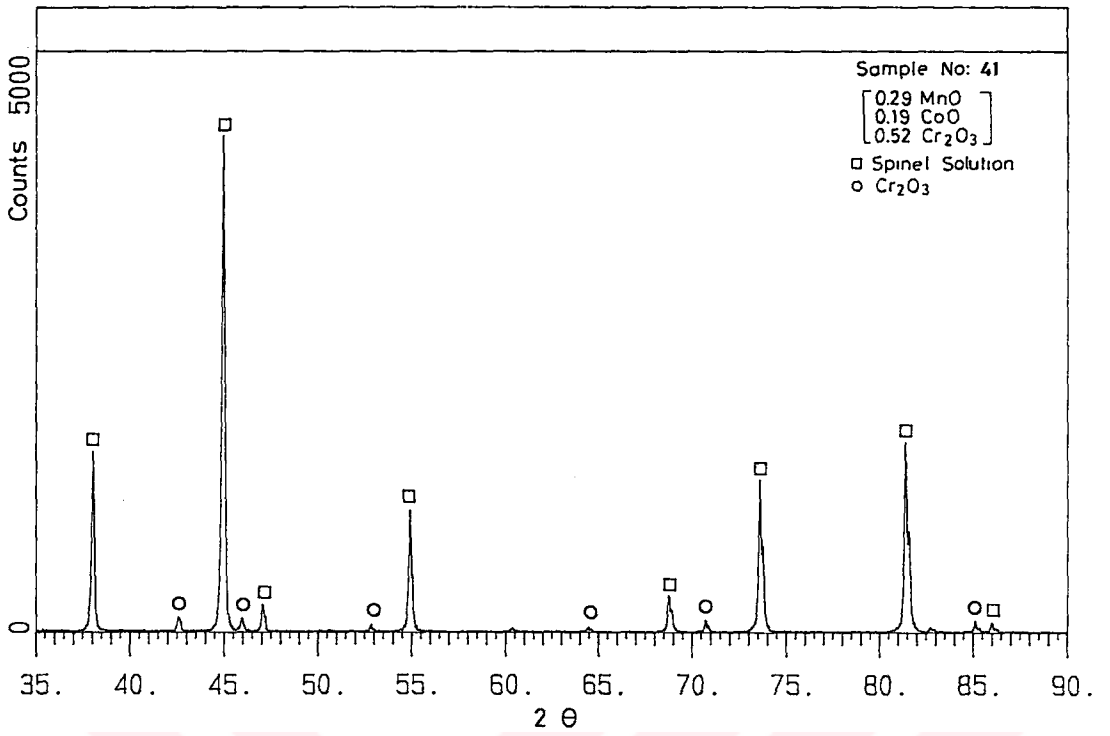

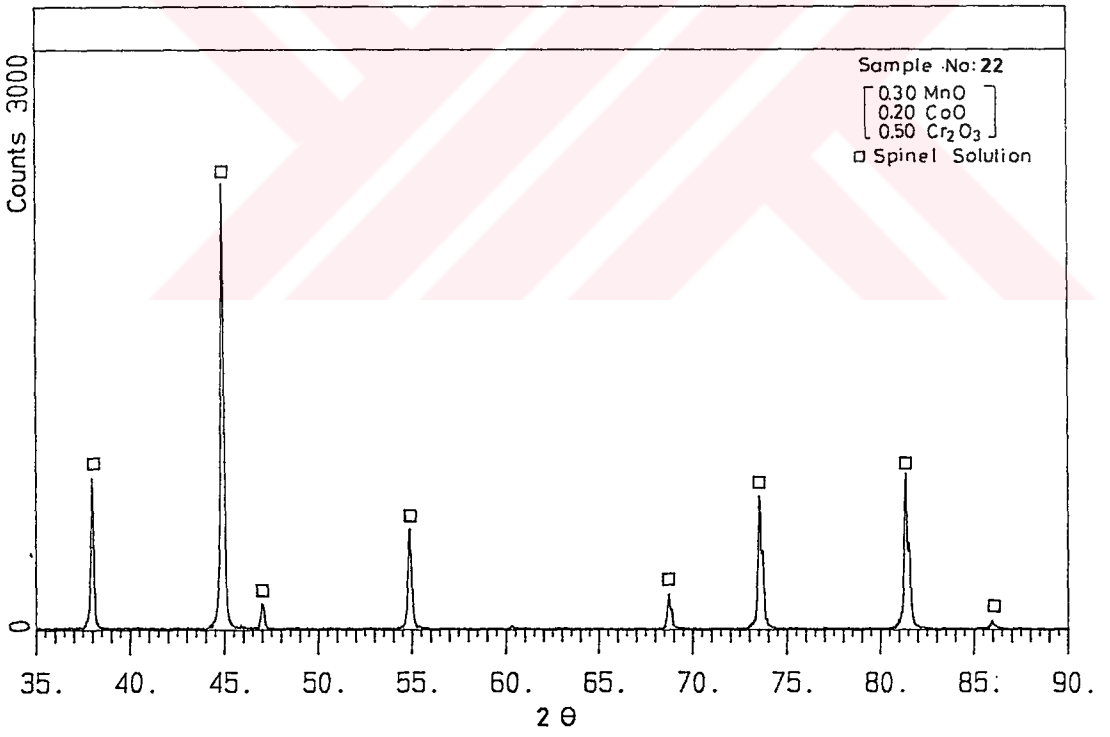

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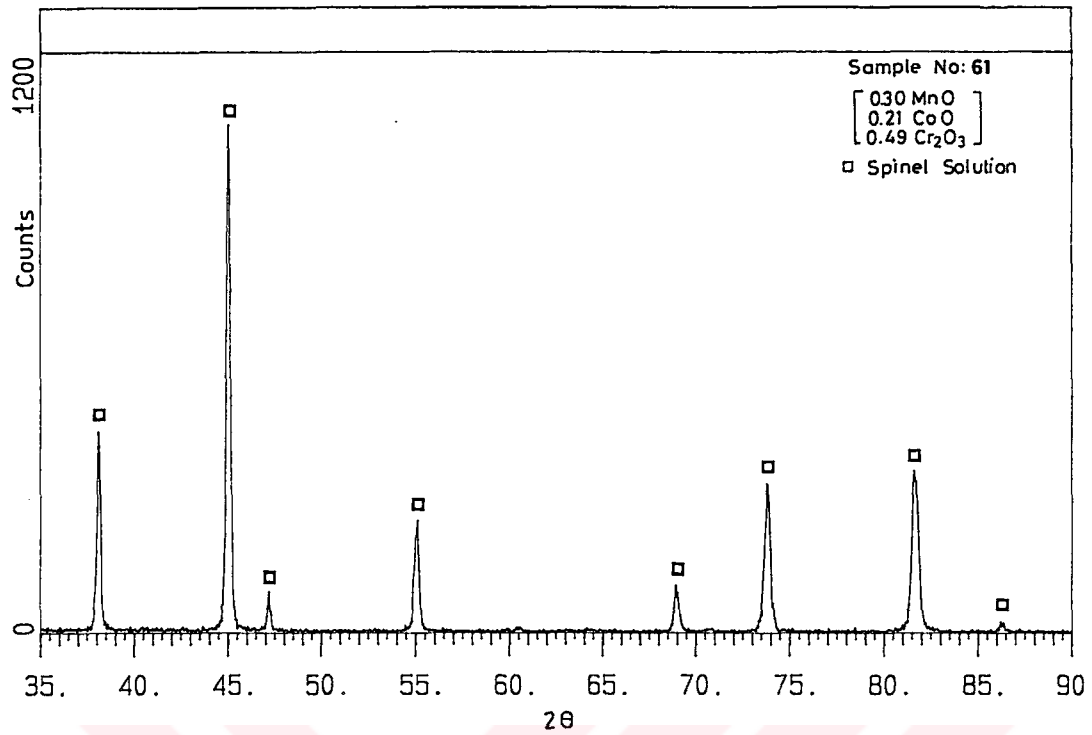

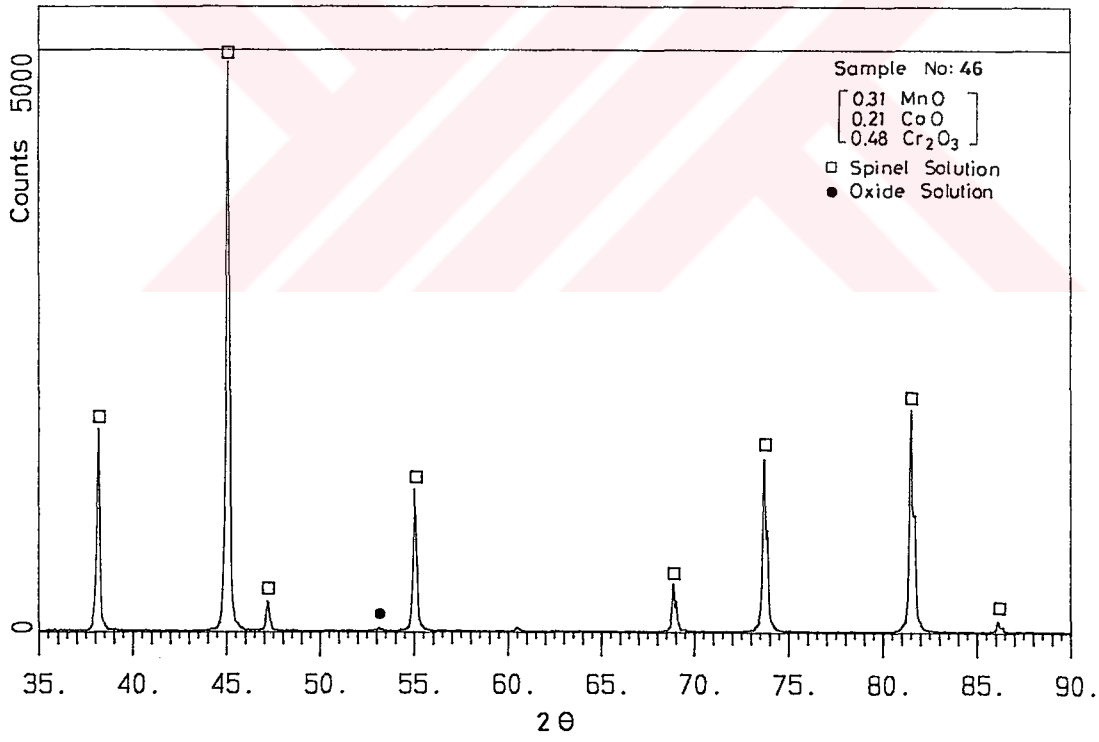

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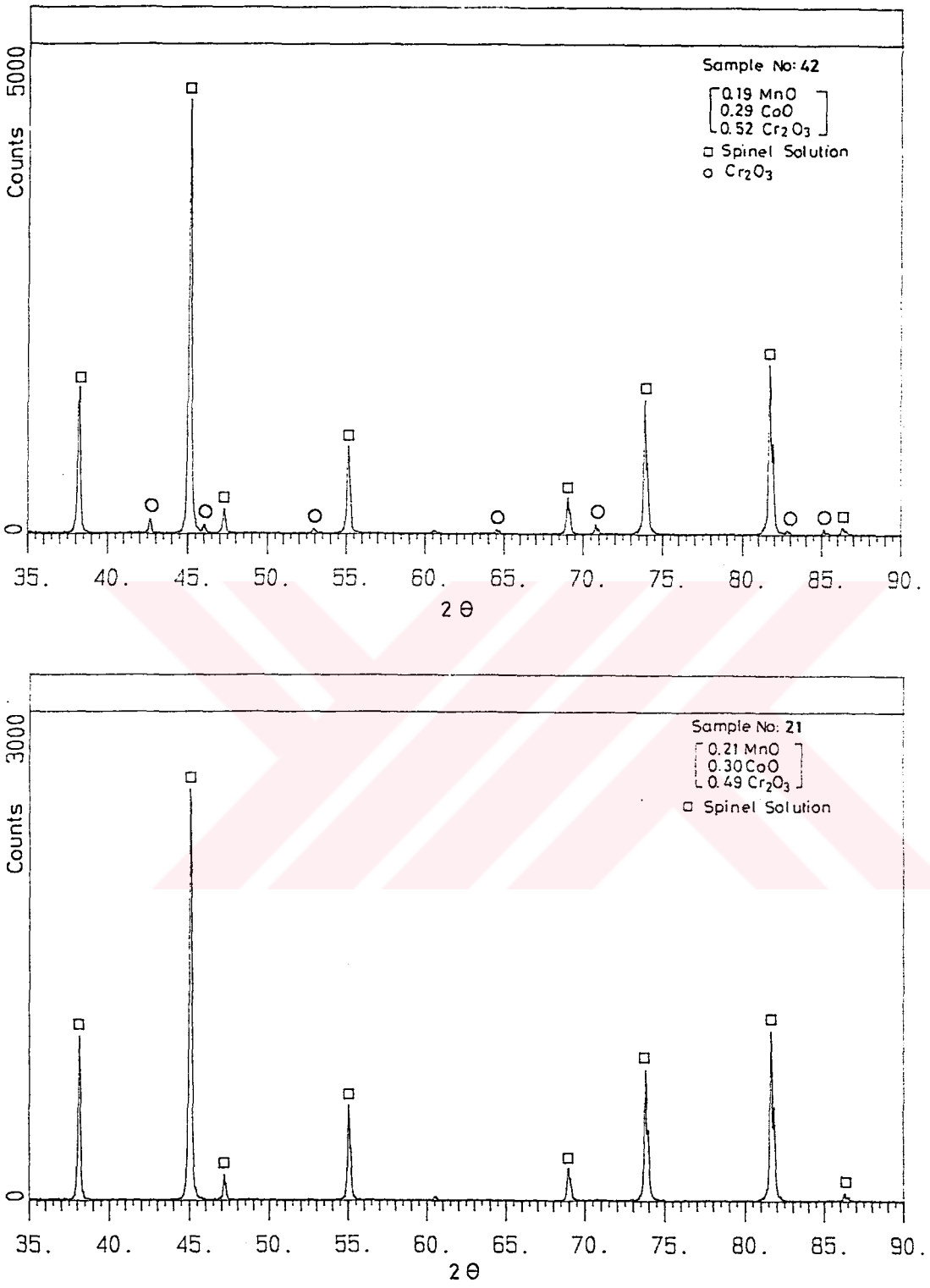

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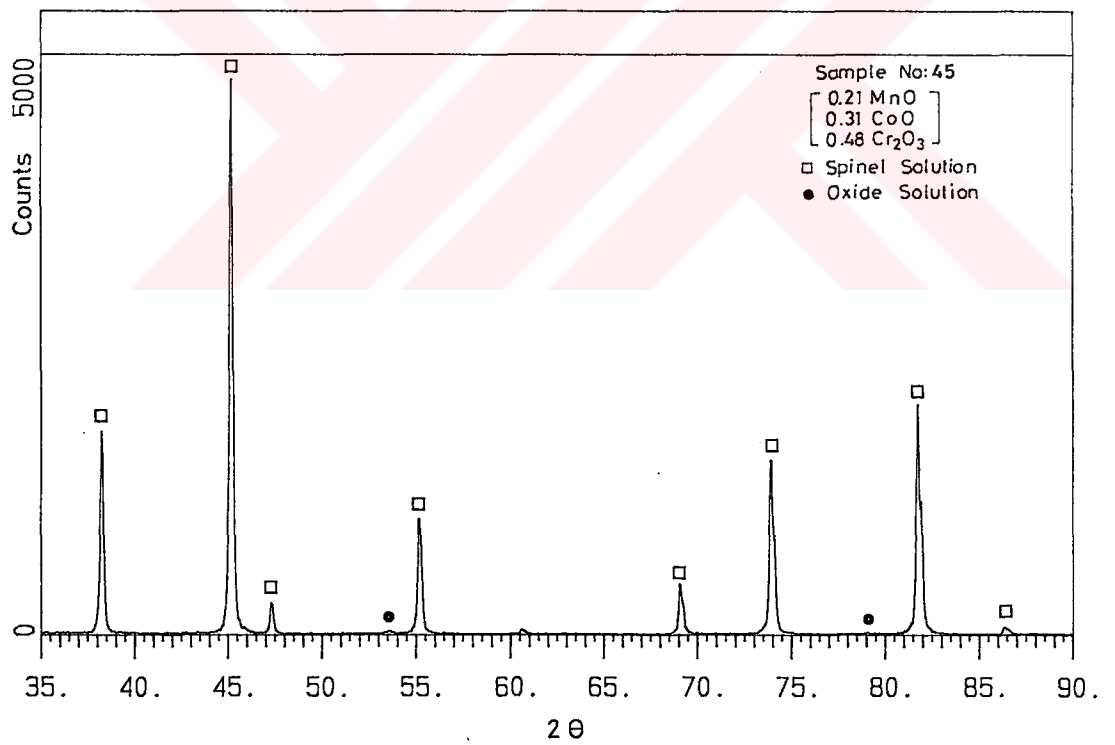

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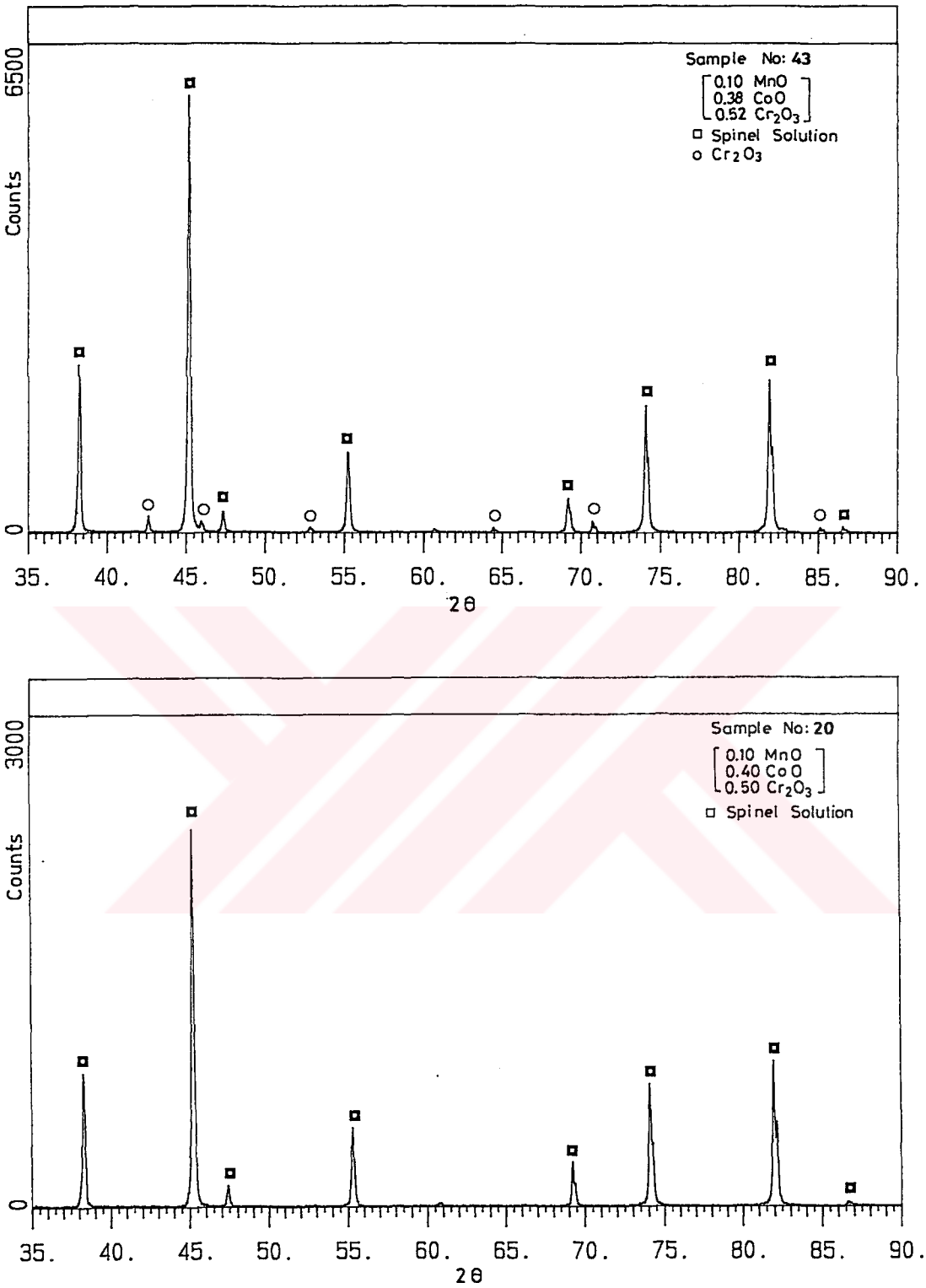

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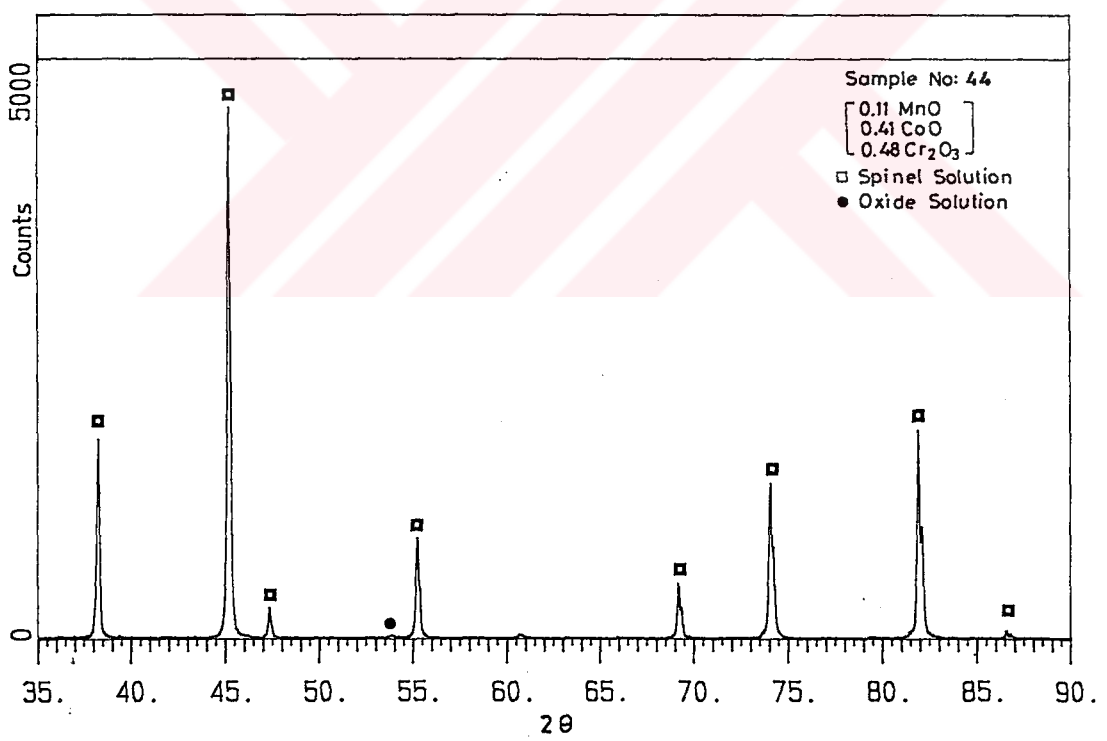

Figure 24 . (continued)

(Mn,Co)O phase boundary shown in Figure 23 was constracted by passing it through approximately midway between the pairs indicated above.

4.9. Conjugation Lines Between Spinel and Manganese-Cobalt Oxide Solid Solutions

A conjugation line, or a tie line is a line, which connects the compositions of phases that are in equilibrium. The phases which are located at the termini of a conjugation line share the same thermodynamic properties. Thus, when the directions of conjugation lines are established, the thermodynamic activities measured or calculated for the phase at one terminal of conjugation line can be carried to the conjugate phase at the other terminal.

The directions of conjugation lines between coexisting (Mn,Co) O solid solutions and the ternary spinel phase were established in the present study by measurement of cobalt oxide activities in two- phase mixtures of the MnO-CoO-Cr_2O_3 system. The compositions selected for this purpose are given in Table 18 and shown in Figure 25, as samples numbered from 11 to 18.

The determination of cobalt oxide activities in these two-phase mixtures were done by establishing the oxygen partial pressures at which metallic cobalt would start precipitating from them in gas equilibration experiments. The volumetric ratios of CO_2/H_2 in the gas mixture and the imposed oxygen partial pressures on condensed phases for each sample are given in Table 18.

Table 18. Data for the Determination of Conjugation Lines Between Coexisting (Mn,Co)O and $(Mn,Co)Cr_2O_4$ Solid Solutions.

Sample No	Sample Composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	N_{MnO}	Imposed Gas Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
11	0.05	0.25	0.70	1.217	9.9540	SS
				1.168	10.0021	SS
				1.132	10.0381	SS
				1.075	10.0991	SS + Co
				1.038	10.1395	SS + Co
12	0.15	0.25	0.60	2.908	8.9865	SS
				2.883	8.9953	SS
				2.834	9.0132	SS
				2.700	9.0621	SS
				2.650	9.0839	SS
				2.614	9.0987	SS
				2.480	9.1555	SS
				2.441	9.1716	SS + Co
13	0.20	0.25	0.55	3.868	8.6933	SS
				3.351	8.8396	SS
				3.200	8.8489	SS
				3.284	8.8602	SS
				3.181	8.8930	SS
				3.066	8.9313	SS
				3.029	8.9437	SS + Co

Table 18. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	N_{MnO}	Imposed Gas Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
				2.968	8.9648	SS + Co
14	0.30	0.25	0.45	4.163	8.6198	SS
				3.887	8.6886	SS
				3.784	8.7155	SS
				3.736	8.7284	SS + Co
				3.628	8.7583	SS + Co
15	0.40	0.25	0.35	3.958	8.6701	SS + Co
				4.133	8.6270	SS + Co
				4.187	8.6141	SS + Co
				4.325	8.5818	SS
16	0.50	0.25	0.25	5.394	8.3649	SS
				5.334	8.3757	SS
				5.250	8.3910	SS
				5.190	8.4022	SS + Co
17	0.60	0.25	0.15	5.768	8.2999	SS
				5.662	8.3179	SS + Co
				5.489	8.3479	SS + Co
				5.471	8.3511	SS + Co
				4.904	8.4576	SS + Co

Table 18. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	$N_{Cr_2O_3}$	N_{MnO}	Imposed Gas Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
18	0.65	0.25	0.10	6.387	8.2021	SS
				6.120	8.2431	SS
				5.989	8.2638	SS
				5.906	8.2773	SS + Co

SS : (Mn,Co)O + $(Mn,Co)Cr_2O_4$ Solid Solution.

Co : Metallic Cobalt Precipitate.

The activities of CoO in the two-phase (Mn,Co)O+Spinel mixtures calculated from the data in Table 18 through the use of Eqn.(29) are summarized in Table 19.

The conjugation lines shown in Figure 25 were constructed, as the iso-CoO activity line by combining the data given in Figure 16 and Table 19.

4.10. Activities of CoO in Ternary Spinel Solutions

The activities of CoO in various samples within the ternary spinel solid solution area were determined by the procedure described in Section 4.6 for cobalt chromite solutions. The compositions of the samples prepared for this purpose are given in Table 20.

The single phase ternary spinel solid solutions were equilibrated at 1300 °C with gas atmospheres of variable CO_2/H_2 ratio until metallic cobalt precipitation was observed. The CO_2/H_2 gas mixing ratios and corresponding partial pressures of oxygen in the gas phase are given in Table 20, together with the phases present under the imposed conditions of temperature and P_{O_2}.

The activities of CoO calculated with the aid of Eqn.(29), by using the data given in Table 20 are summarized in Table 21. These measured CoO activities were combined with the known activities of CoO at the terminals of (Mn,Co)O+ Spinel conjugation lines in order to construct the iso-cobalt oxide activity curves within the ternary spinel field as shown in Figure 26.

Table 19. Activities of CoO in Spinel + Oxide Field at 1300 °C.

Sample No	Sample Composition (mole fraction)			Equilibrium $-\log P_{O_2}$	Cobalt Oxide Activity a_{CoO}
	N_{CoO}	$N_{Cr_2O_3}$	N_{MnO}		
11	0.05	0.25	0.70	10.0681	0.1140
12	0.15	0.25	0.60	9.1608	0.3243
13	0.20	0.25	0.55	8.9374	0.4190
14	0.30	0.25	0.45	8.7219	0.5370
15	0.40	0.25	0.35	8.5978	0.6195
16	0.50	0.25	0.25	8.3966	0.7810
17	0.60	0.25	0.15	8.3089	0.8640
18	0.65	0.25	0.10	8.2705	0.9040

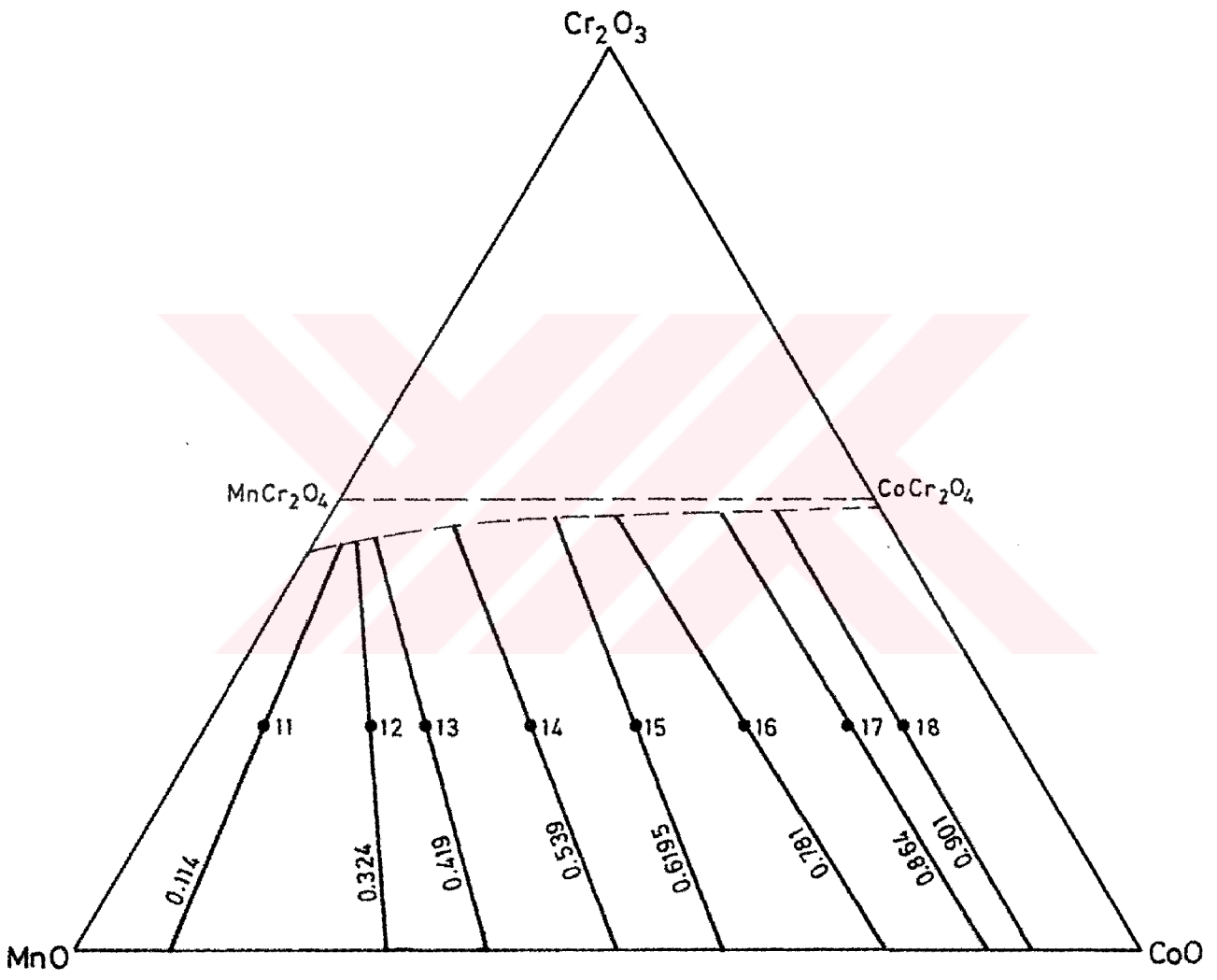

Figure 25. Conjugation Lines Connecting the Compositions of coexisting (Mn,Co)O and Ternary Spinel Solutions at 1300 °C. The number on the Lines Indicate the Compositions Given in Table 4 and 14.

Table 20. Data Obtained in Quenching Experiments in the System MnO-CoO-Cr_2O_3.

Sample No	Sample Composition (mole fraction) N_{CoO}	N_{MnO}	$N_{Cr_2O_3}$	Gas Mixing Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
20	0.40	0.10	0.50	0.529	10.9150	SS + Co
				0.532	10.8965	SS + Co
				0.577	10.8194	SS
21	0.30	0.20	0.50	0.383	11.2560	SS + Co
				0.398	11.2276	SS + Co
				0.440	11.1449	SS + Co
				0.460	11.0693	SS
				0.630	10.7171	SS
22	0.20	0.30	0.50	0.365	11.3192	SS
				0.354	11.3519	SS
				0.340	11.3866	SS
				0.328	11.4220	SS + Co
23	0.10	0.40	0.50	0.154	12.1819	SS + Co
				0.194	11.9540	SS + Trace Co
				0.230	11.7736	SS
47	0.11	0.41	0.48	1.670	9.6198	SS
				1.490	9.7261	SS
				1.415	9.7791	SS
				1.349	9.8355	SS

Table 20. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	N_{MnO}	$N_{Cr_2O_3}$	Gas Mixing Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
				1.139	10.0308	SS
				0.820	10.4203	SS
				0.793	10.4553	SS
				0.470	11.0455	SS
				0.450	11.0938	SS + Co
				0.440	11.1449	SS + Co
50	0.11	0.42	0.47	0.849	10.3757	SS + Co
				1.038	10.1395	SS + Co
				1.770	9.5251	SS + Co
				1.929	9.4287	SS
49	0.05	0.49	0.46	0.140	12.2734	SS + Co
				0.181	12.0235	SS + Co
				0.341	11.3860	SS + Co
				0.376	11.2876	SS + Co
				0.460	11.0693	SS + Co
				0.520	10.9354	SS + Co
				0.726	10.5561	SS + Co
				0.760	10.5042	SS + Co
				0.784	10.4672	SS + Co
				0.825	10.4089	SS + Co

Table 20. (continued)

Sample No	Sample Composition (mole fraction) N_{CoO}	N_{MnO}	$N_{Cr_2O_3}$	Gas Mixing Ratio $r = \frac{CO_2}{H_2}$	$-\log P_{O_2}$	Phases Present
				0.994	10.1906	SS
48	0.05	0.47	0.48	0.480	11.0218	SS
				0.430	11.1444	SS
				0.400	11.2271	SS
				0.374	11.2871	SS + Co
61	0.21	0.30	0.49	0.340	11.3866	SS + Co
				0.460	11.0693	SS + Co
				0.510	10.9563	SS + Co
				0.550	10.8754	SS

SS ; Spinel Solid Solution

Co ; Metallic Cobalt Precipitate

Table 21. Activities of CoO in Ternary Spinel Solutions of the MnO-CoO-Cr_2O_3 System at 1300°C.

Sample No	Sample Composition (mole fraction)			Equilibrium $-\log P_{O_2}$	Cobalt Oxide Activity
	N_{CoO}	N_{MnO}	$N_{Cr_2O_3}$		
20	0.40	0.10	0.50	10.8564	0.0460
21	0.30	0.20	0.50	11.0938	0.0350
22	0.20	0.30	0.50	11.4107	0.0243
23	0.10	0.40	0.50	11.9540	0.0130
47	0.11	0.41	0.48	11.0693	0.0360
50	0.11	0.42	0.47	9.4775	0.2250
49	0.05	0.49	0.46	10.2929	0.0880
48	0.05	0.47	0.48	11.2566	0.0290
61	0.21	0.30	0.49	10.9150	0.0430

4.11 Conjugation Lines in the Spinel + Cr_2O_3 Two-Phase Area.

As stated earlier in Section 4.8., on the stability field of ternary spinel solid solutions, the join $MnCr_2O_4$-$CoCr_2O_4$ defines the phase boundary between the stability field of the ternary spinel area and Cr_2O_3. In view of the presumption that Cr_2O_3 does not dissolve either CoO or MnO in any substantial degree, the conjugation lines in the two-phase Spinel + Cr_2O_3 field must all merge at Cr_2O_3 apex of the MnO-CoO-Cr_2O_3 composition triangle.

In order to verify the presumed directions of conjugation lines, and also provide a check on the location of the Spinel + Cr_2O_3 phase boundary, four Samples marked as 31, 32, 33, and 34 in Table 22 were prepared. These samples were fired initially at 1300 °C for 48 hours each under a gas phase of $P_{O_2}=10^{-8}$ atm so that the two-phase assemblages were formed in all of them. The samples were then subjected to cobalt precipitation experiments with gas mixtures as shown in Table 22. The data obtained in these runs were used to determine the activities of CoO in the two-phase Spinel + Cr_2O_3 mixtures selected.

The results obtained on CoO activities in the samples designated from 31 to 34 are summarized in Table 23, and these values are inscribed in brackets on the conjugation lines passing through the two- phase samples in Fig 26. Note that the CoO activity measured in these samples are, within limits of experimental error, the same as those that were measured at their terminals on the $MnCr_2O_4$-$CoCr_2O_4$ join. Thus, the sample pairs (34,20), (33,21), (32,22), and (31,40) possess the same CoO activity of the conjugation line which they lie.

Table 22. Data Obtained in Quenching Experiments in the System MnO-CoO-Cr_2O_3.

Sample No	Sample Composition (mole fraction)			Gas Mixing Ratio	$-\log P_{O_2}$	Phases Present
	N_{CoO}	N_{MnO}	$N_{Cr_2O_3}$	$r = \frac{CO_2}{H_2}$		
34	0.32	0.08	0.60	0.519	10.9354	SS + Co
				0.532	10.8965	SS + Co
				0.577	10.8194	SS
33	0.24	0.16	0.60	0.440	11.1449	SS + Trace Co
				0.499	10.9978	SS
				0.567	10.8377	SS
				0.622	10.7333	SS
32	0.16	0.24	0.60	0.326	11.4562	SS + Co
				0.337	11.4193	SS
31	0.08	0.32	0.60	0.135	12.2769	SS + Co
				0.144	12.2708	SS + Co
				0.154	12.1819	SS + Co
				0.171	12.0974	SS + Co
				0.220	11.7736	SS

Table 23. Activities of CoO in MnO-CoO-Cr_2O_3 system at 1300°C.

Sample No	Sample Composition (mole fraction)			Equilibrium $-\log P_{O_2}$	Cobalt Oxide Activity
	N_{CoO}	N_{MnO}	$N_{Cr_2O_3}$		
34	0.32	0.08	0.60	10.8565	0.0460
33	0.24	0.16	0.60	11.1189	0.0340
32	0.16	0.24	0.60	11.4215	0.0240
31	0.08	0.32	0.60	11.9540	0.0130

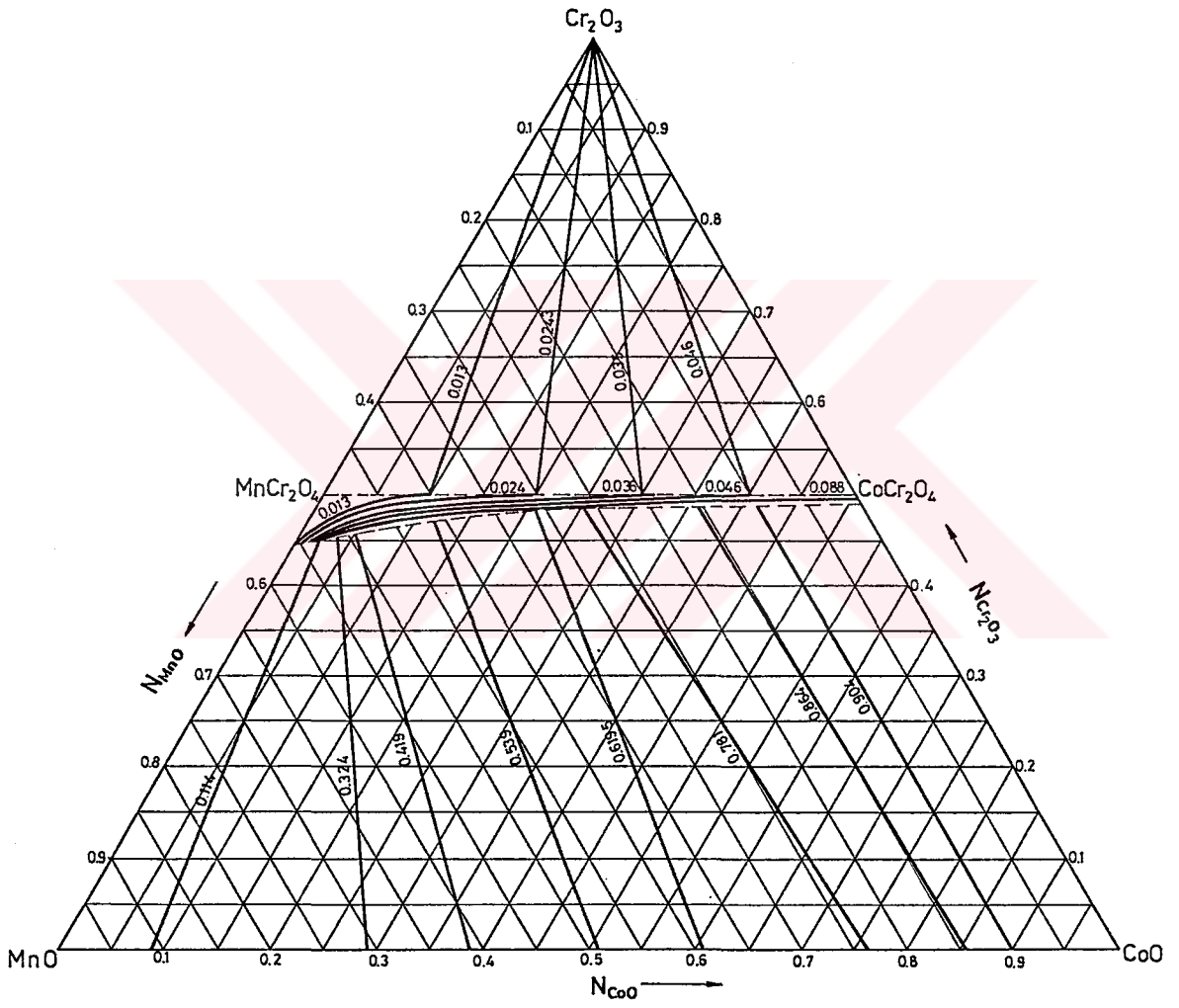

Figure 26. The System MnO-CoO-Cr_2O_3 at 1300 °C.

4.12 Thermodynamics of Mixed Spinel Solid Solutions.

Figure 26 can be regarded as a map that shows iso-CoO activities in various phases and phase assemblages of the MnO-CoO-Cr_2O_3 system at 1300 °C. The diagram that resulted from the studies of the present work is unique in that it represents the first of its kind in which the presence of a mixed spinel solid solution field was established in the Mn-Co-Cr-O system with well-defined boundaries. Narrow as it might be, the existence of such a ternary spinel field alters completely the classical approach of thermodynamic treatment of data obtained for such systems.

Within the past thirty years, thermodynamic properties of a large number of spinel solid solutions were deduced mainly by Carl Wagner's [28] classical treatment of conjugation data between coexisting oxide and spinel solid solution pairs of ternary oxide systems. The essential requisite of Wagner's method is that each of these solutions must be perfectly stoichiometric. Hence, the method becomes inapplicable when either member of the solution pair exhibits substantial deviation from stoichiometry.

The elegance, and probably the inherent comforting simplicity, of Wagner's method [28] led many researchers to neglect the effects of nonstoichiometry in their calculations concerning thermodynamics of spinel solutions. Recently, Timuçin and Muan [29], in their work on MnO-NiO-Al_2O_3 system, proposed an alternative but rigorous, thermodynamic methodology for the treatment of cases involving non-stoichiometric spinel phases. In the present study the essential elements of this more recent methodology [29], which are simply

multicomponent solution thermodynamics, were used to derive information on the thermodynamics of spinel phases that are presented in the following sections.

4.12.1 Activity-Composition Relations in $MnCr_2O_4$ - $CoCr_2O_4$ Solutions

The activities of $CoCr_2O_4$ in the stoichiometric $(Mn,Co)Cr_2O_4$ solid solution series, across the $MnCr_2O_4$-$CoCr_2O_4$ join, were obtained from the measured activities of CoO along this join by considering the following reaction:

$$CoO + Cr_2O_3 = CoCr_2O_4 \qquad (11)$$

The equilibrium constant for reaction (11) is :

$$K_{11} = \frac{a_{CoCr_2O_4}}{a_{CoO} \cdot a_{Cr_2O_3}} \qquad (43)$$

The value for K_{11} at 1300 °C could be calculated from data presented in Section 4.6. for the CoO-Cr_2O_3 system, viz.:

a_{CoO} =0.056 at $a_{Cr_2O_3}$=1, and $a_{CoCr_2O_4}$=1.

Inserting these values into Eqn (43), gave :

$$K_{11} = \frac{1}{0.056}$$

Using the above value for K_{11} Eqn.(43) could be rearranged for $a_{CoCr_2O_4}$ as follows:

$$a_{CoCr_2O_4} = \frac{1}{0.056} * a_{CoO} * a_{Cr_2O_3} \qquad (44)$$

Noting that $a_{Cr_2O_3}$=1 for stoichiometric spinel solutions, we have :

$$a_{CoCr_2O_4} = \frac{a_{CoO}}{0.056} \qquad (45)$$

where a_{CoO} represents the cobalt oxide activity in the spinel solid solution. The activities of CoO that were measured along the $MnCr_2O_4$-$CoCr_2O_4$ join, and given previously in Table 21, were used to draw the smoothened a_{CoO} versus $N_{CoCr_2O_4}$ curve shown in Figure 27.

The activities of CoO picked from Figure 27 and the values of $a_{CoCr_2O_4}$ calculated by their use in Eqn.(45) are listed in Table 24. The manganese chromite activities $a_{MnCr_2O_4}$, in the spinel solutions were obtained from the following Gibbs-Duhem treatment of activity coefficients with α function [23] :

$$\ln\gamma_{MnCr_2O_4} = -N_{MnCr_2O_4} * N_{CoCr_2O_4} * \alpha_{CoCr_2O_4} - \int_{N_{MnCr_2O_4}=1}^{N_{MnCr_2O_4}=N_{MnCr_2O_4}} \alpha_{CoCr_2O_4} * dN_{MnCr_2O_4} \qquad (46)$$

where,

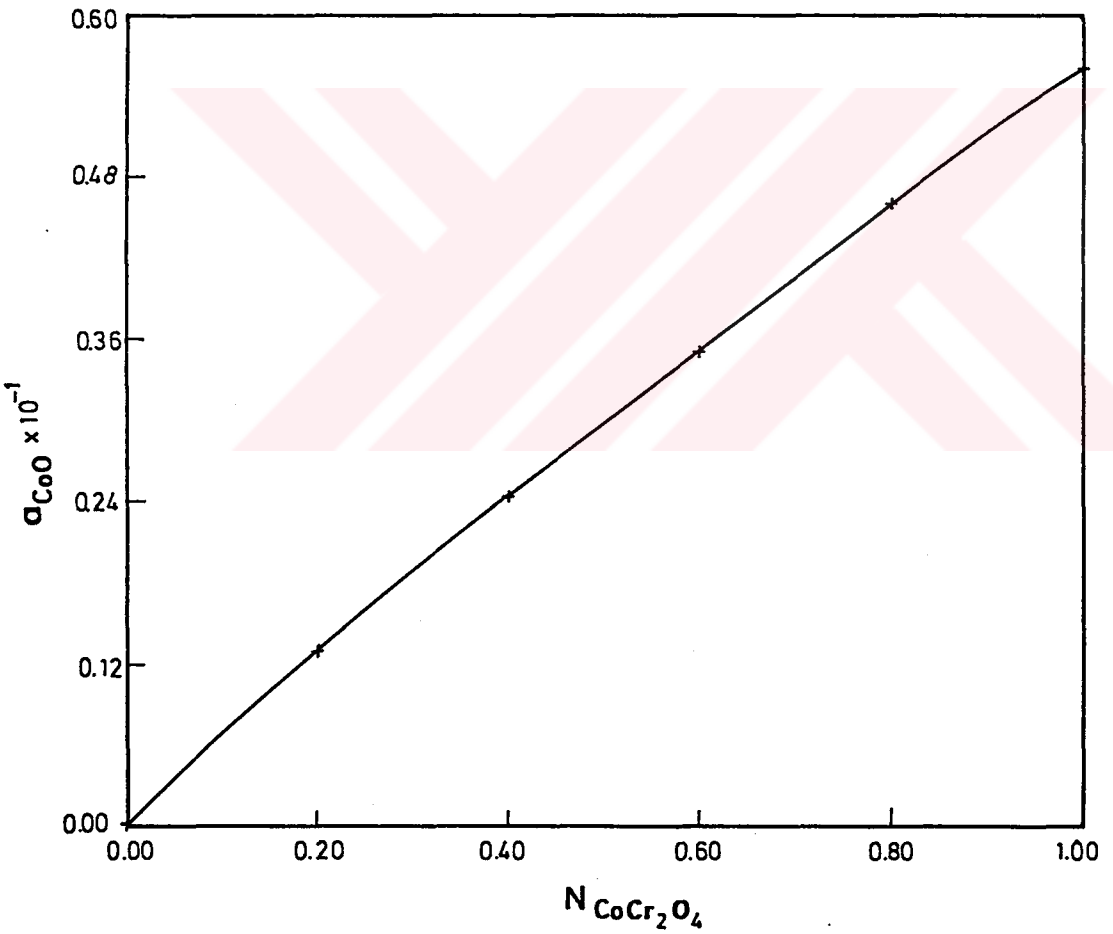

Figure 27. Variation of CoO Activity with Composition Along the Ternary Stoichiometric Spinel Solid Solutions.

$$\alpha_{CoCr_2O_4} = \frac{\ln \gamma_{CoCr_2O_4}}{\left(1 - N_{CoCr_2O_4}\right)^2}$$

The integral in Eqn.(46) was evaluated graphically, and the activity coefficients of $MnCr_2O_4$ were converted into $a_{MnCr_2O_4}$ as listed in Table 24.

Figure 28 shows the variation of spinel component activities in the stoichiometric mixed spinel solutions of the MnO-CoO-Cr_2O_3 system at 1300 °C. The stoichiometric spinels exhibit a positive deviation from ideal solution behavior.

The free energy of formation of mixed spinel solutions, ΔG^M, from $CoCr_2O_4$ and $MnCr_2O_4$, was evaluated at each solution composition by using the values of $a_{CoCr_2O_4}$ and $a_{MnCr_2O_4}$ from Table 24 in the following equation :

$$\Delta G^M = RT[N_{CoCr_2O_4} \ln a_{CoCr_2O_4} + N_{MnCr_2O_4} \ln a_{MnCr_2O_4}] \quad (47)$$

The calculated values for ΔG^M are given in the last column of Table 24. The free energy-composition plot for stoichiometric spinel solid solutions is shown in Figure 29.

4.12.2 The Free Energy of Formation of $MnCr_2O_4$

The formation of the manganese chromite spinel compound, $MnCr_2O_4$, from its binary oxides MnO and Cr_2O_3 can be described by the following reaction :

$$MnO + Cr_2O_3 = MnCr_2O_4 \quad (48)$$

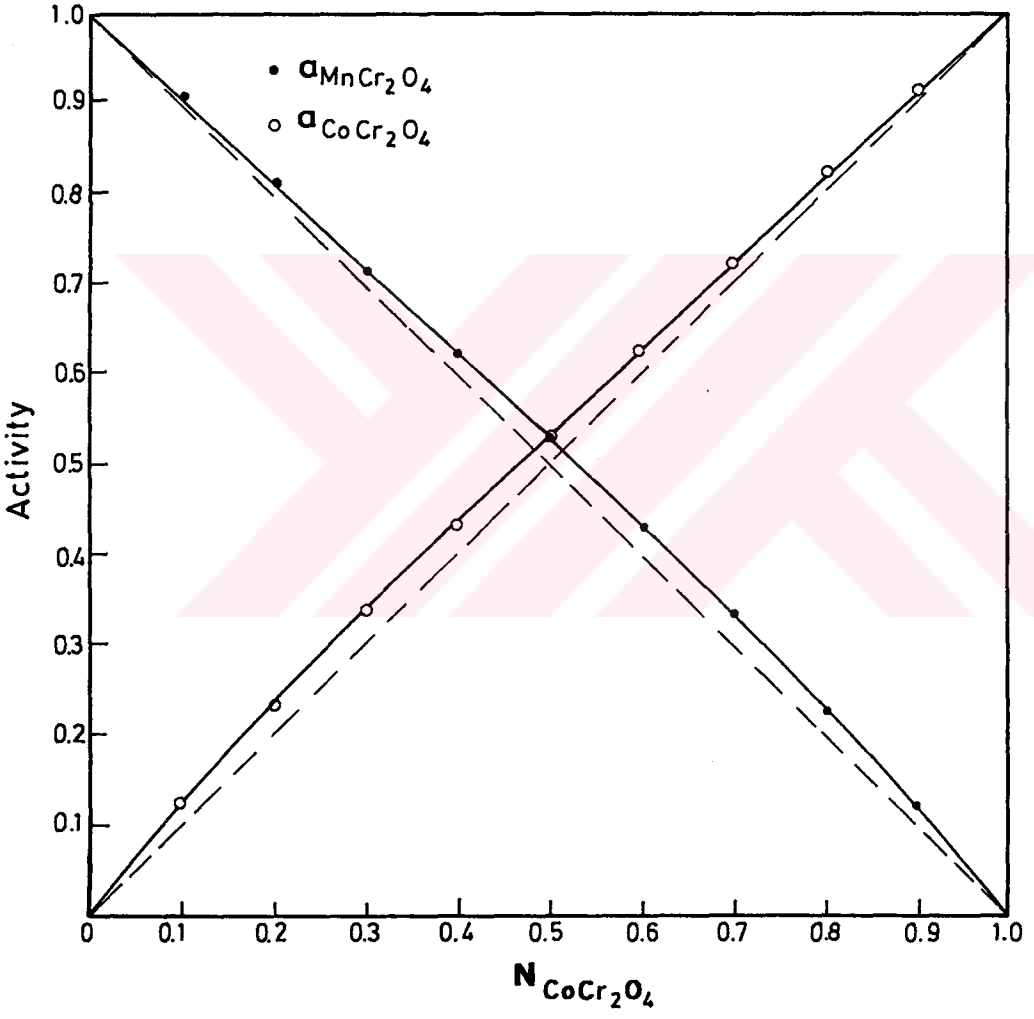

Figure 28. Activities of $CoCr_2O_4$ and $MnCr_2O_4$ as a Function of Composition in the System $MnCr_2O_4$ - $CoCr_2O_4$ Solid Solutions at 1300 °C.

Table 24. Activities of $CoCr_2O_4$ and $MnCr_2O_4$ as a Function of Composition in Stoichiometric $MnCr_2O_4$ - $CoCr_2O_4$ Solutions, and the Free Energy of Mixing.

Sample Composition (mole fraction)					
$N_{CoCr_2O_4}$	$N_{MnCr_2O_4}$	a_{CoO}	$a_{CoCr_2O_4}$	$a_{MnCr_2O_4}$	ΔG^M kJ
1.0	0.0	0.0560	1.000	0.000	0
0.9	0.1	0.0513	0.916	0.120	-3.806
0.8	0.2	0.0460	0.821	0.224	-5.978
0.7	0.3	0.0405	0.722	0.330	-7.319
0.6	0.4	0.0350	0.625	0.432	-8.079
0.5	0.5	0.0296	0.529	0.530	-8.315
0.4	0.6	0.0243	0.434	0.622	-8.092
0.3	0.7	0.0188	0.336	0.715	-7.350
0.2	0.8	0.0130	0.232	0.807	-6.065
0.1	0.9	0.0067	0.120	0.902	-3.987
0.0	1.0	0.0000	0.000	1.000	0

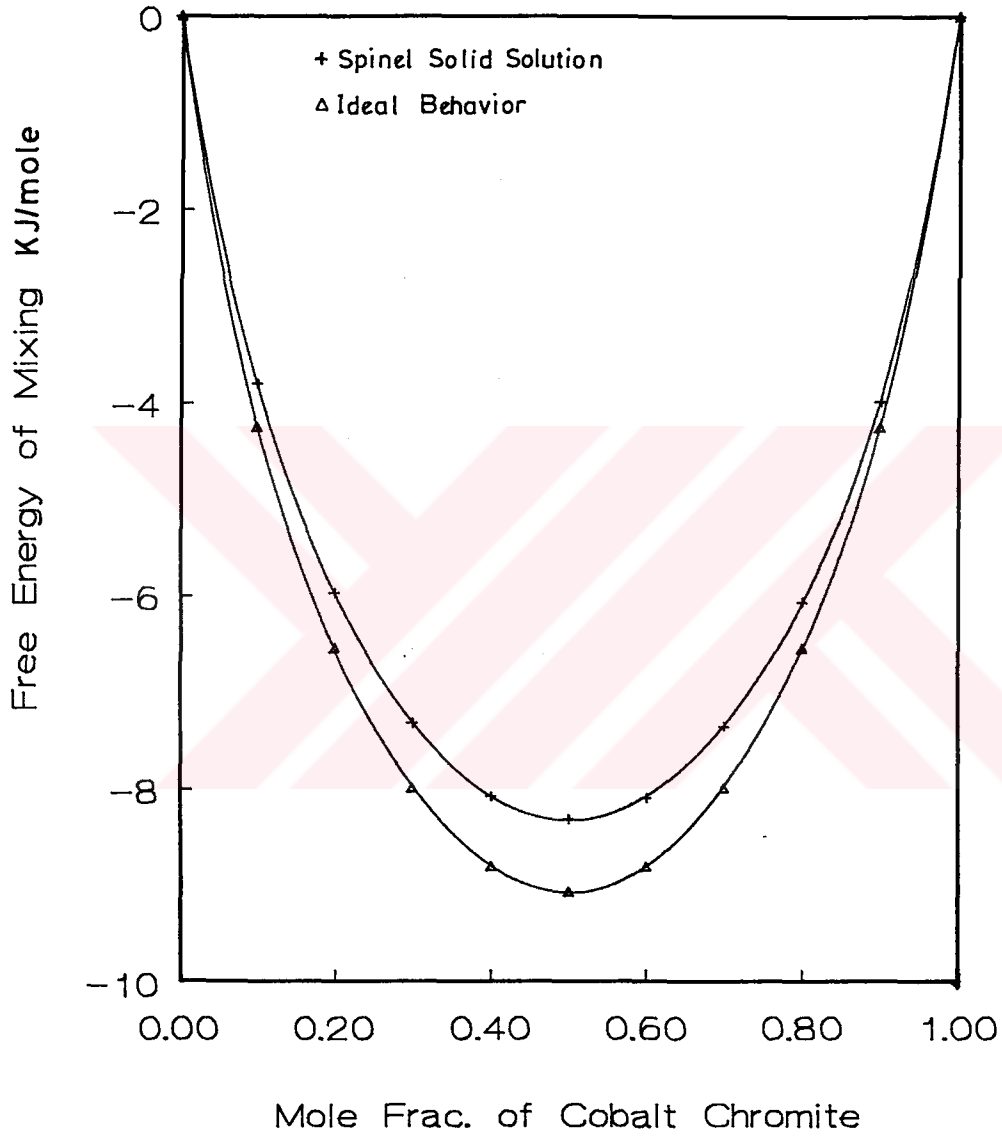

Figure 29. Free Energy of Mixing-Composition Plot for Stoichiometric Spinel Solid Solutions at 1300 °C.

The standard free energy change for Reaction (48) is given by:

$$\Delta G^{o}_{MnCr_2O_4} = -RT\ln\frac{a_{MnCr_2O_4}}{a_{MnO}\cdot a_{Cr_2O_3}} \qquad (49)$$

where the terms in the activity quotient refer to the activities of the species indicated in the stoichiometric spinel solutions. In order to evaluate $\Delta G^{o}_{MnCr_2O_4}$ from Eqn (49), all the parameters except a_{MnO} are known. Therefore a knowledge on how the MnO activities would change with composition across the $MnCr_2O_4$-$CoCr_2O_4$ spinel solutions was necessary.

The multicomponent-solution thermodynamics, characterized typically in this case, by ternary Gibbs-Duhem treatment of the known CoO activity data provided the necessary information about the MnO activities in the spinel field of the MnO-CoO-Cr_2O_3 system. Among the known ternary Gibbs-Duhem methods, the one suggested by Schuhmann [30] was used in the present study, due to its simplicity and the amenability of the data for the Gibbs-Schuhmann treatment.

The Gibbs-Schuhmann equation, for the calculation of MnO activities from data on a_{CoO} can be written as follows:

$$\log a_{MnO} = \left[\log a^{I}_{MnO} - \int_{\log a^{I}_{CoO}}^{\log a^{II}_{CoO}} \left(\frac{\partial n_{CoO}}{\partial n_{MnO}}\right)_{a_{CoO}, n_{MnO}} d\log a_{CoO} \right]_{n_{MnO}/n_{Cr_2O_3}} \qquad (50)$$

Various terms in this equation and the details of processing the equation are explained in the original paper [30]. Briefly, the calculation method followed in the present study consisted of using Fig.26 with the following sequential steps:

(1) An integration path with constant $n_{MnO}/n_{Cr_2O_3}$ ratio was selected. This path was a straight line radiating from the CoO corner and cutting the opposite side the MnO-CoO-Cr_2O_3 triangle at the selected n_{MnO}/n_{CoO} molar ratio,

(2) The points at which the selected integration path cut the iso-CoO activity curves in the curves in the spinel area were marked and then at each of these points tangents were constructed to the CoO activity curves. The intersection point of a tangent with the MnO-CoO side of the triangle would give the value of the $\partial n_{CoO}/\partial n_{MnO}$, known as the tangent-intercept term.

(3) After obtaining all possible tangent-intercepts Eqn.(50) was evaluated graphically along the selected path. The integration started from the Spinel + (Mn,Co)O boundary and terminated at the Spinel + Cr_2O_3 boundary.

(4) The term a^I_{MnO} represented the activity of MnO on the Spinel + (Mn,Co)O phase boundary; the values of a^I_{MnO} were known from the directions of conjugation lines inside the Spinel + (Mn,Co)O two phase field. The integration procedure described above was performed along the integration paths of $n_{MnO}/n_{Cr_2O_3}$=0.52/0.48, $n_{MnO}/n_{Cr_2O_3}$=0.50/0.50, $n_{MnO}/n_{Cr_2O_3}$=0.475/0.525, and $n_{MnO}/n_{Cr_2O_3}$=0.555/0.445. The results on the calculated MnO activities are given in Table 25.

Table 25. Activity calculations of MnO in the MnO-CoO-Cr_2O_3 System

Integration path : $\frac{n_{MnO}}{n_{Cr_2O_3}} = \frac{0.52}{0.48}$

a_{CoO}	$-\log a_{CoO}$	$-\frac{\partial n_{CoO}}{\partial n_{MnO}}$	$-\log a_{MnO}$	a_{MnO}
0.013	1.886	0.307	0.8900	0.129
0.024	1.620	0.345	0.8030	0.157
0.036	1.444	0.442	0.7340	0.185
0.046	1.337	0.485	0.6840	0.207
0.088	1.056	0.530	0.3586	0.438
0.400	0.398	0.560	0.1804	0.660

Integration path : $\frac{n_{MnO}}{n_{Cr_2O_3}} = \frac{0.50}{0.50}$

a_{CoO}	$-\log a_{CoO}$	$-\frac{\partial n_{CoO}}{\partial n_{MnO}}$	$-\log a_{MnO}$	a_{MnO}
0.013	1.886	0.412	1.1166	0.076
0.024	1.620	0.452	0.9929	0.102
0.036	1.444	0.530	0.9075	0.124
0.046	1.337	0.600	0.8470	0.142
0.088	1.056	0.620	0.6747	0.212
0.465	0.333	0.630	0.2250	0.595

Integration path : $\frac{n_{MnO}}{n_{Cr_2O_3}} = \frac{0.475}{0.525}$

a_{CoO}	$-\log a_{CoO}$	$-\frac{\partial n_{CoO}}{\partial n_{MnO}}$	$-\log a_{MnO}$	a_{MnO}
0.013	1.886	0.510	1.3080	0.049
0.024	1.620	0.542	1.1670	0.068
0.036	1.444	0.632	1.1049	0.086
0.046	1.337	0.654	0.9960	0.100
0.088	1.056	0.685	0.8110	0.156
0.525	0.280	0.695	0.272	0.534

Integration path : $\frac{n_{MnO}}{n_{Cr_2O_3}} = \frac{0.445}{0.555}$

a_{CoO}	$-\log a_{CoO}$	$-\frac{\partial n_{CoO}}{\partial n_{MnO}}$	$-\log a_{MnO}$	a_{MnO}
0.013	1.886	0.671	1.4966	0.032
0.024	1.620	0.695	1.3152	0.048
0.036	1.444	0.716	1.1893	0.065
0.046	1.337	0.725	1.1123	0.077
0.088	1.056	0.736	0.9110	0.123
0.565	0.248	0.742	0.3140	0.485

The calculations on MnO activities inside the ternary spinel field revealed that at the terminals where the last two integration paths cut the stoichiometric $MnCr_2O_4$-$CoCr_2O_4$ solid solutions. The MnO activities were calculated as 0.0355 and 0.0375 for $N_{MnCr_2O_4}$= 0.90 and $N_{MnCr_2O_4}$= 0.95, respectively. Activity of MnO for the stoichiometric $MnCr_2O_4$ compound was obtained by extrapolating these values to $N_{MnCr_2O_4}$= 1.00. Hence it was reasonable to assign a_{MnO}=0.0395 for the stoichiometric $MnCr_2O_4$ compound.

Taking a_{MnO}=0.0395 and $a_{Cr_2O_3}$=1 at the composition point of $MnCr_2O_4$, the standard free energy of formation of $MnCr_2O_4$ from its binary oxides MnO and Cr_2O_3 at 1300 °C was calculated as -42278 J/mole from Eqn.(49).

Jacob and Fitzner [19] made an indirect estimate for $\Delta G^{o}_{MnCr_2O_4}$ at 1100 °C by using the Wagner's treatment of conjugation lines mentioned earlier. Their value for $\Delta G^{o}_{MnCr_2O_4}$ at 1100 °C was -59015 J/mole. A similar method was used by Tsai and Muan [31] in the system $MnCr_2O_4$-$MnAl_2O_4$; they obtained a value of $\Delta G^{o}_{MnCr_2O_4}$ = -52600 J/mole at 1600 °C. The discrepancies between $\Delta G^{o}_{MnCr_2O_4}$ values of the present study and those of earlier investigators [19,31] can be attributed largely to the incorrect methodology used in their calculations. It should be pointed out that N.Koç and M. Timuçin [32] has obtained a value of -41588 J/mole for $\Delta G^{o}_{MnCr_2O_4}$ at 1300 °C in their earlier studies on the thermodynamics of the system NiO-MnO-Cr_2O_3.

4.13 Cation Distribution Model

Many of the properties of spinel solutions are related to cation distribution and charges in the end- members. Because of the very high octahedral site preference of Cr^{+3}, the system $CoCr_2O_4$ - $MnCr_2O_4$ has normal distribution at low temperature and exhibits increasing cation exchange between nonequivalent crystallographic sites with temperature. Contribution to the activities of spinel components from distribution of the cations Co^{+2},Mn^{+2},Cr^{+3} among the tetrahedral and octahedral lattice positions in the spinel structure can be estimated by models developed for cation distribution. The lattice molecule in $CoCr_2O_4$-$MnCr_2O_4$ solid solution can be represented as;

$$\left(Co_a^{+2}Mn_b^{+2}Cr_c^{+3}\right)\left[Co_d^{+2}Mn_e^{+2}Cr_f^{+3}\right]O_4$$

where ( ) and [ ] denote the tetrahedral and octahedral sites, respectively. The parameter a to f show the cation concentrations. The cation concentration per lattice molecule a to f may be solved for by writing appropriate site balance, charge balance, and mass balance relations. In the present study, six equations were selected as follows;

Two site balance equations,

$$a + b + c = 1 \text{ (for tetrahedral positions)} \quad (52)$$

$$d + e + f = 2 \text{ (for octahedral positions)} \quad (53)$$

An equation for charge balance,

$$2(a + b + d + e) + 3(c + f) = 8 \quad (54)$$

An equation for mass balance of Co^{+2}, involving the mole fraction $N_{CoCr_2O_4}$ of $CoCr_2O_4$ in the solution,

$$a + d = N_{CoCr_2O_4} \quad (55)$$

Two nonlinear equations for ion exchange equilibria,

$$(Co^{+2}) + [Cr^{+3}] = (Cr^{+3}) + [Co^{+2}] \text{ with } K_{Co}^{CD} = \frac{c \cdot d}{a \cdot f} \quad (56)$$

$$(Mn^{+2}) + [Cr^{+3}] = (Cr^{+3}) + [Mn^{+2}] \text{ with } K_{Mn}^{CD} = \frac{e \cdot c}{b \cdot f} \quad (57)$$

Where K_{Co}^{CD} and K_{Mn}^{CD} are cation exchange equilibrium constants. In the present study, values of K_{Co}^{CD} and K_{Mn}^{CD} necessary for the complete solution of the parameters a to f through Eqn.(52) to (57) were obtained by considering two models available for cation distribution.

The first model was developed by Jacob and co workers [19,33,34,35] . According to this model, the differences in the octahedral site preference energies of Co^{+2},Mn^{+2} and Cr^{+3} are equal to the enthalpy change for the exchange reactions, and independent of cation concentration. They assume ideal Temkin mixing of cations on each cation sublattice of the spinel, and the cation distribution can be related to differences in the octahedral site preference energies. In the present study, the octahedral site preference energies of the ions, Co^{+2}, Mn^{+2} and Cr^{+3} estimated by

Dunitz and Orgel [36] , are used for determining the values of K_{Co}^{CD} and K_{Mn}^{CD}. The octahedral site preference energies used to calculate the cation distribution in the spinel systems investigated here are, 0, -30.962, -157.737 kJ for Mn^{+2}, Co^{+2} and Cr^{+3} respectively. The enthalpy change for the exchange equilibria for the two solid solution systems reduced from the site preference energies are,

$$\Delta H_{Co}^{CD} = -RT\ln K_{Co}^{CD} = 126775 \text{ J} \tag{58}$$

$$\Delta H_{Mn}^{CD} = -RT\ln K_{Mn}^{CD} = 157737 \text{ J} \tag{59}$$

The values of K_{Co}^{CD} and K_{Mn}^{CD} were calculated from Eqn. (58) and Eqn. (59) at 1300 °C and these were used to solve for the values of concentration parameter a to f. The results obtained for the concentrations of ions on various spinel sites are tabulated in Table 26 and are shown graphically in Figure 30. These concentrations are used to calculate the free energy of mixing of spinel solid solutions by methods similar to those described by Jacob, Alcock and Fitzner [35]. Free energy change due to disordering is;

$$\Delta G_{CD} = d \cdot \Delta H_{CoCr_2O_4}^{int.} + e \cdot \Delta H_{MnCr_2O_4}^{int.} - TS_c \tag{60}$$

S_c is configurational entropy of the spinel solution and it is written as;

$$S_c = -R\sum_i b^s N_i^s \ln N_i^s \tag{61}$$

where N_i^s is the fraction of the species i in the site "s" and b^s is the number of sites of type "s" per formula unit. Free energy of mixing of spinel solid solution is;

$$\Delta G_{mix.} = \Delta G_{CD} - N_{CoCr_2O_4}\Delta G_{CoCr_2O_4} - (1 - N_{CoCr_2O_4})\Delta G_{MnCr_2O_4} \quad (62)$$

Values of free energy of mixing of $CoCr_2O_4$-$MnCr_2O_4$ solid solution are given in Table 26 and resulting curve is in Figure 32.

The second model considered for cation distribution was that developed by O'Neill and Navrotsky [37]. This model takes into account the temperature and composition dependence of cation exchange constants in terms of empirical energy parameters tabulated for various spinels. The distribution parameters a to f for the spinel cations were calculated also following the method described by O'Neill and Navrotsky [37]. The expressions are;

$$-RT\ln\frac{d\cdot c}{a\cdot f} = \alpha_{Co^{+2}-Cr^{+3}} - T\sigma_{Co^{+2}-Cr^{+3}} + 2\beta\cdot c \quad (63)$$

$$-RT\ln\frac{e\cdot c}{b\cdot f} = \alpha_{Mn^{+2}-Cr^{+3}} - T\sigma_{Mn^{+2}-Cr^{+3}} + 2\beta\cdot c \quad (64)$$

where β is a constant typically about -20 kJ/mole for 2/3 spinel.α's are site preference enthalpies, σ's are the electronic contribution of entropy. In the present study O'Neill and Navrotsky's tabulated values were used for α and σ. α values of Co^{+2}, Mn^{+2} and Cr^{+3} are 20, 45 and -160 kJ respectively and $\sigma_{Cr}{}^{+3}$ is -9.1, σ values for Mn^{+2} and Co^{+2} are zero. By substituting the related parameters into equation 63 and 64 at temperature 1300 °C we obtain;

Table 26. Cation Distriibution Model Calculation of Free Energy of Mixing for $CoCr_2O_4$ -$MnCr_2O_4$ at 1300°C. (Model1)

$N_{CoCr_2O_4}$	Tetrahedral			Octahedral			ΔG_{mix} (KJ/mole)
	(Co^{+2})	(Mn^{+2})	(Cr^{+3})	[Co^{+2}]	[Mn^{+2}]	[Cr^{+3}]	
0.0	0.0000	0.9966	0.0034	0.000	0.0034	1.9966	0
0.1	0.0975	0.8978	0.0047	0.0025	0.0022	1.9953	-4.374
0.2	0.1958	0.7984	0.0058	0.0042	0.0016	1.9942	-6.673
0.3	0.2946	0.6988	0.0067	0.0054	0.0012	1.9933	-8.099
0.4	0.3935	0.5991	0.0074	0.0065	$9.2822*10^{-4}$	1.9926	-8.914
0.5	0.4926	0.4993	0.0081	0.0074	$7.0623*10^{-4}$	1.9919	-9.162
0.6	0.5917	0.3995	0.0088	0.0083	$5.2308*10^{-4}$	1.9912	-8.902
0.7	0.6910	0.2996	0.0094	0.0090	$3.6695*10^{-4}$	1.9906	-8.069
0.8	0.7903	0.1998	0.0100	0.0097	$2.0362*10^{-4}$	1.9900	-6.626
0.9	0.8896	0.0999	0.0105	0.0104	$1.0938*10^{-4}$	1.9895	-4.326
1.0	0.9890	0.000	0.0110	0.0110	0.0000	1.9890	0

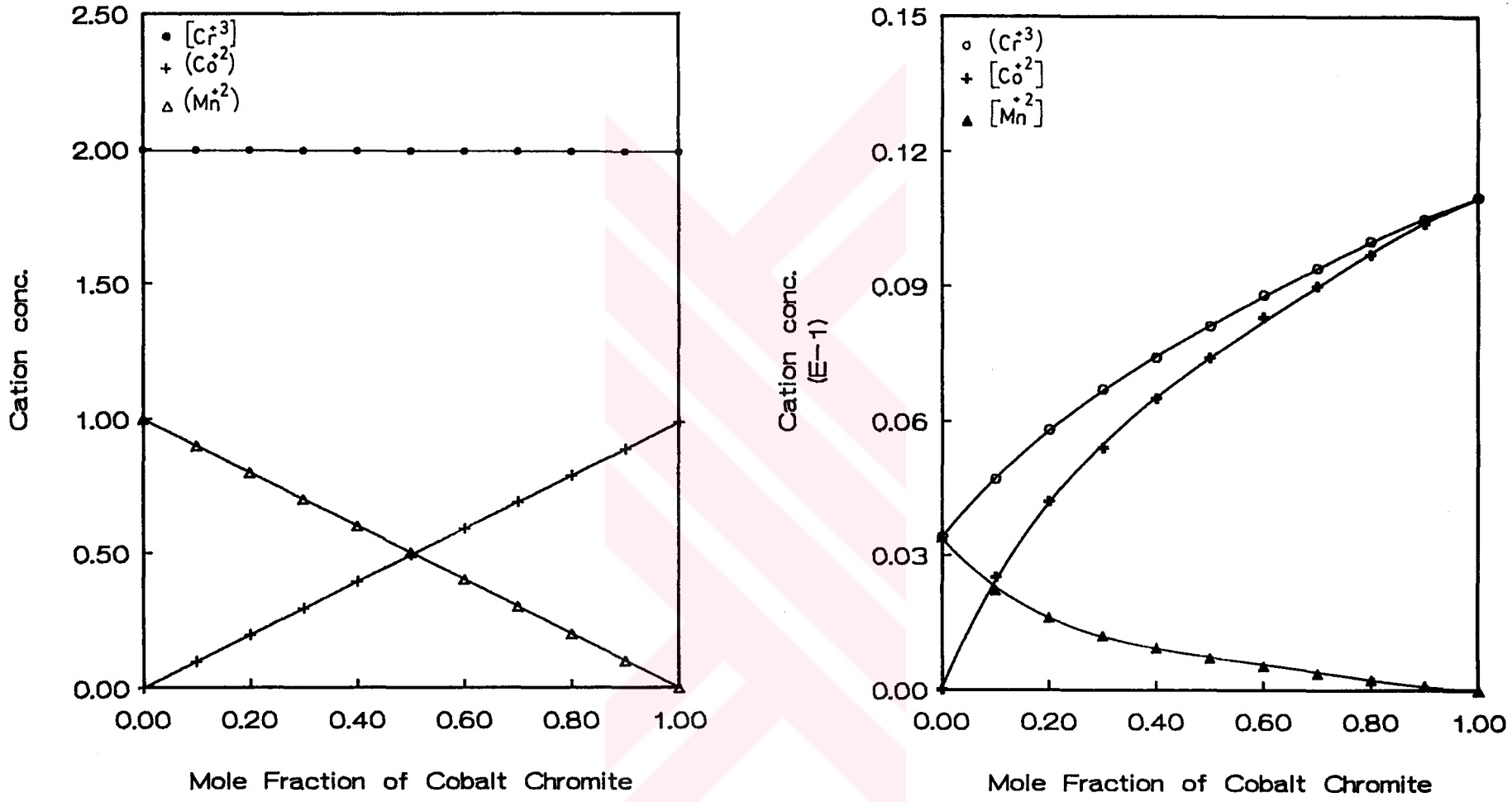

Figure 30. Variation of Cation Concentrations in the Tetrahedral and Octahedral Sites of the $MnCr_2O_4$ - $CoCr_2O_4$ Spinel Solutions as a Function of Composition at 1300 ^{o} C. (Model 1)

$$\ln\frac{d\cdot c}{a\cdot f} = -12.6655 + 3.05859\cdot c \qquad (65)$$

$$\ln\frac{e\cdot c}{b\cdot f} = -14.5771 + 3.05859\cdot c \qquad (66)$$

Numerical solutions of Eqns. 52-55 and 65-66 for each mole fraction of $CoCr_2O_4$ give the concentration of ions in tetrahedral and octahedral site at 1300 °C. The results of the cation distribution analysis at 1300 °C are given in Table 27 and shown in Figure 31.

The change in the distribution of cations will be accompanied by a free energy change, $\Delta G_{(\text{cation distribution})}$, which will be defined relative to a standard state of zero order. The free energy change of the system on disordering is ;

$$\Delta G_{(c.d)} = \Delta G_{CD} - TS_c \qquad (67)$$

where ΔG_{CD} is the nonconfigurational contribution to the free energy of disordering S_c is the configurational entropy. The nonconfigurational entropy is negligible, so the free energy of cation distribution, $\Delta G_{CD,N}$ for $CoCr_2O_4$ - $MnCr_2O_4$ solid solution series would be ;

$$\begin{aligned}\Delta G_{CD,N} = {} & d(\alpha_{Co^{+2}-Cr^{+3}} - T\cdot\sigma_{Co^{+2}-Cr^{+3}} + \beta\cdot c) \\ & + e(\alpha_{Mn^{+2}-Cr^{+3}} - T\cdot\sigma_{Mn^{+2}-Cr^{+3}} + \beta\cdot c) \\ & + RT\left[a\ln a + b\ln b + c\ln c + d\ln\frac{d}{2} + e\ln\frac{e}{2} + f\ln\frac{f}{2}\right]\end{aligned} \qquad (68)$$

Table 27. Cation Distriibution Model Calculation of Free Energy of Mixing for $CoCr_2O_4$ -$MnCr_2O_4$ at 1300°C. (Model 2)

$N_{CoCr_2O_4}$	Tetrahedral			Octahedral			ΔG_{mix} (KJ/mole)
	(Co^{+2})	(Mn^{+2})	(Cr^{+3})	[Co^{+2}]	[Mn^{+2}]	[Cr^{+3}]	
0.0	0.0000	0.9990	$9.671*10^{-4}$	0.0000	$9.671*10^{-4}$	1.9990	0
0.1	0.0995	0.8993	0.0012	$5.194*10^{-4}$	$6.942*10^{-4}$	1.9988	-4.299
0.2	0.1991	0.7995	0.0014	$8.899*10^{-4}$	$5.283*10^{-4}$	1.9986	-6.588
0.3	0.2988	0.6996	0.0016	0.0012	$4.107*10^{-4}$	1.9984	-8.028
0.4	0.3986	0.5997	0.0018	0.0014	$3.199*10^{-4}$	1.9982	-8.836
0.5	0.4983	0.4998	0.0019	0.0017	$2.461*10^{-4}$	1.9981	-9.904
0.6	0.5981	0.3999	0.0020	0.0019	$1.837*10^{-4}$	1.9980	-8.883
0.7	0.6980	0.2999	0.0022	0.0020	$1.297*10^{-4}$	1.9978	-8.007
0.8	0.7978	0.1999	0.0023	0.0022	$8.191*10^{-4}$	1.9977	-6.556
0.9	0.8976	0.0999	0.0024	0.0024	$3.900*10^{-5}$	1.9976	-4.257
1.0	0.9975	0.0000	0.0025	0.0025	0.000	1.9975	0

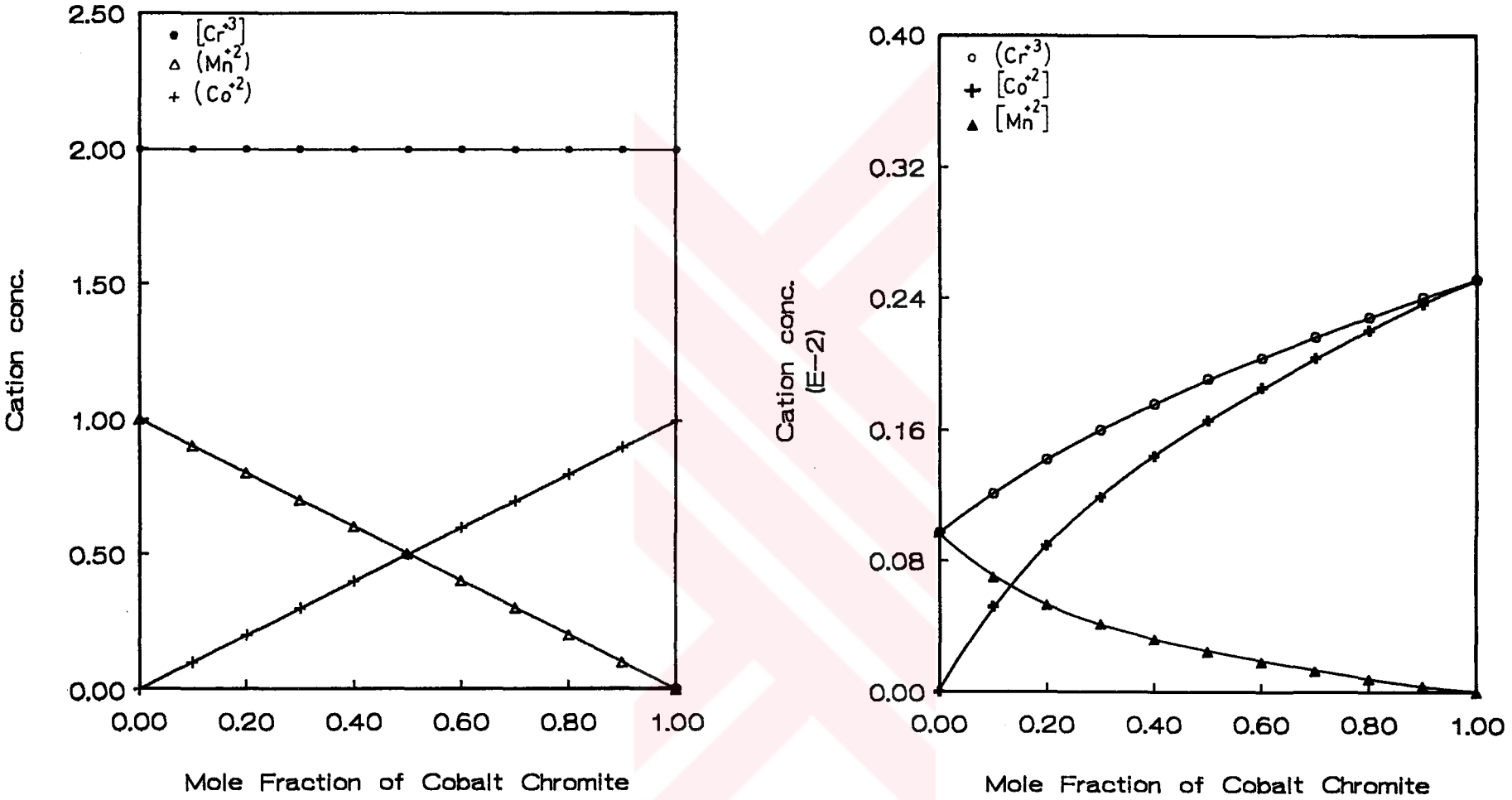

Figure 31. Variation of Cation Concentrations in the Tetrahedral and Octahedral Sites of the $MnCr_2O_4$ - $CoCr_2O_4$ Spinel Solutions as a Function of Composition at 1300 ° C. (Model 2)

The free energy of mixing at each point $N = N_{CoCr_2O_4}$, is then ;

$$\Delta G_{mix} = \Delta G_{CD;N} - N\Delta G_{CD,CoCr_2O_4} - (1-N)\Delta G_{CD;MnCr_2O_4} \qquad (69)$$

where $\Delta G_{CD,CoCr_2O_4}$ and $\Delta G_{CD,MnCr_2O_4}$ are free energy change of cation disordering in end members $CoCr_2O_4$ and $MnCr_2O_4$, respectively.

The results obtained for the concentrations of ions on various spinel sites are tabulated in Table 27 and are shown graphically in Figure 32. The free energy curves given in Fig.32 show that the mixing energies calculated from both models are closer to the ideal behavior of spinel solutions. The differences between the experimental and theoretical free energies of mixing may be attributed largely to the empirical site energies used in these models. The site preference energies assigned in 1957 by Dunitz and Orgel [36] to various cations in the spinel lattice, and the empirical cation interchange energy parameters, α, β, and σ derived by O'Neill and Navrotsky [37] may need revisions in light of the new data emerging on the thermodynamics of spinel phases so that experimental results can be verified by theoretical calculations.

4.14 Structural Studies in $CoCr_2O_4$ and $MnCr_2O_4$

The structural studies on $CoCr_2O_4$ and $MnCr_2O_4$ in the present thesis were concentrated on the determination of the cation distribution parameter "x". For this purpose quantitative x-ray diffraction methods described by Azaroff [38]

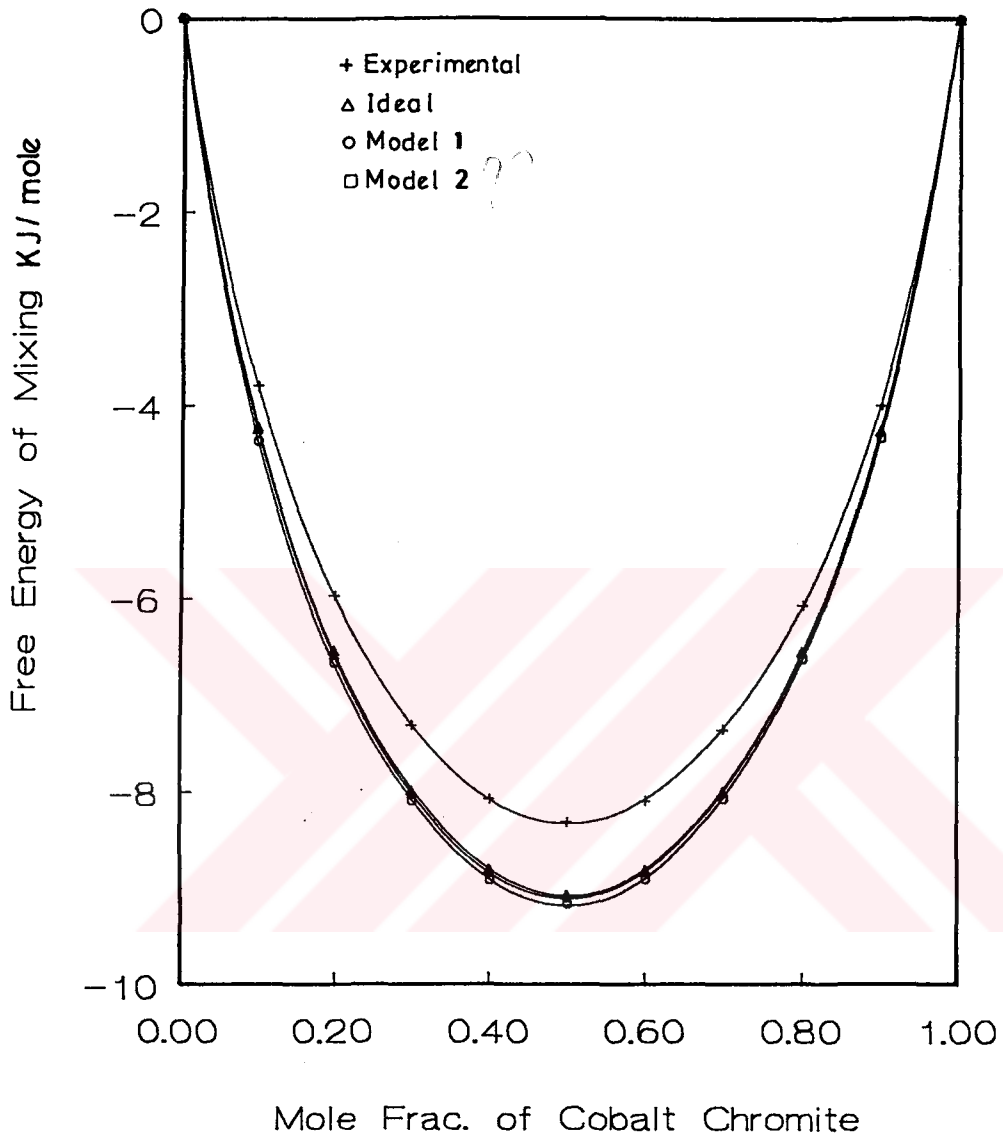

Figure 32. Gibbs Free Energy of Mixing in $MnCr_2O_4$ - $CoCr_2O_4$ Solid Solutions at 1300 °C.

Model 1 is from Jacob and co-workers [19,33,34,35]

Model 2 is from O'Neill and Navrotsky [36].

was used. This method was taken and almost standardized by a number of previous investigators [39,40,41] for the analysis of the spinel structure.

Inside the spinel unit cell, the tetrahedral cations A and the octahedral cations B occupy fixed positions on 8a and 16d lattice positions, respectively [38,42]. The coordinates (u,v,w) for these positions are given as follows :

8a tetrahedral positions : $\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{7}{8},\frac{7}{8},\frac{7}{8}$

16d octahedral positions : $\frac{1}{2},\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}$

The separations between cations are, consequently, dependent only on the unit cell dimensions. The anions in the spinel structure, on the other hand, occupy the general positions 32e. For a complete description of the locations of oxygen ions in an oxide spinel an additional parameter designated as "u" and known as "oxygen parameter" is necessary. The atom positions of oxygen in the spinel structure are given in terms of "u" as follows [38,42];

$$32e:\ u,u,u;\ u,\left(\frac{1}{4}-u\right),\left(\frac{1}{4}-u\right);\ \left(\frac{1}{4}-u\right),u,\left(\frac{1}{4}-u\right);\ \left(\frac{1}{4}-u\right),\left(\frac{1}{4}-u\right),u;$$
$$\bar{u},\bar{u},\bar{u};\ \bar{u},\left(\frac{3}{4}+u\right),\left(\frac{3}{4}+u\right);\ \left(\frac{3}{4}+u\right),\bar{u},\left(\frac{3}{4}+u\right);\ \left(\frac{3}{4}+u\right),\left(\frac{3}{4}+u\right),\bar{u}$$

Hence for an oxide spinel of general formula $(A_{1-x}B_x)[A_xB_{2-x}]O_4$ the structure would be made certain by determining the values of the disorder parameter "x" and the oxygen parameter "u". It should be pointed out that if the origin of the unit cell is taken as the center of symmetry, when u equals 0.250 the

oxygen anions are arranged in ideal cubic closest-packing. The values for "u" in actual spinels range between 0.240 and 0.275 [42,43].

The input for the structural studies in this thesis was the x-ray diffraction pattern of the spinel on which rather lengthy multiple iterative calculations were performed in order to obtain a consistent set of structural parameters x and u which defined the positions of cations and anions in the spinel lattice.

The basic equations used in the structural analysis were as follows:

1) The x-ray diffraction intensity from a single- phase powder specimen:

$$I = \left(\frac{I_o e}{m^2 c^4}\right)\left(\frac{\lambda^3 A}{32\pi r}\right)\left(\frac{1}{V^2}\right)\left(\frac{e^{-2M}}{2\mu}\right)\left[|F|^2 p\left(\frac{1+\mathrm{Cos}^2 2\theta \mathrm{Cos}^2 2\alpha}{\mathrm{Sin}^2\theta \mathrm{Cos}\theta}\right)\right] \quad (70)$$

2) The equation for the calculated structure factor $|F_c|$:

$$|F_c|^2_{hkl} = \left[\sum_1^n f_n \mathrm{Cos}2\pi(hu_n + kv_n + lw_n)\right]^2 \quad (71)$$

3) The equation for the residual parameter R:

$$R = \frac{\sum\big||F_o| - |F_c|\big|}{\sum|F_o|} \quad (72)$$

The experimental part of the structure determinations were manifested in Eqn (70). The significance of various terms in this equation have been described

in detail by Cullity [44]. The first four terms of the equation involve parameters pertinent to the diffraction system and the sample; these can be lumped into a single parameter so that the equation can be regarded as one which permits to calculate the structure factor $|F_o|$ from the intensity of refraction I from a plane of known (h,k,l) and the diffraction angles belonging to this plane.

In the present study the structural analyses were performed by picking the planes (220), (311), (222), (400), (422), (440), (531), (620), (533), (622), (444), (642), and (800) ; these were sufficient for the analysis as suggested in earlier similar studies. The structure factor $|F_o|$ calculated from Eqn.(70) is called the first crude "observed structure factor" and is designated as $|F_o|'$. In the present study diffraction patterns of $MnCr_2O_4$ and $CoCr_2O_4$ were obtained at a speed of 1/4 °/min and they are given in Fig. 35. The values of $|F_o|'$ for the spinels $MnCr_2O_4$ and $CoCr_2O_4$, as determined for the above planes from the diffraction patterns are given in Table 28.

The second step in the analysis was to obtain the "calculated structure factors" $|F_c|$. This was done, again for the refraction planes selected, by using Eqn.(71).The $|F_c|$ equations, as a function of u and x, for all the planes considered are summarized in Table 29. The mean values for the atomic scattering factors f_A, f_B, and f_O in these equations were taken from X-Ray International Tables [42] and were corrected for dispersion in accordance with the following equation given by Azaroff [38]:

$$(f)^2 = (f_o + \Delta f')^2 + (\Delta f'')^2 \qquad (73)$$

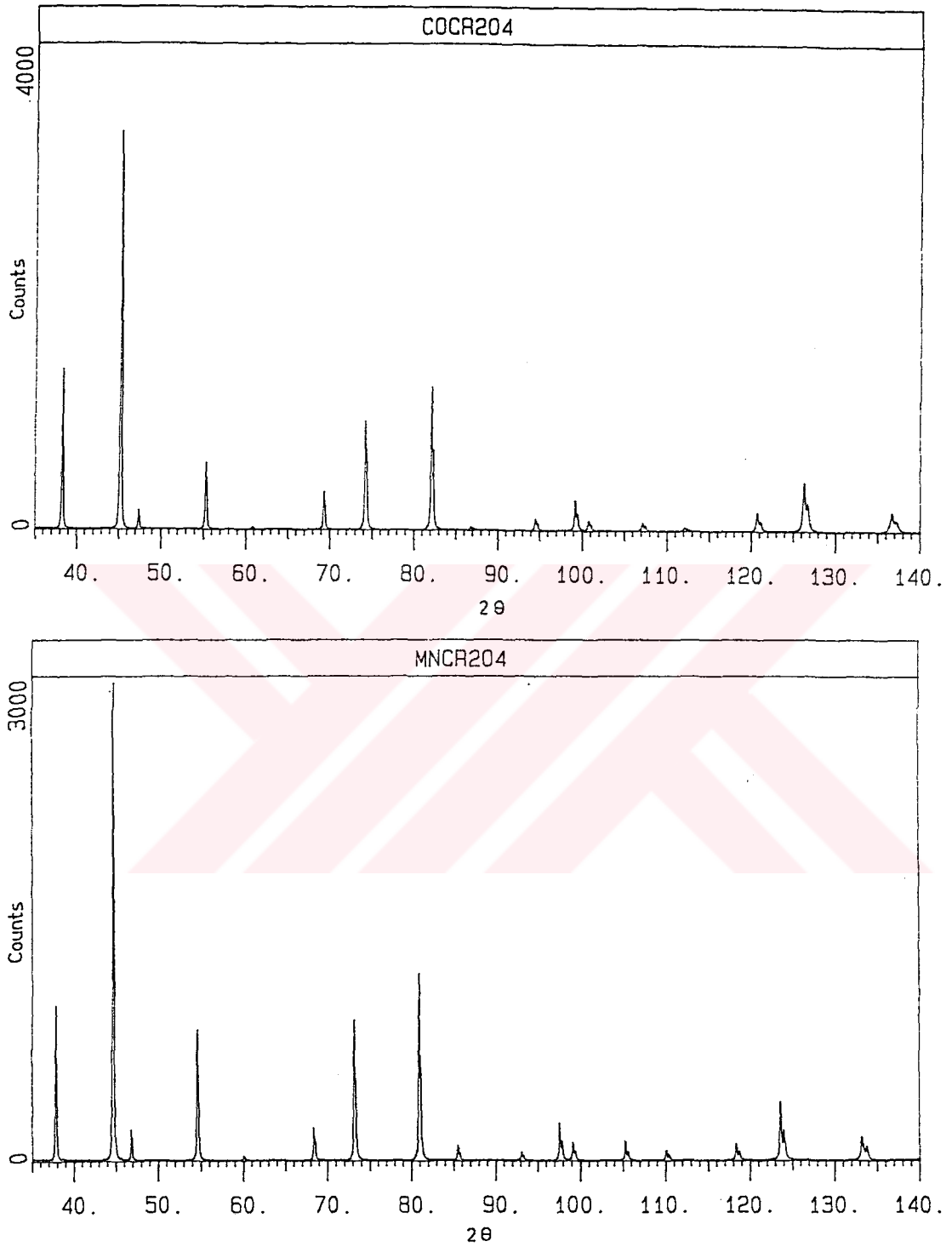

Figure 33. X-ray Diffraction Patterns for $MnCr_2O_4$ and $CoCr_2O_4$.

Table 28. Observed Structure Factors for $MnCr_2O_4$ and $CoCr_2O_4$

	$MnCr_2O_4$		$CoCr_2O_4$	
hkl	2θ	|Fo|'	2θ	|Fo|'
220	37.875	6.8454	38.314	8.2562
311	44.749	10.5249	45.283	11.6297
222	46.860	4.6977	47.427	4.6207
400	54.672	14.3518	55.355	12.8403
422	68.455	4.7287	69.371	6.2361
440	81.009	19.0950	82.182	11.8127
531	85.573	2.7315	86.861	1.6852
620	93.161	3.3917	94.610	4.9121
533	97.692	6.9401	99.293	7.7690
622	99.209	4.9152	100.857	4.7922
444	105.407	8.7119	107.248	7.5993
642	118.478	3.5476	120.860	4.6499
800	133.449	12.91707	136.833	14.0929

Table 29. Structure Factors $|Fc|$ for all Site in the Spinel $(A_{1-x}B_x)[A_xB_{2-x}]O_4$

Diffraction line hkl	Structure Factor; $\sum_1^n f_n \mathrm{Cos}2\pi(hu+kv+lw)$		
	8a Tetrahedral	16d Octahedral	32e Oxygen
220	$-8[(1-x)f_A+xf_B]$	0	$4f_O[-4+2\mathrm{Cos}2\pi\cdot 4u+\mathrm{Cos}2\pi\cdot(1-4u)+\mathrm{Cos}2\pi\cdot(3+4u)]$
311	$-5.6568[(1-x)f_A+xf_B]$	$-4[(2-x)f_A+xf_B]$	$4f_O[2\mathrm{Cos}2\pi\cdot 5u+2\mathrm{Cos}2\pi\cdot(1-3u)+2\mathrm{Cos}2\pi\cdot(3+3u)+\mathrm{Cos}2\pi\cdot(u+0.5)+\mathrm{Cos}2\pi\cdot(1.5-u)]$
222	0	$8[(2-x)f_B+xf_A]$	$4f_O[2\mathrm{Cos}2\pi\cdot 6u+2\mathrm{Cos}2\pi\cdot(1-2u)+\mathrm{Cos}2\pi\cdot(1+2u)+2\mathrm{Cos}2\pi(2u+3)+\mathrm{Cos}2\pi\cdot(3-2u)]$
400	$-8[(1-x)f_A+xf_B]$	$8[(2-x)f_B+xf_A]$	$8f_O[2\mathrm{Cos}2\pi\cdot 4u+\mathrm{Cos}2\pi\cdot(1-4u)+\mathrm{Cos}2\pi\cdot(3+4u)]$
422	$8[(1-x)f_A+xf_B]$	0	$8f_O[1+\mathrm{Cos}2\pi\cdot 8u+\mathrm{Cos}2\pi\cdot(1.5-4u)+\mathrm{Cos}2\pi\cdot(4.5-4u)]$
440	$8[(1-x)f_A+xf_B]$	$8[(2-x)f_B+xf_A]$	$4f_O[4+2\mathrm{Cos}2\pi\cdot 8u+\mathrm{Cos}2\pi\cdot(2-8u)+\mathrm{Cos}2\pi\cdot(6+8u)]$
531	$5.6568[(1-x)f_A+xf_B]$	$-8[(2-x)f_B+xf_A]$	$4f_O[2\mathrm{Cos}2\pi\cdot 9u+\mathrm{Cos}2\pi\cdot(1+u)+\mathrm{Cos}2\pi\cdot(1.5+3u)+\mathrm{Cos}2\pi\cdot(2-7u)+\mathrm{Cos}2\pi\cdot(3-u)+\mathrm{Cos}2\pi\cdot(4.5+3u)+\mathrm{Cos}2\pi\cdot(6-7u)]$

Table 29. (continued)

Diffraction line hkl	Structure Factor; $\sum_{1}^{n} f_n \mathrm{Cos}2\pi(hu+kv+lw)$		
	8a Tetrahedral	16d Octahedral	32e Oxygen
620	$8[(1-x)f_A + xf_B]$	0	$4f_O[2\mathrm{Cos}2\pi\cdot 8u + \mathrm{Cos}2\pi\cdot(0.5+4u) + 2\mathrm{Cos}2\pi\cdot(1.5-4u) + \mathrm{Cos}2\pi\cdot(4.5+4u) + \mathrm{Cos}2\pi\cdot(2-8u) + \mathrm{Cos}2\pi\cdot(6+8u)]$
533	$-5.6568[(1-x)f_A + xf_B]$	$-8[(2-x)f_B + xf_A]$	$4f_O[2\mathrm{Cos}2\pi\cdot 11u + \mathrm{Cos}2\pi\cdot(1.5-u) + 2\mathrm{Cos}2\pi\cdot(2-5u) + 2\mathrm{Cos}2\pi\cdot(6+5u) + \mathrm{Cos}2\pi\cdot(4.5+u)]$
622	0	$8[(2-x)f_B + xf_A]$	$4f_O[2\mathrm{Cos}2\pi\cdot 10u + \mathrm{Cos}2\pi\cdot(1+2u) + 2\mathrm{Cos}2\pi\cdot(2-6u) + \mathrm{Cos}2\pi\cdot(3-2u) + 2\mathrm{Cos}2\pi\cdot(6+6u)]$
444	$-8[(1-x)f_A + xf_B]$	$8[(2-x)f_B + xf_A]$	$4f_O[2\mathrm{Cos}2\pi\cdot 12u + 3\mathrm{Cos}2\pi\cdot(2-4u) + 3\mathrm{Cos}2\pi\cdot(6+4u)]$
642	$-8[(1-x)f_A + xf_B]$	0	$8f_O[-1+\mathrm{Cos}2\pi\cdot 12u + \mathrm{Cos}2\pi\cdot(2-6u) + \mathrm{Cos}2\pi\cdot(6+6u)]$
800	$8[(1-x)f_A + xf_B]$	$8[(2-x)f_B + xf_A]$	$8f_O[2\mathrm{Cos}2\pi\cdot 8u + \mathrm{Cos}2\pi\cdot(2-8u) + \mathrm{Cos}2\pi\cdot(6+8u)]$

where f_o is the mean atomic scattering factor and, $\Delta f'$ and $\Delta f''$ are the real and the imaginary parts of the dispersion corrections [38]. Figure 34 shows the variation of the atomic scattering factors with $\sin\theta/\lambda$ and Table 30 gives the values of the correction factors.

Table 30. Real and Imaginary Dispersion Corrections for Atomic Scattering Factors.

Element	FeKα	
	$\Delta f'$	$\Delta f''$
O	0.069	0.052
Cr	-1.973	3.533
Mn	- 3.367	0.481
Co	- 1.627	0.662

The third step in the analysis was to ascertain the values of the " true observed structure factors", designated as $|F_o|$. The true observed structure factor $|F_o|$ was calculated for each refraction by correcting the crude observed structure factor $|F_o|'$ with the scale constant K and the Debye temperature factor B through the use of the following equation [38]

$$|F_o| = K|F_o|' \cdot e^{B\frac{\sin^2\theta}{\lambda^2}} \qquad (74)$$

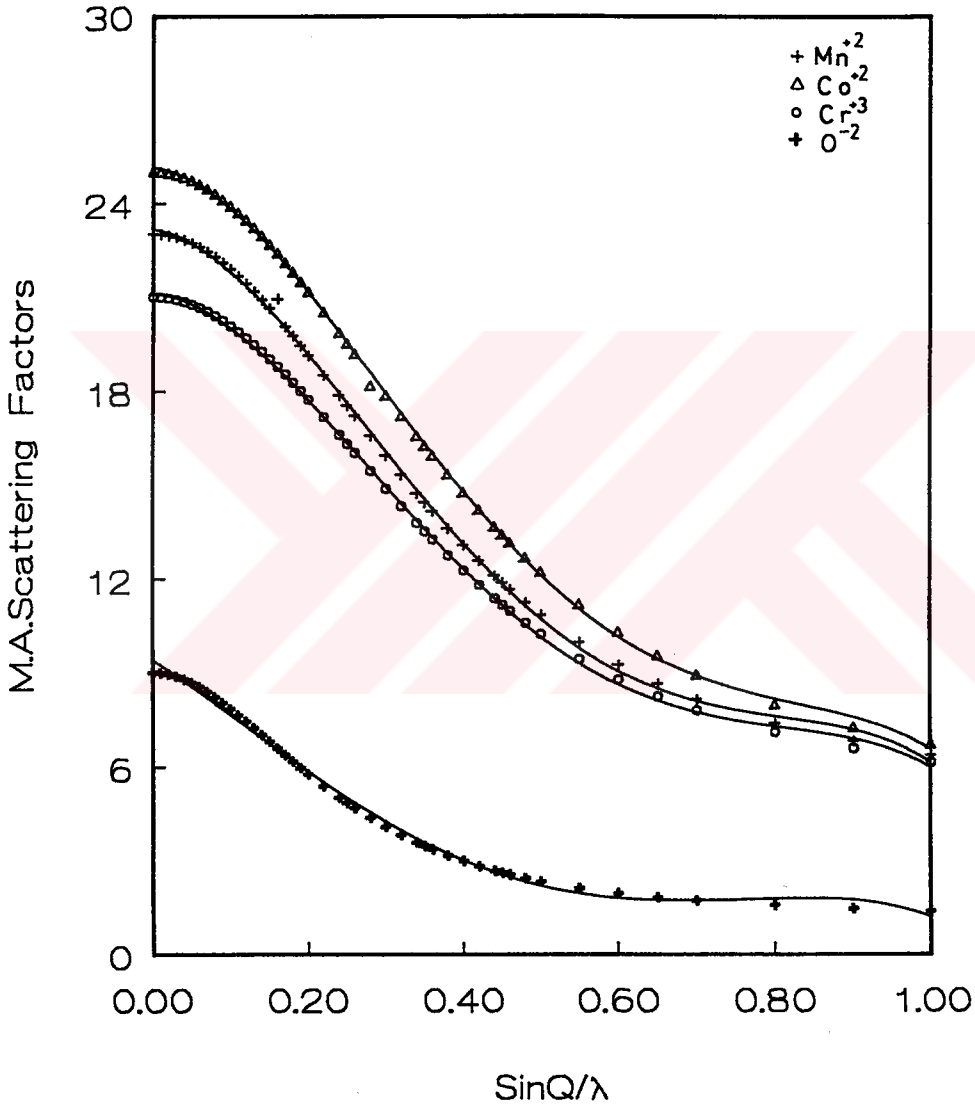

Figure 34. Mean Atomic Scattering Factors in Electrons for Chemically Significant Ions.

The factors K and B modify the crude structure factor $|Fo|'$. The values of these two correction terms could be obtained by solving the equation which relates $|F_o|'$ to $|F_c|$ [38] ;

$$K|F_o|' = |F_c| e^{-B\frac{\sin^2\theta}{\lambda^2}} \qquad (75)$$

Rearranging the terms and taking the natural logarithm of both sides, the following equation could be written :

$$\ln\frac{|F_o|'}{|F_c|} = \ln\frac{1}{K} - B\frac{\sin^2\theta}{\lambda^2} \qquad (76)$$

Table 29 shows that the integrated intensities of the diffraction lines from (440) and (800) planes are independent of the cation distribution parameter x and are functions only of u. X-ray data belonging to these planes could be used for estimating the values of the scale constant K and the temperature factor B. A plot of the left side of Eqn.(76) against ($\sin^2\theta/\lambda^2$) for these two particular refractions would yield a straight line of slope (-B) and the intercept at $\theta=0^o$ would be the scale constant "K". This procedure, devised first by A.J.C.Wilson [45] has been used commonly to scale experimentally measured intensities before comparing them with calculated values.

The values of K and B obtained by the procedure given above were used in Eqn.(75) to calculate the true observed structure factors $|Fo|$. The expression for the residuals, Eqn (72), describes the essence of the iteration

procedure. The residual R for a selected combination of u and x should approach zero or be at a minimum value if this combination fits the structure of the spinel.

The calculations performed for $|Fc|$ and $|Fo|$ by the multiple iteration procedure described above are given in Tables A.1 and A.2 of the Appendix. In the insert of table captions the parameter selected for the iteration and the corresponding values of B and K are indicated.

In general, during iterations, the u and x values were altered by increments of 0.0001 and 0.001, respectively. The residuals "R" determined by using the information contained in these tables are given in Tables A.3 and A.4. for cobalt chromite and manganese chromite, respectively. The pair (u,x) found to yield the minimum of R value was taken as the optimized solution of the structure.

Referring to these tables the structural parameters for $MnCr_2O_4$ and $CoCr_2O_4$ are tabulated in Table 30.

Table 30. Structural parameters for $MnCr_2O_4$ and $CoCr_2O_4$.

	B	K	u	x
$MnCr_2O_4$	0.50290	20.06425	0.2671	0.000
$CoCr_2O_4$	0.35014	19.69118	0.2628	0.071

While, no high temperature data are readily available for comparison, R.J. Bovabard and A Wold [46] has published a value of u=0.2641 and x=0.00 for $MnCr_2O_4$, Tretjakow and Schmalzried [9] gave a value of u= 0.261 for $CoCr_2O_4$; both at room temperature. The results for "x" given in Table 30 indicate that the compound $MnCr_2O_4$ is a perfectly normal spinel, whereas there is a slight tendency for the site exchange of cations in the compound $CoCr_2O_4$.

CHAPTER V

CONCLUSIONS

Oxide systems containing spinel phases are potential candidates for the production of a variety of functional ceramics useful particularly in the electronic device industry. Such systems are equally important in refractory technology since many of the new generation of refractories contain spinels of chromium or aluminum which possess exceptional thermal and chemical stability. Knowledge on phase equilibria and thermodynamics of phases that develop in these materials at high temperatures is essential for their processing and property development. The objective of the present thesis was to generate such information for the system MnO-CoO-Cr_2O_3 at 1300 °C.

The results of the experimental work carried out in this thesis showed that the system was characterized by the presence of two unbroken series of solid solutions; one of them being MnO-CoO series with the rock-salt structure and the other was the $MnCr_2O_4$ - $CoCr_2O_4$ solutions having spinel structure. The experiments were performed to measure the activities of CoO in both of these solutions and in their mixtures mainly by using the gas equilibration technique. The results for the MnO-CoO series were supplemented by emf measurements using a solid ionic conductor as electrolyte. In addition to the determination of activities

phase boundaries in the system were delineated which permitted to define the stability areas as a function of composition and oxygen partial pressure.

The results on CoO activity measurements in the MnO-CoO binary revealed that these solutions exhibit slight to moderate deviations from ideal behavior at 1300 °C. Regarding the activity-composition relationships in this system, the finding of the present work were in excellent agreement with those deduced by extrapolations of the data obtained by previous researchers at lower temperatures.

The spinel solid solutions in the system were found to be completely stoichiometric with respect to Cr_2O_3 but they would tend to dissolve an excess of the divalent oxides giving rise to a narrow band of ternary spinel solid solutions. The isoactivity curves for CoO in these solutions were constructed from the experimental CoO activity data. The phase boundary where the ternary spinels were saturated with MnO-CoO solid solution was determined by optical microscopy and x-ray diffraction analyses on quenched samples. The isoactivity curves of CoO in the ternary spinel field were helpful in locating this boundary precisely.

The extent of nonstoichiometry in the $CoCr_2O_4$ spinel was shown by accurate CoO activity measurements inside the very narrow spinel field of the CoO-Cr_2O_3 binary. These measurements permitted to calculate the free energy of formation of $CoCr_2O_4$ compound from its oxides, CoO and Cr_2O_3, as -37636 J/mole at 1300 °C.

The activities of $CoCr_2O_4$ in the stoichiometric $MnCr_2O_4$-$CoCr_2O_4$ solid solutions were obtained by combining the calculated stability of $CoCr_2O_4$ with the activities of CoO measured across this join. The results indicated that the stoichiometric ternary spinel solutions exhibit positive deviations from ideality at 1300 °C. This was in contrast to the predictions made by using the cation distribution models available in the literature for spinel solutions. Since the models tested were based upon empirical energy parameters assigned some forty years ago revisions in the generally accepted values of these parameters are necessary in order to use them for a sound estimate of the thermodynamic behavior of other spinel systems.

No information was available in the previous literature on a direct determination of the stability of the compound $MnCr_2O_4$. The present study did not yield a direct value for the $\Delta G^{o}_{MnCr_2O_4}$ either. However, the Gibbs-Duhem treatment of the data on the CoO activities in the ternary spinel field allowed to make an estimate for this quantity at 1300 °C. The free energy of formation of $MnCr_2O_4$ from MnO and Cr_2O_3 at the temperature of the present work was calculated as -42278 J/mole. This value was considerably higher than those of other two earlier estimates but close to the one determined at 1300 °C in a study conducted on the system NiO-MnO-Cr_2O_3. The present value, -42278 J/mole, indicates that the compound $MnCr_2O_4$ is more stable than $CoCr_2O_4$. This is verified by the directions of conjugation lines between coexisting MnO-CoO solid solutions and ternary spinel solutions ; i.e., they converge towards the $MnCr_2O_4$ composition point.

In addition to the phase equilibria and thermodynamic studies mentioned above the structures of $MnCr_2O_4$ and $CoCr_2O_4$ spinels were examined in terms of the cation distribution parameter "x" and the oxygen parameter "u". These studies were based upon quantitative x-ray diffraction methods involving the comparison of calculated and measured diffraction intensities from selected crystallographic planes of the spinel lattice. A computer program was developed so that multiple successive iterations could be performed during the structural analyses. The results indicated that, within limits of analytical procedures, the disorder parameter x for the $MnCr_2O_4$ spinel was zero so that this compound could be regarded as a perfect normal spinel. In the cobalt spinel the disorder parameter x was found as 0.071 which showed that there was a slight tendency for the exchange of cations between tetrahedral and octahedral lattice sites.

Because of the volatility of CoO at high temperatures and the similar propensity of Cr_2O_3 to volatilize, the system $MnO\text{-}CoO\text{-}Cr_2O_3$ could not be studied at temperatures higher than 1300 °C. At the lower temperatures the time to attain equilibrium was rather too long. Therefore in the present work no information could be generated on the temperature dependence of equilibria and thermodynamics of the system. However, in the future a high temperature in-situ x-ray study on the binary and ternary spinels could yield quite valuable information on disorder parameter x and the energetics of cation exchange reactions. It should be emphasized that the disorder parameters reported in this thesis were determined on quenched spinel samples. Thus the actual disorder prevailing at 1300 °C was likely changed and parameters reflect the situation only at room temperature.

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APPENDIX

APPENDIX A. TABLES

Table A.1.1. Calculated and Observed Structure Factor for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2500, B=-0.56087, K=19.75001)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.008	240.202	73.146	257.258	131.528	433.541	13.539	109.880	163.522	76.787	160.032	94.544	316.728
0.010	163.723	239.557	72.064	257.771	131.295	433.541	13.785	109.688	163.484	76.970	160.380	94.387	316.728
0.020	163.437	238.913	70.983	258.284	131.063	433.541	14.031	109.496	163.445	77.153	160.728	94.230	316.728
0.030	163.152	238.268	69.902	258.797	130.830	433.541	14.277	109.304	163.407	77.335	161.076	94.072	316.728
0.040	162.867	237.624	68.820	259.310	130.598	433.541	14.523	109.113	163.369	77.518	161.423	93.915	316.728
0.050	162.581	236.979	67.739	259.823	130.365	433.541	14.769	108.921	163.330	77.701	161.771	93.758	316.728
0.060	162.296	236.335	66.658	260.336	130.133	433.541	15.015	108.729	163.292	77.884	162.119	93.601	316.728
0.070	162.010	235.690	65.576	260.849	129.900	433.541	15.261	108.537	163.254	78.066	162.467	93.444	316.728
0.080	161.725	235.046	64.495	261.363	129.668	433.541	15.507	108.345	163.215	78.249	162.815	93.286	316.728
0.090	161.440	234.401	63.413	261.876	129.435	433.541	15.753	108.153	163.177	78.432	163.163	93.129	316.728
0.100	161.154	233.757	62.332	262.389	129.202	433.541	15.999	107.962	163.139	78.614	163.510	92.972	316.728
0.110	160.869	233.112	61.251	262.902	128.970	433.541	16.245	107.770	163.100	78.797	163.858	92.815	316.728
0.120	160.584	232.468	60.169	263.415	128.737	433.541	16.491	107.578	163.062	78.980	164.206	92.658	316.728
0.130	160.298	231.823	59.088	263.928	128.505	433.541	16.737	107.386	163.024	79.163	164.554	92.500	316.728
0.140	160.013	231.179	58.007	264.441	128.272	433.541	16.983	107.194	162.986	79.345	164.902	92.343	316.728
0.150	159.728	230.534	56.925	264.954	128.040	433.541	17.229	107.002	162.947	79.528	165.250	92.186	316.728
0.160	159.442	229.890	55.844	265.468	127.807	433.541	17.475	106.811	162.909	79.711	165.597	92.029	316.728
0.170	159.157	229.245	54.763	265.981	127.574	433.541	17.721	106.619	162.871	79.893	165.945	91.872	316.728
0.180	158.872	228.601	53.681	266.494	127.342	433.541	17.968	106.427	162.832	80.076	166.293	91.714	316.728
0.190	158.586	227.956	52.600	267.007	127.109	433.541	18.214	106.235	162.794	80.259	166.641	91.557	316.728
0.200	158.301	227.312	51.519	267.520	126.877	433.541	18.460	106.043	162.756	80.442	166.989	91.400	316.728
|Fo|	165.705	234.831	93.491	261.906	129.270	433.541	35.718	105.170	167.349	103.435	165.354	102.827	316.728

Table A.1.2. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2504, B=-0.56066, K=19.74994)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.013	239.965	73.152	257.249	131.525	433.529	13.958	109.872	163.398	76.801	160.018	94.550	316.712
0.010	163.728	239.321	72.071	257.763	131.292	433.529	14.204	109.680	163.360	76.983	160.366	94.393	316.712
0.020	163.442	238.676	70.990	258.276	131.059	433.529	14.450	109.489	163.321	77.166	160.714	94.236	316.712
0.030	163.157	238.032	69.908	258.789	130.827	433.529	14.696	109.297	163.283	77.349	161.062	94.079	316.712
0.040	162.872	237.387	68.827	259.302	130.594	433.529	14.942	109.105	163.245	77.532	161.409	93.922	316.712
0.050	162.586	236.743	67.746	259.815	130.362	433.529	15.188	108.913	163.206	77.714	161.757	93.764	316.712
0.060	162.301	236.098	66.664	260.328	130.129	433.529	15.434	108.721	163.168	77.897	162.105	93.607	316.712
0.070	162.016	235.454	65.583	260.841	129.897	433.529	15.680	108.529	163.130	78.080	162.453	93.450	316.712
0.080	161.730	234.809	64.502	261.354	129.664	433.529	15.926	108.338	163.091	78.262	162.801	93.293	316.712
0.090	161.445	234.165	63.420	261.868	129.432	433.529	16.172	108.146	163.053	78.445	163.149	93.136	316.712
0.100	161.160	233.520	62.339	262.381	129.199	433.529	16.418	107.954	163.015	78.628	163.496	92.978	316.712
0.110	160.874	232.876	61.258	262.894	128.966	433.529	16.664	107.762	162.977	78.811	163.844	92.821	316.712
0.120	160.589	232.231	60.176	263.407	128.734	433.529	16.910	107.570	162.938	78.993	164.192	92.664	316.712
0.130	160.303	231.587	59.095	263.920	128.501	433.529	17.156	107.378	162.900	79.176	164.540	92.507	316.712
0.140	160.018	230.942	58.014	264.433	128.269	433.529	17.402	107.187	162.862	79.359	164.888	92.350	316.712
0.150	159.733	230.298	56.932	264.946	128.036	433.529	17.648	106.995	162.823	79.541	165.236	92.192	316.712
0.160	159.447	229.654	55.851	265.459	127.804	433.529	17.894	106.803	162.785	79.724	165.583	92.035	316.712
0.170	159.162	229.009	54.769	265.973	127.571	433.529	18.141	106.611	162.747	79.907	165.931	91.878	316.712
0.180	158.877	228.365	53.688	266.486	127.339	433.529	18.387	106.419	162.708	80.090	166.279	91.721	316.712
0.190	158.591	227.720	52.607	266.999	127.106	433.529	18.633	106.227	162.670	80.272	166.627	91.564	316.712
0.200	158.306	227.076	51.525	267.512	126.873	433.529	18.879	106.035	162.632	80.455	166.975	91.406	316.712
|Fo|	165.704	234.828	93.490	261.902	129.268	433.529	35.717	105.167	167.344	103.431	165.348	102.822	316.712

Table A.1.3. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2508, B=-0.56003, K=19.74979)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.029	239.731	73.173	257.225	131.514	433.494	14.375	109.849	163.273	76.841	159.976	94.570	316.663
0.010	163.743	239.087	72.092	257.738	131.282	433.494	14.621	109.657	163.234	77.024	160.324	94.412	316.663
0.020	163.458	238.442	71.010	258.251	131.049	433.494	14.867	109.465	163.196	77.206	160.672	94.255	316.663
0.030	163.173	237.798	69.929	258.764	130.817	433.494	15.113	109.274	163.158	77.389	161.020	94.098	316.663
0.040	162.887	237.153	68.847	259.278	130.584	433.494	15.360	109.082	163.120	77.572	161.367	93.941	316.663
0.050	162.602	236.509	67.766	259.791	130.352	433.494	15.606	108.890	163.081	77.755	161.715	93.784	316.663
0.060	162.316	235.864	66.685	260.304	130.119	433.494	15.852	108.698	163.043	77.937	162.063	93.626	316.663
0.070	162.031	235.220	65.603	260.817	129.887	433.494	16.098	108.506	163.005	78.120	162.411	93.469	316.663
0.080	161.746	234.575	64.522	261.330	129.654	433.494	16.344	108.314	162.966	78.303	162.759	93.312	316.663
0.090	161.460	233.931	63.441	261.843	129.421	433.494	16.590	108.123	162.928	78.485	163.107	93.155	316.663
0.100	161.175	233.286	62.359	262.356	129.189	433.494	16.836	107.931	162.890	78.668	163.454	92.998	316.663
0.110	160.890	232.642	61.278	262.869	128.956	433.494	17.082	107.739	162.851	78.851	163.802	92.840	316.663
0.120	160.604	231.997	60.197	263.383	128.724	433.494	17.328	107.547	162.813	79.034	164.150	92.683	316.663
0.130	160.319	231.353	59.115	263.896	128.491	433.494	17.574	107.355	162.775	79.216	164.498	92.526	316.663
0.140	160.034	230.708	58.034	264.409	128.259	433.494	17.820	107.163	162.737	79.399	164.846	92.369	316.663
0.150	159.748	230.064	56.953	264.922	128.026	433.494	18.066	106.971	162.698	79.582	165.194	92.212	316.663
0.160	159.463	229.419	55.871	265.435	127.794	433.494	18.312	106.780	162.660	79.765	165.542	92.054	316.663
0.170	159.178	228.775	54.790	265.948	127.561	433.494	18.558	106.588	162.622	79.947	165.889	91.897	316.663
0.180	158.892	228.131	53.709	266.461	127.328	433.494	18.804	106.396	162.583	80.130	166.237	91.740	316.663
0.190	158.607	227.486	52.627	266.974	127.096	433.494	19.050	106.204	162.545	80.313	166.585	91.583	316.663
0.200	158.321	226.842	51.546	267.487	126.863	433.494	19.296	106.012	162.507	80.495	166.933	91.426	316.663
|Fo|	165.699	234.820	93.487	261.891	129.260	433.494	35.714	105.156	167.326	103.420	165.328	102.809	316.663

Table A.1.4. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2512, B=-0.55904, K=19.74931)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.054	239.495	73.207	257.184	131.498	433.434	14.793	109.809	163.150	76.909	159.858	94.603	316.584
0.010	163.769	238.850	72.126	257.698	131.265	433.434	15.039	109.617	163.112	77.092	160.206	94.446	316.584
0.020	163.484	238.206	71.044	258.211	131.032	433.434	15.285	109.425	163.074	77.275	160.554	94.288	316.584
0.030	163.198	237.561	69.963	258.724	130.800	433.434	15.531	109.234	163.035	77.458	160.902	94.131	316.584
0.040	162.913	236.917	68.882	259.237	130.567	433.434	15.777	109.042	162.997	77.640	161.250	93.974	316.584
0.050	162.628	236.272	67.800	259.750	130.335	433.434	16.023	108.850	162.959	77.823	161.598	93.817	316.584
0.060	162.342	235.628	66.719	260.263	130.102	433.434	16.269	108.658	162.920	78.006	161.945	93.660	316.584
0.070	162.057	234.983	65.637	260.776	129.870	433.434	16.515	108.466	162.882	78.189	162.293	93.502	316.584
0.080	161.772	234.339	64.556	261.289	129.637	433.434	16.761	108.274	162.844	78.371	162.641	93.345	316.584
0.090	161.486	233.694	63.475	261.803	129.405	433.434	17.008	108.083	162.805	78.554	162.989	93.188	316.584
0.100	161.201	233.050	62.393	262.316	129.172	433.434	17.254	107.891	162.767	78.737	163.337	93.031	316.584
0.110	160.915	232.406	61.312	262.829	128.939	433.434	17.500	107.699	162.729	78.919	163.685	92.874	316.584
0.120	160.630	231.761	60.231	263.342	128.707	433.434	17.746	107.507	162.690	79.102	164.032	92.716	316.584
0.130	160.345	231.117	59.149	263.855	128.474	433.434	17.992	107.315	162.652	79.285	164.380	92.559	316.584
0.140	160.059	230.472	58.068	264.368	128.242	433.434	18.238	107.123	162.614	79.468	164.728	92.402	316.584
0.150	159.774	229.828	56.987	264.881	128.009	433.434	18.484	106.932	162.576	79.650	165.076	92.245	316.584
0.160	159.489	229.183	55.905	265.394	127.777	433.434	18.730	106.740	162.537	79.833	165.424	92.088	316.584
0.170	159.203	228.539	54.824	265.907	127.544	433.434	18.976	106.548	162.499	80.016	165.772	91.930	316.584
0.180	158.918	227.894	53.743	266.421	127.311	433.434	19.222	106.356	162.461	80.198	166.120	91.773	316.584
0.190	158.633	227.250	52.661	266.934	127.079	433.434	19.468	106.164	162.422	80.381	166.467	91.616	316.584
0.200	158.347	226.605	51.580	267.447	126.846	433.434	19.714	105.972	162.384	80.564	166.815	91.459	316.584
|Fo|	165.691	234.805	93.481	261.870	129.245	433.434	35.709	105.139	167.296	103.401	165.296	102.786	316.584

Table A.1.5. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2516, B=-0.55757, K=19.74895)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.091	239.261	73.255	257.125	131.474	433.353	15.211	109.755	163.029	77.005	159.806	94.648	316.470
0.010	163.805	238.616	72.173	257.639	131.241	433.353	15.457	109.563	162.990	77.188	160.154	94.491	316.470
0.020	163.520	237.972	71.092	258.152	131.009	433.353	15.703	109.371	162.952	77.370	160.502	94.333	316.470
0.030	163.234	237.327	70.011	258.665	130.776	433.353	15.949	109.179	162.914	77.553	160.850	94.176	316.470
0.040	162.949	236.683	68.929	259.178	130.544	433.353	16.195	108.988	162.876	77.736	161.197	94.019	316.470
0.050	162.664	236.038	67.848	259.691	130.311	433.353	16.441	108.796	162.837	77.918	161.545	93.862	316.470
0.060	162.378	235.394	66.767	260.204	130.079	433.353	16.687	108.604	162.799	78.101	161.893	93.705	316.470
0.070	162.093	234.749	65.685	260.717	129.846	433.353	16.933	108.412	162.761	78.284	162.241	93.547	316.470
0.080	161.808	234.105	64.604	261.230	129.613	433.353	17.179	108.220	162.722	78.467	162.589	93.390	316.470
0.090	161.522	233.460	63.522	261.744	129.381	433.353	17.425	108.028	162.684	78.649	162.937	93.233	316.470
0.100	161.237	232.816	62.441	262.257	129.148	433.353	17.671	107.837	162.646	78.832	163.284	93.076	316.470
0.110	160.952	232.171	61.360	262.770	128.916	433.353	17.917	107.645	162.607	79.015	163.632	92.919	316.470
0.120	160.666	231.527	60.278	263.283	128.683	433.353	18.163	107.453	162.569	79.198	163.980	92.761	316.470
0.130	160.381	230.882	59.197	263.796	128.451	433.353	18.409	107.261	162.531	79.380	164.328	92.604	316.470
0.140	160.096	230.238	58.116	264.309	128.218	433.353	18.656	107.069	162.492	79.563	164.676	92.447	316.470
0.150	159.810	229.594	57.034	264.822	127.985	433.353	18.902	106.877	162.454	79.746	165.024	92.290	316.470
0.160	159.525	228.949	55.953	265.335	127.753	433.353	19.148	106.686	162.416	79.928	165.371	92.133	316.470
0.170	159.239	228.305	54.872	265.849	127.520	433.353	19.394	106.494	162.378	80.111	165.719	91.975	316.470
0.180	158.954	227.660	53.790	266.362	127.288	433.353	19.640	106.302	162.339	80.294	166.067	91.818	316.470
0.190	158.669	227.016	52.709	266.875	127.055	433.353	19.886	106.110	162.301	80.477	166.415	91.661	316.470
0.200	158.383	226.371	51.628	267.388	126.823	433.353	20.132	105.918	162.263	80.659	166.763	91.504	316.470
IFoI	165.681	234.787	93.473	261.843	129.227	433.353	35.702	105.115	167.255	103.375	165.251	102.753	316.470

Table A.1.6. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2520, B=-0.55574, K=19.74825)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.140	239.024	73.318	257.052	131.443	433.247	15.627	109.685	162.907	77.127	159.679	94.705	316.326
0.010	163.854	238.380	72.237	257.565	131.211	433.247	15.873	109.494	162.869	77.310	160.027	94.548	316.326
0.020	163.569	237.735	71.156	258.079	130.978	433.247	16.119	109.302	162.831	77.493	160.375	94.391	316.326
0.030	163.284	237.091	70.074	258.592	130.746	433.247	16.365	109.110	162.792	77.675	160.723	94.234	316.326
0.040	162.998	236.446	68.993	259.105	130.513	433.247	16.611	108.918	162.754	77.858	161.070	94.077	316.326
0.050	162.713	235.802	67.911	259.618	130.281	433.247	16.857	108.726	162.716	78.041	161.418	93.919	316.326
0.060	162.427	235.158	66.830	260.131	130.048	433.247	17.103	108.534	162.677	78.224	161.766	93.762	316.326
0.070	162.142	234.513	65.749	260.644	129.816	433.247	17.349	108.342	162.639	78.406	162.114	93.605	316.326
0.080	161.857	233.869	64.667	261.157	129.583	433.247	17.596	108.151	162.601	78.589	162.462	93.448	316.326
0.090	161.571	233.224	63.586	261.670	129.350	433.247	17.842	107.959	162.563	78.772	162.810	93.291	316.326
0.100	161.286	232.580	62.505	262.184	129.118	433.247	18.088	107.767	162.524	78.954	163.157	93.133	316.326
0.110	161.001	231.935	61.423	262.697	128.885	433.247	18.334	107.575	162.486	79.137	163.505	92.976	316.326
0.120	160.715	231.291	60.342	263.210	128.653	433.247	18.580	107.383	162.448	79.320	163.853	92.819	316.326
0.130	160.430	230.646	59.261	263.723	128.420	433.247	18.826	107.191	162.409	79.503	164.201	92.662	316.326
0.140	160.145	230.002	58.179	264.236	128.188	433.247	19.072	107.000	162.371	79.685	164.549	92.505	316.326
0.150	159.859	229.357	57.098	264.749	127.955	433.247	19.318	106.808	162.333	79.868	164.897	92.347	316.326
0.160	159.574	228.713	56.017	265.262	127.722	433.247	19.564	106.616	162.294	80.051	165.244	92.190	316.326
0.170	159.288	228.068	54.935	265.775	127.490	433.247	19.810	106.424	162.256	80.233	165.592	92.033	316.326
0.180	159.003	227.424	53.854	266.288	127.257	433.247	20.056	106.232	162.218	80.416	165.940	91.876	316.326
0.190	158.718	226.779	52.773	266.802	127.025	433.247	20.302	106.040	162.180	80.599	166.288	91.719	316.326
0.200	158.432	226.135	51.691	267.315	126.792	433.247	20.548	105.849	162.141	80.782	166.636	91.561	316.326
|Fo|	165.666	234.762	93.462	261.806	129.202	433.247	35.692	105.083	167.202	103.342	165.193	102.712	316.326

Table A.1.7. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x)
(u=0.2524, B=-0.55351, K=19.74742)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.196	238.788	73.393	256.963	131.405	433.117	16.043	109.599	162.790	77.276	159.524	94.777	316.150
0.010	163.911	238.144	72.312	257.476	131.172	433.117	16.289	109.407	162.751	77.459	159.872	94.620	316.150
0.020	163.626	237.499	71.231	257.989	130.939	433.117	16.536	109.215	162.713	77.642	160.220	94.463	316.150
0.030	163.340	236.855	70.149	258.502	130.707	433.117	16.782	109.023	162.675	77.825	160.568	94.306	316.150
0.040	163.055	236.210	69.068	259.015	130.474	433.117	17.028	108.832	162.636	78.007	160.915	94.148	316.150
0.050	162.770	235.566	67.986	259.528	130.242	433.117	17.274	108.640	162.598	78.190	161.263	93.991	316.150
0.060	162.484	234.921	66.905	260.042	130.009	433.117	17.520	108.448	162.560	78.373	161.611	93.834	316.150
0.070	162.199	234.277	65.824	260.555	129.777	433.117	17.766	108.256	162.521	78.555	161.959	93.677	316.150
0.080	161.913	233.632	64.742	261.068	129.544	433.117	18.012	108.064	162.483	78.738	162.307	93.520	316.150
0.090	161.628	232.988	63.661	261.581	129.312	433.117	18.258	107.872	162.445	78.921	162.655	93.362	316.150
0.100	161.343	232.343	62.580	262.094	129.079	433.117	18.504	107.681	162.407	79.104	163.002	93.205	316.150
0.110	161.057	231.699	61.498	262.607	128.846	433.117	18.750	107.489	162.368	79.286	163.350	93.048	316.150
0.120	160.772	231.054	60.417	263.120	128.614	433.117	18.996	107.297	162.330	79.469	163.698	92.891	316.150
0.130	160.487	230.410	59.336	263.633	128.381	433.117	19.242	107.105	162.292	79.652	164.046	92.734	316.150
0.140	160.201	229.765	58.254	264.147	128.149	433.117	19.488	106.913	162.253	79.834	164.394	92.576	316.150
0.150	159.916	229.121	57.173	264.660	127.916	433.117	19.734	106.721	162.215	80.017	164.742	92.419	316.150
0.160	159.631	228.476	56.092	265.173	127.684	433.117	19.980	106.530	162.177	80.200	165.090	92.262	316.150
0.170	159.345	227.832	55.010	265.686	127.451	433.117	20.226	106.338	162.138	80.383	165.437	92.105	316.150
0.180	159.060	227.187	53.929	266.199	127.218	433.117	20.472	106.146	162.100	80.565	165.785	91.948	316.150
0.190	158.775	226.543	52.848	266.712	126.986	433.117	20.718	105.954	162.062	80.748	166.133	91.790	316.150
0.200	158.489	225.898	51.766	267.225	126.753	433.117	20.965	105.762	162.024	80.931	166.481	91.633	316.150
|Fo|	165.648	234.732	93.449	261.761	129.171	433.117	35.681	105.045	167.137	103.301	165.122	102.661	316.150

Table A.1.8. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder x.
(u=0.2528, B=-0.55084, K=19.74651)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.263	238.552	73.482	256.855	131.361	432.964	16.458	109.497	162.674	77.452	159.341	94.861	315.941
0.010	163.978	237.907	72.400	257.368	131.128	432.964	16.704	109.305	162.636	77.635	159.689	94.703	315.941
0.020	163.693	237.263	71.319	257.881	130.895	432.964	16.950	109.113	162.598	77.818	160.037	94.546	315.941
0.030	163.407	236.618	70.238	258.395	130.663	432.964	17.197	108.922	162.559	78.001	160.385	94.389	315.941
0.040	163.122	235.974	69.156	258.908	130.430	432.964	17.443	108.730	162.521	78.183	160.733	94.232	315.941
0.050	162.837	235.329	68.075	259.421	130.198	432.964	17.689	108.538	162.483	78.366	161.080	94.075	315.941
0.060	162.551	234.685	66.994	259.934	129.965	432.964	17.935	108.346	162.445	78.549	161.428	93.917	315.941
0.070	162.266	234.040	65.912	260.447	129.733	432.964	18.181	108.154	162.406	78.732	161.776	93.760	315.941
0.080	161.981	233.396	64.831	260.960	129.500	432.964	18.427	107.962	162.368	78.914	162.124	93.603	315.941
0.090	161.695	232.751	63.750	261.473	129.268	432.964	18.673	107.771	162.330	79.097	162.472	93.446	315.941
0.100	161.410	232.107	62.668	261.986	129.035	432.964	18.919	107.579	162.291	79.280	162.820	93.289	315.941
0.110	161.124	231.462	61.587	262.499	128.802	432.964	19.165	107.387	162.253	79.462	163.167	93.131	315.941
0.120	160.839	230.818	60.506	263.013	128.570	432.964	19.411	107.195	162.215	79.645	163.515	92.974	315.941
0.130	160.554	230.173	59.424	263.526	128.337	432.964	19.657	107.003	162.176	79.828	163.863	92.817	315.941
0.140	160.268	229.529	58.343	264.039	128.105	432.964	19.903	106.811	162.138	80.011	164.211	92.660	315.941
0.150	159.983	228.884	57.262	264.552	127.872	432.964	20.149	106.620	162.100	80.193	164.559	92.503	315.941
0.160	159.698	228.240	56.180	265.065	127.640	432.964	20.395	106.428	162.061	80.376	164.907	92.345	315.941
0.170	159.412	227.595	55.099	265.578	127.407	432.964	20.641	106.236	162.023	80.559	165.254	92.188	315.941
0.180	159.127	226.951	54.018	266.091	127.175	432.964	20.887	106.044	161.985	80.741	165.602	92.031	315.941
0.190	158.842	226.306	52.936	266.604	126.942	432.964	21.133	105.852	161.947	80.924	165.950	91.874	315.941
0.200	158.556	225.662	51.855	267.118	126.709	432.964	21.379	105.660	161.908	81.107	166.298	91.717	315.941
|Fo|	165.628	234.696	93.434	261.709	129.136	432.964	35.667	105.000	167.060	103.252	165.039	102.601	315.941

Table A.1.9. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2532, B=-0.54773, K=19.74560)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.341	238.315	73.586	256.731	131.310	432.789	16.872	109.381	162.562	77.656	159.131	94.957	315.701
0.010	164.055	237.671	72.505	257.244	131.077	432.789	17.118	109.189	162.523	77.838	159.479	94.800	315.701
0.020	163.770	237.026	71.424	257.757	130.845	432.789	17.364	108.997	162.485	78.021	159.827	94.642	315.701
0.030	163.485	236.382	70.342	258.271	130.612	432.789	17.610	108.806	162.447	78.204	160.175	94.485	315.701
0.040	163.199	235.737	69.261	258.784	130.380	432.789	17.856	108.614	162.408	78.386	160.523	94.328	315.701
0.050	162.914	235.093	68.180	259.297	130.147	432.789	18.102	108.422	162.370	78.569	160.871	94.171	315.701
0.060	162.629	234.448	67.098	259.810	129.915	432.789	18.348	108.230	162.332	78.752	161.218	94.014	315.701
0.070	162.343	233.804	66.017	260.323	129.682	432.789	18.594	108.038	162.293	78.935	161.566	93.856	315.701
0.080	162.058	233.159	64.936	260.836	129.449	432.789	18.840	107.846	162.255	79.117	161.914	93.699	315.701
0.090	161.773	232.515	63.854	261.349	129.217	432.789	19.086	107.655	162.217	79.300	162.262	93.542	315.701
0.100	161.487	231.870	62.773	261.862	128.984	432.789	19.332	107.463	162.179	79.483	162.610	93.385	315.701
0.110	161.202	231.226	61.691	262.375	128.752	432.789	19.579	107.271	162.140	79.665	162.958	93.228	315.701
0.120	160.917	230.581	60.610	262.889	128.519	432.789	19.825	107.079	162.102	79.848	163.306	93.070	315.701
0.130	160.631	229.937	59.529	263.402	128.287	432.789	20.071	106.887	162.064	80.031	163.653	92.913	315.701
0.140	160.346	229.292	58.447	263.915	128.054	432.789	20.317	106.695	162.025	80.214	164.001	92.756	315.701
0.150	160.060	228.648	57.366	264.428	127.821	432.789	20.563	106.504	161.987	80.396	164.349	92.599	315.701
0.160	159.775	228.003	56.285	264.941	127.589	432.789	20.809	106.312	161.949	80.579	164.697	92.442	315.701
0.170	159.490	227.359	55.203	265.454	127.356	432.789	21.055	106.120	161.910	80.762	165.045	92.284	315.701
0.180	159.204	226.715	54.122	265.967	127.124	432.789	21.301	105.928	161.872	80.944	165.393	92.127	315.701
0.190	158.919	226.070	53.041	266.480	126.891	432.789	21.547	105.736	161.834	81.127	165.740	91.970	315.701
0.200	158.634	225.426	51.959	266.994	126.659	432.789	21.793	105.544	161.796	81.310	166.088	91.813	315.701
|Fo|	165.606	234.657	93.417	261.650	129.095	432.789	35.651	104.948	166.972	103.197	164.942	102.532	315.701

Table A.1.10. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2536, B=0.54773, K=19.74560)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.431	238.079	73.702	256.593	131.252	432.590	17.283	109.248	162.453	77.885	158.893	95.065	315.429
0.010	164.146	237.434	72.621	257.106	131.020	432.590	17.529	109.057	162.414	78.068	159.240	94.908	315.429
0.020	163.860	236.790	71.539	257.619	130.787	432.590	17.775	108.865	162.376	78.251	159.588	94.750	315.429
0.030	163.575	236.145	70.458	258.132	130.555	432.590	18.021	108.673	162.338	78.434	159.936	94.593	315.429
0.040	163.290	235.501	69.377	258.645	130.322	432.590	18.267	108.481	162.299	78.616	160.284	94.436	315.429
0.050	163.004	234.856	68.295	259.159	130.090	432.590	18.513	108.289	162.261	78.799	160.632	94.279	315.429
0.060	162.719	234.212	67.214	259.672	129.857	432.590	18.759	108.097	162.223	78.982	160.980	94.122	315.429
0.070	162.434	233.567	66.133	260.185	129.624	432.590	19.005	107.906	162.184	79.164	161.328	93.964	315.429
0.080	162.148	232.923	65.051	260.698	129.392	432.590	19.251	107.714	162.146	79.347	161.675	93.807	315.429
0.090	161.863	232.278	63.970	261.211	129.159	432.590	19.497	107.522	162.108	79.530	162.023	93.650	315.429
0.100	161.578	231.634	62.889	261.724	128.927	432.590	19.743	107.330	162.070	79.713	162.371	93.493	315.429
0.110	161.292	230.990	61.807	262.237	128.694	432.590	19.989	107.138	162.031	79.895	162.719	93.336	315.429
0.120	161.007	230.345	60.726	262.750	128.462	432.590	20.235	106.946	161.993	80.078	163.067	93.178	315.429
0.130	160.721	229.701	59.645	263.264	128.229	432.590	20.481	106.754	161.955	80.261	163.415	93.021	315.429
0.140	160.436	229.056	58.563	263.777	127.997	432.590	20.727	106.563	161.916	80.443	163.762	92.864	315.429
0.150	160.151	228.412	57.482	264.290	127.764	432.590	20.974	106.371	161.878	80.626	164.110	92.707	315.429
0.160	159.865	227.767	56.401	264.803	127.531	432.590	21.220	106.179	161.840	80.809	164.458	92.550	315.429
0.170	159.580	227.123	55.319	265.316	127.299	432.590	21.466	105.987	161.801	80.992	164.806	92.392	315.429
0.180	159.295	226.478	54.238	265.829	127.066	432.590	21.712	105.795	161.763	81.174	165.154	92.235	315.429
0.190	159.009	225.834	53.157	266.342	126.834	432.590	21.958	105.603	161.725	81.357	165.502	92.078	315.429
0.200	158.724	225.189	52.075	266.855	126.601	432.590	22.204	105.412	161.687	81.540	165.849	91.921	315.429
|Fo|	165.579	234.610	93.398	261.582	129.048	432.590	35.634	104.889	166.872	103.134	164.834	102.454	315.429

Table A.1.11. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2540, B=0.54037, K=19.74306)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.529	237.840	73.834	256.436	131.188	432.367	17.693	109.101	162.347	78.142	158.627	95.187	315.125
0.010	164.244	237.196	72.753	256.950	130.956	432.367	17.940	108.910	162.309	78.325	158.975	95.030	315.125
0.020	163.958	236.551	71.671	257.463	130.723	432.367	18.186	108.718	162.271	78.508	159.323	94.872	315.125
0.030	163.673	235.907	70.590	257.976	130.490	432.367	18.432	108.526	162.232	78.690	159.671	94.715	315.125
0.040	163.388	235.262	69.509	258.489	130.258	432.367	18.678	108.334	162.194	78.873	160.018	94.558	315.125
0.050	163.102	234.618	68.427	259.002	130.025	432.367	18.924	108.142	162.156	79.056	160.366	94.401	315.125
0.060	162.817	233.973	67.346	259.515	129.793	432.367	19.170	107.950	162.117	79.239	160.714	94.244	315.125
0.070	162.532	233.329	66.264	260.028	129.560	432.367	19.416	107.759	162.079	79.421	161.062	94.086	315.125
0.080	162.246	232.684	65.183	260.541	129.328	432.367	19.662	107.567	162.041	79.604	161.410	93.929	315.125
0.090	161.961	232.040	64.102	261.055	129.095	432.367	19.908	107.375	162.003	79.787	161.758	93.772	315.125
0.100	161.676	231.395	63.020	261.568	128.863	432.367	20.154	107.183	161.964	79.969	162.105	93.615	315.125
0.110	161.390	230.751	61.939	262.081	128.630	432.367	20.400	106.991	161.926	80.152	162.453	93.458	315.125
0.120	161.105	230.106	60.858	262.594	128.397	432.367	20.646	106.799	161.888	80.335	162.801	93.300	315.125
0.130	160.819	229.462	59.776	263.107	128.165	432.367	20.892	106.608	161.849	80.518	163.149	93.143	315.125
0.140	160.534	228.817	58.695	263.620	127.932	432.367	21.138	106.416	161.811	80.700	163.497	92.986	315.125
0.150	160.249	228.173	57.614	264.133	127.700	432.367	21.384	106.224	161.773	80.883	163.845	92.829	315.125
0.160	159.963	227.528	56.532	264.646	127.467	432.367	21.630	106.032	161.734	81.066	164.192	92.672	315.125
0.170	159.678	226.884	55.451	265.160	127.235	432.367	21.876	105.840	161.696	81.248	164.540	92.514	315.125
0.180	159.393	226.239	54.370	265.673	127.002	432.367	22.122	105.648	161.658	81.431	164.888	92.357	315.125
0.190	159.107	225.595	53.288	266.186	126.769	432.367	22.369	105.457	161.619	81.614	165.236	92.200	315.125
0.200	158.822	224.950	52.207	266.699	126.537	432.367	22.615	105.265	161.581	81.797	165.584	92.043	315.125
|Fo|	165.549	234.558	93.376	261.506	128.997	432.367	35.614	104.824	166.761	103.063	164.712	102.367	315.125

Table A.1.12. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2544, B=-0.53605, K=19.74170)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.638	237.601	73.977	256.264	131.117	432.122	18.101	108.939	162.246	78.425	158.335	95.320	314.790
0.010	164.352	236.957	72.896	256.777	130.885	432.122	18.348	108.747	162.207	78.607	158.682	95.163	314.790
0.020	164.067	236.312	71.814	257.290	130.652	432.122	18.594	108.555	162.169	78.790	159.030	95.006	314.790
0.030	163.781	235.668	70.733	257.803	130.419	432.122	18.840	108.364	162.131	78.973	159.378	94.849	314.790
0.040	163.496	235.023	69.652	258.316	130.187	432.122	19.086	108.172	162.092	79.156	159.726	94.692	314.790
0.050	163.211	234.379	68.570	258.829	129.954	432.122	19.332	107.980	162.054	79.338	160.074	94.534	314.790
0.060	162.925	233.734	67.489	259.342	129.722	432.122	19.578	107.788	162.016	79.521	160.422	94.377	314.790
0.070	162.640	233.090	66.408	259.856	129.489	432.122	19.824	107.596	161.978	79.704	160.769	94.220	314.790
0.080	162.355	232.446	65.326	260.369	129.257	432.122	20.070	107.404	161.939	79.887	161.117	94.063	314.790
0.090	162.069	231.801	64.245	260.882	129.024	432.122	20.316	107.212	161.901	80.069	161.465	93.906	314.790
0.100	161.784	231.157	63.164	261.395	128.792	432.122	20.562	107.021	161.863	80.252	161.813	93.748	314.790
0.110	161.499	230.512	62.082	261.908	128.559	432.122	20.808	106.829	161.824	80.435	162.161	93.591	314.790
0.120	161.213	229.868	61.001	262.421	128.326	432.122	21.054	106.637	161.786	80.617	162.509	93.434	314.790
0.130	160.928	229.223	59.919	262.934	128.094	432.122	21.300	106.445	161.748	80.800	162.857	93.277	314.790
0.140	160.642	228.579	58.838	263.447	127.861	432.122	21.546	106.253	161.709	80.983	163.204	93.120	314.790
0.150	160.357	227.934	57.757	263.960	127.629	432.122	21.792	106.061	161.671	81.166	163.552	92.962	314.790
0.160	160.072	227.290	56.675	264.474	127.396	432.122	22.038	105.870	161.633	81.348	163.900	92.805	314.790
0.170	159.786	226.645	55.594	264.987	127.164	432.122	22.284	105.678	161.595	81.531	164.248	92.648	314.790
0.180	159.501	226.001	54.513	265.500	126.931	432.122	22.530	105.486	161.556	81.714	164.596	92.491	314.790
0.190	159.216	225.356	53.431	266.013	126.698	432.122	22.777	105.294	161.518	81.896	164.944	92.334	314.790
0.200	158.930	224.712	52.350	266.526	126.466	432.122	23.023	105.102	161.480	82.079	165.291	92.176	314.790
|Fo|	165.517	234.502	93.352	261.423	128.940	432.122	35.592	104.750	166.638	102.986	164.577	102.271	314.790

Table A.1.13. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2548, B=-0.53137, K=19.74002)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.759	237.363	74.136	256.077	131.039	431.853	18.508	108.761	162.149	78.734	158.014	95.466	314.424
0.010	164.473	236.718	73.055	256.590	130.807	431.853	18.754	108.569	162.111	78.917	158.362	95.309	314.424
0.020	164.188	236.074	71.973	257.103	130.574	431.853	19.000	108.378	162.072	79.100	158.710	95.151	314.424
0.030	163.903	235.429	70.892	257.616	130.342	431.853	19.246	108.186	162.034	79.282	159.058	94.994	314.424
0.040	163.617	234.785	69.811	258.129	130.109	431.853	19.492	107.994	161.996	79.465	159.406	94.837	314.424
0.050	163.332	234.140	68.729	258.642	129.877	431.853	19.738	107.802	161.958	79.648	159.753	94.680	314.424
0.060	163.047	233.496	67.648	259.155	129.644	431.853	19.984	107.610	161.919	79.830	160.101	94.523	314.424
0.070	162.761	232.851	66.567	259.669	129.411	431.853	20.230	107.418	161.881	80.013	160.449	94.365	314.424
0.080	162.476	232.207	65.485	260.182	129.179	431.853	20.477	107.226	161.843	80.196	160.797	94.208	314.424
0.090	162.191	231.562	64.404	260.695	128.946	431.853	20.723	107.035	161.804	80.379	161.145	94.051	314.424
0.100	161.905	230.918	63.323	261.208	128.714	431.853	20.969	106.843	161.766	80.561	161.493	93.894	314.424
0.110	161.620	230.273	62.241	261.721	128.481	431.853	21.215	106.651	161.728	80.744	161.840	93.737	314.424
0.120	161.334	229.629	61.160	262.234	128.249	431.853	21.461	106.459	161.689	80.927	162.188	93.579	314.424
0.130	161.049	228.984	60.079	262.747	128.016	431.853	21.707	106.267	161.651	81.110	162.536	93.422	314.424
0.140	160.764	228.340	58.997	263.260	127.783	431.853	21.953	106.075	161.613	81.292	162.884	93.265	314.424
0.150	160.478	227.695	57.916	263.774	127.551	431.853	22.199	105.884	161.574	81.475	163.232	93.108	314.424
0.160	160.193	227.051	56.834	264.287	127.318	431.853	22.445	105.692	161.536	81.658	163.580	92.951	314.424
0.170	159.908	226.406	55.753	264.800	127.086	431.853	22.691	105.500	161.498	81.840	163.928	92.793	314.424
0.180	159.622	225.762	54.672	265.313	126.853	431.853	22.937	105.308	161.460	82.023	164.275	92.636	314.424
0.190	159.337	225.117	53.590	265.826	126.621	431.853	23.183	105.116	161.421	82.206	164.623	92.479	314.424
0.200	159.052	224.473	52.509	266.339	126.388	431.853	23.429	104.924	161.383	82.389	164.971	92.322	314.424
IFoI	165.481	234.439	93.325	261.330	128.877	431.853	35.568	104.672	166.503	102.901	164.430	102.166	314.424

Table A.1.14. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2552, B=-0.52624, K=19.73835)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	164.888	237.124	74.306	255.871	130.956	431.561	18.913	108.568	162.057	79.070	157.668	95.623	314.026
0.010	164.602	236.479	73.225	256.385	130.724	431.561	19.159	108.376	162.019	79.253	158.016	95.466	314.026
0.020	164.317	235.835	72.144	256.898	130.491	431.561	19.405	108.184	161.981	79.436	158.364	95.309	314.026
0.030	164.032	235.190	71.062	257.411	130.259	431.561	19.651	107.992	161.942	79.619	158.712	95.151	314.026
0.040	163.746	234.546	69.981	257.924	130.026	431.561	19.898	107.800	161.904	79.801	159.060	94.994	314.026
0.050	163.461	233.902	68.900	258.437	129.794	431.561	20.144	107.609	161.866	79.984	159.407	94.837	314.026
0.060	163.176	233.257	67.818	258.950	129.561	431.561	20.390	107.417	161.828	80.167	159.755	94.680	314.026
0.070	162.890	232.613	66.737	259.463	129.329	431.561	20.636	107.225	161.789	80.350	160.103	94.523	314.026
0.080	162.605	231.968	65.656	259.976	129.096	431.561	20.882	107.033	161.751	80.532	160.451	94.365	314.026
0.090	162.320	231.324	64.574	260.490	128.863	431.561	21.128	106.841	161.713	80.715	160.799	94.208	314.026
0.100	162.034	230.679	63.493	261.003	128.631	431.561	21.374	106.649	161.674	80.898	161.147	94.051	314.026
0.110	161.749	230.035	62.412	261.516	128.398	431.561	21.620	106.458	161.636	81.080	161.494	93.894	314.026
0.120	161.463	229.390	61.330	262.029	128.166	431.561	21.866	106.266	161.598	81.263	161.842	93.737	314.026
0.130	161.178	228.746	60.249	262.542	127.933	431.561	22.112	106.074	161.559	81.446	162.190	93.579	314.026
0.140	160.893	228.101	59.168	263.055	127.701	431.561	22.358	105.882	161.521	81.629	162.538	93.422	314.026
0.150	160.607	227.457	58.086	263.568	127.468	431.561	22.604	105.690	161.483	81.811	162.886	93.265	314.026
0.160	160.322	226.812	57.005	264.081	127.236	431.561	22.850	105.498	161.444	81.994	163.234	93.108	314.026
0.170	160.037	226.168	55.923	264.594	127.003	431.561	23.096	105.307	161.406	82.177	163.581	92.951	314.026
0.180	159.751	225.523	54.842	265.108	126.770	431.561	23.342	105.115	161.368	82.359	163.929	92.793	314.026
0.190	159.466	224.879	53.761	265.621	126.538	431.561	23.588	104.923	161.330	82.542	164.277	92.636	314.026
0.200	159.181	224.234	52.679	266.134	126.305	431.561	23.834	104.731	161.291	82.725	164.625	92.479	314.026
|Fo|	165.443	234.371	93.297	261.231	128.809	431.561	35.542	104.586	166.357	102.808	164.271	102.052	314.026

Table A.1.15. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2556, B=-0.52066, K=19.73670)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	165.030	236.883	74.493	255.650	130.865	431.248	19.316	108.360	161.971	79.432	157.294	95.792	313.596
0.010	164.744	236.238	73.411	256.163	130.633	431.248	19.562	108.168	161.932	79.615	157.642	95.635	313.596
0.020	164.459	235.594	72.330	256.676	130.400	431.248	19.808	107.977	161.894	79.798	157.990	95.478	313.596
0.030	164.174	234.949	71.249	257.189	130.167	431.248	20.054	107.785	161.856	79.981	158.338	95.320	313.596
0.040	163.888	234.305	70.167	257.702	129.935	431.248	20.300	107.593	161.817	80.163	158.686	95.163	313.596
0.050	163.603	233.660	69.086	258.215	129.702	431.248	20.546	107.401	161.779	80.346	159.033	95.006	313.596
0.060	163.318	233.016	68.005	258.729	129.470	431.248	20.792	107.209	161.741	80.529	159.381	94.849	313.596
0.070	163.032	232.371	66.923	259.242	129.237	431.248	21.038	107.017	161.703	80.712	159.729	94.692	313.596
0.080	162.747	231.727	65.842	259.755	129.005	431.248	21.284	106.826	161.664	80.894	160.077	94.534	313.596
0.090	162.461	231.083	64.761	260.268	128.772	431.248	21.530	106.634	161.626	81.077	160.425	94.377	313.596
0.100	162.176	230.438	63.679	260.781	128.540	431.248	21.776	106.442	161.588	81.260	160.773	94.220	313.596
0.110	161.891	229.794	62.598	261.294	128.307	431.248	22.022	106.250	161.549	81.442	161.120	94.063	313.596
0.120	161.605	229.149	61.517	261.807	128.074	431.248	22.268	106.058	161.511	81.625	161.468	93.906	313.596
0.130	161.320	228.505	60.435	262.320	127.842	431.248	22.514	105.866	161.473	81.808	161.816	93.748	313.596
0.140	161.035	227.860	59.354	262.834	127.609	431.248	22.761	105.675	161.434	81.991	162.164	93.591	313.596
0.150	160.749	227.216	58.272	263.347	127.377	431.248	23.007	105.483	161.396	82.173	162.512	93.434	313.596
0.160	160.464	226.571	57.191	263.860	127.144	431.248	23.253	105.291	161.358	82.356	162.860	93.277	313.596
0.170	160.179	225.927	56.110	264.373	126.912	431.248	23.499	105.099	161.319	82.539	163.208	93.120	313.596
0.180	159.893	225.282	55.028	264.886	126.679	431.248	23.745	104.907	161.281	82.721	163.555	92.962	313.596
0.190	159.608	224.638	53.947	265.399	126.447	431.248	23.991	104.715	161.243	82.904	163.903	92.805	313.596
0.200	159.323	223.993	52.866	265.912	126.214	431.248	24.237	104.524	161.205	83.087	164.251	92.648	313.596
|Fo|	165.403	234.300	93.267	261.126	128.736	431.248	35.514	104.493	166.199	102.709	164.099	101.928	313.596

Table A.1.16. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2560, B=-0.51471, K=19.73481)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	165.179	236.644	74.690	255.412	130.769	430.912	19.714	108.139	161.890	79.820	156.895	95.973	313.136
0.010	164.894	236.000	73.609	255.925	130.536	430.912	19.960	107.947	161.852	80.003	157.242	95.816	313.136
0.020	164.609	235.355	72.528	256.438	130.304	430.912	20.206	107.755	161.814	80.186	157.590	95.658	313.136
0.030	164.323	234.711	71.446	256.951	130.071	430.912	20.452	107.563	161.775	80.368	157.938	95.501	313.136
0.040	164.038	234.066	70.365	257.465	129.839	430.912	20.698	107.371	161.737	80.551	158.286	95.344	313.136
0.050	163.753	233.422	69.284	257.978	129.606	430.912	20.944	107.179	161.699	80.734	158.634	95.187	313.136
0.060	163.467	232.777	68.202	258.491	129.373	430.912	21.190	106.988	161.660	80.916	158.982	95.030	313.136
0.070	163.182	232.133	67.121	259.004	129.141	430.912	21.436	106.796	161.622	81.099	159.330	94.872	313.136
0.080	162.896	231.488	66.040	259.517	128.908	430.912	21.682	106.604	161.584	81.282	159.677	94.715	313.136
0.090	162.611	230.844	64.958	260.030	128.676	430.912	21.929	106.412	161.545	81.465	160.025	94.558	313.136
0.100	162.326	230.199	63.877	260.543	128.443	430.912	22.175	106.220	161.507	81.647	160.373	94.401	313.136
0.110	162.040	229.555	62.795	261.056	128.211	430.912	22.421	106.028	161.469	81.830	160.721	94.244	313.136
0.120	161.755	228.910	61.714	261.570	127.978	430.912	22.667	105.837	161.430	82.013	161.069	94.086	313.136
0.130	161.470	228.266	60.633	262.083	127.745	430.912	22.913	105.645	161.392	82.196	161.417	93.929	313.136
0.140	161.184	227.621	59.551	262.596	127.513	430.912	23.159	105.453	161.354	82.378	161.764	93.772	313.136
0.150	160.899	226.977	58.470	263.109	127.280	430.912	23.405	105.261	161.316	82.561	162.112	93.615	313.136
0.160	160.614	226.332	57.389	263.622	127.048	430.912	23.651	105.069	161.277	82.744	162.460	93.458	313.136
0.170	160.328	225.688	56.307	264.135	126.815	430.912	23.897	104.877	161.239	82.926	162.808	93.300	313.136
0.180	160.043	225.043	55.226	264.648	126.583	430.912	24.143	104.685	161.201	83.109	163.156	93.143	313.136
0.190	159.758	224.399	54.145	265.161	126.350	430.912	24.389	104.494	161.162	83.292	163.504	92.986	313.136
0.200	159.472	223.754	53.063	265.674	126.118	430.912	24.635	104.302	161.124	83.475	163.851	92.829	313.136
|Fo|	165.358	234.223	93.234	261.011	128.657	430.912	35.484	104.394	166.031	102.603	163.915	101.796	313.136

Table A.1.17. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2564, B=-0.50836, K=19.73275)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	165.339	236.401	74.902	255.158	130.666	430.552	20.111	107.900	161.816	80.235	156.469	96.165	312.646
0.010	165.054	235.756	73.820	255.671	130.433	430.552	20.357	107.708	161.777	80.417	156.817	96.008	312.646
0.020	164.769	235.112	72.739	256.184	130.201	430.552	20.603	107.516	161.739	80.600	157.165	95.851	312.646
0.030	164.483	234.467	71.658	256.697	129.968	430.552	20.849	107.325	161.701	80.783	157.513	95.694	312.646
0.040	164.198	233.823	70.576	257.210	129.735	430.552	21.095	107.133	161.663	80.966	157.861	95.536	312.646
0.050	163.913	233.178	69.495	257.724	129.503	430.552	21.341	106.941	161.624	81.148	158.209	95.379	312.646
0.060	163.627	232.534	68.414	258.237	129.270	430.552	21.587	106.749	161.586	81.331	158.556	95.222	312.646
0.070	163.342	231.889	67.332	258.750	129.038	430.552	21.833	106.557	161.548	81.514	158.904	95.065	312.646
0.080	163.056	231.245	66.251	259.263	128.805	430.552	22.079	106.365	161.509	81.696	159.252	94.908	312.646
0.090	162.771	230.600	65.169	259.776	128.573	430.552	22.325	106.174	161.471	81.879	159.600	94.750	312.646
0.100	162.486	229.956	64.088	260.289	128.340	430.552	22.571	105.982	161.433	82.062	159.948	94.593	312.646
0.110	162.200	229.311	63.007	260.802	128.107	430.552	22.818	105.790	161.394	82.245	160.296	94.436	312.646
0.120	161.915	228.667	61.925	261.315	127.875	430.552	23.064	105.598	161.356	82.427	160.644	94.279	312.646
0.130	161.630	228.022	60.844	261.829	127.642	430.552	23.310	105.406	161.318	82.610	160.991	94.122	312.646
0.140	161.344	227.378	59.763	262.342	127.410	430.552	23.556	105.214	161.280	82.793	161.339	93.964	312.646
0.150	161.059	226.733	58.681	262.855	127.177	430.552	23.802	105.023	161.241	82.976	161.687	93.807	312.646
0.160	160.774	226.089	57.600	263.368	126.945	430.552	24.048	104.831	161.203	83.158	162.035	93.650	312.646
0.170	160.488	225.444	56.519	263.881	126.712	430.552	24.294	104.639	161.165	83.341	162.383	93.493	312.646
0.180	160.203	224.800	55.437	264.394	126.480	430.552	24.540	104.447	161.126	83.524	162.731	93.336	312.646
0.190	159.917	224.156	54.356	264.907	126.247	430.552	24.786	104.255	161.088	83.706	163.078	93.178	312.646
0.200	159.632	223.511	53.275	265.420	126.014	430.552	25.032	104.063	161.050	83.889	163.426	93.021	312.646
IFoI	165.311	234.139	93.198	260.889	128.574	430.552	35.452	104.287	165.850	102.489	163.718	101.656	312.656

Table A.1.18. Calculated and Observed Structure for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2568, B=-0.50158, K=19.73065)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	165.512	236.160	75.129	254.890	130.557	430.170	20.505	107.649	161.749	80.674	156.017	96.368	312.125
0.010	165.227	235.515	74.047	255.403	130.325	430.170	20.751	107.457	161.711	80.856	156.365	96.211	312.125
0.020	164.941	234.871	72.966	255.916	130.092	430.170	20.997	107.265	161.672	81.039	156.713	96.054	312.125
0.030	164.656	234.226	71.885	256.429	129.860	430.170	21.243	107.073	161.634	81.222	157.061	95.897	312.125
0.040	164.371	233.582	70.803	256.942	129.627	430.170	21.489	106.881	161.596	81.405	157.409	95.740	312.125
0.050	164.085	232.937	69.722	257.455	129.395	430.170	21.735	106.690	161.557	81.587	157.757	95.582	312.125
0.060	163.800	232.293	68.641	257.968	129.162	430.170	21.981	106.498	161.519	81.770	158.104	95.425	312.125
0.070	163.515	231.648	67.559	258.482	128.929	430.170	22.227	106.306	161.481	81.953	158.452	95.268	312.125
0.080	163.229	231.004	66.478	258.995	128.697	430.170	22.474	106.114	161.442	82.136	158.800	95.111	312.125
0.090	162.944	230.359	65.397	259.508	128.464	430.170	22.720	105.922	161.404	82.318	159.148	94.954	312.125
0.100	162.659	229.715	64.315	260.021	128.232	430.170	22.966	105.730	161.366	82.501	159.496	94.796	312.125
0.110	162.373	229.070	63.234	260.534	127.999	430.170	23.212	105.539	161.328	82.684	159.844	94.639	312.125
0.120	162.088	228.426	62.153	261.047	127.767	430.170	23.458	105.347	161.289	82.866	160.191	94.482	312.125
0.130	161.803	227.781	61.071	261.560	127.534	430.170	23.704	105.155	161.251	83.049	160.539	94.325	312.125
0.140	161.517	227.137	59.990	262.073	127.302	430.170	23.950	104.963	161.213	83.232	160.887	94.168	312.125
0.150	161.232	226.492	58.909	262.587	127.069	430.170	24.196	104.771	161.174	83.415	161.235	94.010	312.125
0.160	160.946	225.848	57.827	263.100	126.836	430.170	24.442	104.579	161.136	83.597	161.583	93.853	312.125
0.170	160.661	225.203	56.746	263.613	126.604	430.170	24.688	104.388	161.098	83.780	161.931	93.696	312.125
0.180	160.376	224.559	55.664	264.126	126.371	430.170	24.934	104.196	161.059	83.963	162.279	93.539	312.125
0.190	160.090	223.914	54.583	264.639	126.139	430.170	25.180	104.004	161.021	84.145	162.626	93.382	312.125
0.200	159.805	223.270	53.502	265.152	125.906	430.170	25.426	103.812	160.983	84.328	162.974	93.224	312.125
|Fo|	165.261	234.052	93.161	260.759	128.485	430.170	35.418	104.175	165.659	102.368	163.509	101.506	312.125

Table A.1.19. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2572, B=-0.49440, K=19.72845)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	165.693	235.916	75.367	254.603	130.442	429.767	20.896	107.382	161.688	81.138	155.541	96.582	311.574
0.010	165.407	235.272	74.286	255.116	130.210	429.767	21.142	107.190	161.650	81.321	155.889	96.425	311.574
0.020	165.122	234.627	73.205	255.629	129.977	429.767	21.389	106.998	161.612	81.504	156.237	96.268	311.574
0.030	164.837	233.983	72.123	256.142	129.745	429.767	21.635	106.806	161.573	81.687	156.584	96.111	311.574
0.040	164.551	233.338	71.042	256.656	129.512	429.767	21.881	106.615	161.535	81.869	156.932	95.953	311.574
0.050	164.266	232.694	69.961	257.169	129.280	429.767	22.127	106.423	161.497	82.052	157.280	95.796	311.574
0.060	163.981	232.049	68.879	257.682	129.047	429.767	22.373	106.231	161.458	82.235	157.628	95.639	311.574
0.070	163.695	231.405	67.798	258.195	128.815	429.767	22.619	106.039	161.420	82.418	157.976	95.482	311.574
0.080	163.410	230.760	66.717	258.708	128.582	429.767	22.865	105.847	161.382	82.600	158.324	95.325	311.574
0.090	163.125	230.116	65.635	259.221	128.349	429.767	23.111	105.655	161.343	82.783	158.671	95.167	311.574
0.100	162.839	229.471	64.554	259.734	128.117	429.767	23.357	105.464	161.305	82.966	159.019	95.010	311.574
0.110	162.554	228.827	63.472	260.247	127.884	429.767	23.603	105.272	161.267	83.148	159.367	94.853	311.574
0.120	162.268	228.182	62.391	260.761	127.652	429.767	23.849	105.080	161.229	83.331	159.715	94.696	311.574
0.130	161.983	227.538	61.310	261.274	127.419	429.767	24.095	104.888	161.190	83.514	160.063	94.539	311.574
0.140	161.698	226.893	60.228	261.787	127.187	429.767	24.341	104.696	161.152	83.697	160.411	94.381	311.574
0.150	161.412	226.249	59.147	262.300	126.954	429.767	24.587	104.504	161.114	83.879	160.759	94.224	311.574
0.160	161.127	225.604	58.066	262.813	126.721	429.767	24.833	104.313	161.075	84.062	161.106	94.067	311.574
0.170	160.842	224.960	56.984	263.326	126.489	429.767	25.079	104.121	161.037	84.245	161.454	93.910	311.574
0.180	160.556	224.316	55.903	263.839	126.256	429.767	25.325	103.929	160.999	84.427	161.802	93.753	311.574
0.190	160.271	223.671	54.822	264.352	126.024	429.767	25.571	103.737	160.960	84.610	162.150	93.595	311.574
0.200	159.986	223.027	53.740	264.866	125.791	429.767	25.818	103.545	160.922	84.793	162.498	93.438	311.574
|Fo|	165.209	233.959	93.122	260.623	128.391	429.767	35.382	104.055	165.456	102.240	163.288	101.348	311.574

Table A.1.20. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2576, B=-0.48677, K=19.72623)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	165.884	235.673	75.619	254.300	130.321	429.342	21.285	107.101	161.634	81.629	155.039	96.808	310.992
0.010	165.598	235.028	74.538	254.813	130.088	429.342	21.531	106.909	161.595	81.812	155.387	96.651	310.992
0.020	165.313	234.384	73.457	255.327	129.856	429.342	21.777	106.717	161.557	81.994	155.734	96.494	310.992
0.030	165.028	233.739	72.375	255.840	129.623	429.342	22.023	106.525	161.519	82.177	156.082	96.336	310.992
0.040	164.742	233.095	71.294	256.353	129.390	429.342	22.269	106.334	161.480	82.360	156.430	96.179	310.992
0.050	164.457	232.450	70.213	256.866	129.158	429.342	22.515	106.142	161.442	82.542	156.778	96.022	310.992
0.060	164.172	231.806	69.131	257.379	128.925	429.342	22.761	105.950	161.404	82.725	157.126	95.865	310.992
0.070	163.886	231.161	68.050	257.892	128.693	429.342	23.007	105.758	161.366	82.908	157.474	95.708	310.992
0.080	163.601	230.517	66.969	258.405	128.460	429.342	23.253	105.566	161.327	83.091	157.822	95.550	310.992
0.090	163.315	229.872	65.887	258.918	128.228	429.342	23.499	105.374	161.289	83.273	158.169	95.393	310.992
0.100	163.030	229.228	64.806	259.431	127.995	429.342	23.746	105.183	161.251	83.456	158.517	95.236	310.992
0.110	162.745	228.584	63.725	259.945	127.763	429.342	23.992	104.991	161.212	83.639	158.865	95.079	310.992
0.120	162.459	227.939	62.643	260.458	127.530	429.342	24.238	104.799	161.174	83.822	159.213	94.922	310.992
0.130	162.174	227.295	61.562	260.971	127.297	429.342	24.484	104.607	161.136	84.004	159.561	94.764	310.992
0.140	161.889	226.650	60.481	261.484	127.065	429.342	24.730	104.415	161.097	84.187	159.909	94.607	310.992
0.150	161.603	226.006	59.399	261.997	126.832	429.342	24.976	104.223	161.059	84.370	160.256	94.450	310.992
0.160	161.318	225.361	58.318	262.510	126.600	429.342	25.222	104.032	161.021	84.552	160.604	94.293	310.992
0.170	161.033	224.717	57.237	263.023	126.367	429.342	25.468	103.840	160.982	84.735	160.952	94.136	310.992
0.180	160.747	224.072	56.155	263.536	126.135	429.342	25.714	103.648	160.944	84.918	161.300	93.978	310.992
0.190	160.462	223.428	55.074	264.050	125.902	429.342	25.960	103.456	160.906	85.101	161.648	93.821	310.992
0.200	160.177	222.783	53.992	264.563	125.669	429.342	26.206	103.264	160.868	85.283	161.996	93.664	310.992
IFoI	165.154	233.863	93.081	260.479	128.292	429.342	35.344	103.929	165.242	102.105	163.055	101.181	310.992

Table A.1.21. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2580, B=-0.47879 K=19.72373)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	166.088	235.427	75.885	253.981	130.192	428.893	21.669	106.806	161.588	82.144	154.512	97.043	310.381
0.010	165.802	234.783	74.804	254.494	129.960	428.893	21.915	106.614	161.550	82.326	154.860	96.886	310.381
0.020	165.517	234.138	73.723	255.007	129.727	428.893	22.162	106.422	161.511	82.509	155.208	96.729	310.381
0.030	165.231	233.494	72.641	255.521	129.494	428.893	22.408	106.230	161.473	82.692	155.556	96.572	310.381
0.040	164.946	232.849	71.560	256.034	129.262	428.893	22.654	106.038	161.435	82.875	155.904	96.414	310.381
0.050	164.661	232.205	70.478	256.547	129.029	428.893	22.900	105.847	161.396	83.057	156.251	96.257	310.381
0.060	164.375	231.560	69.397	257.060	128.797	428.893	23.146	105.655	161.358	83.240	156.599	96.100	310.381
0.070	164.090	230.916	68.316	257.573	128.564	428.893	23.392	105.463	161.320	83.423	156.947	95.943	310.381
0.080	163.805	230.271	67.234	258.086	128.332	428.893	23.638	105.271	161.281	83.606	157.295	95.786	310.381
0.090	163.519	229.627	66.153	258.599	128.099	428.893	23.884	105.079	161.243	83.788	157.643	95.628	310.381
0.100	163.234	228.982	65.072	259.112	127.867	428.893	24.130	104.887	161.205	83.971	157.991	95.471	310.381
0.110	162.949	228.338	63.990	259.625	127.634	428.893	24.376	104.696	161.166	84.154	158.338	95.314	310.381
0.120	162.663	227.693	62.909	260.139	127.401	428.893	24.622	104.504	161.128	84.336	158.686	95.157	310.381
0.130	162.378	227.049	61.828	260.652	127.169	428.893	24.868	104.312	161.090	84.519	159.034	95.000	310.381
0.140	162.093	226.404	60.746	261.165	126.936	428.893	25.114	104.120	161.052	84.702	159.382	94.842	310.381
0.150	161.807	225.760	59.665	261.678	126.704	428.893	25.360	103.928	161.013	84.885	159.730	94.685	310.381
0.160	161.522	225.115	58.584	262.191	126.471	428.893	25.606	103.736	160.975	85.067	160.078	94.528	310.381
0.170	161.236	224.471	57.502	262.704	126.239	428.893	25.852	103.545	160.937	85.250	160.426	94.371	310.381
0.180	160.951	223.826	56.421	263.217	126.006	428.893	26.098	103.353	160.898	85.433	160.773	94.214	310.381
0.190	160.666	223.182	55.340	263.730	125.774	428.893	26.344	103.161	160.860	85.615	161.121	94.056	310.381
0.200	160.380	222.537	54.258	264.244	125.541	428.893	26.590	102.969	160.822	85.798	161.469	93.899	310.381
|Fo|	165.095	233.759	93.037	260.327	128.187	428.893	35.304	103.797	165.018	101.963	162.809	101.005	310.381

Table A.1.22. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2584, B=0.47033, K=19.72135)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	166.299	235.181	76.162	253.648	130.060	428.424	22.050	106.496	161.551	82.684	153.961	97.289	309.740
0.010	166.014	234.537	75.081	254.161	129.828	428.424	22.296	106.305	161.512	82.867	154.309	97.132	309.740
0.020	165.728	233.892	74.000	254.674	129.595	428.424	22.542	106.113	161.474	83.050	154.657	96.975	309.740
0.030	165.443	233.248	72.918	255.187	129.363	428.424	22.788	105.921	161.436	83.232	155.005	96.818	309.740
0.040	165.158	232.603	71.837	255.700	129.130	428.424	23.034	105.729	161.397	83.415	155.352	96.660	309.740
0.050	164.872	231.959	70.756	256.213	128.897	428.424	23.280	105.537	161.359	83.598	155.700	96.503	309.740
0.060	164.587	231.314	69.674	256.727	128.665	428.424	23.526	105.345	161.321	83.781	156.048	96.346	309.740
0.070	164.302	230.670	68.593	257.240	128.432	428.424	23.772	105.154	161.283	83.963	156.396	96.189	309.740
0.080	164.016	230.025	67.512	257.753	128.200	428.424	24.018	104.962	161.244	84.146	156.744	96.032	309.740
0.090	163.731	229.381	66.430	258.266	127.967	428.424	24.264	104.770	161.206	84.329	157.092	95.874	309.740
0.100	163.446	228.736	65.349	258.779	127.735	428.424	24.510	104.578	161.168	84.512	157.439	95.717	309.740
0.110	163.160	228.092	64.268	259.292	127.502	428.424	24.756	104.386	161.129	84.694	157.787	95.560	309.740
0.120	162.875	227.448	63.186	259.805	127.270	428.424	25.002	104.194	161.091	84.877	158.135	95.403	309.740
0.130	162.589	226.803	62.105	260.318	127.037	428.424	25.248	104.003	161.053	85.060	158.483	95.246	309.740
0.140	162.304	226.159	61.023	260.832	126.804	428.424	25.494	103.811	161.014	85.242	158.831	95.088	309.740
0.150	162.019	225.514	59.942	261.345	126.572	428.424	25.740	103.619	160.976	85.425	159.179	94.931	309.740
0.160	161.733	224.870	58.861	261.858	126.339	428.424	25.987	103.427	160.938	85.608	159.527	94.774	309.740
0.170	161.448	224.225	57.779	262.371	126.107	428.424	26.233	103.235	160.899	85.791	159.874	94.617	309.740
0.180	161.163	223.581	56.698	262.884	125.874	428.424	26.479	103.043	160.861	85.973	160.222	94.460	309.740
0.190	160.877	222.936	55.617	263.397	125.642	428.424	26.725	102.852	160.823	86.156	160.570	94.302	309.740
0.200	160.592	222.292	54.535	263.910	125.409	428.424	26.971	102.660	160.785	86.339	160.918	94.145	309.740
IFoI	165.035	233.653	92.992	260.169	128.078	428.424	35.262	103.658	164.782	101.815	162.552	100.821	309.740

Table A.1.23. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2588, B=-0.46148, K=19.71883)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	166.521	234.933	76.455	253.296	129.920	427.933	22.427	106.173	161.521	83.248	153.386	97.544	309.070
0.010	166.236	234.289	75.374	253.809	129.687	427.933	22.673	105.981	161.483	83.431	153.734	97.386	309.070
0.020	165.950	233.644	74.293	254.322	129.455	427.933	22.919	105.789	161.444	83.614	154.081	97.229	309.070
0.030	165.665	233.000	73.211	254.836	129.222	427.933	23.165	105.597	161.406	83.796	154.429	97.072	309.070
0.040	165.380	232.355	72.130	255.349	128.990	427.933	23.411	105.406	161.368	83.979	154.777	96.915	309.070
0.050	165.094	231.711	71.049	255.862	128.757	427.933	23.657	105.214	161.329	84.162	155.125	96.758	309.070
0.060	164.809	231.066	69.967	256.375	128.525	427.933	23.903	105.022	161.291	84.344	155.473	96.600	309.070
0.070	164.523	230.422	68.886	256.888	128.292	427.933	24.149	104.830	161.253	84.527	155.821	96.443	309.070
0.080	164.238	229.777	67.805	257.401	128.059	427.933	24.396	104.638	161.214	84.710	156.168	96.286	309.070
0.090	163.953	229.133	66.723	257.914	127.827	427.933	24.642	104.446	161.176	84.893	156.516	96.129	309.070
0.100	163.667	228.488	65.642	258.427	127.594	427.933	24.888	104.255	161.138	85.075	156.864	95.972	309.070
0.110	163.382	227.844	64.561	258.941	127.362	427.933	25.134	104.063	161.100	85.258	157.212	95.814	309.070
0.120	163.097	227.199	63.479	259.454	127.129	427.933	25.380	103.871	161.061	85.441	157.560	95.657	309.070
0.130	162.811	226.555	62.398	259.967	126.897	427.933	25.626	103.679	161.023	85.623	157.908	95.500	309.070
0.140	162.526	225.910	61.317	260.480	126.664	427.933	25.872	103.487	160.985	85.806	158.255	95.343	309.070
0.150	162.241	225.266	60.235	260.993	126.432	427.933	26.118	103.295	160.946	85.989	158.603	95.186	309.070
0.160	161.955	224.621	59.154	261.506	126.199	427.933	26.364	103.104	160.908	86.172	158.951	95.028	309.070
0.170	161.670	223.977	58.072	262.019	125.966	427.933	26.610	102.912	160.870	86.354	159.299	94.871	309.070
0.180	161.385	223.333	56.991	262.532	125.734	427.933	26.856	102.720	160.831	86.537	159.647	94.714	309.070
0.190	161.099	222.688	55.910	263.045	125.501	427.933	27.102	102.528	160.793	86.720	159.995	94.557	309.070
0.200	160.814	222.044	54.828	263.559	125.269	427.933	27.348	102.336	160.755	86.902	160.342	94.400	309.070
|Fo|	164.972	233.542	92.945	260.003	127.964	427.933	35.219	103.513	164.535	101.659	162.283	100.629	309.070

Table A.1.24. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2592, B=-0.45221, K=19.71631)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	166.756	234.685	76.760	252.930	129.776	427.422	22.802	105.837	161.500	83.838	152.787	97.809	308.370
0.010	166.470	234.041	75.678	253.443	129.544	427.422	23.048	105.645	161.462	84.020	153.135	97.652	308.370
0.020	166.185	233.396	74.597	253.957	129.311	427.422	23.294	105.453	161.423	84.203	153.483	97.494	308.370
0.030	165.900	232.752	73.516	254.470	129.079	427.422	23.540	105.261	161.385	84.386	153.830	97.337	308.370
0.040	165.614	232.107	72.434	254.983	128.846	427.422	23.786	105.069	161.347	84.568	154.178	97.180	308.370
0.050	165.329	231.463	71.353	255.496	128.613	427.422	24.032	104.877	161.308	84.751	154.526	97.023	308.370
0.060	165.044	230.818	70.272	256.009	128.381	427.422	24.278	104.685	161.270	84.934	154.874	96.866	308.370
0.070	164.758	230.174	69.190	256.522	128.148	427.422	24.524	104.494	161.232	85.117	155.222	96.708	308.370
0.080	164.473	229.529	68.109	257.035	127.916	427.422	24.770	104.302	161.193	85.299	155.570	96.551	308.370
0.090	164.188	228.885	67.028	257.548	127.683	427.422	25.016	104.110	161.155	85.482	155.917	96.394	308.370
0.100	163.902	228.240	65.946	258.062	127.451	427.422	25.262	103.918	161.117	85.665	156.265	96.237	308.370
0.110	163.617	227.596	64.865	258.575	127.218	427.422	25.508	103.726	161.078	85.847	156.613	96.080	308.370
0.120	163.331	226.951	63.784	259.088	126.985	427.422	25.754	103.534	161.040	86.030	156.961	95.922	308.370
0.130	163.046	226.307	62.702	259.601	126.753	427.422	26.001	103.343	161.002	86.213	157.309	95.765	308.370
0.140	162.761	225.662	61.621	260.114	126.520	427.422	26.247	103.151	160.964	86.396	157.657	95.608	308.370
0.150	162.475	225.018	60.540	260.627	126.288	427.422	26.493	102.959	160.925	86.578	158.004	95.451	308.370
0.160	162.190	224.373	59.458	261.140	126.055	427.422	26.739	102.767	160.887	86.761	158.352	95.294	308.370
0.170	161.905	223.729	58.377	261.653	125.823	427.422	26.985	102.575	160.849	86.944	158.700	95.136	308.370
0.180	161.619	223.084	57.296	262.167	125.590	427.422	27.231	102.383	160.810	87.127	159.048	94.979	308.370
0.190	161.334	222.440	56.214	262.680	125.358	427.422	27.477	102.192	160.772	87.309	159.396	94.822	308.370
0.200	161.049	221.795	55.133	263.193	125.125	427.422	27.723	102.000	160.734	87.492	159.744	94.665	308.370
IFoI	164.907	233.426	92.896	259.831	127.845	427.422	35.173	103.362	164.278	101.497	162.003	100.428	308.370

Table A.1.25. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2596, B=-0.45221, K=19.71631)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	166.998	234.435	77.080	252.548	129.626	426.889	23.171	105.486	161.487	84.450	152.166	98.084	307.642
0.010	166.713	233.790	75.999	253.061	129.393	426.889	23.417	105.294	161.449	84.633	152.514	97.927	307.642
0.020	166.428	233.146	74.917	253.574	129.161	426.889	23.663	105.102	161.411	84.816	152.862	97.769	307.642
0.030	166.142	232.501	73.836	254.088	128.928	426.889	23.909	104.910	161.373	84.998	153.209	97.612	307.642
0.040	165.857	231.857	72.755	254.601	128.695	426.889	24.155	104.719	161.334	85.181	153.557	97.455	307.642
0.050	165.572	231.212	71.673	255.114	128.463	426.889	24.401	104.527	161.296	85.364	153.905	97.298	307.642
0.060	165.286	230.568	70.592	255.627	128.230	426.889	24.647	104.335	161.258	85.547	154.253	97.141	307.642
0.070	165.001	229.923	69.511	256.140	127.998	426.889	24.893	104.143	161.219	85.729	154.601	96.983	307.642
0.080	164.715	229.279	68.429	256.653	127.765	426.889	25.139	103.951	161.181	85.912	154.949	96.826	307.642
0.090	164.430	228.634	67.348	257.166	127.533	426.889	25.385	103.759	161.143	86.095	155.296	96.669	307.642
0.100	164.145	227.990	66.267	257.679	127.300	426.889	25.632	103.568	161.104	86.277	155.644	96.512	307.642
0.110	163.859	227.345	65.185	258.193	127.068	426.889	25.878	103.376	161.066	86.460	155.992	96.355	307.642
0.120	163.574	226.701	64.104	258.706	126.835	426.889	26.124	103.184	161.028	86.643	156.340	96.197	307.642
0.130	163.289	226.056	63.023	259.219	126.602	426.889	26.370	102.992	160.989	86.826	156.688	96.040	307.642
0.140	163.003	225.412	61.941	259.732	126.370	426.889	26.616	102.800	160.951	87.008	157.036	95.883	307.642
0.150	162.718	224.767	60.860	260.245	126.137	426.889	26.862	102.608	160.913	87.191	157.384	95.726	307.642
0.160	162.433	224.123	59.779	260.758	125.905	426.889	27.108	102.416	160.875	87.374	157.731	95.569	307.642
0.170	162.147	223.478	58.697	261.271	125.672	426.889	27.354	102.225	160.836	87.557	158.079	95.411	307.642
0.180	161.862	222.834	57.616	261.784	125.440	426.889	27.600	102.033	160.798	87.739	158.427	95.254	307.642
0.190	161.576	222.190	56.534	262.298	125.207	426.889	27.846	101.841	160.760	87.922	158.775	95.097	307.642
0.200	161.291	221.545	55.453	262.811	124.975	426.889	28.092	101.649	160.721	88.105	159.123	94.940	307.642
|Fo|	164.840	233.306	92.845	259.652	127.722	426.889	35.125	103.204	164.011	101.328	161.710	100.219	307.642

Table A.1.26. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2600, B=-0.43248, K=19.71083)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	167.251	234.184	77.412	252.150	129.470	426.334	23.536	105.122	161.485	85.086	151.521	98.367	306.886
0.010	166.966	233.540	76.330	252.663	129.238	426.334	23.782	104.931	161.447	85.269	151.868	98.210	306.886
0.020	166.680	232.895	75.249	253.176	129.005	426.334	24.028	104.739	161.408	85.452	152.216	98.053	306.886
0.030	166.395	232.251	74.168	253.689	128.772	426.334	24.274	104.547	161.370	85.634	152.564	97.896	306.886
0.040	166.110	231.606	73.086	254.202	128.540	426.334	24.520	104.355	161.332	85.817	152.912	97.738	306.886
0.050	165.824	230.962	72.005	254.715	128.307	426.334	24.766	104.163	161.293	86.000	153.260	97.581	306.886
0.060	165.539	230.317	70.924	255.229	128.075	426.334	25.012	103.971	161.255	86.183	153.608	97.424	306.886
0.070	165.254	229.673	69.842	255.742	127.842	426.334	25.258	103.780	161.217	86.365	153.955	97.267	306.886
0.080	164.968	229.028	68.761	256.255	127.610	426.334	25.504	103.588	161.179	86.548	154.303	97.110	306.886
0.090	164.683	228.384	67.680	256.768	127.377	426.334	25.750	103.396	161.140	86.731	154.651	96.952	306.886
0.100	164.398	227.739	66.598	257.281	127.145	426.334	25.996	103.204	161.102	86.913	154.999	96.795	306.886
0.110	164.112	227.095	65.517	257.794	126.912	426.334	26.243	103.012	161.064	87.096	155.347	96.638	306.886
0.120	163.827	226.450	64.436	258.307	126.679	426.334	26.489	102.820	161.025	87.279	155.695	96.481	306.886
0.130	163.541	225.806	63.354	258.820	126.447	426.334	26.735	102.629	160.987	87.462	156.042	96.324	306.886
0.140	163.256	225.162	62.273	259.334	126.214	426.334	26.981	102.437	160.949	87.644	156.390	96.166	306.886
0.150	162.971	224.517	61.192	259.847	125.982	426.334	27.227	102.245	160.910	87.827	156.738	96.009	306.886
0.160	162.685	223.873	60.110	260.360	125.749	426.334	27.473	102.053	160.872	88.010	157.086	95.852	306.886
0.170	162.400	223.228	59.029	260.873	125.517	426.334	27.719	101.861	160.834	88.192	157.434	95.695	306.886
0.180	162.115	222.584	57.948	261.386	125.284	426.334	27.965	101.669	160.795	88.375	157.782	95.538	306.886
0.190	161.829	221.939	56.866	261.899	125.052	426.334	28.211	101.477	160.757	88.558	158.129	95.380	306.886
0.200	161.544	221.295	55.785	262.412	124.819	426.334	28.457	101.286	160.719	88.741	158.477	95.223	306.886
IFoI	164.768	233.180	92.291	259.465	127.953	426.334	35.076	103.040	163.732	101.152	161.407	100.001	306.886

Table A.1.27. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2604, B=-0.42195, K=19.70816)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	167.514	233.934	77.755	251.735	129.310	425.760	23.898	104.745	161.492	85.747	150.854	98.659	306.102
0.010	167.229	233.289	76.673	252.248	129.077	425.760	24.144	104.553	161.454	85.929	151.202	98.502	306.102
0.020	166.944	232.645	75.592	252.761	128.844	425.760	24.390	104.361	161.416	86.112	151.550	98.345	306.102
0.030	166.658	232.000	74.511	253.275	128.612	425.760	24.636	104.169	161.377	86.295	151.898	98.187	306.102
0.040	166.373	231.356	73.429	253.788	128.379	425.760	24.882	103.977	161.339	86.477	152.245	98.030	306.102
0.050	166.088	230.711	72.348	254.301	128.147	425.760	25.128	103.786	161.301	86.660	152.593	97.873	306.102
0.060	165.802	230.067	71.267	254.814	127.914	425.760	25.374	103.594	161.263	86.843	152.941	97.716	306.102
0.070	165.517	229.422	70.185	255.327	127.682	425.760	25.621	103.402	161.224	87.026	153.289	97.559	306.102
0.080	165.231	228.778	69.104	255.840	127.449	425.760	25.867	103.210	161.186	87.208	153.637	97.401	306.102
0.090	164.946	228.134	68.023	256.353	127.216	425.760	26.113	103.018	161.148	87.391	153.985	97.244	306.102
0.100	164.661	227.489	66.941	256.866	126.984	425.760	26.359	102.826	161.109	87.574	154.333	97.087	306.102
0.110	164.375	226.845	65.860	257.380	126.751	425.760	26.605	102.635	161.071	87.757	154.680	96.930	306.102
0.120	164.090	226.200	64.779	257.893	126.519	425.760	26.851	102.443	161.033	87.939	155.028	96.773	306.102
0.130	163.805	225.556	63.697	258.406	126.286	425.760	27.097	102.251	160.994	88.122	155.376	96.615	306.102
0.140	163.519	224.911	62.616	258.919	126.054	425.760	27.343	102.059	160.956	88.305	155.724	96.458	306.102
0.150	163.234	224.267	61.535	259.432	125.821	425.760	27.589	101.867	160.918	88.487	156.072	96.301	306.102
0.160	162.949	223.622	60.453	259.945	125.589	425.760	27.835	101.675	160.880	88.670	156.420	96.144	306.102
0.170	162.663	222.978	59.372	260.458	125.356	425.760	28.081	101.484	160.841	88.853	156.767	95.987	306.102
0.180	162.378	222.333	58.291	260.971	125.123	425.760	28.327	101.292	160.803	89.036	157.115	95.829	306.102
0.190	162.092	221.689	57.209	261.485	124.891	425.760	28.573	101.100	160.765	89.218	157.463	95.672	306.102
0.200	161.807	221.044	56.128	261.998	124.658	425.760	28.819	100.908	160.726	89.401	157.811	95.515	306.102
|Fo|	164.696	233.051	92.732	259.272	127.459	425.760	35.025	102.870	163.443	100.970	161.092	99.776	306.102

Table A.1.28. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2608, B=-0.41101, K=19.70538)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	167.785	233.679	78.114	251.304	129.142	425.164	24.255	104.356	161.510	86.430	150.166	98.960	305.288
0.010	167.500	233.034	77.032	251.817	128.910	425.164	24.501	104.164	161.471	86.613	150.513	98.802	305.288
0.020	167.215	232.390	75.951	252.331	128.677	425.164	24.747	103.972	161.433	86.796	150.861	98.645	305.288
0.030	166.929	231.745	74.870	252.844	128.444	425.164	24.993	103.780	161.395	86.978	151.209	98.488	305.288
0.040	166.644	231.101	73.788	253.357	128.212	425.164	25.239	103.588	161.357	87.161	151.557	98.331	305.288
0.050	166.358	230.456	72.707	253.870	127.979	425.164	25.485	103.396	161.318	87.344	151.905	98.174	305.288
0.060	166.073	229.812	71.626	254.383	127.747	425.164	25.731	103.204	161.280	87.527	152.253	98.016	305.288
0.070	165.788	229.167	70.544	254.896	127.514	425.164	25.977	103.013	161.242	87.709	152.600	97.859	305.288
0.080	165.502	228.523	69.463	255.409	127.282	425.164	26.223	102.821	161.203	87.892	152.948	97.702	305.288
0.090	165.217	227.878	68.382	255.922	127.049	425.164	26.469	102.629	161.165	88.075	153.296	97.545	305.288
0.100	164.932	227.234	67.300	256.436	126.817	425.164	26.715	102.437	161.127	88.257	153.644	97.388	305.288
0.110	164.646	226.589	66.219	256.949	126.584	425.164	26.961	102.245	161.088	88.440	153.992	97.230	305.288
0.120	164.361	225.945	65.138	257.462	126.351	425.164	27.207	102.053	161.050	88.623	154.340	97.073	305.288
0.130	164.076	225.300	64.056	257.975	126.119	425.164	27.454	101.862	161.012	88.806	154.688	96.916	305.288
0.140	163.790	224.656	62.975	258.488	125.886	425.164	27.700	101.670	160.973	88.988	155.035	96.759	305.288
0.150	163.505	224.011	61.894	259.001	125.654	425.164	27.946	101.478	160.935	89.171	155.383	96.602	305.288
0.160	163.219	223.367	60.812	259.514	125.421	425.164	28.192	101.286	160.897	89.354	155.731	96.444	305.288
0.170	162.934	222.723	59.731	260.027	125.189	425.164	28.438	101.094	160.859	89.536	156.079	96.287	305.288
0.180	162.649	222.078	58.649	260.541	124.956	425.164	28.684	100.902	160.820	89.719	156.427	96.130	305.288
0.190	162.363	221.434	57.568	261.054	124.723	425.164	28.930	100.711	160.782	89.902	156.775	95.973	305.288
0.200	162.078	220.789	56.487	261.567	124.491	425.164	29.176	100.519	160.744	90.085	157.122	95.816	305.288
|Fo|	164.621	232.918	92.680	259.073	127.321	425.164	34.972	102.694	163.144	100.781	160.765	99.542	305.288

Table A.1.29. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2612, B=-0.2612, K=19.70258)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	168.069	233.426	78.484	250.857	128.971	424.549	24.607	103.952	161.537	87.136	149.455	99.269	304.449
0.010	167.784	232.782	77.403	251.370	128.739	424.549	24.853	103.760	161.499	87.319	149.803	99.111	304.449
0.020	167.498	232.137	76.321	251.883	128.506	424.549	25.099	103.568	161.460	87.501	150.151	98.954	304.449
0.030	167.213	231.493	75.240	252.397	128.274	424.549	25.345	103.377	161.422	87.684	150.498	98.797	304.449
0.040	166.928	230.848	74.159	252.910	128.041	424.549	25.592	103.185	161.384	87.867	150.846	98.640	304.449
0.050	166.642	230.204	73.077	253.423	127.809	424.549	25.838	102.993	161.345	88.049	151.194	98.483	304.449
0.060	166.357	229.559	71.996	253.936	127.576	424.549	26.084	102.801	161.307	88.232	151.542	98.325	304.449
0.070	166.072	228.915	70.915	254.449	127.343	424.549	26.330	102.609	161.269	88.415	151.890	98.168	304.449
0.080	165.786	228.270	69.833	254.962	127.111	424.549	26.576	102.417	161.231	88.598	152.238	98.011	304.449
0.090	165.501	227.626	68.752	255.475	126.878	424.549	26.822	102.226	161.192	88.780	152.586	97.854	304.449
0.100	165.215	226.981	67.671	255.988	126.646	424.549	27.068	102.034	161.154	88.963	152.933	97.697	304.449
0.110	164.930	226.337	66.589	256.502	126.413	424.549	27.314	101.842	161.116	89.146	153.281	97.539	304.449
0.120	164.645	225.692	65.508	257.015	126.181	424.549	27.560	101.650	161.077	89.329	153.629	97.382	304.449
0.130	164.359	225.048	64.426	257.528	125.948	424.549	27.806	101.458	161.039	89.511	153.977	97.225	304.449
0.140	164.074	224.403	63.345	258.041	125.715	424.549	28.052	101.266	161.001	89.694	154.325	97.068	304.449
0.150	163.789	223.759	62.264	258.554	125.483	424.549	28.298	101.074	160.962	89.877	154.673	96.911	304.449
0.160	163.503	223.114	61.182	259.067	125.250	424.549	28.544	100.883	160.924	90.059	155.020	96.753	304.449
0.170	163.218	222.470	60.101	259.580	125.018	424.549	28.790	100.691	160.886	90.242	155.368	96.596	304.449
0.180	162.933	221.825	59.020	260.093	124.785	424.549	29.036	100.499	160.848	90.425	155.716	96.439	304.449
0.190	162.647	221.181	57.938	260.606	124.553	424.549	29.282	100.307	160.809	90.608	156.064	96.282	304.449
0.200	162.362	220.536	56.857	261.120	124.320	424.549	29.528	100.115	160.771	90.790	156.412	96.125	304.449
IFoI	164.544	232.780	92.621	258.867	127.179	424.549	34.917	102.512	162.835	100.586	160.427	99.301	304.449

Table A.1.30. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2616, B=-0.38792, K=19.69976)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	168.363	233.169	78.866	250.396	128.794	423.914	24.954	103.924	161.575	87.865	148.725	99.585	303.581
0.010	168.078	232.524	77.784	250.909	128.561	423.914	25.200	103.732	161.537	88.047	149.072	99.428	303.581
0.020	167.792	231.880	76.703	251.422	128.329	423.914	25.446	103.540	161.499	88.230	149.420	99.271	303.581
0.030	167.507	231.235	75.622	251.935	128.096	423.914	25.692	103.348	161.461	88.413	149.768	99.114	303.581
0.040	167.222	230.591	74.540	252.448	127.864	423.914	25.938	103.156	161.422	88.596	150.116	98.956	303.581
0.050	166.936	229.946	73.459	252.961	127.631	423.914	26.184	102.965	161.384	88.778	150.464	98.799	303.581
0.060	166.651	229.302	72.378	253.475	127.398	423.914	26.431	102.773	161.346	88.961	150.812	98.642	303.581
0.070	166.366	228.657	71.296	253.988	127.166	423.914	26.677	102.581	161.307	89.144	151.159	98.485	303.581
0.080	166.080	228.013	70.215	254.501	126.933	423.914	26.923	102.389	161.269	89.327	151.507	98.328	303.581
0.090	165.795	227.368	69.134	255.014	126.701	423.914	27.169	102.197	161.231	89.509	151.855	98.170	303.581
0.100	165.510	226.724	68.052	255.527	126.468	423.914	27.415	102.005	161.192	89.692	152.203	98.013	303.581
0.110	165.224	226.079	66.971	256.040	126.236	423.914	27.661	101.813	161.154	89.875	152.551	97.856	303.581
0.120	164.939	225.435	65.889	256.553	126.003	423.914	27.907	101.622	161.116	90.057	152.899	97.699	303.581
0.130	164.653	224.790	64.808	257.066	125.771	423.914	28.153	101.430	161.077	90.240	153.246	97.542	303.581
0.140	164.368	224.146	63.727	257.579	125.538	423.914	28.399	101.238	161.039	90.423	153.594	97.384	303.581
0.150	164.083	223.501	62.645	258.093	125.305	423.914	28.645	101.046	161.001	90.606	153.942	97.227	303.581
0.160	163.797	222.857	61.564	258.606	125.073	423.914	28.891	100.854	160.963	90.788	154.290	97.070	303.581
0.170	163.512	222.212	60.483	259.119	124.840	423.914	29.137	100.662	160.924	90.971	154.638	96.913	303.581
0.180	163.227	221.568	59.401	259.632	124.608	423.914	29.383	100.471	160.886	91.154	154.986	96.756	303.581
0.190	162.941	220.923	58.320	260.145	124.375	423.914	29.629	100.279	160.848	91.336	155.333	96.598	303.581
0.200	162.656	220.279	57.239	260.658	124.143	423.914	29.875	100.087	160.809	91.519	155.681	96.441	303.581
|Fo|	164.465	232.639	92.561	258.655	127.031	423.914	34.860	102.324	162.516	100.385	160.079	99.052	303.581

Table A.1.31. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2620, B=-0.37575, K=19.69685)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	168.665	232.911	79.263	249.918	128.613	423.259	25.297	103.109	161.624	88.614	147.973	99.908	302.687
0.010	168.380	232.267	78.182	250.431	128.380	423.259	25.543	102.917	161.585	88.797	148.321	99.751	302.687
0.020	168.094	231.622	77.101	250.944	128.148	423.259	25.789	102.725	161.547	88.980	148.669	99.594	302.687
0.030	167.809	230.978	76.019	251.458	127.915	423.259	26.035	102.534	161.509	89.163	149.017	99.437	302.687
0.040	167.524	230.333	74.938	251.971	127.683	423.259	26.281	102.342	161.471	89.345	149.364	99.279	302.687
0.050	167.238	229.689	73.856	252.484	127.450	423.259	26.527	102.150	161.432	89.528	149.712	99.122	302.687
0.060	166.953	229.044	72.775	252.997	127.217	423.259	26.773	101.958	161.394	89.711	150.060	98.965	302.687
0.070	166.668	228.400	71.694	253.510	126.985	423.259	27.019	101.766	161.356	89.893	150.408	98.808	302.687
0.080	166.382	227.755	70.612	254.023	126.752	423.259	27.265	101.574	161.317	90.076	150.756	98.651	302.687
0.090	166.097	227.111	69.531	254.536	126.520	423.259	27.511	101.383	161.279	90.259	151.104	98.493	302.687
0.100	165.811	226.466	68.450	255.049	126.287	423.259	27.758	101.191	161.241	90.442	151.451	98.336	302.687
0.110	165.526	225.822	67.368	255.562	126.055	423.259	28.004	100.999	161.202	90.624	151.799	98.179	302.687
0.120	165.241	225.177	66.287	256.076	125.822	423.259	28.250	100.807	161.164	90.807	152.147	98.022	302.687
0.130	164.955	224.533	65.206	256.589	125.590	423.259	28.496	100.615	161.126	90.990	152.495	97.865	302.687
0.140	164.670	223.888	64.124	257.102	125.357	423.259	28.742	100.423	161.087	91.173	152.843	97.707	302.687
0.150	164.385	223.244	63.043	257.615	125.124	423.259	28.988	100.231	161.049	91.355	153.191	97.550	302.687
0.160	164.099	222.599	61.962	258.128	124.892	423.259	29.234	100.040	161.011	91.538	153.539	97.393	302.687
0.170	163.814	221.955	60.880	258.641	124.659	423.259	29.480	99.848	160.973	91.721	153.886	97.236	302.687
0.180	163.529	221.310	59.799	259.154	124.427	423.259	29.726	99.656	160.934	91.903	154.234	97.079	302.687
0.190	163.243	220.666	58.718	259.667	124.194	423.259	29.972	99.464	160.896	92.086	154.582	96.921	302.687
0.200	162.958	220.021	57.636	260.181	123.962	423.259	30.218	99.272	160.858	92.269	154.930	96.764	302.687
|Fo|	164.384	232.493	92.499	258.436	126.879	423.259	34.802	102.130	162.186	100.177	159.719	98.794	302.687

Table A.1.32. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2624, B=-0.36315, K=19.69401)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	168.980	232.651	79.672	249.424	128.427	422.585	25.636	102.668	161.684	89.387	147.202	100.239	301.766
0.010	168.694	232.007	78.591	249.937	128.194	422.585	25.882	102.476	161.646	89.570	147.550	100.081	301.766
0.020	168.409	231.362	77.509	250.451	127.962	422.585	26.128	102.285	161.608	89.753	147.898	99.924	301.766
0.030	168.124	230.718	76.428	250.964	127.729	422.585	26.374	102.093	161.570	89.936	148.245	99.767	301.766
0.040	167.838	230.073	75.347	251.477	127.497	422.585	26.620	101.901	161.531	90.118	148.593	99.610	301.766
0.050	167.553	229.429	74.265	251.990	127.264	422.585	26.866	101.709	161.493	90.301	148.941	99.453	301.766
0.060	167.268	228.784	73.184	252.503	127.031	422.585	27.112	101.517	161.455	90.484	149.289	99.295	301.766
0.070	166.982	228.140	72.103	253.016	126.799	422.585	27.358	101.325	161.416	90.666	149.637	99.138	301.766
0.080	166.697	227.495	71.021	253.529	126.566	422.585	27.604	101.134	161.378	90.849	149.985	98.981	301.766
0.090	166.412	226.851	69.940	254.042	126.334	422.585	27.850	100.942	161.340	91.032	150.332	98.824	301.766
0.100	166.126	226.206	68.859	254.555	126.101	422.585	28.096	100.750	161.301	91.215	150.680	98.667	301.766
0.110	165.841	225.562	67.777	255.069	125.869	422.585	28.342	100.558	161.263	91.397	151.028	98.509	301.766
0.120	165.555	224.917	66.696	255.582	125.636	422.585	28.588	100.366	161.225	91.580	151.376	98.352	301.766
0.130	165.270	224.273	65.615	256.095	125.404	422.585	28.834	100.174	161.186	91.763	151.724	98.195	301.766
0.140	164.985	223.628	64.533	256.608	125.171	422.585	29.080	99.983	161.148	91.945	152.072	98.038	301.766
0.150	164.699	222.984	63.452	257.121	124.938	422.585	29.326	99.791	161.110	92.128	152.419	97.881	301.766
0.160	164.414	222.340	62.371	257.634	124.706	422.585	29.572	99.599	161.072	92.311	152.767	97.723	301.766
0.170	164.129	221.695	61.289	258.147	124.473	422.585	29.819	99.407	161.033	92.494	153.115	97.566	301.766
0.180	163.843	221.051	60.208	258.660	124.241	422.585	30.065	99.215	160.995	92.676	153.463	97.409	301.766
0.190	163.558	220.406	59.126	259.174	124.008	422.585	30.311	99.023	160.957	92.859	153.811	97.252	301.766
0.200	163.273	219.762	58.045	259.687	123.776	422.585	30.557	98.831	160.918	93.042	154.159	97.095	301.766
IFoI	164.301	232.344	92.435	258.212	126.723	422.585	34.741	101.930	161.847	99.963	159.349	98.530	301.766

Table A.1.33. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2625, B=-0.35990, K=19.69344)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	169.060	232.588	79.777	249.300	128.380	422.414	25.719	102.556	161.701	89.584	147.006	100.323	301.532
0.010	168.774	231.944	78.695	249.813	128.147	422.414	25.965	102.364	161.662	89.767	147.354	100.166	301.532
0.020	168.489	231.299	77.614	250.327	127.914	422.414	26.211	102.172	161.624	89.950	147.702	100.009	301.532
0.030	168.204	230.655	76.533	250.840	127.682	422.414	26.457	101.981	161.586	90.132	148.050	99.851	301.532
0.040	167.918	230.010	75.451	251.353	127.449	422.414	26.703	101.789	161.547	90.315	148.397	99.694	301.532
0.050	167.633	229.366	74.370	251.866	127.217	422.414	26.949	101.597	161.509	90.498	148.745	99.537	301.532
0.060	167.348	228.721	73.289	252.379	126.984	422.414	27.195	101.405	161.471	90.681	149.093	99.380	301.532
0.061	167.319	228.657	73.180	252.430	126.961	422.414	27.220	101.386	161.467	90.699	149.128	99.364	301.532
0.062	167.291	228.592	73.072	252.482	126.938	422.414	27.244	101.367	161.463	90.717	149.163	99.348	301.532
0.063	167.262	228.528	72.964	252.533	126.914	422.414	27.269	101.348	161.459	90.735	149.198	99.333	301.532
0.064	167.233	228.463	72.856	252.584	126.891	422.414	27.294	101.328	161.455	90.754	149.232	99.317	301.532
0.065	167.205	228.399	72.748	252.636	126.868	422.414	27.318	101.309	161.452	90.772	149.267	99.301	301.532
0.066	167.176	228.334	72.640	252.687	126.845	422.414	27.343	101.290	161.448	90.790	149.302	99.286	301.532
0.067	167.148	228.270	72.532	252.738	126.821	422.414	27.367	101.271	161.444	90.808	149.337	99.270	301.532
0.068	167.119	228.206	72.423	252.790	126.798	422.414	27.392	101.252	161.440	90.827	149.371	99.254	301.532
0.069	167.091	228.141	72.315	252.841	126.775	422.414	27.417	101.232	161.436	90.845	149.406	99.238	301.532
0.070	167.062	228.077	72.207	252.892	126.752	422.414	27.441	101.213	161.432	90.863	149.441	99.223	301.532
0.071	167.034	228.012	72.099	252.943	126.728	422.414	27.466	101.194	161.429	90.882	149.476	99.207	301.532
0.072	167.005	227.948	71.991	252.995	126.705	422.414	27.490	101.175	161.425	90.900	149.511	99.191	301.532
0.073	166.977	227.883	71.883	253.046	126.682	422.414	27.515	101.156	161.421	90.918	149.545	99.175	301.532
0.074	166.948	227.819	71.775	253.097	126.659	422.414	27.540	101.137	161.417	90.936	149.580	99.160	301.532
IFoI	164.281	232.307	92.420	258.156	126.684	422.414	34.726	101.879	161.761	99.909	159.255	98.642	301.532

Table A.1.34. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2626, B=-0.35668, K=19.69266)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	169.140	232.523	79.881	249.172	128.332	422.241	25.802	102.444	161.718	89.782	146.809	100.406	301.296
0.010	168.854	231.878	78.800	249.685	128.100	422.241	26.048	102.252	161.680	89.965	147.157	100.249	301.296
0.020	168.569	231.234	77.718	250.198	127.867	422.241	26.294	102.060	161.641	90.148	147.505	100.092	301.296
0.030	168.284	230.589	76.637	250.712	127.634	422.241	26.540	101.868	161.603	90.331	147.853	99.935	301.296
0.040	167.998	229.945	75.556	251.225	127.402	422.241	26.786	101.677	161.565	90.513	148.201	99.778	301.296
0.050	167.713	229.300	74.474	251.738	127.169	422.241	27.032	101.485	161.526	90.696	148.548	99.620	301.296
0.060	167.428	228.656	73.393	252.251	126.937	422.241	27.278	101.293	161.488	90.879	148.896	99.463	301.296
0.061	167.399	228.591	73.285	252.302	126.914	422.241	27.303	101.274	161.484	90.897	148.931	99.448	301.296
0.062	167.371	228.527	73.177	252.354	126.890	422.241	27.328	101.255	161.480	90.915	148.966	99.432	301.296
0.063	167.342	228.462	73.069	252.405	126.867	422.241	27.352	101.235	161.477	90.934	149.001	99.416	301.296
0.064	167.313	228.398	72.960	252.456	126.844	422.241	27.377	101.216	161.473	90.952	149.035	99.400	301.296
0.065	167.285	228.333	72.852	252.508	126.821	422.241	27.402	101.197	161.469	90.970	149.070	99.385	301.296
0.066	167.256	228.269	72.744	252.559	126.797	422.241	27.426	101.178	161.465	90.988	149.105	99.369	301.296
0.067	167.228	228.205	72.636	252.610	126.774	422.241	27.451	101.159	161.461	91.007	149.140	99.353	301.296
0.068	167.199	228.140	72.528	252.661	126.751	422.241	27.475	101.139	161.457	91.025	149.175	99.337	301.296
0.069	167.171	228.076	72.420	252.713	126.727	422.241	27.500	101.120	161.454	91.043	149.209	99.322	301.296
0.070	167.142	228.011	72.312	252.764	126.704	422.241	27.525	101.101	161.450	91.061	149.244	99.306	301.296
0.071	167.114	227.947	72.204	252.815	126.681	422.241	27.549	101.082	161.446	91.080	149.279	99.290	301.296
0.072	167.085	227.882	72.095	252.867	126.658	422.241	27.574	101.063	161.442	91.098	149.314	99.275	301.296
0.073	167.057	227.818	71.987	252.918	126.634	422.241	27.598	101.044	161.438	91.116	149.348	99.259	301.296
0.074	167.028	227.753	71.879	252.969	126.611	422.241	27.623	101.024	161.434	91.135	149.383	99.243	301.296
IFoI	164.259	232.268	92.403	258.098	126.644	422.241	34.711	101.828	161.674	99.854	159.160	98.394	301.296

Table A.1.35. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2627, B=-0.35339, K=19.69202)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	169.220	232.457	79.986	249.044	128.285	422.067	25.885	102.331	161.736	89.982	146.611	100.491	301.058
0.010	168.934	231.813	78.904	249.557	128.052	422.067	26.131	102.139	161.698	90.164	146.959	100.334	301.058
0.020	168.649	231.168	77.823	250.070	127.820	422.067	26.378	101.947	161.660	90.347	147.307	100.177	301.058
0.030	168.364	230.524	76.742	250.584	127.587	422.067	26.624	101.755	161.622	90.530	147.655	100.019	301.058
0.040	168.078	229.879	75.660	251.097	127.355	422.067	26.870	101.563	161.583	90.713	148.003	99.862	301.058
0.050	167.793	229.235	74.579	251.610	127.122	422.067	27.116	101.371	161.545	90.895	148.350	99.705	301.058
0.060	167.508	228.590	73.498	252.123	126.889	422.067	27.362	101.180	161.507	91.078	148.698	99.548	301.058
0.061	167.479	228.526	73.389	252.174	126.866	422.067	27.386	101.160	161.503	91.096	148.733	99.532	301.058
0.062	167.451	228.461	73.281	252.226	126.843	422.067	27.411	101.141	161.499	91.115	148.768	99.516	301.058
0.063	167.422	228.397	73.173	252.277	126.820	422.067	27.436	101.122	161.495	91.133	148.803	99.501	301.058
0.064	167.393	228.332	73.065	252.328	126.796	422.067	27.460	101.103	161.491	91.151	148.837	99.485	301.058
0.065	167.365	228.268	72.957	252.379	126.773	422.067	27.485	101.084	161.488	91.169	148.872	99.469	301.058
0.066	167.336	228.203	72.849	252.431	126.750	422.067	27.509	101.064	161.484	91.188	148.907	99.453	301.058
0.067	167.308	228.139	72.741	252.482	126.727	422.067	27.534	101.045	161.480	91.206	148.942	99.438	301.058
0.068	167.279	228.075	72.632	252.533	126.703	422.067	27.559	101.026	161.476	91.224	148.977	99.422	301.058
0.069	167.251	228.010	72.524	252.585	126.680	422.067	27.583	101.007	161.472	91.242	149.011	99.406	301.058
0.070	167.222	227.946	72.416	252.636	126.657	422.067	27.608	100.988	161.468	91.261	149.046	99.391	301.058
0.071	167.194	227.881	72.308	252.687	126.634	422.067	27.632	100.968	161.465	91.279	149.081	99.375	301.058
0.072	167.165	227.817	72.200	252.739	126.610	422.067	27.657	100.949	161.461	91.297	149.116	99.359	301.058
0.073	167.137	227.752	72.092	252.790	126.587	422.067	27.682	100.930	161.457	91.316	149.150	99.343	301.058
0.074	167.108	227.688	71.984	252.841	126.564	422.067	27.706	100.911	161.453	91.334	149.185	99.328	301.058
IFoI	164.238	232.231	92.387	258.041	126.604	422.067	34.695	101.776	161.586	99.798	159.065	98.326	301.058

Table A.1.36. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2628, B=-0.35014, K=19.69118)

	|Fcl|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	169.302	232.392	80.092	248.916	128.236	421.891	25.969	102.216	161.755	90.181	146.412	100.576	300.819
0.010	169.017	231.747	79.011	249.429	128.003	421.891	26.215	102.024	161.717	90.364	146.760	100.419	300.819
0.020	168.732	231.103	77.930	249.942	127.771	421.891	26.461	101.832	161.678	90.546	147.108	100.262	300.819
0.030	168.446	230.458	76.848	250.455	127.538	421.891	26.707	101.640	161.640	90.729	147.456	100.105	300.819
0.040	168.161	229.814	75.767	250.969	127.306	421.891	26.953	101.448	161.602	90.912	147.803	99.948	300.819
0.050	167.876	229.169	74.686	251.482	127.073	421.891	27.199	101.257	161.564	91.095	148.151	99.790	300.819
0.060	167.590	228.525	73.604	251.995	126.840	421.891	27.445	101.065	161.525	91.277	148.499	99.633	300.819
0.061	167.562	228.460	73.496	252.046	126.817	421.891	27.470	101.046	161.521	91.296	148.534	99.618	300.819
0.062	167.533	228.396	73.388	252.097	126.794	421.891	27.494	101.026	161.518	91.314	148.569	99.602	300.819
0.063	167.505	228.331	73.280	252.149	126.771	421.891	27.519	101.007	161.514	91.332	148.603	99.586	300.819
0.064	167.476	228.267	73.172	252.200	126.747	421.891	27.543	100.988	161.510	91.350	148.638	99.570	300.819
0.065	167.447	228.202	73.064	252.251	126.724	421.891	27.568	100.969	161.506	91.369	148.673	99.555	300.819
0.066	167.419	228.138	72.955	252.303	126.701	421.891	27.593	100.950	161.502	91.387	148.708	99.539	300.819
0.067	167.390	228.073	72.847	252.354	126.678	421.891	27.617	100.931	161.498	91.405	148.743	99.523	300.819
0.068	167.362	228.009	72.739	252.405	126.654	421.891	27.642	100.911	161.495	91.424	148.777	99.508	300.819
0.069	167.333	227.945	72.631	252.457	126.631	421.891	27.666	100.892	161.491	91.442	148.812	99.492	300.819
0.070	167.305	227.880	72.523	252.508	126.608	421.891	27.691	100.873	161.487	91.460	148.847	99.476	300.819
0.071	167.276	227.816	72.415	252.559	126.585	421.891	27.716	100.854	161.483	91.478	148.882	99.460	300.819
0.072	167.248	227.751	72.307	252.611	126.561	421.891	27.740	100.835	161.479	91.497	148.916	99.445	300.819
0.073	167.219	227.687	72.199	252.662	126.538	421.891	27.765	100.815	161.475	91.515	148.951	99.429	300.819
0.074	167.191	227.622	72.090	252.713	126.515	421.891	27.789	100.796	161.472	91.533	148.986	99.413	300.819
|Fol|	164.216	232.191	92.370	257.982	126.563	421.891	34.679	101.724	161.498	99.743	158.969	98.257	300.819

Table A.1.37. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2629, B=-0.34682, K=19.69047)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	169.385	232.326	80.199	248.786	128.188	421.715	26.051	102.101	161.775	90.384	146.212	100.661	300.579
0.010	169.100	231.681	79.118	249.299	127.956	421.715	26.297	101.909	161.737	90.567	146.559	100.504	300.579
0.020	168.814	231.037	78.036	249.812	127.723	421.715	26.543	101.717	161.698	90.750	146.907	100.347	300.579
0.030	168.529	230.393	76.955	250.325	127.491	421.715	26.789	101.526	161.660	90.932	147.255	100.189	300.579
0.040	168.243	229.748	75.874	250.839	127.258	421.715	27.035	101.334	161.622	91.115	147.603	100.032	300.579
0.050	167.958	229.104	74.792	251.352	127.026	421.715	27.281	101.142	161.583	91.298	147.951	99.875	300.579
0.060	167.673	228.459	73.711	251.865	126.793	421.715	27.527	100.950	161.545	91.480	148.299	99.718	300.579
0.061	167.644	228.395	73.603	251.916	126.770	421.715	27.551	100.931	161.541	91.499	148.333	99.702	300.579
0.062	167.616	228.330	73.495	251.967	126.747	421.715	27.576	100.912	161.537	91.517	148.368	99.686	300.579
0.063	167.587	228.266	73.387	252.019	126.723	421.715	27.601	100.893	161.534	91.535	148.403	99.671	300.579
0.064	167.559	228.201	73.279	252.070	126.700	421.715	27.625	100.873	161.530	91.553	148.438	99.655	300.579
0.065	167.530	228.137	73.170	252.121	126.677	421.715	27.650	100.854	161.526	91.572	148.473	99.639	300.579
0.066	167.502	228.072	73.062	252.173	126.654	421.715	27.675	100.835	161.522	91.590	148.507	99.623	300.579
0.067	167.473	228.008	72.954	252.224	126.630	421.715	27.699	100.816	161.518	91.608	148.542	99.608	300.579
0.068	167.444	227.943	72.846	252.275	126.607	421.715	27.724	100.797	161.514	91.627	148.577	99.592	300.579
0.069	167.416	227.879	72.738	252.327	126.584	421.715	27.748	100.777	161.511	91.645	148.612	99.576	300.579
0.070	167.387	227.815	72.630	252.378	126.561	421.715	27.773	100.758	161.507	91.663	148.646	99.561	300.579
0.071	167.359	227.750	72.522	252.429	126.537	421.715	27.798	100.739	161.503	91.681	148.681	99.545	300.579
0.072	167.330	227.686	72.413	252.481	126.514	421.715	27.822	100.720	161.499	91.700	148.716	99.529	300.579
0.073	167.302	227.621	72.305	252.532	126.491	421.715	27.847	100.701	161.495	91.718	148.751	99.513	300.579
0.074	167.273	227.557	72.197	252.583	126.467	421.715	27.871	100.682	161.491	91.736	148.786	99.498	300.579
IFoI	164.194	232.152	92.354	257.923	126.522	421.715	34.664	101.672	161.409	99.687	158.972	98.188	300.579

Table A.1.38. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2632, B=-0.33667, K=19.68850)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	169.635	232.129	80.526	248.392	128.041	421.180	26.296	101.753	161.838	90.997	145.602	100.920	299.847
0.010	169.350	231.485	79.445	248.905	127.809	421.180	26.542	101.561	161.800	91.179	145.950	100.763	299.847
0.020	169.064	230.840	78.364	249.418	127.576	421.180	26.788	101.369	161.761	91.362	146.298	100.605	299.847
0.030	168.779	230.196	77.282	249.931	127.344	421.180	27.034	101.178	161.723	91.545	146.646	100.448	299.847
0.040	168.494	229.551	76.201	250.444	127.111	421.180	27.280	100.986	161.685	91.728	146.994	100.291	299.847
0.050	168.208	228.907	75.120	250.957	126.879	421.180	27.526	100.794	161.647	91.910	147.342	100.134	299.847
0.060	167.923	228.262	74.038	251.470	126.646	421.180	27.773	100.602	161.608	92.093	147.689	99.977	299.847
0.070	167.638	227.618	72.957	251.984	126.413	421.180	28.019	100.410	161.570	92.276	148.037	99.819	299.847
0.080	167.352	226.973	71.875	252.497	126.181	421.180	28.265	100.218	161.532	92.459	148.385	99.662	299.847
0.090	167.067	226.329	70.794	253.010	125.948	421.180	28.511	100.027	161.493	92.641	148.733	99.505	299.847
0.100	166.782	225.685	69.713	253.523	125.716	421.180	28.757	99.835	161.455	92.824	149.081	99.348	299.847
0.110	166.496	225.040	68.631	254.036	125.483	421.180	29.003	99.643	161.417	93.007	149.429	99.191	299.847
0.120	166.211	224.396	67.550	254.549	125.251	421.180	29.249	99.451	161.378	93.189	149.776	99.033	299.847
0.130	165.925	223.751	66.469	255.062	125.018	421.180	29.495	99.259	161.340	93.372	150.124	98.876	299.847
0.140	165.640	223.107	65.387	255.575	124.785	421.180	29.741	99.067	161.302	93.555	150.472	98.719	299.847
0.150	165.355	222.462	64.306	256.089	124.553	421.180	29.987	98.876	161.264	93.738	150.820	98.562	299.847
0.160	165.069	221.818	63.225	256.602	124.320	421.180	30.233	98.684	161.225	93.920	151.168	98.405	299.847
0.170	164.784	221.173	62.143	257.115	124.088	421.180	30.479	98.492	161.187	94.103	151.516	98.247	299.847
0.180	164.499	220.529	61.062	257.628	123.855	421.180	30.725	98.300	161.149	94.286	151.863	98.090	299.847
0.190	164.213	219.884	59.981	258.141	123.623	421.180	30.971	98.108	161.110	94.468	152.211	97.933	299.847
0.200	163.928	219.240	58.899	258.654	123.390	421.180	31.217	97.916	161.072	94.651	152.559	97.776	299.847
IFoI	164.130	232.036	92.304	257.747	126.399	421.180	34.616	101.514	161.140	99.517	158.578	97.978	299.847

Table A.1.39. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2636, B=-0.32284, K=19.68564)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	169.978	231.865	80.974	247.851	127.842	420.449	26.618	101.277	161.932	91.833	144.775	101.268	298.849
0.010	169.693	231.220	79.892	248.364	127.609	420.449	26.864	101.086	161.894	92.016	145.123	101.111	298.849
0.020	169.408	230.576	78.811	248.877	127.377	420.449	27.110	100.894	161.856	92.199	145.471	100.954	298.849
0.030	169.122	229.931	77.730	249.390	127.144	420.449	27.356	100.702	161.817	92.381	145.819	100.797	298.849
0.040	168.837	229.287	76.648	249.904	126.912	420.449	27.602	100.510	161.779	92.564	146.167	100.640	298.849
0.050	168.552	228.642	75.567	250.417	126.679	420.449	27.848	100.318	161.741	92.747	146.514	100.482	298.849
0.060	168.266	227.998	74.486	250.930	126.446	420.449	28.094	100.126	161.702	92.930	146.862	100.325	298.849
0.070	167.981	227.353	73.404	251.443	126.214	420.449	28.341	99.935	161.664	93.112	147.210	100.168	298.849
0.080	167.695	226.709	72.323	251.956	125.981	420.449	28.587	99.743	161.626	93.295	147.558	100.011	298.849
0.090	167.410	226.065	71.242	252.469	125.749	420.449	28.833	99.551	161.587	93.478	147.906	99.854	298.849
0.100	167.125	225.420	70.160	252.982	125.516	420.449	29.079	99.359	161.549	93.660	148.254	99.696	298.849
0.110	166.839	224.776	69.079	253.495	125.284	420.449	29.325	99.167	161.511	93.843	148.601	99.539	298.849
0.120	166.554	224.131	67.998	254.009	125.051	420.449	29.571	98.975	161.473	94.026	148.949	99.382	298.849
0.130	166.269	223.487	66.916	254.522	124.819	420.449	29.817	98.784	161.434	94.209	149.297	99.225	298.849
0.140	165.983	222.842	65.835	255.035	124.586	420.449	30.063	98.592	161.396	94.391	149.645	99.068	298.849
0.150	165.698	222.198	64.754	255.548	124.353	420.449	30.309	98.400	161.358	94.574	149.993	98.910	298.849
0.160	165.413	221.553	63.672	256.061	124.121	420.449	30.555	98.208	161.319	94.757	150.341	98.753	298.849
0.170	165.127	220.909	62.591	256.574	123.888	420.449	30.801	98.016	161.281	94.940	150.688	98.596	298.849
0.180	164.842	220.264	61.510	257.087	123.656	420.449	31.047	97.824	161.243	95.122	151.036	98.439	298.849
0.190	164.556	219.620	60.428	257.600	123.423	420.449	31.293	97.633	161.204	95.305	151.384	98.282	298.849
0.200	164.271	218.975	59.347	258.113	123.191	420.449	31.539	97.441	161.166	95.488	151.732	98.124	298.849
|Fo|	164.041	231.875	92.236	257.505	126.230	420.449	34.551	101.297	160.772	99.285	158.176	97.691	298.849

Table A.1.40: Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2640, B=-0.30854, K=19.68295)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	170.332	231.600	81.433	247.296	127.637	419.701	26.935	100.790	162.039	92.689	143.931	101.623	297.826
0.010	170.046	230.956	80.351	247.809	127.405	419.701	27.181	100.598	162.000	92.872	144.278	101.466	297.826
0.020	169.761	230.311	79.270	248.322	127.172	419.701	27.427	100.407	161.962	93.055	144.626	101.309	297.826
0.030	169.476	229.667	78.189	248.836	126.940	419.701	27.673	100.215	161.924	93.238	144.974	101.152	297.826
0.040	169.190	229.022	77.107	249.349	126.707	419.701	27.919	100.023	161.886	93.420	145.322	100.995	297.826
0.050	168.905	228.378	76.026	249.862	126.474	419.701	28.165	99.831	161.847	93.603	145.670	100.837	297.826
0.060	168.620	227.734	74.945	250.375	126.242	419.701	28.411	99.639	161.809	93.786	146.018	100.680	297.826
0.070	168.334	227.089	73.863	250.888	126.009	419.701	28.657	99.447	161.771	93.968	146.365	100.523	297.826
0.080	168.049	226.445	72.782	251.401	125.777	419.701	28.903	99.256	161.732	94.151	146.713	100.366	297.826
0.090	167.764	225.800	71.701	251.914	125.544	419.701	29.149	99.064	161.694	94.334	147.061	100.209	297.826
0.100	167.478	225.156	70.619	252.427	125.312	419.701	29.395	98.872	161.656	94.517	147.409	100.051	297.826
0.110	167.193	224.511	69.538	252.941	125.079	419.701	29.641	98.680	161.617	94.699	147.757	99.894	297.826
0.120	166.907	223.867	68.456	253.454	124.846	419.701	29.887	98.488	161.579	94.882	148.105	99.737	297.826
0.130	166.622	223.222	67.375	253.967	124.614	419.701	30.133	98.296	161.541	95.065	148.452	99.580	297.826
0.140	166.337	222.578	66.294	254.480	124.381	419.701	30.379	98.104	161.503	95.247	148.800	99.423	297.826
0.150	166.051	221.933	65.212	254.993	124.149	419.701	30.625	97.913	161.464	95.430	149.148	99.265	297.826
0.160	165.766	221.289	64.131	255.506	123.916	419.701	30.871	97.721	161.426	95.613	149.496	99.108	297.826
0.170	165.481	220.644	63.050	256.019	123.684	419.701	31.117	97.529	161.388	95.796	149.844	98.951	297.826
0.180	165.195	220.000	61.968	256.532	123.451	419.701	31.364	97.337	161.349	95.978	150.192	98.794	297.826
0.190	164.910	219.355	60.887	257.045	123.219	419.701	31.610	97.145	161.311	96.161	150.539	98.637	297.826
0.200	164.625	218.711	59.806	257.559	122.986	419.701	31.856	96.953	161.273	96.344	150.887	98.479	297.826
|Fo|	163.951	231.713	92.166	257.258	126.057	419.701	34.484	101.075	160.395	99.047	157.764	97.396	297.826

Table A.1.41. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2644, B=-0.29386, K=19.68017)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	170.693	231.334	81.903	246.725	127.431	418.933	27.245	100.293	162.159	93.566	143.068	101.983	296.778
0.010	170.408	230.689	80.822	247.238	127.198	418.933	27.491	100.101	162.121	93.749	143.416	101.826	296.778
0.020	170.122	230.045	79.740	247.751	126.966	418.933	27.738	99.909	162.082	93.932	143.764	101.668	296.778
0.030	169.837	229.400	78.659	248.264	126.733	418.933	27.984	99.717	162.044	94.114	144.112	101.511	296.778
0.040	169.552	228.756	77.578	248.778	126.501	418.933	28.230	99.525	162.006	94.297	144.460	101.354	296.778
0.050	169.266	228.111	76.496	249.291	126.268	418.933	28.476	99.334	161.967	94.480	144.808	101.197	296.778
0.060	168.981	227.467	75.415	249.804	126.036	418.933	28.722	99.142	161.929	94.663	145.155	101.040	296.778
0.070	168.695	226.822	74.333	250.317	125.803	418.933	28.968	98.950	161.891	94.845	145.503	100.882	296.778
0.080	168.410	226.178	73.252	250.830	125.570	418.933	29.214	98.758	161.853	95.028	145.851	100.725	296.778
0.090	168.125	225.533	72.171	251.343	125.338	418.933	29.460	98.566	161.814	95.211	146.199	100.568	296.778
0.100	167.839	224.889	71.089	251.856	125.105	418.933	29.706	98.374	161.776	95.393	146.547	100.411	296.778
0.110	167.554	224.244	70.008	252.369	124.873	418.933	29.952	98.182	161.738	95.576	146.895	100.254	296.778
0.120	167.269	223.600	68.927	252.883	124.640	418.933	30.198	97.991	161.699	95.759	147.243	100.096	296.778
0.130	166.983	222.955	67.845	253.396	124.408	418.933	30.444	97.799	161.661	95.942	147.590	99.939	296.778
0.140	166.698	222.311	66.764	253.909	124.175	418.933	30.690	97.607	161.623	96.124	147.938	99.782	296.778
0.150	166.413	221.666	65.683	254.422	123.943	418.933	30.936	97.415	161.584	96.307	148.286	99.625	296.778
0.160	166.127	221.022	64.601	254.935	123.710	418.933	31.182	97.223	161.546	96.490	148.634	99.468	296.778
0.170	165.842	220.377	63.520	255.448	123.477	418.933	31.428	97.031	161.508	96.672	148.982	99.310	296.778
0.180	165.557	219.733	62.439	255.961	123.245	418.933	31.674	96.840	161.469	96.855	149.330	99.153	296.778
0.190	165.271	219.088	61.357	256.474	123.012	418.933	31.920	96.648	161.431	97.038	149.677	98.996	296.778
0.200	164.986	218.444	60.276	256.987	122.780	418.933	32.167	96.456	161.393	97.221	150.025	98.839	296.778
|Fo|	163.859	231.564	92.095	257.005	125.879	418.933	34.415	100.847	160.008	98.803	157.343	97.095	296.778

Table A.1.42. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2648, B=-0.27874, K=19.67758)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	171.065	231.064	82.387	246.138	127.220	418.149	27.552	99.785	162.290	94.463	142.189	102.346	295.707
0.010	170.779	230.420	81.305	246.651	126.987	418.149	27.798	99.593	162.252	94.645	142.537	102.189	295.707
0.020	170.494	229.775	80.224	247.164	126.754	418.149	28.044	99.401	162.214	94.828	142.885	102.032	295.707
0.030	170.208	229.131	79.143	247.677	126.522	418.149	28.290	99.209	162.175	95.011	143.232	101.875	295.707
0.040	169.923	228.487	78.061	248.190	126.289	418.149	28.536	99.018	162.137	95.194	143.580	101.718	295.707
0.050	169.638	227.842	76.980	248.703	126.057	418.149	28.782	98.826	162.099	95.376	143.928	101.560	295.707
0.060	169.352	227.198	75.899	249.216	125.824	418.149	29.028	98.634	162.060	95.559	144.276	101.403	295.707
0.070	169.067	226.553	74.817	249.730	125.592	418.149	29.274	98.442	162.022	95.742	144.624	101.246	295.707
0.080	168.782	225.909	73.736	250.243	125.359	418.149	29.521	98.250	161.984	95.924	144.972	101.089	295.707
0.090	168.496	225.264	72.655	250.756	125.126	418.149	29.767	98.058	161.946	96.107	145.319	100.932	295.707
0.100	168.211	224.620	71.573	251.269	124.894	418.149	30.013	97.866	161.907	96.290	145.667	100.774	295.707
0.110	167.926	223.975	70.492	251.782	124.661	418.149	30.259	97.675	161.869	96.473	146.015	100.617	295.707
0.120	167.640	223.331	69.411	252.295	124.429	418.149	30.505	97.483	161.831	96.655	146.363	100.460	295.707
0.130	167.355	222.686	68.329	252.808	124.196	418.149	30.751	97.291	161.792	96.838	146.711	100.303	295.707
0.140	167.069	222.042	67.248	253.321	123.964	418.149	30.997	97.099	161.754	97.021	147.059	100.146	295.707
0.150	166.784	221.397	66.167	253.834	123.731	418.149	31.243	96.907	161.716	97.203	147.406	99.988	295.707
0.160	166.499	220.753	65.085	254.348	123.499	418.149	31.489	96.715	161.677	97.386	147.754	99.831	295.707
0.170	166.213	220.108	64.004	254.861	123.266	418.149	31.735	96.524	161.639	97.569	148.102	99.674	295.707
0.180	165.928	219.464	62.922	255.374	123.033	418.149	31.981	96.332	161.601	97.752	148.450	99.517	295.707
0.190	165.643	218.819	61.841	255.887	122.801	418.149	32.227	96.140	161.563	97.934	148.798	99.360	295.707
0.200	165.357	218.175	60.760	256.400	122.568	418.149	32.473	95.948	161.524	98.117	149.146	99.202	295.707
IFoI	163.766	231.377	92.023	256.748	125.699	418.149	34.345	100.615	159.613	98.553	156.912	96.787	295.707

Table A.1.43. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2652, B=-0.26322, K=19.67492)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	171.446	230.793	82.882	245.536	127.003	417.347	27.852	99.265	162.434	95.379	141.295	102.715	294.612
0.010	171.161	230.148	81.801	246.049	126.771	417.347	28.098	99.074	162.396	95.561	141.643	102.558	294.612
0.020	170.876	229.504	80.719	246.562	126.538	417.347	28.344	98.882	162.357	95.744	141.991	102.401	294.612
0.030	170.590	228.859	79.638	247.075	126.305	417.347	28.590	98.690	162.319	95.927	142.339	102.244	294.612
0.040	170.305	228.215	78.557	247.589	126.073	417.347	28.836	98.498	162.281	96.110	142.687	102.086	294.612
0.050	170.020	227.571	77.475	248.102	125.840	417.347	29.082	98.306	162.242	96.292	143.035	101.929	294.612
0.060	169.734	226.926	76.394	248.615	125.608	417.347	29.328	98.114	162.204	96.475	143.382	101.772	294.612
0.070	169.449	226.282	75.313	249.128	125.375	417.347	29.574	97.923	162.166	96.658	143.730	101.615	294.612
0.080	169.163	225.637	74.231	249.641	125.143	417.347	29.820	97.731	162.128	96.840	144.078	101.458	294.612
0.090	168.878	224.993	73.150	250.154	124.910	417.347	30.066	97.539	162.089	97.023	144.426	101.300	294.612
0.100	168.593	224.348	72.069	250.667	124.677	417.347	30.312	97.347	162.051	97.206	144.774	101.143	294.612
0.110	168.307	223.704	70.987	251.180	124.445	417.347	30.558	97.155	162.013	97.389	145.122	100.986	294.612
0.120	168.022	223.059	69.906	251.693	124.212	417.347	30.805	96.963	161.974	97.571	145.469	100.829	294.612
0.130	167.737	222.415	68.824	252.207	123.980	417.347	31.051	96.771	161.936	97.754	145.817	100.672	294.612
0.140	167.451	221.770	67.743	252.720	123.747	417.347	31.297	96.580	161.898	97.937	146.165	100.514	294.612
0.150	167.166	221.126	66.662	253.233	123.515	417.347	31.543	96.388	161.859	98.119	146.513	100.357	294.612
0.160	166.881	220.481	65.580	253.746	123.282	417.347	31.789	96.196	161.821	98.302	146.861	100.200	294.612
0.170	166.595	219.837	64.499	254.259	123.050	417.347	32.035	96.004	161.783	98.485	147.209	100.043	294.612
0.180	166.310	219.192	63.418	254.772	122.817	417.347	32.281	95.812	161.745	98.668	147.556	99.886	294.612
0.190	166.025	218.548	62.336	255.285	122.584	417.347	32.527	95.620	161.706	98.850	147.904	99.728	294.612
0.200	165.739	217.903	61.255	255.798	122.352	417.347	32.773	95.429	161.668	99.033	148.252	99.571	294.612
IFoI	163.671	231.204	91.949	256.484	125.513	417.347	34.274	100.377	159.209	98.298	156.470	96.471	294.612

Table A.1.44. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2656, B=-0.24728, K=19.67240)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	171.839	230.521	83.389	244.920	126.785	416.528	28.145	98.737	162.591	96.313	140.385	103.087	293.494
0.010	171.553	229.877	82.307	245.433	126.552	416.528	28.391	98.545	162.553	96.496	140.733	102.930	293.494
0.020	171.268	229.232	81.226	245.946	126.320	416.528	28.637	98.353	162.515	96.678	141.081	102.773	293.494
0.030	170.982	228.588	80.145	246.460	126.087	416.528	28.883	98.161	162.476	96.861	141.429	102.616	293.494
0.040	170.697	227.944	79.063	246.973	125.855	416.528	29.129	97.970	162.438	97.044	141.777	102.459	293.494
0.050	170.412	227.299	77.982	247.486	125.622	416.528	29.375	97.778	162.400	97.227	142.125	102.301	293.494
0.060	170.126	226.655	76.901	247.999	125.390	416.528	29.621	97.586	162.362	97.409	142.472	102.144	293.494
0.070	169.841	226.010	75.819	248.512	125.157	416.528	29.867	97.394	162.323	97.592	142.820	101.987	293.494
0.080	169.556	225.366	74.738	249.025	124.924	416.528	30.113	97.202	162.285	97.775	143.168	101.830	293.494
0.090	169.270	224.721	73.656	249.538	124.692	416.528	30.359	97.010	162.247	97.957	143.516	101.673	293.494
0.100	168.985	224.077	72.575	250.051	124.459	416.528	30.605	96.819	162.208	98.140	143.864	101.515	293.494
0.110	168.700	223.432	71.494	250.565	124.227	416.528	30.851	96.627	162.170	98.323	144.212	101.358	293.494
0.120	168.414	222.788	70.412	251.078	123.994	416.528	31.097	96.435	162.132	98.506	144.560	101.201	293.494
0.130	168.129	222.143	69.331	251.591	123.762	416.528	31.343	96.243	162.093	98.688	144.907	101.044	293.494
0.140	167.844	221.499	68.250	252.104	123.529	416.528	31.589	96.051	162.055	98.871	145.255	100.887	293.494
0.150	167.558	220.854	67.168	252.617	123.297	416.528	31.836	95.859	162.017	99.054	145.603	100.729	293.494
0.160	167.273	220.210	66.087	253.130	123.064	416.528	32.082	95.668	161.978	99.236	145.951	100.572	293.494
0.170	166.987	219.565	65.006	253.643	122.831	416.528	32.328	95.476	161.940	99.419	146.299	100.415	293.494
0.180	166.702	218.921	63.924	254.156	122.599	416.528	32.574	95.284	161.902	99.602	146.647	100.258	293.494
0.190	166.417	218.276	62.843	254.669	122.366	416.528	32.820	95.092	161.864	99.785	146.994	100.101	293.494
0.200	166.131	217.632	61.762	255.183	122.134	416.528	33.066	94.900	161.825	99.967	147.342	99.943	293.494
IFoI	163.576	231.029	91.874	256.216	125.325	416.528	34.201	100.134	158.796	98.038	156.020	96.149	293.494

Table A.1.45. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2660, B=-0.23089, K=19.66997)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	172.241	230.245	83.909	244.288	126.563	415.692	28.433	98.198	162.761	97.266	139.460	103.463	292.352
0.010	171.956	229.601	82.827	244.801	126.331	415.692	28.679	98.006	162.723	97.448	139.808	103.306	292.352
0.020	171.670	228.956	81.746	245.314	126.098	415.692	28.925	97.814	162.684	97.631	140.156	103.148	292.352
0.030	171.385	228.312	80.665	245.827	125.866	415.692	29.172	97.623	162.646	97.814	140.504	102.991	292.352
0.040	171.100	227.667	79.583	246.341	125.633	415.692	29.418	97.431	162.608	97.997	140.852	102.834	292.352
0.050	170.814	227.023	78.502	246.854	125.401	415.692	29.664	97.239	162.570	98.179	141.200	102.677	292.352
0.060	170.529	226.378	77.421	247.367	125.168	415.692	29.910	97.047	162.531	98.362	141.547	102.520	292.352
0.070	170.244	225.734	76.339	247.880	124.936	415.692	30.156	96.855	162.493	98.545	141.895	102.362	292.352
0.080	169.958	225.089	75.258	248.393	124.703	415.692	30.402	96.663	162.455	98.727	142.243	102.205	292.352
0.090	169.673	224.445	74.177	248.906	124.470	415.692	30.648	96.472	162.416	98.910	142.591	102.048	292.352
0.100	169.387	223.800	73.095	249.419	124.238	415.692	30.894	96.280	162.378	99.093	142.939	101.891	292.352
0.110	169.102	223.156	72.014	249.932	124.005	415.692	31.140	96.088	162.340	99.276	143.287	101.734	292.352
0.120	168.817	222.511	70.933	250.446	123.773	415.692	31.386	95.896	162.301	99.458	143.635	101.576	292.352
0.130	168.531	221.867	69.851	250.959	123.540	415.692	31.632	95.704	162.263	99.641	143.982	101.419	292.352
0.140	168.246	221.222	68.770	251.472	123.308	415.692	31.878	95.512	162.225	99.824	144.330	101.262	292.352
0.150	167.961	220.578	67.689	251.985	123.075	415.692	32.124	95.321	162.187	100.006	144.678	101.105	292.352
0.160	167.675	219.934	66.607	252.498	122.842	415.692	32.370	95.129	162.148	100.189	145.026	100.948	292.352
0.170	167.390	219.289	65.526	253.011	122.610	415.692	32.616	94.937	162.110	100.372	145.374	100.790	292.352
0.180	167.105	218.645	64.445	253.524	122.377	415.692	32.862	94.745	162.072	100.555	145.722	100.633	292.352
0.190	166.819	218.000	63.363	254.037	122.145	415.692	33.108	94.553	162.033	100.737	146.069	100.476	292.352
0.200	166.534	217.356	62.282	254.550	121.912	415.692	33.354	94.361	161.995	100.920	146.417	100.319	292.352
IFoI	163.479	230.851	91.798	255.943	125.132	415.692	34.126	99.886	158.375	97.772	155.560	95.821	292.352

Table A.1.46. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2664, B=-0.21413, K=19.66757)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	172.651	229.969	84.440	243.640	126.339	414.840	28.715	97.649	162.944	98.237	138.523	103.841	291.190
0.010	172.366	229.325	83.359	244.153	126.106	414.840	28.961	97.457	162.906	98.419	138.870	103.684	291.190
0.020	172.081	228.680	82.278	244.666	125.873	414.840	29.207	97.265	162.868	98.602	139.218	103.527	291.190
0.030	171.795	228.036	81.196	245.179	125.641	414.840	29.453	97.074	162.830	98.785	139.566	103.370	291.190
0.040	171.510	227.391	80.115	245.692	125.408	414.840	29.699	96.882	162.791	98.968	139.914	103.213	291.190
0.050	171.224	226.747	79.034	246.205	125.176	414.840	29.945	96.690	162.753	99.150	140.262	103.055	291.190
0.060	170.939	226.102	77.952	246.718	124.943	414.840	30.191	96.498	162.715	99.333	140.610	102.898	291.190
0.070	170.654	225.458	76.871	247.232	124.711	414.840	30.437	96.306	162.676	99.516	140.957	102.741	291.190
0.080	170.368	224.813	75.790	247.745	124.478	414.840	30.683	96.114	162.638	99.698	141.305	102.584	291.190
0.090	170.083	224.169	74.708	248.258	124.246	414.840	30.930	95.922	162.600	99.881	141.653	102.427	291.190
0.100	169.798	223.524	73.627	248.771	124.013	414.840	31.176	95.731	162.561	100.064	142.001	102.269	291.190
0.110	169.512	222.880	72.546	249.284	123.780	414.840	31.422	95.539	162.523	100.247	142.349	102.112	291.190
0.120	169.227	222.235	71.464	249.797	123.548	414.840	31.668	95.347	162.485	100.429	142.697	101.955	291.190
0.130	168.942	221.591	70.383	250.310	123.315	414.840	31.914	95.155	162.447	100.612	143.045	101.798	291.190
0.140	168.656	220.946	69.301	250.823	123.083	414.840	32.160	94.963	162.408	100.795	143.392	101.641	291.190
0.150	168.371	220.302	68.220	251.337	122.850	414.840	32.406	94.771	162.370	100.977	143.740	101.483	291.190
0.160	168.086	219.657	67.139	251.850	122.618	414.840	32.652	94.580	162.332	101.160	144.088	101.326	291.190
0.170	167.800	219.013	66.057	252.363	122.385	414.840	32.898	94.388	162.293	101.343	144.436	101.169	291.190
0.180	167.515	218.368	64.976	252.876	122.152	414.840	33.144	94.196	162.255	101.526	144.784	101.012	291.190
0.190	167.229	217.724	63.895	253.389	121.920	414.840	33.390	94.004	162.217	101.708	145.132	100.855	291.190
0.200	166.944	217.079	62.813	253.902	121.687	414.840	33.636	93.812	162.178	101.891	145.479	100.697	291.190
IFoI	163.380	230.670	91.270	255.665	124.936	414.840	34.050	99.633	157.945	97.501	155.091	95.486	291.190

Table A.1.47. Calculated and Observed Structure Factors for Cobalt Chromite with respesct to Degree of Disorder (x).
(u=0.2668, B=-0.19691, K=19.66534)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	173.072	229.691	84.983	242.977	126.110	413.972	28.990	97.091	163.141	99.225	137.570	104.222	290.004
0.010	172.786	229.046	83.902	243.490	125.878	413.972	29.236	96.899	163.103	99.408	137.917	104.065	290.004
0.020	172.501	228.402	82.821	244.003	125.645	413.972	29.482	96.707	163.065	99.590	138.265	103.908	290.004
0.030	172.216	227.757	81.739	244.516	125.413	413.972	29.728	96.515	163.027	99.773	138.613	103.750	290.004
0.040	171.930	227.113	80.658	245.030	125.180	413.972	29.974	96.324	162.988	99.956	138.961	103.593	290.004
0.050	171.645	226.468	79.577	245.543	124.947	413.972	30.220	96.132	162.950	100.138	139.309	103.436	290.004
0.060	171.360	225.824	78.495	246.056	124.715	413.972	30.466	95.940	162.912	100.321	139.657	103.279	290.004
0.070	171.074	225.179	77.414	246.569	124.482	413.972	30.712	95.748	162.873	100.504	140.005	103.122	290.004
0.080	170.789	224.535	76.333	247.082	124.250	413.972	30.958	95.556	162.835	100.687	140.352	102.964	290.004
0.090	170.504	223.890	75.251	247.595	124.017	413.972	31.204	95.364	162.797	100.869	140.700	102.807	290.004
0.100	170.218	223.246	74.170	248.108	123.785	413.972	31.450	95.173	162.758	101.052	141.048	102.650	290.004
0.110	169.933	222.601	73.088	248.621	123.552	413.972	31.696	94.981	162.720	101.235	141.396	102.493	290.004
0.120	169.648	221.957	72.007	249.135	123.320	413.972	31.942	94.789	162.682	101.417	141.744	102.336	290.004
0.130	169.362	221.312	70.926	249.648	123.087	413.972	32.189	94.597	162.644	101.600	142.092	102.178	290.004
0.140	169.077	220.668	69.844	250.161	122.854	413.972	32.435	94.405	162.605	101.783	142.439	102.021	290.004
0.150	168.791	220.023	68.763	250.674	122.622	413.972	32.681	94.213	162.567	101.966	142.787	101.864	290.004
0.160	168.506	219.379	67.682	251.187	122.389	413.972	32.927	94.021	162.529	102.148	143.135	101.707	290.004
0.170	168.221	218.734	66.600	251.700	122.157	413.972	33.173	93.830	162.490	102.331	143.483	101.550	290.004
0.180	167.935	218.090	65.519	252.213	121.924	413.972	33.419	93.638	162.452	102.514	143.831	101.392	290.004
0.190	167.650	217.445	64.438	252.726	121.692	413.972	33.665	93.446	162.414	102.697	144.179	101.235	290.004
0.200	167.365	216.801	63.356	253.240	121.459	413.972	33.911	93.254	162.375	102.879	144.526	101.078	290.004
|Fo|	163.281	230.487	91.642	255.384	124.737	413.972	33.972	99.375	157.507	97.224	154.613	95.144	290.004

Table A.1.48. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2672, B=-0.17927, K=19.66331)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	173.503	229.410	85.538	242.239	125.879	413.089	29.259	96.524	163.351	100.231	136.605	104.606	288.798
0.010	173.217	228.765	84.456	242.752	125.646	413.089	29.505	96.332	163.313	100.414	136.953	104.449	288.798
0.020	172.932	228.121	83.375	243.266	125.414	413.089	29.751	96.140	163.274	100.597	137.301	104.292	288.798
0.030	172.647	227.476	82.294	243.779	125.181	413.089	29.997	95.948	163.236	100.780	137.649	104.134	288.798
0.040	172.361	226.832	81.212	244.292	124.948	413.089	30.243	95.756	163.198	100.962	137.996	103.977	288.798
0.050	172.076	226.187	80.131	244.805	124.716	413.089	30.489	95.565	163.159	101.145	138.344	103.820	288.798
0.060	171.791	225.543	79.050	245.318	124.483	413.089	30.735	95.373	163.121	101.328	138.692	103.663	288.798
0.070	171.505	224.898	77.968	245.831	124.251	413.089	30.981	95.181	163.083	101.510	139.040	103.506	288.798
0.080	171.220	224.254	76.887	246.344	124.018	413.089	31.227	94.989	163.044	101.693	139.388	103.348	288.798
0.090	170.934	223.609	75.805	246.857	123.786	413.089	31.474	94.797	163.006	101.876	139.736	103.191	288.798
0.100	170.649	222.965	74.724	247.371	123.553	413.089	31.720	94.605	162.968	102.059	140.083	103.034	288.798
0.110	170.364	222.320	73.643	247.884	123.320	413.089	31.966	94.414	162.929	102.241	140.431	102.877	288.798
0.120	170.078	221.676	72.561	248.397	123.088	413.089	32.212	94.222	162.891	102.424	140.779	102.720	288.798
0.130	169.793	221.031	71.480	248.910	122.855	413.089	32.458	94.030	162.853	102.607	141.127	102.562	288.798
0.140	169.508	220.387	70.399	249.423	122.623	413.089	32.704	93.838	162.815	102.789	141.475	102.405	288.798
0.150	169.222	219.742	69.317	249.936	122.390	413.089	32.950	93.646	162.776	102.972	141.823	102.248	288.798
0.160	168.937	219.098	68.236	250.449	122.158	413.089	33.196	93.454	162.738	103.155	142.170	102.091	288.798
0.170	168.652	218.453	67.155	250.962	121.925	413.089	33.442	93.263	162.700	103.338	142.518	101.934	288.798
0.180	168.366	217.809	66.073	251.475	121.693	413.089	33.688	93.071	162.661	103.520	142.866	101.776	288.798
0.190	168.081	217.165	64.992	251.989	121.460	413.089	33.934	92.879	162.623	103.703	143.214	101.619	288.798
0.200	167.795	216.520	63.911	252.502	121.227	413.089	34.180	92.687	162.585	103.886	143.562	101.462	288.798
|Fo|	163.181	230.303	91.563	255.098	124.534	413.089	33.893	99.113	157.061	96.943	154.127	94.797	288.798

Table A.1.49. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2676, B=-0.16119, K=19.66140)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	173.941	229.127	86.106	241.607	125.645	412.191	29.523	95.949	163.469	101.254	135.629	104.990	287.569
0.010	173.656	228.482	85.024	242.120	125.413	412.191	29.769	95.757	163.430	101.436	135.977	104.833	287.569
0.020	173.371	227.838	83.943	242.633	125.180	412.191	30.015	95.565	163.392	101.619	136.324	104.675	287.569
0.030	173.085	227.193	82.861	243.147	124.948	412.191	30.261	95.373	163.354	101.802	136.672	104.518	287.569
0.040	172.800	226.549	81.780	243.660	124.715	412.191	30.507	95.182	163.315	101.985	137.020	104.361	287.569
0.050	172.515	225.904	80.699	244.173	124.482	412.191	30.753	94.990	163.277	102.167	137.368	104.204	287.569
0.060	172.229	225.260	79.617	244.686	124.250	412.191	30.999	94.798	163.239	102.350	137.716	104.047	287.569
0.070	171.944	224.615	78.536	245.199	124.017	412.191	31.245	94.606	163.200	102.533	138.064	103.889	287.569
0.080	171.658	223.971	77.455	245.712	123.785	412.191	31.491	94.414	163.162	102.715	138.411	103.732	287.569
0.090	171.373	223.326	76.373	246.225	123.552	412.191	31.737	94.222	163.124	102.898	138.759	103.575	287.569
0.100	171.088	222.682	75.292	246.738	123.320	412.191	31.983	94.031	163.086	103.081	139.107	103.418	287.569
0.110	170.802	222.037	74.211	247.252	123.087	412.191	32.229	93.839	163.047	103.264	139.455	103.261	287.569
0.120	170.517	221.393	73.129	247.765	122.855	412.191	32.475	93.647	163.009	103.446	139.803	103.103	287.569
0.130	170.232	220.748	72.048	248.278	122.622	412.191	32.721	93.455	162.971	103.629	140.151	102.946	287.569
0.140	169.946	220.104	70.967	248.791	122.389	412.191	32.967	93.263	162.932	103.812	140.499	102.789	287.569
0.150	169.661	219.459	69.885	249.304	122.157	412.191	33.214	93.071	162.894	103.995	140.846	102.632	287.569
0.160	169.376	218.815	68.804	249.817	121.924	412.191	33.460	92.879	162.856	104.177	141.194	102.475	287.569
0.170	169.090	218.170	67.723	250.330	121.692	412.191	33.706	92.688	162.817	104.360	141.542	102.317	287.569
0.180	168.805	217.526	66.641	250.843	121.459	412.191	33.952	92.496	162.779	104.543	141.890	102.160	287.569
0.190	168.519	216.881	65.560	251.356	121.227	412.191	34.198	92.304	162.741	104.725	142.238	102.003	287.569
0.200	168.234	216.237	64.479	251.870	120.994	412.191	34.444	92.112	162.702	104.908	142.586	101.846	287.569
IFoI	163.081	230.116	91.483	254.809	124.328	412.191	33.813	98.846	156.607	96.657	153.631	94.443	287.569

Table A.1.50. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2680, B=-0.14275, K=19.65943)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	174.390	228.843	86.683	240.900	125.409	411.276	29.779	95.364	163.232	102.292	134.640	105.376	286.322
0.010	174.105	228.199	85.601	241.413	125.176	411.276	30.026	95.172	163.194	102.475	134.988	105.219	286.322
0.020	173.820	227.554	84.520	241.926	124.943	411.276	30.272	94.980	163.155	102.657	135.335	105.062	286.322
0.030	173.534	226.910	83.438	242.439	124.711	411.276	30.518	94.788	163.117	102.840	135.683	104.904	286.322
0.040	173.249	226.265	82.357	242.952	124.478	411.276	30.764	94.596	163.079	103.023	136.031	104.747	286.322
0.050	172.963	225.621	81.276	243.465	124.246	411.276	31.010	94.405	163.040	103.206	136.379	104.590	286.322
0.060	172.678	224.976	80.194	243.979	124.013	411.276	31.256	94.213	163.002	103.388	136.727	104.433	286.322
0.070	172.393	224.332	79.113	244.492	123.781	411.276	31.502	94.021	162.964	103.571	137.075	104.276	286.322
0.080	172.107	223.687	78.032	245.005	123.548	411.276	31.748	93.829	162.925	103.754	137.422	104.118	286.322
0.090	171.822	223.043	76.950	245.518	123.316	411.276	31.994	93.637	162.887	103.937	137.770	103.961	286.322
0.100	171.537	222.398	75.869	246.031	123.083	411.276	32.240	93.445	162.849	104.119	138.118	103.804	286.322
0.110	171.251	221.754	74.788	246.544	122.850	411.276	32.486	93.253	162.811	104.302	138.466	103.647	286.322
0.120	170.966	221.110	73.706	247.057	122.618	411.276	32.732	93.062	162.772	104.485	138.814	103.490	286.322
0.130	170.681	220.465	72.625	247.570	122.385	411.276	32.978	92.870	162.734	104.667	139.162	103.332	286.322
0.140	170.395	219.821	71.544	248.084	122.153	411.276	33.224	92.678	162.696	104.850	139.509	103.175	286.322
0.150	170.110	219.176	70.462	248.597	121.920	411.276	33.470	92.486	162.657	105.033	139.857	103.018	286.322
0.160	169.824	218.532	69.381	249.110	121.688	411.276	33.716	92.294	162.619	105.216	140.205	102.861	286.322
0.170	169.539	217.887	68.300	249.623	121.455	411.276	33.962	92.102	162.581	105.398	140.553	102.704	286.322
0.180	169.254	217.243	67.218	250.136	121.222	411.276	34.208	91.911	162.542	105.581	140.901	102.546	286.322
0.190	168.968	216.598	66.137	250.649	120.990	411.276	34.455	91.719	162.504	105.764	141.249	102.389	286.322
0.200	168.683	215.954	65.056	251.162	120.757	411.276	34.701	91.527	162.466	105.946	141.596	102.232	286.322
|Fo|	162.978	229.926	91.401	254.513	124.118	411.276	33.731	98.574	156.146	96.365	153.128	94.083	286.322

Table A.1.51. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2688, B=-0.10454, K=19.65631

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	175.316	228.265	87.873	239.443	124.930	409.406	30.272	94.171	162.717	104.418	132.631	106.149	283.767
0.010	175.031	227.621	86.792	239.956	124.697	409.406	30.518	93.980	162.678	104.600	132.979	105.992	283.767
0.020	174.746	226.976	85.710	240.469	124.465	409.406	30.764	93.788	162.640	104.783	133.327	105.835	283.767
0.030	174.460	226.332	84.629	240.982	124.232	409.406	31.010	93.596	162.602	104.966	133.675	105.678	283.767
0.040	174.175	225.687	83.548	241.495	124.000	409.406	31.256	93.404	162.563	105.148	134.023	105.520	283.767
0.050	173.890	225.043	82.466	242.008	123.767	409.406	31.502	93.212	162.525	105.331	134.370	105.363	283.767
0.060	173.604	224.398	81.385	242.521	123.535	409.406	31.748	93.020	162.487	105.514	134.718	105.206	283.767
0.070	173.319	223.754	80.303	243.034	123.302	409.406	31.995	92.829	162.448	105.697	135.066	105.049	283.767
0.080	173.034	223.109	79.222	243.548	123.070	409.406	32.241	92.637	162.410	105.879	135.414	104.892	283.767
0.090	172.748	222.465	78.141	244.061	122.837	409.406	32.487	92.445	162.372	106.062	135.762	104.734	283.767
0.100	172.463	221.820	77.059	244.574	122.604	409.406	32.733	92.253	162.333	106.245	136.110	104.577	283.767
0.110	172.178	221.176	75.978	245.087	122.372	409.406	32.979	92.061	162.295	106.427	136.457	104.420	283.767
0.120	171.892	220.531	74.897	245.600	122.139	409.406	33.225	91.869	162.257	106.610	136.805	104.263	283.767
0.130	171.607	219.887	73.815	246.113	121.907	409.406	33.471	91.678	162.219	106.793	137.153	104.106	283.767
0.140	171.321	219.242	72.734	246.626	121.674	409.406	33.717	91.486	162.180	106.976	137.501	103.948	283.767
0.150	171.036	218.598	71.653	247.139	121.442	409.406	33.963	91.294	162.142	107.158	137.849	103.791	283.767
0.160	170.751	217.953	70.571	247.652	121.209	409.406	34.209	91.102	162.104	107.341	138.197	103.634	283.767
0.170	170.465	217.309	69.490	248.166	120.977	409.406	34.455	90.910	162.065	107.524	138.544	103.477	283.767
0.180	170.180	216.664	68.409	248.679	120.744	409.406	34.701	90.718	162.027	107.706	138.892	103.320	283.767
0.190	169.895	216.020	67.327	249.192	120.511	409.406	34.947	90.526	161.989	107.889	139.240	103.162	283.767
0.200	169.609	215.376	66.246	249.705	120.279	409.406	35.193	90.335	161.950	108.072	139.588	103.005	283.767
IFoI	162.774	229.543	91.236	253.914	123.689	409.406	33.564	98.017	155.200	95.769	152.096	93.346	283.767

Table A.1.52. Calculated and Observed Structure Factors for Cobalt Chromite with respect to Degree of Disorder (x).
(u=0.2700, B=-0.04410, K=19.65289)

	|Fcl												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	176.774	227.385	89.742	237.146	124.196	406.497	30.962	92.326	161.838	107.715	129.549	107.307	279.795
0.010	176.489	226.741	88.661	237.659	123.964	406.497	31.208	92.134	161.800	107.897	129.896	107.150	279.795
0.020	176.204	226.096	87.580	238.172	123.731	406.497	31.454	91.942	161.761	108.080	130.244	106.993	279.795
0.030	175.918	225.452	86.498	238.685	123.498	406.497	31.700	91.750	161.723	108.263	130.592	106.836	279.795
0.040	175.633	224.807	85.417	239.198	123.266	406.497	31.946	91.558	161.685	108.446	130.940	106.678	279.795
0.050	175.347	224.163	84.336	239.711	123.033	406.497	32.192	91.366	161.647	108.628	131.288	106.521	279.795
0.060	175.062	223.518	83.254	240.225	122.801	406.497	32.438	91.175	161.608	108.811	131.636	106.364	279.795
0.070	174.777	222.874	82.173	240.738	122.568	406.497	32.684	90.983	161.570	108.994	131.983	106.207	279.795
0.080	174.491	222.229	81.092	241.251	122.336	406.497	32.930	90.791	161.532	109.176	132.331	106.050	279.795
0.090	174.206	221.585	80.010	241.764	122.103	406.497	33.176	90.599	161.493	109.359	132.679	105.892	279.795
0.100	173.921	220.940	78.929	242.277	121.871	406.497	33.422	90.407	161.455	109.542	133.027	105.735	279.795
0.110	173.635	220.296	77.848	242.790	121.638	406.497	33.668	90.215	161.417	109.725	133.375	105.578	279.795
0.120	173.350	219.651	76.766	243.303	121.405	406.497	33.914	90.024	161.378	109.907	133.723	105.421	279.795
0.130	173.065	219.007	75.685	243.816	121.173	406.497	34.161	89.832	161.340	110.090	134.071	105.264	279.795
0.140	172.779	218.362	74.604	244.329	120.940	406.497	34.407	89.640	161.302	110.273	134.418	105.106	279.795
0.150	172.494	217.718	73.522	244.843	120.708	406.497	34.653	89.448	161.264	110.455	134.766	104.949	279.795
0.160	172.208	217.073	72.441	245.356	120.475	406.497	34.899	89.256	161.225	110.638	135.114	104.792	279.795
0.170	171.923	216.429	71.360	245.869	120.243	406.497	35.145	89.064	161.187	110.821	135.462	104.635	279.795
0.180	171.638	215.784	70.278	246.382	120.010	406.497	35.391	88.873	161.149	111.004	135.810	104.478	279.795
0.190	171.352	215.140	69.197	246.895	119.778	406.497	35.637	88.681	161.110	111.186	136.158	104.320	279.795
0.200	171.067	214.496	68.115	247.408	119.545	406.497	35.883	88.489	161.072	111.369	136.505	104.163	279.795
|Fol	162.464	228.956	91.983	252.990	123.025	406.497	33.303	97.152	153.729	94.840	150.490	92.200	279.795

Table A.2.1. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).

(u=0.2500, B=-0.57012, K=20.08096)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.107	219.647	73.701	289.158	102.944	408.822	33.826	82.926	145.569	77.171	189.195	69.184	294.862
0.001	134.109	219.600	73.589	289.150	102.950	408.822	33.816	82.934	145.571	77.162	189.176	69.194	294.862
0.002	134.111	219.553	73.477	289.141	102.956	408.822	33.807	82.943	145.573	77.153	189.157	69.205	294.862
0.003	134.112	219.506	73.365	289.133	102.962	408.822	33.797	82.951	145.575	77.144	189.138	69.215	294.862
0.004	134.114	219.459	73.253	289.124	102.968	408.822	33.788	82.960	145.577	77.135	189.118	69.226	294.862
0.005	134.116	219.412	73.140	289.115	102.975	408.822	33.778	82.969	145.579	77.126	189.099	69.236	294.862
0.006	134.118	219.365	73.028	289.107	102.981	408.822	33.768	82.977	145.581	77.116	189.080	69.247	294.862
0.007	134.119	219.318	72.916	289.098	102.987	408.822	33.759	82.986	145.582	77.107	189.061	69.257	294.862
0.008	134.121	219.271	72.804	289.090	102.993	408.822	33.749	82.995	145.584	77.098	189.042	69.268	294.862
0.009	134.123	219.224	72.692	289.081	102.999	408.822	33.740	83.003	145.586	77.089	189.022	69.278	294.862
0.010	134.125	219.176	72.580	289.072	103.005	408.822	33.730	83.012	145.588	77.080	189.003	69.289	294.862
0.020	134.142	218.706	71.459	288.986	103.066	408.822	33.634	83.098	145.607	76.989	188.811	69.394	294.862
0.030	134.159	218.236	70.339	288.900	103.127	408.822	33.539	83.185	145.625	76.897	188.619	69.498	294.862
0.040	134.177	217.765	69.218	288.814	103.188	408.822	33.443	83.271	145.644	76.806	188.427	69.603	294.862
0.050	134.194	217.295	68.097	288.728	103.249	408.822	33.347	83.357	145.663	76.715	188.235	69.708	294.862
0.060	134.212	216.824	66.976	288.642	103.310	408.822	33.252	83.444	145.681	76.623	188.043	69.813	294.862
0.070	134.229	216.354	65.856	288.556	103.371	408.822	33.156	83.530	145.700	76.532	187.851	69.917	294.862
0.080	134.246	215.883	64.735	288.470	103.432	408.822	33.060	83.616	145.719	76.441	187.659	70.022	294.862
0.090	134.264	215.413	63.614	288.384	103.493	408.822	32.964	83.703	145.737	76.349	187.467	70.127	294.862
0.100	134.281	214.943	62.494	288.298	103.554	408.822	32.869	83.789	145.756	76.258	187.275	70.232	294.862
|Fo|	139.679	216.054	96.628	297.580	99.632	408.822	58.834	73.792	151.898	107.793	192.596	79.696	294.862

Table A.2.2. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2504, B=-0.5989, K=20.08090)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.112	219.409	73.708	289.150	102.941	408.811	34.250	82.918	145.444	77.185	189.181	69.191	294.846
0.001	134.114	219.362	73.596	289.142	102.947	408.811	34.241	82.926	145.446	77.176	189.162	69.201	294.846
0.002	134.116	219.315	73.483	289.133	102.953	408.811	34.231	82.935	145.448	77.167	189.143	69.211	294.846
0.003	134.118	219.268	73.371	289.124	102.959	408.811	34.222	82.944	145.449	77.157	189.123	69.222	294.846
0.004	134.119	219.221	73.259	289.116	102.965	408.811	34.212	82.952	145.451	77.148	189.104	69.232	294.846
0.005	134.121	219.174	73.147	289.107	102.971	408.811	34.203	82.961	145.453	77.139	189.085	69.243	294.846
0.006	134.123	219.126	73.035	289.099	102.977	408.811	34.193	82.970	145.455	77.130	189.066	69.253	294.846
0.007	134.125	219.079	72.923	289.090	102.983	408.811	34.183	82.978	145.457	77.121	189.047	69.264	294.846
0.008	134.126	219.032	72.811	289.081	102.989	408.811	34.174	82.987	145.459	77.112	189.027	69.274	294.846
0.009	134.128	218.985	72.699	289.073	102.995	408.811	34.164	82.995	145.461	77.103	189.008	69.285	294.846
0.010	134.130	218.938	72.587	289.064	103.002	408.811	34.155	83.004	145.462	77.094	188.989	69.295	294.846
0.020	134.147	218.468	71.466	288.978	103.063	408.811	34.059	83.090	145.481	77.002	188.797	69.400	294.846
0.030	134.165	217.997	70.345	288.892	103.124	408.811	33.963	83.177	145.500	76.911	188.605	69.505	294.846
0.040	134.182	217.527	69.225	288.806	103.185	408.811	33.868	83.263	145.518	76.820	188.413	69.610	294.846
0.050	134.199	217.057	68.104	288.720	103.246	408.811	33.772	83.349	145.537	76.728	188.221	69.714	294.846
0.060	134.217	216.586	66.983	288.634	103.307	408.811	33.676	83.436	145.556	76.637	188.029	69.819	294.846
0.070	134.234	216.116	65.863	288.548	103.368	408.811	33.580	83.522	145.574	76.546	187.837	69.924	294.846
0.080	134.252	215.645	64.742	288.462	103.429	408.811	33.485	83.608	145.593	76.454	187.645	70.029	294.846
0.090	134.269	215.175	63.621	288.376	103.490	408.811	33.389	83.695	145.612	76.363	187.452	70.133	294.846
0.100	134.286	214.704	62.500	288.290	103.551	408.811	33.293	83.781	145.630	76.272	187.260	70.238	294.846
|Fo|	139.678	216.051	96.626	297.575	99.630	408.811	58.832	73.789	151.893	107.789	192.588	79.692	294.846

Table A.2.3. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2508, B=-0.56918, K=20.08079)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.128	219.173	73.728	289.126	102.930	408.775	34.674	82.894	145.317	77.226	189.138	69.210	294.797
0.001	134.130	219.126	73.616	289.117	102.936	408.775	34.664	82.903	145.319	77.217	189.119	69.220	294.797
0.002	134.131	219.079	73.504	289.108	102.943	408.775	34.655	82.912	145.321	77.207	189.100	69.231	294.797
0.003	134.133	219.032	73.392	289.100	102.949	408.775	34.645	82.920	145.323	77.198	189.081	69.241	294.797
0.004	134.135	218.985	73.280	289.091	102.955	408.775	34.635	82.929	145.324	77.189	189.062	69.252	294.797
0.005	134.137	218.938	73.168	289.083	102.961	408.775	34.626	82.937	145.326	77.180	189.042	69.262	294.797
0.006	134.138	218.891	73.056	289.074	102.967	408.775	34.616	82.946	145.328	77.171	189.023	69.273	294.797
0.007	134.140	218.844	72.944	289.065	102.973	408.775	34.607	82.955	145.330	77.162	189.004	69.283	294.797
0.008	134.142	218.797	72.831	289.057	102.979	408.775	34.597	82.963	145.332	77.153	188.985	69.294	294.797
0.009	134.144	218.750	72.719	289.048	102.985	408.775	34.588	82.972	145.334	77.144	188.966	69.304	294.797
0.010	134.145	218.702	72.607	289.040	102.991	408.775	34.578	82.981	145.336	77.134	188.946	69.315	294.797
0.020	134.163	218.232	71.487	288.954	103.052	408.775	34.482	83.067	145.354	77.043	188.754	69.420	294.797
0.030	134.180	217.762	70.366	288.868	103.113	408.775	34.387	83.153	145.373	76.952	188.562	69.524	294.797
0.040	134.198	217.291	69.245	288.782	103.174	408.775	34.291	83.240	145.392	76.860	188.370	69.629	294.797
0.050	134.215	216.821	68.124	288.696	103.235	408.775	34.195	83.326	145.410	76.769	188.178	69.734	294.797
0.060	134.232	216.350	67.004	288.610	103.296	408.775	34.099	83.412	145.429	76.678	187.986	69.839	294.797
0.070	134.250	215.880	65.883	288.524	103.357	408.775	34.004	83.499	145.448	76.586	187.794	69.943	294.797
0.080	134.267	215.409	64.762	288.438	103.418	408.775	33.908	83.585	145.466	76.495	187.602	70.048	294.797
0.090	134.285	214.939	63.642	288.352	103.479	408.775	33.812	83.671	145.485	76.404	187.410	70.153	294.797
0.100	134.302	214.469	62.521	288.266	103.540	408.775	33.717	83.758	145.504	76.312	187.218	70.258	294.797
IFoI	139.674	216.044	96.623	297.561	99.623	408.775	58.626	73.781	151.875	107.776	192.564	79.680	294.797

Table A.2.4. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2512, B=-0.56806, K=20.08033)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.154	218.935	73.762	289.085	102.913	408.715	35.097	82.854	145.193	77.295	189.066	69.244	294.716
0.001	134.156	218.888	73.650	289.076	102.919	408.715	35.087	82.862	145.194	77.286	189.047	69.254	294.716
0.002	134.157	218.841	73.538	289.067	102.925	408.715	35.078	82.871	145.196	77.277	189.028	69.265	294.716
0.003	134.159	218.794	73.426	289.059	102.932	408.715	35.068	82.880	145.198	77.268	189.009	69.275	294.716
0.004	134.161	218.747	73.314	289.050	102.938	408.715	35.059	82.888	145.200	77.259	188.990	69.285	294.716
0.005	134.163	218.700	73.202	289.042	102.944	408.715	35.049	82.897	145.202	77.250	188.970	69.296	294.716
0.006	134.164	218.652	73.090	289.033	102.950	408.715	35.039	82.906	145.204	77.240	188.951	69.306	294.716
0.007	134.166	218.605	72.978	289.024	102.956	408.715	35.030	82.914	145.206	77.231	188.932	69.317	294.716
0.008	134.168	218.558	72.866	289.016	102.962	408.715	35.020	82.923	145.208	77.222	188.913	69.327	294.716
0.009	134.170	218.511	72.753	289.007	102.968	408.715	35.011	82.931	145.209	77.213	188.894	69.338	294.716
0.010	134.171	218.464	72.641	288.999	102.974	408.715	35.001	82.940	145.211	77.204	188.874	69.348	294.716
0.020	134.189	217.994	71.521	288.913	103.035	408.715	34.905	83.026	145.230	77.113	188.682	69.453	294.716
0.030	134.206	217.523	70.400	288.827	103.096	408.715	34.810	83.113	145.249	77.021	188.490	69.558	294.716
0.040	134.224	217.053	69.279	288.741	103.157	408.715	34.714	83.199	145.267	76.930	188.298	69.663	294.716
0.050	134.241	216.583	68.158	288.655	103.218	408.715	34.618	83.285	145.286	76.839	188.106	69.767	294.716
0.060	134.258	216.112	67.038	288.569	103.279	408.715	34.523	83.372	145.305	76.747	187.914	69.872	294.716
0.070	134.276	215.642	65.917	288.483	103.340	408.715	34.427	83.458	145.323	76.656	187.722	69.977	294.716
0.080	134.293	215.171	64.796	288.397	103.401	408.715	34.331	83.544	145.342	76.565	187.530	70.082	294.716
0.090	134.311	214.701	63.676	288.311	103.462	408.715	34.235	83.631	145.361	76.473	187.338	70.186	294.716
0.100	134.328	214.230	62.555	288.225	103.523	408.715	34.140	83.717	145.379	76.382	187.146	70.291	294.716
IFoI	139.667	216.030	96.616	297.536	99.612	408.715	58.817	73.768	151.846	107.755	192.523	79.661	294.716

Table A.2.5. Calculated and Observed Structure Factors for Manganese Chromite with repect to Degree of Disorder (x).
(u=0.2516, B=-0.56639, K=20.08004)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.190	218.699	73.810	289.025	102.889	408.632	35.520	82.799	145.070	77.392	188.966	69.289	294.601
0.001	134.192	218.652	73.698	289.017	102.895	408.632	35.511	82.807	145.071	77.383	188.947	69.300	294.601
0.002	134.194	218.605	73.586	289.008	102.901	408.632	35.501	82.816	145.073	77.374	188.928	69.310	294.601
0.003	134.195	218.558	73.474	288.999	102.908	408.632	35.491	82.825	145.075	77.365	188.908	69.321	294.601
0.004	134.197	218.511	73.361	288.991	102.914	408.632	35.482	82.833	145.077	77.355	188.889	69.331	294.601
0.005	134.199	218.464	73.249	288.982	102.920	408.632	35.472	82.842	145.079	77.346	188.870	69.341	294.601
0.006	134.201	218.417	73.137	288.974	102.926	408.632	35.463	82.851	145.081	77.337	188.851	69.352	294.601
0.007	134.202	218.370	73.025	288.965	102.932	408.632	35.453	82.859	145.083	77.328	188.832	69.362	294.601
0.008	134.204	218.323	72.913	288.956	102.938	408.632	35.444	82.868	145.084	77.319	188.812	69.373	294.601
0.009	134.206	218.276	72.801	288.948	102.944	408.632	35.434	82.877	145.086	77.310	188.793	69.383	294.601
0.010	134.208	218.229	72.689	288.939	102.950	408.632	35.424	82.885	145.088	77.301	188.774	69.394	294.601
0.020	134.225	217.758	71.568	288.853	103.011	408.632	35.329	82.972	145.107	77.209	188.582	69.499	294.601
0.030	134.242	217.288	70.448	288.767	103.072	408.632	35.233	83.058	145.126	77.118	188.390	69.603	294.601
0.040	134.260	216.817	69.327	288.681	103.133	408.632	35.137	83.144	145.144	77.027	188.198	69.708	294.601
0.050	134.277	216.347	68.206	288.595	103.194	408.632	35.042	83.230	145.163	76.935	188.006	69.813	294.601
0.060	134.295	215.876	67.085	288.509	103.255	408.632	34.946	83.317	145.181	76.844	187.814	69.918	294.601
0.070	134.312	215.406	65.965	288.423	103.316	408.632	34.850	83.403	145.200	76.753	187.622	70.022	294.601
0.080	134.329	214.936	64.844	288.337	103.377	408.632	34.754	83.489	145.219	76.661	187.430	70.127	294.601
0.090	134.347	214.465	63.723	288.251	103.438	408.632	34.659	83.576	145.237	76.570	187.237	70.232	294.601
0.100	134.364	213.995	62.603	288.165	103.499	408.632	34.563	83.662	145.256	76.479	187.045	70.337	294.601
IFoI	139.658	216.013	96.608	297.504	99.596	408.632	58.804	73.750	151.805	107.726	192.466	79.633	294.601

Table A.2.6. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2520, B=-0.56432, K=20.07941

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.240	218.461	73.873	288.951	102.858	408.524	35.942	82.728	144.946	77.516	188.837	69.348	294.455
0.001	134.241	218.414	73.761	288.943	102.865	408.524	35.932	82.737	144.948	77.507	188.818	69.358	294.455
0.002	134.243	218.367	73.649	288.934	102.871	408.524	35.923	82.746	144.950	77.498	188.799	69.369	294.455
0.003	134.245	218.320	73.537	288.926	102.877	408.524	35.913	82.754	144.952	77.488	188.780	69.379	294.455
0.004	134.247	218.273	73.425	288.917	102.883	408.524	35.904	82.763	144.954	77.479	188.760	69.390	294.455
0.005	134.248	218.226	73.313	288.908	102.889	408.524	35.894	82.771	144.956	77.470	188.741	69.400	294.455
0.006	134.250	218.179	73.201	288.900	102.895	408.524	35.884	82.780	144.958	77.461	188.722	69.410	294.455
0.007	134.252	218.131	73.089	288.891	102.901	408.524	35.875	82.789	144.960	77.452	188.703	69.421	294.455
0.008	134.254	218.084	72.977	288.883	102.907	408.524	35.865	82.797	144.961	77.443	188.684	69.431	294.455
0.009	134.255	218.037	72.865	288.874	102.913	408.524	35.856	82.806	144.963	77.434	188.664	69.442	294.455
0.010	134.257	217.990	72.753	288.865	102.919	408.524	35.846	82.815	144.965	77.425	188.645	69.452	294.455
0.020	134.274	217.520	71.632	288.779	102.980	408.524	35.750	82.901	144.984	77.333	188.453	69.557	294.455
0.030	134.292	217.049	70.511	288.693	103.041	408.524	35.655	82.987	145.002	77.242	188.261	69.662	294.455
0.040	134.309	216.579	69.390	288.607	103.103	408.524	35.559	83.074	145.021	77.151	188.069	69.767	294.455
0.050	134.327	216.109	68.270	288.521	103.164	408.524	35.463	83.160	145.040	77.059	187.877	69.871	294.455
0.060	134.344	215.638	67.149	288.435	103.225	408.524	35.368	83.246	145.058	76.968	187.685	69.976	294.455
0.070	134.361	215.168	66.028	288.349	103.286	408.524	35.272	83.333	145.077	76.877	187.493	70.081	294.455
0.080	134.379	214.697	64.908	288.263	103.347	408.524	35.176	83.419	145.096	76.785	187.301	70.186	294.455
0.090	134.396	214.227	63.787	288.177	103.408	408.524	35.080	83.505	145.114	76.694	187.109	70.290	294.455
0.100	134.414	213.756	62.666	288.091	103.469	408.524	34.985	83.592	145.133	76.603	186.917	70.395	294.455
IFoI	139.645	215.989	96.597	297.460	99.576	408.524	58.787	73.726	151.754	107.788	192.393	79.599	294.455

Table A.2.7. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2524, B=-0.56179, K=20.07867)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.297	218.223	73.948	288.861	102.819	408.393	36.364	82.641	144.827	77.667	188.680	69.420	294.277
0.001	134.298	218.176	73.836	288.853	102.825	408.393	36.354	82.649	144.829	77.658	188.661	69.431	294.277
0.002	134.300	218.129	73.724	288.844	102.831	408.393	36.345	82.658	144.831	77.649	188.642	69.441	294.277
0.003	134.302	218.081	73.612	288.835	102.837	408.393	36.335	82.667	144.833	77.640	188.623	69.452	294.277
0.004	134.304	218.034	73.500	288.827	102.844	408.393	36.325	82.675	144.835	77.631	188.603	69.462	294.277
0.005	134.305	217.987	73.388	288.818	102.850	408.393	36.316	82.684	144.836	77.622	188.584	69.473	294.277
0.006	134.307	217.940	73.276	288.810	102.856	408.393	36.306	82.693	144.838	77.612	188.565	69.483	294.277
0.007	134.309	217.893	73.164	288.801	102.862	408.393	36.297	82.701	144.840	77.603	188.546	69.494	294.277
0.008	134.311	217.846	73.052	288.792	102.868	408.393	36.287	82.710	144.842	77.594	188.527	69.504	294.277
0.009	134.312	217.799	72.940	288.784	102.874	408.393	36.278	82.718	144.844	77.585	188.507	69.514	294.277
0.010	134.314	217.752	72.828	288.775	102.880	408.393	36.268	82.727	144.846	77.576	188.488	69.525	294.277
0.020	134.332	217.282	71.707	288.689	102.941	408.393	36.172	82.813	144.864	77.485	188.296	69.630	294.277
0.030	134.349	216.811	70.586	288.603	103.002	408.393	36.077	82.900	144.883	77.393	188.104	69.734	294.277
0.040	134.366	216.341	69.465	288.517	103.063	408.393	35.981	82.986	144.902	77.302	187.912	69.839	294.277
0.050	134.384	215.870	68.345	288.431	103.124	408.393	35.885	83.072	144.920	77.211	187.720	69.944	294.277
0.060	134.401	215.400	67.224	288.345	103.185	408.393	35.789	83.159	144.939	77.119	187.528	70.049	294.277
0.070	134.419	214.930	66.103	288.259	103.246	408.393	35.694	83.245	144.958	77.028	187.336	70.153	294.277
0.080	134.436	214.459	64.982	288.173	103.307	408.393	35.598	83.331	144.976	76.937	187.144	70.258	294.277
0.090	134.453	213.989	63.862	288.087	103.368	408.393	35.502	83.418	144.995	76.845	186.952	70.363	294.277
0.100	134.471	213.518	62.741	288.001	103.429	408.393	35.407	83.504	145.014	76.754	186.760	70.468	294.277
|Fo|	139.630	215.960	96.583	297.407	99.551	408.393	58.767	73.697	151.690	107.642	192.304	79.556	294.277

Table A.2.8. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2528, B=-0.55877, K=20.07787)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.364	217.984	74.037	288.753	102.775	408.238	36.784	82.537	144.710	77.846	188.495	69.505	294.065
0.001	134.366	217.937	73.925	288.744	102.781	408.238	36.774	82.546	144.712	77.837	188.475	69.515	294.065
0.002	134.368	217.890	73.813	288.735	102.787	408.238	36.765	82.555	144.714	77.827	188.456	69.526	294.065
0.003	134.369	217.843	73.701	288.727	102.793	408.238	36.755	82.563	144.716	77.818	188.437	69.536	294.065
0.004	134.371	217.796	73.589	288.718	102.799	408.238	36.746	82.572	144.718	77.809	188.418	69.547	294.065
0.005	134.373	217.749	73.476	288.710	102.805	408.238	36.736	82.581	144.720	77.800	188.399	69.557	294.065
0.006	134.375	217.702	73.364	288.701	102.811	408.238	36.727	82.589	144.722	77.791	188.379	69.568	294.065
0.007	134.376	217.655	73.252	288.692	102.817	408.238	36.717	82.598	144.723	77.782	188.360	69.578	294.065
0.008	134.378	217.608	73.140	288.684	102.823	408.238	36.708	82.607	144.725	77.773	188.341	69.589	294.065
0.009	134.380	217.561	73.028	288.675	102.830	408.238	36.698	82.615	144.727	77.764	188.322	69.599	294.065
0.010	134.382	217.514	72.916	288.667	102.836	408.238	36.688	82.624	144.729	77.754	188.303	69.609	294.065
0.020	134.399	217.044	71.795	288.581	102.897	408.238	36.593	82.710	144.748	77.663	188.111	69.714	294.065
0.030	134.416	216.573	70.675	288.495	102.958	408.238	36.497	82.796	144.766	77.572	187.919	69.819	294.065
0.040	134.434	216.103	69.554	288.409	103.019	408.238	36.401	82.883	144.785	77.480	187.726	69.924	294.065
0.050	134.451	215.632	68.433	288.323	103.080	408.238	36.306	82.969	144.804	77.389	187.534	70.028	294.065
0.060	134.469	215.162	67.312	288.237	103.141	408.238	36.210	83.055	144.822	77.298	187.342	70.133	294.065
0.070	134.486	214.691	66.192	288.151	103.202	408.238	36.114	83.142	144.841	77.206	187.150	70.238	294.065
0.080	134.503	214.221	65.071	288.065	103.263	408.238	36.018	83.228	144.860	77.115	186.958	70.343	294.065
0.090	134.521	213.751	63.950	287.979	103.324	408.238	35.923	83.314	144.878	77.024	186.766	70.447	294.065
0.100	134.538	213.280	62.830	287.893	103.385	408.238	35.827	83.401	144.897	76.932	186.574	70.552	294.065
|Fo|	139.613	215.926	96.567	297.344	99.521	408.238	58.743	73.663	151.615	107.587	192.198	79.506	294.065

Table A.2.9. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2532, B=-0.55524, K=20.07711)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.442	217.746	74.141	288.628	102.723	408.061	37.203	82.420	144.596	78.052	188.282	69.602	293.821
0.001	134.444	217.699	74.138	288.619	102.729	408.061	37.193	82.429	144.598	78.042	188.263	69.613	293.821
0.002	134.446	217.652	74.135	288.610	102.735	408.061	37.184	82.437	144.600	78.033	188.244	69.623	293.821
0.003	134.447	217.605	74.133	288.602	102.742	408.061	37.174	82.446	144.602	78.024	188.224	69.634	293.821
0.004	134.449	217.558	74.130	288.593	102.748	408.061	37.165	82.454	144.604	78.015	188.205	69.644	293.821
0.005	134.451	217.511	74.127	288.585	102.754	408.061	37.155	82.463	144.605	78.006	188.186	69.655	293.821
0.006	134.453	217.464	74.124	288.576	102.760	408.061	37.146	82.472	144.607	77.997	188.167	69.665	293.821
0.007	134.454	217.417	74.121	288.567	102.766	408.061	37.136	82.480	144.609	77.988	188.148	69.676	293.821
0.008	134.456	217.370	74.118	288.559	102.772	408.061	37.126	82.489	144.611	77.978	188.128	69.686	293.821
0.009	134.458	217.323	74.115	288.550	102.778	408.061	37.117	82.498	144.613	77.969	188.109	69.697	293.821
0.010	134.459	217.276	74.112	288.542	102.784	408.061	37.107	82.506	144.615	77.960	188.090	69.707	293.821
0.020	134.477	216.805	74.083	288.456	102.845	408.061	37.012	82.593	144.633	77.869	187.898	69.812	293.821
0.030	134.494	216.335	74.055	288.370	102.906	408.061	36.916	82.679	144.652	77.778	187.706	69.916	293.821
0.040	134.512	215.865	74.026	288.284	102.967	408.061	36.820	82.765	144.671	77.686	187.514	70.021	293.821
0.050	134.529	215.394	73.997	288.198	103.028	408.061	36.725	82.852	144.689	77.595	187.322	70.126	293.821
0.060	134.546	214.924	73.968	288.112	103.089	408.061	36.629	82.938	144.708	77.504	187.130	70.231	293.821
0.070	134.564	214.453	73.939	288.026	103.150	408.061	36.533	83.024	144.727	77.412	186.938	70.335	293.821
0.080	134.581	213.983	73.910	287.940	103.211	408.061	36.437	83.111	144.745	77.321	186.746	70.440	293.821
0.090	134.599	213.512	73.881	287.854	103.272	408.061	36.342	83.197	144.764	77.230	186.553	70.545	293.821
0.100	134.616	213.042	73.852	287.768	103.333	408.061	36.246	83.283	144.783	77.138	186.361	70.650	293.821
|Fo|	139.594	215.889	96.549	297.274	99.488	408.061	58.715	73.623	151.528	107.525	192.077	79.447	293.821

Table A.2.10. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2536, B=-0.55132, K=20.07602)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.533	217.508	74.257	288.488	102.665	407.859	37.619	82.285	144.486	78.285	188.040	69.712	293.546
0.001	134.535	217.461	74.254	288.480	102.671	407.859	37.610	82.294	144.487	78.276	188.021	69.722	293.546
0.002	134.536	217.414	74.251	288.471	102.677	407.859	37.600	82.303	144.489	78.266	188.001	69.733	293.546
0.003	134.538	217.367	74.248	288.463	102.683	407.859	37.591	82.311	144.491	78.257	187.982	69.743	293.546
0.004	134.540	217.320	74.246	288.454	102.690	407.859	37.581	82.320	144.493	78.248	187.963	69.754	293.546
0.005	134.542	217.273	74.243	288.445	102.696	407.859	37.571	82.328	144.495	78.239	187.944	69.764	293.546
0.006	134.543	217.226	74.240	288.437	102.702	407.859	37.562	82.337	144.497	78.230	187.925	69.775	293.546
0.007	134.545	217.179	74.237	288.428	102.708	407.859	37.552	82.346	144.499	78.221	187.905	69.785	293.546
0.008	134.547	217.132	74.234	288.420	102.714	407.859	37.543	82.354	144.500	78.212	187.886	69.795	293.546
0.009	134.549	217.085	74.231	288.411	102.720	407.859	37.533	82.363	144.502	78.202	187.867	69.806	293.546
0.010	134.550	217.038	74.228	288.402	102.726	407.859	37.524	82.372	144.504	78.193	187.848	69.816	293.546
0.020	134.568	216.567	74.199	288.316	102.787	407.859	37.428	82.458	144.523	78.102	187.656	69.921	293.546
0.030	134.585	216.097	74.170	288.230	102.848	407.859	37.332	82.544	144.541	78.011	187.464	70.026	293.546
0.040	134.603	215.626	74.141	288.144	102.909	407.859	37.236	82.631	144.560	77.919	187.272	70.131	293.546
0.050	134.620	215.156	74.113	288.058	102.970	407.859	37.141	82.717	144.579	77.828	187.080	70.235	293.546
0.060	134.637	214.686	74.084	287.972	103.031	407.859	37.045	82.803	144.597	77.737	186.888	70.340	293.546
0.070	134.655	214.215	74.055	287.886	103.092	407.859	36.949	82.890	144.616	77.645	186.695	70.445	293.546
0.080	134.672	213.745	74.026	287.800	103.153	407.859	36.854	82.976	144.635	77.554	186.503	70.550	293.546
0.090	134.690	213.274	73.997	287.714	103.214	407.859	36.758	83.062	144.653	77.463	186.311	70.654	293.546
0.100	134.707	212.804	73.968	287.628	103.275	407.859	36.662	83.149	144.672	77.371	186.119	70.759	293.546
|Fo|	139.571	215.844	96.527	297.192	99.450	407.859	58.683	73.579	151.431	107.454	191.939	79.382	293.546

Table A.2.11. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2540, B=-0.54689, K=20.07488)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.632	217.268	74.389	288.331	102.600	407.633	38.035	82.136	144.379	78.545	187.771	69.835	293.237
0.001	134.633	217.221	74.386	288.322	102.606	407.633	38.026	82.145	144.381	78.536	187.751	69.846	293.237
0.002	134.635	217.173	74.383	288.313	102.612	407.633	38.016	82.154	144.382	78.527	187.732	69.856	293.237
0.003	134.637	217.126	74.380	288.305	102.618	407.633	38.007	82.162	144.384	78.518	187.713	69.867	293.237
0.004	134.639	217.079	74.377	288.296	102.624	407.633	37.997	82.171	144.386	78.509	187.694	69.877	293.237
0.005	134.640	217.032	74.374	288.288	102.631	407.633	37.988	82.179	144.388	78.499	187.675	69.888	293.237
0.006	134.642	216.985	74.371	288.279	102.637	407.633	37.978	82.188	144.390	78.490	187.655	69.898	293.237
0.007	134.644	216.938	74.369	288.270	102.643	407.633	37.968	82.197	144.392	78.481	187.636	69.908	293.237
0.008	134.646	216.891	74.366	288.262	102.649	407.633	37.959	82.205	144.394	78.472	187.617	69.919	293.237
0.009	134.647	216.844	74.363	288.253	102.655	407.633	37.949	82.214	144.396	78.463	187.598	69.929	293.237
0.010	134.649	216.797	74.360	288.245	102.661	407.633	37.940	82.223	144.397	78.454	187.579	69.940	293.237
0.020	134.666	216.327	74.331	288.159	102.722	407.633	37.844	82.309	144.416	78.362	187.386	70.045	293.237
0.030	134.684	215.856	74.302	288.073	102.783	407.633	37.748	82.395	144.435	78.271	187.194	70.149	293.237
0.040	134.701	215.386	74.273	287.987	102.844	407.633	37.653	82.482	144.453	78.180	187.002	70.254	293.237
0.050	134.719	214.915	74.244	287.901	102.905	407.633	37.557	82.568	144.472	78.088	186.810	70.359	293.237
0.060	134.736	214.445	74.215	287.815	102.966	407.633	37.461	82.654	144.491	77.997	186.618	70.464	293.237
0.070	134.753	213.975	74.186	287.729	103.027	407.633	37.365	82.741	144.509	77.906	186.426	70.568	293.237
0.080	134.771	213.504	74.157	287.643	103.088	407.633	37.270	82.827	144.528	77.814	186.234	70.673	293.237
0.090	134.788	213.034	74.129	287.557	103.149	407.633	37.174	82.913	144.547	77.723	186.042	70.778	293.237
0.100	134.806	212.563	74.100	287.471	103.210	407.633	37.078	83.000	144.565	77.632	185.850	70.883	293.237
IFoI	139.546	215.795	96.504	297.102	99.407	407.633	58.648	73.529	151.321	107.374	191.785	79.308	293.237

Table A.2.12. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2544, B=-0.54200, K=20.07372)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.741	217.027	74.532	288.156	102.528	407.385	38.449	81.972	144.276	78.831	187.474	69.971	292.898
0.001	134.742	216.980	74.529	288.148	102.534	407.385	38.439	81.980	144.278	78.822	187.455	69.981	292.898
0.002	134.744	216.933	74.526	288.139	102.540	407.385	38.430	81.989	144.279	78.813	187.436	69.992	292.898
0.003	134.746	216.886	74.523	288.131	102.547	407.385	38.420	81.998	144.281	78.804	187.416	70.002	292.898
0.004	134.748	216.839	74.520	288.122	102.553	407.385	38.410	82.006	144.283	78.795	187.397	70.013	292.898
0.005	134.749	216.792	74.517	288.113	102.559	407.385	38.401	82.015	144.285	78.786	187.378	70.023	292.898
0.006	134.751	216.745	74.514	288.105	102.565	407.385	38.391	82.023	144.287	78.777	187.359	70.033	292.898
0.007	134.753	216.698	74.512	288.096	102.571	407.385	38.382	82.032	144.289	78.768	187.340	70.044	292.898
0.008	134.755	216.651	74.509	288.088	102.577	407.385	38.372	82.041	144.291	78.758	187.320	70.054	292.898
0.009	134.756	216.604	74.506	288.079	102.583	407.385	38.363	82.049	144.293	78.749	187.301	70.065	292.898
0.010	134.758	216.557	74.503	288.070	102.589	407.385	38.353	82.058	144.294	78.740	187.282	70.075	292.898
0.020	134.775	216.086	74.474	287.984	102.650	407.385	38.257	82.144	144.313	78.649	187.090	70.180	292.898
0.030	134.793	215.616	74.445	287.898	102.711	407.385	38.162	82.231	144.332	78.557	186.898	70.285	292.898
0.040	134.810	215.145	74.416	287.812	102.772	407.385	38.066	82.317	144.350	78.466	186.706	70.390	292.898
0.050	134.828	214.675	74.387	287.726	102.833	407.385	37.970	82.403	144.369	78.375	186.514	70.494	292.898
0.060	134.845	214.204	74.358	287.640	102.894	407.385	37.875	82.490	144.388	78.283	186.322	70.599	292.898
0.070	134.862	213.734	74.329	287.554	102.955	407.385	37.779	82.576	144.406	78.192	186.130	70.704	292.898
0.080	134.880	213.264	74.300	287.468	103.016	407.385	37.683	82.662	144.425	78.101	185.938	70.809	292.898
0.090	134.897	212.793	74.272	287.382	103.077	407.385	37.587	82.749	144.444	78.010	185.745	70.913	292.898
0.100	134.915	212.323	74.243	287.296	103.138	407.385	37.492	82.835	144.462	77.918	185.553	71.018	292.898
|Fo|	139.518	215.742	96.478	297.003	99.360	407.385	58.609	73.474	151.200	107.287	191.616	79.227	292.898

Table A.2.13. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2548, B=-0.53669, K=20.07224)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.863	216.787	74.691	287.968	102.450	407.112	38.861	81.791	144.178	79.145	187.149	70.118	292.527
0.001	134.864	216.739	74.688	287.959	102.456	407.112	38.851	81.800	144.180	79.136	187.130	70.128	292.527
0.002	134.866	216.692	74.685	287.951	102.462	407.112	38.842	81.809	144.182	79.127	187.111	70.139	292.527
0.003	134.868	216.645	74.682	287.942	102.468	407.112	38.832	81.817	144.183	79.118	187.092	70.149	292.527
0.004	134.870	216.598	74.679	287.933	102.474	407.112	38.822	81.826	144.185	79.109	187.072	70.160	292.527
0.005	134.871	216.551	74.676	287.925	102.480	407.112	38.813	81.834	144.187	79.099	187.053	70.170	292.527
0.006	134.873	216.504	74.673	287.916	102.486	407.112	38.803	81.843	144.189	79.090	187.034	70.181	292.527
0.007	134.875	216.457	74.670	287.908	102.492	407.112	38.794	81.852	144.191	79.081	187.015	70.191	292.527
0.008	134.877	216.410	74.668	287.899	102.498	407.112	38.784	81.860	144.193	79.072	186.996	70.202	292.527
0.009	134.878	216.363	74.665	287.890	102.504	407.112	38.775	81.869	144.195	79.063	186.976	70.212	292.527
0.010	134.880	216.316	74.662	287.882	102.511	407.112	38.765	81.878	144.196	79.054	186.957	70.223	292.527
0.020	134.897	215.846	74.633	287.796	102.572	407.112	38.669	81.964	144.215	78.962	186.765	70.327	292.527
0.030	134.915	215.375	74.604	287.710	102.633	407.112	38.574	82.050	144.234	78.871	186.573	70.432	292.527
0.040	134.932	214.905	74.575	287.624	102.694	407.112	38.478	82.137	144.252	78.780	186.381	70.537	292.527
0.050	134.950	214.434	74.546	287.538	102.755	407.112	38.382	82.223	144.271	78.689	186.189	70.642	292.527
0.060	134.967	213.964	74.517	287.452	102.816	407.112	38.286	82.309	144.290	78.597	185.997	70.746	292.527
0.070	134.984	213.494	74.488	287.366	102.877	407.112	38.191	82.396	144.308	78.506	185.805	70.851	292.527
0.080	135.002	213.023	74.459	287.280	102.938	407.112	38.095	82.482	144.327	78.415	185.613	70.956	292.527
0.090	135.019	212.553	74.431	287.194	102.999	407.112	37.999	82.568	144.346	78.323	185.421	71.061	292.527
0.100	135.037	212.082	74.402	287.108	103.060	407.112	37.904	82.655	144.364	78.232	185.229	71.165	292.527
|Fo|	139.487	215.682	96.450	296.892	99.308	407.112	58.567	73.414	151.067	107.191	191.430	79.139	292.527

Table A.2.14. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2552, B=-0.53087, K=20.07080)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	134.992	216.546	74.861	287.761	102.366	406.817	39.271	81.595	144.085	79.486	186.798	70.277	292.124
0.001	134.994	216.499	74.858	287.752	102.372	406.817	39.262	81.604	144.087	79.477	186.779	70.288	292.124
0.002	134.996	216.452	74.855	287.744	102.378	406.817	39.252	81.613	144.089	79.468	186.760	70.298	292.124
0.003	134.998	216.405	74.852	287.735	102.384	406.817	39.243	81.621	144.090	79.459	186.741	70.309	292.124
0.004	134.999	216.358	74.849	287.727	102.390	406.817	39.233	81.630	144.092	79.450	186.722	70.319	292.124
0.005	135.001	216.311	74.847	287.718	102.396	406.817	39.223	81.638	144.094	79.440	186.702	70.330	292.124
0.006	135.003	216.264	74.844	287.709	102.402	406.817	39.214	81.647	144.096	79.431	186.683	70.340	292.124
0.007	135.005	216.217	74.841	287.701	102.408	406.817	39.204	81.656	144.098	79.422	186.664	70.351	292.124
0.008	135.006	216.170	74.838	287.692	102.414	406.817	39.195	81.664	144.100	79.413	186.645	70.361	292.124
0.009	135.008	216.123	74.835	287.684	102.421	406.817	39.185	81.673	144.102	79.404	186.626	70.372	292.124
0.010	135.010	216.076	74.832	287.675	102.427	406.817	39.176	81.682	144.104	79.395	186.606	70.382	292.124
0.020	135.027	215.605	74.803	287.589	102.488	406.817	39.080	81.768	144.122	79.303	186.414	70.487	292.124
0.030	135.045	215.135	74.774	287.503	102.549	406.817	38.984	81.854	144.141	79.212	186.222	70.591	292.124
0.040	135.062	214.664	74.745	287.417	102.610	406.817	38.888	81.941	144.159	79.121	186.030	70.696	292.124
0.050	135.079	214.194	74.716	287.331	102.671	406.817	38.793	82.027	144.178	79.029	185.838	70.801	292.124
0.060	135.097	213.723	74.688	287.245	102.732	406.817	38.697	82.113	144.197	78.938	185.646	70.906	292.124
0.070	135.114	213.253	74.659	287.159	102.793	406.817	38.601	82.200	144.215	78.847	185.454	71.010	292.124
0.080	135.132	212.783	74.630	287.073	102.854	406.817	38.506	82.286	144.234	78.756	185.262	71.115	292.124
0.090	135.149	212.312	74.601	286.987	102.915	406.817	38.410	82.372	144.253	78.664	185.070	71.220	292.124
0.100	135.166	211.842	74.572	286.901	102.976	406.817	38.314	82.459	144.271	78.573	184.878	71.325	292.124
|Fo|	139.455	215.618	96.419	296.774	99.253	406.817	58.521	73.348	150.924	107.087	191.229	79.043	292.124

Table A.2.15. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2556, B=-0.52454, K=20.06942)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	135.135	216.303	75.047	287.538	102.273	406.499	39.679	81.385	143.997	79.853	186.419	70.448	291.688
0.001	135.137	216.256	75.044	287.529	102.279	406.499	39.669	81.394	143.999	79.844	186.400	70.459	291.688
0.002	135.139	216.209	75.041	287.520	102.285	406.499	39.660	81.402	144.001	79.835	186.381	70.469	291.688
0.003	135.140	216.162	75.039	287.512	102.292	406.499	39.650	81.411	144.003	79.826	186.362	70.480	291.688
0.004	135.142	216.115	75.036	287.503	102.298	406.499	39.641	81.419	144.004	79.817	186.342	70.490	291.688
0.005	135.144	216.068	75.033	287.495	102.304	406.499	39.631	81.428	144.006	79.807	186.323	70.501	291.688
0.006	135.146	216.021	75.030	287.486	102.310	406.499	39.622	81.437	144.008	79.798	186.304	70.511	291.688
0.007	135.147	215.974	75.027	287.477	102.316	406.499	39.612	81.445	144.010	79.789	186.285	70.522	291.688
0.008	135.149	215.927	75.024	287.469	102.322	406.499	39.602	81.454	144.012	79.780	186.266	70.532	291.688
0.009	135.151	215.880	75.021	287.460	102.328	406.499	39.593	81.463	144.014	79.771	186.246	70.543	291.688
0.010	135.153	215.833	75.018	287.452	102.334	406.499	39.583	81.471	144.016	79.762	186.227	70.553	291.688
0.020	135.170	215.362	74.989	287.366	102.395	406.499	39.488	81.558	144.034	79.670	186.035	70.658	291.688
0.030	135.187	214.892	74.960	287.280	102.456	406.499	39.392	81.644	144.053	79.579	185.843	70.763	291.688
0.040	135.205	214.421	74.932	287.194	102.517	406.499	39.296	81.730	144.072	79.488	185.651	70.867	291.688
0.050	135.222	213.951	74.903	287.108	102.578	406.499	39.200	81.817	144.090	79.397	185.459	70.972	291.688
0.060	135.240	213.481	74.874	287.022	102.639	406.499	39.105	81.903	144.109	79.305	185.267	71.077	291.688
0.070	135.257	213.010	74.845	286.936	102.700	406.499	39.009	81.989	144.128	79.214	185.075	71.182	291.688
0.080	135.274	212.540	74.816	286.850	102.761	406.499	38.913	82.076	144.146	79.123	184.883	71.286	291.688
0.090	135.292	212.069	74.787	286.764	102.822	406.499	38.818	82.162	144.165	79.031	184.691	71.391	291.688
0.100	135.309	211.599	74.758	286.678	102.883	406.499	38.722	82.248	144.184	78.940	184.499	71.496	291.688
IFoI	139.420	215.550	96.387	296.648	99.193	406.499	58.471	73.278	150.769	106.975	191.012	78.939	291.688

Table A.2.16. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2560, B=-0.51779, K=20.06780)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	135.286	216.063	75.245	287.298	102.176	406.158	40.083	81.160	143.915	80.246	186.014	70.632	291.222
0.001	135.288	216.016	75.242	287.289	102.182	406.158	40.073	81.169	143.917	80.237	185.995	70.642	291.222
0.002	135.289	215.969	75.239	287.281	102.188	406.158	40.063	81.177	143.919	80.228	185.976	70.652	291.222
0.003	135.291	215.921	75.236	287.272	102.194	406.158	40.054	81.186	143.921	80.219	185.956	70.663	291.222
0.004	135.293	215.874	75.233	287.263	102.200	406.158	40.044	81.195	143.923	80.210	185.937	70.673	291.222
0.005	135.294	215.827	75.230	287.255	102.206	406.158	40.035	81.203	143.925	80.201	185.918	70.684	291.222
0.006	135.296	215.780	75.227	287.246	102.212	406.158	40.025	81.212	143.927	80.191	185.899	70.694	291.222
0.007	135.298	215.733	75.224	287.238	102.218	406.158	40.016	81.221	143.928	80.182	185.880	70.705	291.222
0.008	135.300	215.686	75.222	287.229	102.225	406.158	40.006	81.229	143.930	80.173	185.860	70.715	291.222
0.009	135.301	215.639	75.219	287.220	102.231	406.158	39.996	81.238	143.932	80.164	185.841	70.726	291.222
0.010	135.303	215.592	75.216	287.212	102.237	406.158	39.987	81.246	143.934	80.155	185.822	70.736	291.222
0.020	135.321	215.122	75.187	287.126	102.298	406.158	39.891	81.333	143.953	80.064	185.630	70.841	291.222
0.030	135.338	214.651	75.158	287.040	102.359	406.158	39.795	81.419	143.971	79.972	185.438	70.946	291.222
0.040	135.355	214.181	75.129	286.954	102.420	406.158	39.700	81.505	143.990	79.881	185.246	71.051	291.222
0.050	135.373	213.710	75.100	286.868	102.481	406.158	39.604	81.592	144.009	79.790	185.054	71.155	291.222
0.060	135.390	213.240	75.071	286.782	102.542	406.158	39.508	81.678	144.027	79.698	184.862	71.260	291.222
0.070	135.408	212.770	75.042	286.696	102.603	406.158	39.413	81.764	144.046	79.607	184.670	71.365	291.222
0.080	135.425	212.299	75.013	286.610	102.664	406.158	39.317	81.851	144.065	79.516	184.478	71.470	291.222
0.090	135.442	211.829	74.985	286.524	102.725	406.158	39.221	81.937	144.083	79.424	184.285	71.574	291.222
0.100	135.460	211.358	74.956	286.438	102.786	406.158	39.125	82.023	144.102	79.333	184.093	71.679	291.222
IFoI	139.383	215.477	96.352	296.512	99.128	406.158	58.418	73.203	150.604	106.855	190.779	78.828	291.222

Table A.2.17. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2564, B=-0.51059, K=20.06603)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	135.447	215.817	75.456	287.042	102.071	405.794	40.485	80.918	143.840	80.667	185.583	70.827	290.725
0.001	135.448	215.770	75.453	287.033	102.077	405.794	40.475	80.927	143.842	80.657	185.564	70.837	290.725
0.002	135.450	215.723	75.450	287.025	102.084	405.794	40.466	80.936	143.844	80.648	185.544	70.848	290.725
0.003	135.452	215.676	75.447	287.016	102.090	405.794	40.456	80.944	143.846	80.639	185.525	70.858	290.725
0.004	135.454	215.629	75.444	287.007	102.096	405.794	40.446	80.953	143.847	80.630	185.506	70.868	290.725
0.005	135.455	215.582	75.441	286.999	102.102	405.794	40.437	80.962	143.849	80.621	185.487	70.879	290.725
0.006	135.457	215.535	75.439	286.990	102.108	405.794	40.427	80.970	143.851	80.612	185.468	70.889	290.725
0.007	135.459	215.488	75.436	286.982	102.114	405.794	40.418	80.979	143.853	80.603	185.448	70.900	290.725
0.008	135.461	215.441	75.433	286.973	102.120	405.794	40.408	80.987	143.855	80.593	185.429	70.910	290.725
0.009	135.462	215.394	75.430	286.964	102.126	405.794	40.399	80.996	143.857	80.584	185.410	70.921	290.725
0.010	135.464	215.347	75.427	286.956	102.132	405.794	40.389	81.005	143.859	80.575	185.391	70.931	290.725
0.020	135.482	214.877	75.398	286.870	102.193	405.794	40.293	81.091	143.877	80.484	185.199	71.036	290.725
0.030	135.499	214.406	75.369	286.784	102.254	405.794	40.198	81.177	143.896	80.393	185.007	71.141	290.725
0.040	135.516	213.936	75.340	286.698	102.315	405.794	40.102	81.264	143.915	80.301	184.815	71.246	290.725
0.050	135.534	213.465	75.311	286.612	102.376	405.794	40.006	81.350	143.933	80.210	184.623	71.350	290.725
0.060	135.551	212.995	75.282	286.526	102.437	405.794	39.910	81.436	143.952	80.119	184.430	71.455	290.725
0.070	135.569	212.524	75.253	286.440	102.499	405.794	39.815	81.523	143.971	80.027	184.238	71.560	290.725
0.080	135.586	212.054	75.225	286.354	102.560	405.794	39.719	81.609	143.989	79.936	184.046	71.665	290.725
0.090	135.603	211.584	75.196	286.268	102.621	405.794	39.623	81.695	144.008	79.845	183.854	71.769	290.725
0.100	135.621	211.113	75.167	286.182	102.682	405.794	39.528	81.782	144.027	79.753	183.662	71.874	290.725
|Fo|	139.342	215.398	96.314	296.366	99.060	405.794	58.361	73.122	150.426	106.726	190.531	78.709	290.725

Table A.2.18. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2568, B=-0.50290, K=20.06425)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	135.621	215.574	75.683	286.771	101.962	405.407	40.884	80.664	143.772	81.112	185.125	71.032	290.197
0.001	135.622	215.527	75.680	286.763	101.968	405.407	40.874	80.672	143.774	81.103	185.105	71.043	290.197
0.002	135.624	215.480	75.677	286.754	101.974	405.407	40.865	80.681	143.776	81.093	185.086	71.053	290.197
0.003	135.626	215.433	75.674	286.745	101.980	405.407	40.855	80.689	143.778	81.084	185.067	71.064	290.197
0.004	135.628	215.386	75.671	286.737	101.986	405.407	40.846	80.698	143.780	81.075	185.048	71.074	290.197
0.005	135.629	215.339	75.668	286.728	101.992	405.407	40.836	80.707	143.781	81.066	185.028	71.085	290.197
0.006	135.631	215.292	75.666	286.720	101.998	405.407	40.827	80.715	143.783	81.057	185.009	71.095	290.197
0.007	135.633	215.245	75.663	286.711	102.005	405.407	40.817	80.724	143.785	81.048	184.990	71.106	290.197
0.008	135.635	215.198	75.660	286.702	102.011	405.407	40.807	80.733	143.787	81.039	184.971	71.116	290.197
0.009	135.636	215.151	75.657	286.694	102.017	405.407	40.798	80.741	143.789	81.029	184.952	71.127	290.197
0.010	135.638	215.104	75.654	286.685	102.023	405.407	40.788	80.750	143.791	81.020	184.932	71.137	290.197
0.020	135.655	214.634	75.625	286.599	102.084	405.407	40.693	80.836	143.809	80.929	184.740	71.242	290.197
0.030	135.673	214.163	75.596	286.513	102.145	405.407	40.597	80.923	143.828	80.838	184.548	71.347	290.197
0.040	135.690	213.693	75.567	286.427	102.206	405.407	40.501	81.009	143.847	80.746	184.356	71.451	290.197
0.050	135.708	213.222	75.538	286.341	102.267	405.407	40.405	81.095	143.865	80.655	184.164	71.556	290.197
0.060	135.725	212.752	75.509	286.255	102.328	405.407	40.310	81.182	143.884	80.564	183.972	71.661	290.197
0.070	135.742	212.281	75.481	286.169	102.389	405.407	40.214	81.268	143.903	80.472	183.780	71.766	290.197
0.080	135.760	211.811	75.452	286.083	102.450	405.407	40.118	81.354	143.921	80.381	183.588	71.870	290.197
0.090	135.777	211.341	75.423	285.997	102.511	405.407	40.023	81.441	143.940	80.290	183.396	71.975	290.197
0.100	135.795	210.870	75.394	285.911	102.572	405.407	39.927	81.527	143.959	80.198	183.204	72.080	290.197
|Fo|	139.300	215.315	96.274	296.211	98.987	405.407	58.301	73.037	150.238	106.590	190.267	78.583	290.197

Table A.2.19. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2572, B=-0.49474, K=20.06241)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	135.802	215.329	75.921	286.482	101.846	404.998	41.280	80.393	143.711	81.583	184.641	71.249	289.639
0.001	135.804	215.282	75.809	286.474	101.852	404.998	41.271	80.402	143.712	81.574	184.622	71.260	289.639
0.002	135.806	215.235	75.697	286.465	101.858	404.998	41.261	80.410	143.714	81.565	184.603	71.270	289.639
0.003	135.808	215.188	75.585	286.457	101.864	404.998	41.252	80.419	143.716	81.555	184.584	71.281	289.639
0.004	135.809	215.141	75.473	286.448	101.870	404.998	41.242	80.428	143.718	81.546	184.565	71.291	289.639
0.005	135.811	215.094	75.361	286.439	101.876	404.998	41.233	80.436	143.720	81.537	184.545	71.301	289.639
0.006	135.813	215.047	75.249	286.431	101.882	404.998	41.223	80.445	143.722	81.528	184.526	71.312	289.639
0.007	135.815	215.000	75.137	286.422	101.888	404.998	41.213	80.454	143.724	81.519	184.507	71.322	289.639
0.008	135.816	214.953	75.025	286.414	101.894	404.998	41.204	80.462	143.726	81.510	184.488	71.333	289.639
0.009	135.818	214.906	74.913	286.405	101.900	404.998	41.194	80.471	143.727	81.501	184.469	71.343	289.639
0.010	135.820	214.859	74.801	286.396	101.907	404.998	41.185	80.479	143.729	81.492	184.449	71.354	289.639
0.020	135.837	214.388	73.680	286.310	101.968	404.998	41.089	80.566	143.748	81.400	184.257	71.459	289.639
0.030	135.855	213.918	72.559	286.224	102.029	404.998	40.993	80.652	143.767	81.309	184.065	71.563	289.639
0.040	135.872	213.448	71.438	286.138	102.090	404.998	40.898	80.738	143.785	81.218	183.873	71.668	289.639
0.050	135.889	212.977	70.318	286.052	102.151	404.998	40.802	80.825	143.804	81.126	183.681	71.773	289.639
0.060	135.907	212.507	69.197	285.966	102.212	404.998	40.706	80.911	143.823	81.035	183.489	71.878	289.639
0.070	135.924	212.036	68.076	285.880	102.273	404.998	40.610	80.997	143.841	80.944	183.297	71.982	289.639
0.080	135.942	211.566	66.956	285.794	102.334	404.998	40.515	81.084	143.860	80.852	183.105	72.087	289.639
0.090	135.959	211.095	65.835	285.708	102.395	404.998	40.419	81.170	143.879	80.761	182.913	72.192	289.639
0.100	135.976	210.625	64.714	285.622	102.456	404.998	40.323	81.256	143.897	80.670	182.721	72.297	289.639
IFoI	139.255	215.227	96.232	296.048	98.909	404.998	58.237	72.946	150.040	106.446	189.988	78.450	289.639

Table A.2.20. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2576, B=-0.48608, K=20.06057)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	135.994	215.084	76.173	286.177	101.722	404.567	41.674	80.108	143.655	82.080	184.132	71.478	289.049
0.001	135.996	215.037	76.170	286.168	101.728	404.567	41.665	80.117	143.657	82.071	184.113	71.488	289.049
0.002	135.998	214.990	76.168	286.160	101.735	404.567	41.655	80.125	143.659	82.062	184.094	71.499	289.049
0.003	136.000	214.943	76.165	286.151	101.741	404.567	41.645	80.134	143.661	82.053	184.075	71.509	289.049
0.004	136.001	214.896	76.162	286.143	101.747	404.567	41.636	80.143	143.663	82.044	184.055	71.520	289.049
0.005	136.003	214.849	76.159	286.134	101.753	404.567	41.626	80.151	143.665	82.034	184.036	71.530	289.049
0.006	136.005	214.802	76.156	286.125	101.759	404.567	41.617	80.160	143.667	82.025	184.017	71.541	289.049
0.007	136.007	214.755	76.153	286.117	101.765	404.567	41.607	80.169	143.668	82.016	183.998	71.551	289.049
0.008	136.008	214.708	76.150	286.108	101.771	404.567	41.598	80.177	143.670	82.007	183.979	71.562	289.049
0.009	136.010	214.661	76.147	286.100	101.777	404.567	41.588	80.186	143.672	81.998	183.959	71.572	289.049
0.010	136.012	214.614	76.144	286.091	101.783	404.567	41.578	80.195	143.674	81.989	183.940	71.582	289.049
0.020	136.029	214.143	76.116	286.005	101.844	404.567	41.483	80.281	143.693	81.897	183.748	71.687	289.049
0.030	136.047	213.673	76.087	285.919	101.905	404.567	41.387	80.367	143.711	81.806	183.556	71.792	289.049
0.040	136.064	213.202	76.058	285.833	101.966	404.567	41.291	80.454	143.730	81.715	183.364	71.897	289.049
0.050	136.081	212.732	76.029	285.747	102.027	404.567	41.196	80.540	143.749	81.623	183.172	72.001	289.049
0.060	136.099	212.261	76.000	285.661	102.088	404.567	41.100	80.626	143.767	81.532	182.980	72.106	289.049
0.070	136.116	211.791	75.971	285.575	102.149	404.567	41.004	80.713	143.786	81.441	182.788	72.211	289.049
0.080	136.134	211.321	75.942	285.489	102.210	404.567	40.908	80.799	143.805	81.349	182.596	72.316	289.049
0.090	136.151	210.850	75.913	285.403	102.271	404.567	40.813	80.885	143.823	81.258	182.404	72.420	289.049
0.100	136.168	210.380	75.884	285.317	102.333	404.567	40.717	80.972	143.842	81.167	182.212	72.525	289.049
|Fo|	139.208	215.135	96.188	295.877	98.828	404.567	58.170	72.851	149.830	106.294	189.693	78.309	289.049

Table A.2.21. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2580, B=0.47702, K=20.05846)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	136.200	214.836	76.439	285.855	101.592	404.113	42.064	79.809	143.609	82.602	183.598	71.716	288.430
0.001	136.201	214.789	76.436	285.847	101.598	404.113	42.054	79.818	143.611	82.593	183.579	71.727	288.430
0.002	136.203	214.742	76.433	285.838	101.605	404.113	42.044	79.826	143.613	82.584	183.560	71.737	288.430
0.003	136.205	214.695	76.430	285.829	101.611	404.113	42.035	79.835	143.614	82.575	183.541	71.748	288.430
0.004	136.207	214.648	76.427	285.821	101.617	404.113	42.025	79.844	143.616	82.566	183.521	71.758	288.430
0.005	136.208	214.601	76.425	285.812	101.623	404.113	42.016	79.852	143.618	82.556	183.502	71.768	288.430
0.006	136.210	214.554	76.422	285.804	101.629	404.113	42.006	79.861	143.620	82.547	183.483	71.779	288.430
0.007	136.212	214.507	76.419	285.795	101.635	404.113	41.997	79.869	143.622	82.538	183.464	71.789	288.430
0.008	136.213	214.460	76.416	285.786	101.641	404.113	41.987	79.878	143.624	82.529	183.445	71.800	288.430
0.009	136.215	214.413	76.413	285.778	101.647	404.113	41.977	79.887	143.626	82.520	183.425	71.810	288.430
0.010	136.217	214.366	76.410	285.769	101.653	404.113	41.968	79.895	143.628	82.511	183.406	71.821	288.430
0.020	136.234	213.896	76.381	285.683	101.714	404.113	41.872	79.982	143.646	82.419	183.214	71.926	288.430
0.030	136.252	213.425	76.352	285.597	101.775	404.113	41.776	80.068	143.665	82.328	183.022	72.030	288.430
0.040	136.269	212.955	76.323	285.511	101.836	404.113	41.681	80.154	143.683	82.237	182.830	72.135	288.430
0.050	136.287	212.484	76.294	285.425	101.897	404.113	41.585	80.241	143.702	82.145	182.638	72.240	288.430
0.060	136.304	212.014	76.266	285.339	101.958	404.113	41.489	80.327	143.721	82.054	182.446	72.345	288.430
0.070	136.321	211.543	76.237	285.253	102.019	404.113	41.394	80.413	143.739	81.963	182.254	72.449	288.430
0.080	136.339	211.073	76.208	285.167	102.080	404.113	41.298	80.500	143.758	81.871	182.062	72.554	288.430
0.090	136.356	210.603	76.179	285.081	102.141	404.113	41.202	80.586	143.777	81.780	181.870	72.659	288.430
0.100	136.374	210.132	76.150	284.995	102.202	404.113	41.107	80.672	143.795	81.689	181.678	72.764	288.430
IFoI	139.158	215.037	96.141	295.695	98.742	404.113	58.099	72.751	149.609	106.134	189.384	78.161	288.430

Table A.2.22. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2584, B=-0.46741, K=20.05651)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	136.412	214.589	76.716	285.519	101.459	403.637	42.449	79.495	143.571	83.150	183.040	71.965	287.780
0.001	136.414	214.542	76.713	285.511	101.465	403.637	42.439	79.504	143.573	83.141	183.020	71.976	287.780
0.002	136.416	214.495	76.710	285.502	101.471	403.637	42.430	79.513	143.575	83.132	183.001	71.986	287.780
0.003	136.418	214.448	76.707	285.493	101.477	403.637	42.420	79.521	143.577	83.123	182.982	71.997	287.780
0.004	136.419	214.401	76.704	285.485	101.483	403.637	42.411	79.530	143.579	83.114	182.963	72.007	287.780
0.005	136.421	214.354	76.702	285.476	101.489	403.637	42.401	79.539	143.581	83.104	182.944	72.018	287.780
0.006	136.423	214.307	76.699	285.468	101.495	403.637	42.391	79.547	143.582	83.095	182.924	72.028	287.780
0.007	136.425	214.260	76.696	285.459	101.502	403.637	42.382	79.556	143.584	83.086	182.905	72.039	287.780
0.008	136.426	214.212	76.693	285.450	101.508	403.637	42.372	79.564	143.586	83.077	182.886	72.049	287.780
0.009	136.428	214.165	76.690	285.442	101.514	403.637	42.363	79.573	143.588	83.068	182.867	72.060	287.780
0.010	136.430	214.118	76.687	285.433	101.520	403.637	42.353	79.582	143.590	83.059	182.847	72.070	287.780
0.020	136.447	213.648	76.658	285.347	101.581	403.637	42.257	79.668	143.608	82.967	182.655	72.175	287.780
0.030	136.465	213.178	76.629	285.261	101.642	403.637	42.162	79.754	143.627	82.876	182.463	72.280	287.780
0.040	136.482	212.707	76.600	285.175	101.703	403.637	42.066	79.841	143.646	82.785	182.271	72.384	287.780
0.050	136.499	212.237	76.571	285.089	101.764	403.637	41.970	79.927	143.664	82.693	182.079	72.489	287.780
0.060	136.517	211.766	76.543	285.003	101.825	403.637	41.875	80.013	143.683	82.602	181.887	72.594	287.780
0.070	136.534	211.296	76.514	284.917	101.886	403.637	41.779	80.100	143.702	82.511	181.695	72.699	287.780
0.080	136.552	210.825	76.485	284.831	101.947	403.637	41.683	80.186	143.720	82.419	181.503	72.803	287.780
0.090	136.569	210.355	76.456	284.745	102.008	403.637	41.587	80.272	143.739	82.328	181.311	72.908	287.780
0.100	136.586	209.885	76.427	284.659	102.069	403.637	41.492	80.359	143.758	82.237	181.119	73.013	287.780
|Fo|	139.107	214.937	96.093	295.507	98.653	403.637	58.025	72.645	149.378	105.966	189.059	78.006	287.780

Table A.2.23. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2588, B=-0.45735, K=20.05445)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	136.636	214.339	77.009	285.165	101.317	403.140	42.831	79.167	143.541	83.722	182.456	72.223	287.100
0.001	136.637	214.292	77.006	285.156	101.323	403.140	42.822	79.176	143.543	83.713	182.437	72.234	287.100
0.002	136.639	214.245	77.003	285.148	101.329	403.140	42.812	79.185	143.545	83.703	182.418	72.244	287.100
0.003	136.641	214.198	77.000	285.139	101.335	403.140	42.803	79.193	143.547	83.694	182.398	72.255	287.100
0.004	136.643	214.151	76.997	285.130	101.341	403.140	42.793	79.202	143.548	83.685	182.379	72.265	287.100
0.005	136.644	214.104	76.994	285.122	101.347	403.140	42.783	79.211	143.550	83.676	182.360	72.276	287.100
0.006	136.646	214.057	76.992	285.113	101.353	403.140	42.774	79.219	143.552	83.667	182.341	72.286	287.100
0.007	136.648	214.010	76.989	285.105	101.360	403.140	42.764	79.228	143.554	83.658	182.322	72.296	287.100
0.008	136.650	213.963	76.986	285.096	101.366	403.140	42.755	79.236	143.556	83.649	182.302	72.307	287.100
0.009	136.651	213.915	76.983	285.087	101.372	403.140	42.745	79.245	143.558	83.640	182.283	72.317	287.100
0.010	136.653	213.868	76.980	285.079	101.378	403.140	42.736	79.254	143.560	83.630	182.264	72.328	287.100
0.020	136.670	213.398	76.951	284.993	101.439	403.140	42.640	79.340	143.578	83.539	182.072	72.433	287.100
0.030	136.688	212.928	76.922	284.907	101.500	403.140	42.544	79.426	143.597	83.448	181.880	72.537	287.100
0.040	136.705	212.457	76.893	284.821	101.561	403.140	42.448	79.513	143.616	83.356	181.688	72.642	287.100
0.050	136.723	211.987	76.864	284.735	101.622	403.140	42.353	79.599	143.634	83.265	181.496	72.747	287.100
0.060	136.740	211.516	76.835	284.649	101.683	403.140	42.257	79.685	143.653	83.174	181.304	72.852	287.100
0.070	136.757	211.046	76.807	284.563	101.744	403.140	42.161	79.772	143.672	83.082	181.112	72.956	287.100
0.080	136.775	210.575	76.778	284.477	101.805	403.140	42.066	79.858	143.690	82.991	180.919	73.061	287.100
0.090	136.792	210.105	76.749	284.391	101.866	403.140	41.970	79.944	143.709	82.900	180.727	73.166	287.100
0.100	136.810	209.635	76.720	284.305	101.927	403.140	41.874	80.031	143.728	82.808	180.535	73.271	287.100
|Fo|	139.054	214.831	96.043	295.310	98.559	403.140	57.947	72.535	149.135	105.791	188.719	77.844	287.100

Table A.2.24. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2592, B=-0.44681, K=20.05243)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	136.872	214.089	77.313	284.796	101.171	402.622	43.211	78.826	143.520	84.319	181.849	72.492	286.392
0.001	136.874	214.042	77.310	284.787	101.178	402.622	43.201	78.835	143.522	84.310	181.830	72.502	286.392
0.002	136.875	213.995	77.307	284.779	101.184	402.622	43.192	78.844	143.523	84.301	181.810	72.513	286.392
0.003	136.877	213.948	77.304	284.770	101.190	402.622	43.182	78.852	143.525	84.292	181.791	72.523	286.392
0.004	136.879	213.901	77.302	284.762	101.196	402.622	43.173	78.861	143.527	84.283	181.772	72.534	286.392
0.005	136.881	213.854	77.299	284.753	101.202	402.622	43.163	78.869	143.529	84.274	181.753	72.544	286.392
0.006	136.882	213.807	77.296	284.744	101.208	402.622	43.153	78.878	143.531	84.265	181.734	72.555	286.392
0.007	136.884	213.760	77.293	284.736	101.214	402.622	43.144	78.887	143.533	84.255	181.714	72.565	286.392
0.008	136.886	213.713	77.290	284.727	101.220	402.622	43.134	78.895	143.535	84.246	181.695	72.576	286.392
0.009	136.888	213.666	77.287	284.719	101.226	402.622	43.125	78.904	143.536	84.237	181.676	72.586	286.392
0.010	136.889	213.618	77.284	284.710	101.232	402.622	43.115	78.913	143.538	84.228	181.657	72.597	286.392
0.020	136.907	213.148	77.255	284.624	101.293	402.622	43.019	78.999	143.557	84.137	181.465	72.701	286.392
0.030	136.924	212.678	77.226	284.538	101.354	402.622	42.924	79.085	143.576	84.045	181.273	72.806	286.392
0.040	136.941	212.207	77.197	284.452	101.415	402.622	42.828	79.172	143.594	83.954	181.081	72.911	286.392
0.050	136.959	211.737	77.169	284.366	101.476	402.622	42.732	79.258	143.613	83.863	180.888	73.016	286.392
0.060	136.976	211.266	77.140	284.280	101.538	402.622	42.637	79.344	143.632	83.771	180.696	73.120	286.392
0.070	136.994	210.796	77.111	284.194	101.599	402.622	42.541	79.431	143.650	83.680	180.504	73.225	286.392
0.080	137.011	210.325	77.082	284.108	101.660	402.622	42.445	79.517	143.669	83.589	180.312	73.330	286.392
0.090	137.028	209.855	77.053	284.022	101.721	402.622	42.350	79.603	143.688	83.497	180.120	73.435	286.392
0.100	137.046	209.385	77.024	283.936	101.782	402.622	42.254	79.690	143.706	83.406	179.928	73.539	286.392
IFoI	138.999	214.722	95.990	295.105	98.462	402.622	57.866	72.421	148.883	105.608	188.365	77.675	286.392

Table A.2.25. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2596, B=-0.43581, K=20.05031)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	137.116	213.837	77.633	284.411	101.019	402.082	43.585	78.471	143.507	84.941	181.219	72.770	285.654
0.001	137.118	213.790	77.630	284.402	101.025	402.082	43.575	78.479	143.509	84.931	181.200	72.781	285.654
0.002	137.119	213.742	77.627	284.393	101.031	402.082	43.566	78.488	143.511	84.922	181.181	72.791	285.654
0.003	137.121	213.695	77.625	284.385	101.037	402.082	43.556	78.497	143.513	84.913	181.162	72.802	285.654
0.004	137.123	213.648	77.622	284.376	101.044	402.082	43.547	78.505	143.515	84.904	181.142	72.812	285.654
0.005	137.125	213.601	77.619	284.368	101.050	402.082	43.537	78.514	143.516	84.895	181.123	72.823	285.654
0.006	137.126	213.554	77.616	284.359	101.056	402.082	43.527	78.523	143.518	84.886	181.104	72.833	285.654
0.007	137.128	213.507	77.613	284.350	101.062	402.082	43.518	78.531	143.520	84.877	181.085	72.844	285.654
0.008	137.130	213.460	77.610	284.342	101.068	402.082	43.508	78.540	143.522	84.867	181.066	72.854	285.654
0.009	137.132	213.413	77.607	284.333	101.074	402.082	43.499	78.549	143.524	84.858	181.046	72.865	285.654
0.010	137.133	213.366	77.604	284.325	101.080	402.082	43.489	78.557	143.526	84.849	181.027	72.875	285.654
0.020	137.151	212.896	77.575	284.239	101.141	402.082	43.393	78.644	143.544	84.758	180.835	72.980	285.654
0.030	137.168	212.425	77.547	284.153	101.202	402.082	43.298	78.730	143.563	84.667	180.643	73.085	285.654
0.040	137.186	211.955	77.518	284.067	101.263	402.082	43.202	78.816	143.582	84.575	180.451	73.189	285.654
0.050	137.203	211.484	77.489	283.981	101.324	402.082	43.106	78.902	143.600	84.484	180.259	73.294	285.654
0.060	137.220	211.014	77.460	283.895	101.385	402.082	43.011	78.989	143.619	84.393	180.067	73.399	285.654
0.070	137.238	210.544	77.431	283.809	101.446	402.082	42.915	79.075	143.638	84.301	179.875	73.504	285.654
0.080	137.255	210.073	77.402	283.723	101.507	402.082	42.819	79.161	143.656	84.210	179.683	73.608	285.654
0.090	137.273	209.603	77.373	283.637	101.568	402.082	42.724	79.248	143.675	84.119	179.491	73.713	285.654
0.100	137.290	209.132	77.344	283.551	101.629	402.082	42.628	79.334	143.694	84.027	179.299	73.818	285.654
|Fo|	138.941	214.608	95.936	294.892	98.360	402.082	57.782	72.301	148.620	105.417	187.996	77.499	285.654

Table A.2.26. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2600, B=-0.42437, K=20.04802)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	137.370	213.584	77.965	284.009	100.862	401.520	43.955	78.102	143.505	85.585	180.565	73.057	284.888
0.001	137.372	213.537	77.962	284.000	100.868	401.520	43.945	78.111	143.506	85.576	180.546	73.068	284.888
0.002	137.374	213.490	77.959	283.992	100.874	401.520	43.936	78.120	143.508	85.567	180.526	73.078	284.888
0.003	137.376	213.443	77.956	283.983	100.880	401.520	43.926	78.128	143.510	85.558	180.507	73.089	284.888
0.004	137.377	213.396	77.953	283.975	100.886	401.520	43.916	78.137	143.512	85.549	180.488	73.099	284.888
0.005	137.379	213.349	77.950	283.966	100.892	401.520	43.907	78.146	143.514	85.540	180.469	73.110	284.888
0.006	137.381	213.302	77.947	283.957	100.898	401.520	43.897	78.154	143.516	85.531	180.450	73.120	284.888
0.007	137.383	213.255	77.945	283.949	100.904	401.520	43.888	78.163	143.518	85.521	180.430	73.131	284.888
0.008	137.384	213.208	77.942	283.940	100.911	401.520	43.878	78.171	143.520	85.512	180.411	73.141	284.888
0.009	137.386	213.161	77.939	283.932	100.917	401.520	43.869	78.180	143.521	85.503	180.392	73.152	284.888
0.010	137.388	213.114	77.936	283.923	100.923	401.520	43.859	78.189	143.523	85.494	180.373	73.162	284.888
0.020	137.405	212.643	77.907	283.837	100.984	401.520	43.763	78.275	143.542	85.403	180.181	73.267	284.888
0.030	137.423	212.173	77.878	283.751	101.045	401.520	43.668	78.361	143.561	85.311	179.989	73.372	284.888
0.040	137.440	211.703	77.849	283.665	101.106	401.520	43.572	78.448	143.579	85.220	179.797	73.476	284.888
0.050	137.457	211.232	77.820	283.579	101.167	401.520	43.476	78.534	143.598	85.129	179.604	73.581	284.888
0.060	137.475	210.762	77.791	283.493	101.228	401.520	43.380	78.620	143.617	85.037	179.412	73.686	284.888
0.070	137.492	210.291	77.762	283.407	101.289	401.520	43.285	78.707	143.635	84.946	179.220	73.791	284.888
0.080	137.510	209.821	77.733	283.321	101.350	401.520	43.189	78.793	143.654	84.855	179.028	73.895	284.888
0.090	137.527	209.350	77.705	283.235	101.411	401.520	43.093	78.879	143.673	84.763	178.836	74.000	284.888
0.100	137.544	208.880	77.676	283.149	101.472	401.520	42.998	78.966	143.691	84.672	178.644	74.105	284.888
|Fo|	138.881	214.489	95.879	294.669	98.254	401.520	57.694	72.177	148.347	105.219	187.612	77.316	284.888

Table A.2.27. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2604, B=-0.41240, K=20.04595)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	137.635	213.332	78.308	283.591	100.699	400.938	44.322	77.719	143.512	86.255	179.889	73.353	284.093
0.001	137.637	213.285	78.305	283.582	100.705	400.938	44.312	77.728	143.514	86.246	179.870	73.364	284.093
0.002	137.639	213.238	78.302	283.574	100.711	400.938	44.302	77.737	143.516	86.237	179.851	73.374	284.093
0.003	137.640	213.191	78.299	283.565	100.717	400.938	44.293	77.745	143.518	86.227	179.831	73.385	284.093
0.004	137.642	213.144	78.296	283.557	100.724	400.938	44.283	77.754	143.520	86.218	179.812	73.395	284.093
0.005	137.644	213.097	78.293	283.548	100.730	400.938	44.274	77.763	143.521	86.209	179.793	73.406	284.093
0.006	137.646	213.050	78.290	283.539	100.736	400.938	44.264	77.771	143.523	86.200	179.774	73.416	284.093
0.007	137.647	213.003	78.287	283.531	100.742	400.938	44.255	77.780	143.525	86.191	179.755	73.427	284.093
0.008	137.649	212.956	78.284	283.522	100.748	400.938	44.245	77.789	143.527	86.182	179.735	73.437	284.093
0.009	137.651	212.909	78.282	283.514	100.754	400.938	44.235	77.797	143.529	86.173	179.716	73.448	284.093
0.010	137.653	212.862	78.279	283.505	100.760	400.938	44.226	77.806	143.531	86.164	179.697	73.458	284.093
0.020	137.670	212.391	78.250	283.419	100.821	400.938	44.130	77.892	143.549	86.072	179.505	73.563	284.093
0.030	137.687	211.921	78.221	283.333	100.882	400.938	44.035	77.978	143.568	85.981	179.313	73.667	284.093
0.040	137.705	211.450	78.192	283.247	100.943	400.938	43.939	78.065	143.587	85.890	179.121	73.772	284.093
0.050	137.722	210.980	78.163	283.161	101.004	400.938	43.843	78.151	143.605	85.798	178.929	73.877	284.093
0.060	137.740	210.509	78.134	283.075	101.065	400.938	43.747	78.237	143.624	85.707	178.737	73.982	284.093
0.070	137.757	210.039	78.105	282.989	101.126	400.938	43.652	78.324	143.643	85.616	178.545	74.086	284.093
0.080	137.774	209.569	78.076	282.903	101.187	400.938	43.556	78.410	143.661	85.524	178.353	74.191	284.093
0.090	137.792	209.098	78.047	282.817	101.248	400.938	43.460	78.496	143.680	85.433	178.161	74.296	284.093
0.100	137.809	208.628	78.018	282.731	101.309	400.938	43.365	78.583	143.699	85.342	177.968	74.401	284.093
|Fo|	138.820	214.368	95.820	294.440	98.145	400.938	57.603	72.048	148.063	105.014	187.215	77.126	284.093

Table A.2.28. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2608, B=-0.39995, K=20.04380)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	137.908	213.075	78.666	283.157	100.530	400.334	44.683	77.325	143.530	86.948	179.191	73.658	283.268
0.001	137.909	213.028	78.554	283.148	100.536	400.334	44.673	77.333	143.532	86.939	179.172	73.668	283.268
0.002	137.911	212.981	78.442	283.139	100.542	400.334	44.664	77.342	143.533	86.930	179.153	73.679	283.268
0.003	137.913	212.934	78.330	283.131	100.548	400.334	44.654	77.351	143.535	86.921	179.133	73.689	283.268
0.004	137.915	212.887	78.218	283.122	100.554	400.334	44.645	77.359	143.537	86.911	179.114	73.700	283.268
0.005	137.916	212.840	78.106	283.114	100.560	400.334	44.635	77.368	143.539	86.902	179.095	73.710	283.268
0.006	137.918	212.793	77.994	283.105	100.566	400.334	44.626	77.377	143.541	86.893	179.076	73.721	283.268
0.007	137.920	212.746	77.882	283.096	100.572	400.334	44.616	77.385	143.543	86.884	179.056	73.731	283.268
0.008	137.922	212.699	77.770	283.088	100.579	400.334	44.606	77.394	143.545	86.875	179.037	73.741	283.268
0.009	137.923	212.652	77.658	283.079	100.585	400.334	44.597	77.403	143.547	86.866	179.018	73.752	283.268
0.010	137.925	212.604	77.546	283.071	100.591	400.334	44.587	77.411	143.548	86.857	178.999	73.762	283.268
0.020	137.942	212.134	76.425	282.985	100.652	400.334	44.492	77.497	143.567	86.765	178.807	73.867	283.268
0.030	137.960	211.664	75.304	282.899	100.713	400.334	44.396	77.584	143.586	86.674	178.615	73.972	283.268
0.040	137.977	211.193	74.183	282.813	100.774	400.334	44.300	77.670	143.604	86.583	178.423	74.077	283.268
0.050	137.995	210.723	73.063	282.727	100.835	400.334	44.204	77.756	143.623	86.491	178.231	74.181	283.268
0.060	138.012	210.252	71.942	282.641	100.896	400.334	44.109	77.843	143.642	86.400	178.039	74.286	283.268
0.070	138.029	209.782	70.821	282.555	100.957	400.334	44.013	77.929	143.660	86.309	177.846	74.391	283.268
0.080	138.047	209.311	69.701	282.469	101.018	400.334	43.917	78.015	143.679	86.217	177.654	74.496	283.268
0.090	138.064	208.841	68.580	282.383	101.079	400.334	43.822	78.102	143.698	86.126	177.462	74.600	283.268
0.100	138.082	208.371	67.459	282.297	101.140	400.334	43.726	78.188	143.716	86.035	177.270	74.705	283.268
|Fo|	138.756	214.242	95.760	294.202	98.031	400.334	57.509	71.914	147.769	104.801	186.802	76.929	283.268

Table A.2.29. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2612, B=-0.38704, K=20.04166)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	138.193	212.820	79.036	282.706	100.357	399.712	45.040	76.916	143.557	87.663	178.470	73.971	282.417
0.001	138.195	212.773	79.034	282.697	100.363	399.712	45.031	76.924	143.559	87.654	178.451	73.981	282.417
0.002	138.197	212.726	79.031	282.689	100.369	399.712	45.021	76.933	143.561	87.645	178.432	73.992	282.417
0.003	138.198	212.679	79.028	282.680	100.375	399.712	45.011	76.942	143.563	87.636	178.413	74.002	282.417
0.004	138.200	212.632	79.025	282.671	100.381	399.712	45.002	76.950	143.565	87.627	178.394	74.013	282.417
0.005	138.202	212.585	79.022	282.663	100.387	399.712	44.992	76.959	143.567	87.618	178.374	74.023	282.417
0.006	138.204	212.538	79.019	282.654	100.394	399.712	44.983	76.968	143.569	87.609	178.355	74.034	282.417
0.007	138.205	212.491	79.016	282.646	100.400	399.712	44.973	76.976	143.570	87.599	178.336	74.044	282.417
0.008	138.207	212.444	79.013	282.637	100.406	399.712	44.964	76.985	143.572	87.590	178.317	74.055	282.417
0.009	138.209	212.397	79.010	282.628	100.412	399.712	44.954	76.994	143.574	87.581	178.298	74.065	282.417
0.010	138.211	212.350	79.008	282.620	100.418	399.712	44.944	77.002	143.576	87.572	178.278	74.076	282.417
0.020	138.228	211.879	78.979	282.534	100.479	399.712	44.849	77.088	143.595	87.481	178.086	74.180	282.417
0.030	138.245	211.409	78.950	282.448	100.540	399.712	44.753	77.175	143.613	87.389	177.894	74.285	282.417
0.040	138.263	210.939	78.921	282.362	100.601	399.712	44.657	77.261	143.632	87.298	177.702	74.390	282.417
0.050	138.280	210.468	78.892	282.276	100.662	399.712	44.562	77.347	143.651	87.207	177.510	74.495	282.417
0.060	138.298	209.998	78.863	282.190	100.723	399.712	44.466	77.434	143.669	87.115	177.318	74.599	282.417
0.070	138.315	209.527	78.834	282.104	100.784	399.712	44.370	77.520	143.688	87.024	177.126	74.704	282.417
0.080	138.332	209.057	78.805	282.018	100.845	399.712	44.274	77.606	143.707	86.933	176.934	74.809	282.417
0.090	138.350	208.586	78.776	281.932	100.906	399.712	44.179	77.693	143.725	86.841	176.742	74.914	282.417
0.100	138.367	208.116	78.747	281.846	100.967	399.712	44.083	77.779	143.744	86.750	176.550	75.018	282.417
IFoI	138.691	214.112	95.698	293.958	97.914	399.712	57.412	71.776	147.466	104.581	186.376	76.726	282.417

Table A.2.30. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2616, B=-0.37365, K=20.03955)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	138.489	212.561	79.418	282.241	100.177	399.068	45.392	76.495	143.596	88.402	177.730	74.292	281.538
0.001	138.491	212.514	79.415	282.232	100.183	399.068	45.382	76.504	143.598	88.393	177.710	74.302	281.538
0.002	138.493	212.467	79.412	282.224	100.190	399.068	45.372	76.512	143.600	88.384	177.691	74.312	281.538
0.003	138.494	212.420	79.409	282.215	100.196	399.068	45.363	76.521	143.602	88.375	177.672	74.323	281.538
0.004	138.496	212.373	79.406	282.206	100.202	399.068	45.353	76.530	143.604	88.366	177.653	74.333	281.538
0.005	138.498	212.326	79.403	282.198	100.208	399.068	45.344	76.538	143.606	88.357	177.634	74.344	281.538
0.006	138.500	212.279	79.401	282.189	100.214	399.068	45.334	76.547	143.607	88.348	177.614	74.354	281.538
0.007	138.501	212.232	79.398	282.181	100.220	399.068	45.325	76.555	143.609	88.338	177.595	74.365	281.538
0.008	138.503	212.185	79.395	282.172	100.226	399.068	45.315	76.564	143.611	88.329	177.576	74.375	281.538
0.009	138.505	212.137	79.392	282.163	100.232	399.068	45.305	76.573	143.613	88.320	177.557	74.386	281.538
0.010	138.507	212.090	79.389	282.155	100.238	399.068	45.296	76.581	143.615	88.311	177.538	74.396	281.538
0.020	138.524	211.620	79.360	282.069	100.299	399.068	45.200	76.668	143.634	88.220	177.346	74.501	281.538
0.030	138.541	211.150	79.331	281.983	100.360	399.068	45.104	76.754	143.652	88.128	177.154	74.606	281.538
0.040	138.559	210.679	79.302	281.897	100.421	399.068	45.009	76.840	143.671	88.037	176.961	74.711	281.538
0.050	138.576	210.209	79.273	281.811	100.482	399.068	44.913	76.927	143.690	87.946	176.769	74.815	281.538
0.060	138.594	209.738	79.244	281.725	100.543	399.068	44.817	77.013	143.708	87.854	176.577	74.920	281.538
0.070	138.611	209.268	79.215	281.639	100.604	399.068	44.722	77.099	143.727	87.763	176.385	75.025	281.538
0.080	138.628	208.797	79.187	281.553	100.665	399.068	44.626	77.186	143.746	87.672	176.193	75.130	281.538
0.090	138.646	208.327	79.158	281.467	100.726	399.068	44.530	77.272	143.764	87.580	176.001	75.234	281.538
0.100	138.663	207.857	79.129	281.381	100.787	399.068	44.435	77.358	143.783	87.489	175.809	75.339	281.538
|Fo|	138.625	213.979	95.633	293.706	97.793	399.068	57.311	71.633	147.152	104.353	185.936	76.516	281.538

Table A.2.31. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2620, B=-0.35979, K=20.03738)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	138.793	212.301	79.815	281.759	99.994	398.404	45.739	76.061	143.645	89.162	176.968	74.619	280.632
0.001	138.795	212.254	79.812	281.751	100.000	398.404	45.729	76.070	143.647	89.153	176.949	74.629	280.632
0.002	138.796	212.207	79.809	281.742	100.006	398.404	45.720	76.078	143.649	89.144	176.929	74.640	280.632
0.003	138.798	212.160	79.807	281.733	100.013	398.404	45.710	76.087	143.651	89.135	176.910	74.650	280.632
0.004	138.800	212.113	79.804	281.725	100.019	398.404	45.701	76.096	143.653	89.126	176.891	74.661	280.632
0.005	138.802	212.066	79.801	281.716	100.025	398.404	45.691	76.104	143.655	89.117	176.872	74.671	280.632
0.006	138.803	212.019	79.798	281.708	100.031	398.404	45.681	76.113	143.656	89.108	176.853	74.682	280.632
0.007	138.805	211.972	79.795	281.699	100.037	398.404	45.672	76.122	143.658	89.099	176.833	74.692	280.632
0.008	138.807	211.925	79.792	281.690	100.043	398.404	45.662	76.130	143.660	89.089	176.814	74.703	280.632
0.009	138.809	211.878	79.789	281.682	100.049	398.404	45.653	76.139	143.662	89.080	176.795	74.713	280.632
0.010	138.810	211.831	79.786	281.673	100.055	398.404	45.643	76.148	143.664	89.071	176.776	74.723	280.632
0.020	138.828	211.361	79.757	281.587	100.116	398.404	45.547	76.234	143.683	88.980	176.584	74.828	280.632
0.030	138.845	210.890	79.728	281.501	100.177	398.404	45.452	76.320	143.701	88.888	176.392	74.933	280.632
0.040	138.863	210.420	79.700	281.415	100.238	398.404	45.356	76.407	143.720	88.797	176.200	75.038	280.632
0.050	138.880	209.949	79.671	281.329	100.299	398.404	45.260	76.493	143.739	88.706	176.007	75.142	280.632
0.060	138.897	209.479	79.642	281.243	100.360	398.404	45.165	76.579	143.757	88.614	175.815	75.247	280.632
0.070	138.915	209.008	79.613	281.157	100.421	398.404	45.069	76.665	143.776	88.523	175.623	75.352	280.632
0.080	138.932	208.538	79.584	281.071	100.482	398.404	44.973	76.752	143.795	88.432	175.431	75.457	280.632
0.090	138.950	208.068	79.555	280.985	100.543	398.404	44.878	76.838	143.813	88.341	175.239	75.562	280.632
0.100	138.967	207.597	79.526	280.899	100.604	398.404	44.782	76.924	143.832	88.249	175.047	75.666	280.632
|Fo|	138.556	213.841	95.567	293.445	97.669	398.404	57.207	71.486	146.829	104.119	185.482	76.299	280.632

Table A.2.32. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2624, B=-0.34542, K=20.03534)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	139.110	212.040	80.224	281.261	99.806	397.721	46.082	75.614	143.707	89.946	176.186	74.954	279.698
0.001	139.111	211.993	80.221	281.253	99.812	397.721	46.072	75.623	143.709	89.937	176.167	74.964	279.698
0.002	139.113	211.946	80.218	281.244	99.818	397.721	46.063	75.632	143.711	89.928	176.147	74.974	279.698
0.003	139.115	211.899	80.215	281.235	99.824	397.721	46.053	75.640	143.712	89.919	176.128	74.985	279.698
0.004	139.117	211.852	80.212	281.227	99.830	397.721	46.044	75.649	143.714	89.910	176.109	74.995	279.698
0.005	139.118	211.805	80.209	281.218	99.837	397.721	46.034	75.657	143.716	89.900	176.090	75.006	279.698
0.006	139.120	211.757	80.207	281.210	99.843	397.721	46.025	75.666	143.718	89.891	176.071	75.016	279.698
0.007	139.122	211.710	80.204	281.201	99.849	397.721	46.015	75.675	143.720	89.882	176.051	75.027	279.698
0.008	139.124	211.663	80.201	281.192	99.855	397.721	46.005	75.683	143.722	89.873	176.032	75.037	279.698
0.009	139.125	211.616	80.198	281.184	99.861	397.721	45.996	75.692	143.724	89.864	176.013	75.048	279.698
0.010	139.127	211.569	80.195	281.175	99.867	397.721	45.986	75.701	143.725	89.855	175.994	75.058	279.698
0.020	139.144	211.099	80.166	281.089	99.928	397.721	45.891	75.787	143.744	89.763	175.802	75.163	279.698
0.030	139.162	210.628	80.137	281.003	99.989	397.721	45.795	75.873	143.763	89.672	175.610	75.268	279.698
0.040	139.179	210.158	80.108	280.917	100.050	397.721	45.699	75.960	143.781	89.581	175.418	75.373	279.698
0.050	139.197	209.688	80.079	280.831	100.111	397.721	45.603	76.046	143.800	89.489	175.225	75.477	279.698
0.060	139.214	209.217	80.050	280.745	100.172	397.721	45.508	76.132	143.819	89.398	175.033	75.582	279.698
0.070	139.231	208.747	80.022	280.659	100.233	397.721	45.412	76.219	143.837	89.307	174.841	75.687	279.698
0.080	139.249	208.276	79.993	280.573	100.294	397.721	45.316	76.305	143.856	89.215	174.649	75.792	279.698
0.090	139.266	207.806	79.964	280.487	100.355	397.721	45.221	76.391	143.875	89.124	174.457	75.896	279.698
0.100	139.284	207.335	79.935	280.401	100.416	397.721	45.125	76.478	143.893	89.033	174.265	76.001	279.698
IFoI	138.486	213.701	95.500	293.179	97.540	397.721	57.101	71.335	146.495	103.877	185.014	76.076	279.698

Table A.2.33. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2628, B=-0.33058, K=20.03334)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	139.434	211.778	80.644	280.749	99.613	397.018	46.419	75.156	143.778	90.751	175.385	75.296	278.739
0.001	139.436	211.731	80.641	280.740	99.619	397.018	46.410	75.164	143.780	90.742	175.366	75.306	278.739
0.002	139.438	211.684	80.638	280.732	99.625	397.018	46.400	75.173	143.782	90.733	175.346	75.317	278.739
0.003	139.439	211.637	80.635	280.723	99.631	397.018	46.391	75.182	143.784	90.723	175.327	75.327	278.739
0.004	139.441	211.590	80.632	280.715	99.637	397.018	46.381	75.190	143.786	90.714	175.308	75.338	278.739
0.005	139.443	211.543	80.629	280.706	99.643	397.018	46.372	75.199	143.788	90.705	175.289	75.348	278.739
0.006	139.445	211.496	80.627	280.697	99.649	397.018	46.362	75.207	143.790	90.696	175.270	75.359	278.739
0.007	139.446	211.449	80.624	280.689	99.655	397.018	46.352	75.216	143.791	90.687	175.250	75.369	278.739
0.008	139.448	211.402	80.621	280.680	99.661	397.018	46.343	75.225	143.793	90.678	175.231	75.380	278.739
0.009	139.450	211.355	80.618	280.672	99.668	397.018	46.333	75.233	143.795	90.669	175.212	75.390	278.739
0.010	139.452	211.308	80.615	280.663	99.674	397.018	46.324	75.242	143.797	90.659	175.193	75.401	278.739
0.020	139.469	210.837	80.586	280.577	99.735	397.018	46.228	75.328	143.816	90.568	175.001	75.505	278.739
0.030	139.486	210.367	80.557	280.491	99.796	397.018	46.132	75.415	143.834	90.477	174.809	75.610	278.739
0.040	139.504	209.896	80.528	280.405	99.857	397.018	46.037	75.501	143.853	90.385	174.617	75.715	278.739
0.050	139.521	209.426	80.499	280.319	99.918	397.018	45.941	75.587	143.872	90.294	174.425	75.820	278.739
0.060	139.539	208.955	80.470	280.233	99.979	397.018	45.845	75.674	143.890	90.203	174.232	75.924	278.739
0.070	139.556	208.485	80.442	280.147	100.040	397.018	45.749	75.760	143.909	90.112	174.040	76.029	278.739
0.080	139.573	208.015	80.413	280.061	100.101	397.018	45.654	75.846	143.928	90.020	173.848	76.134	278.739
0.090	139.591	207.544	80.384	279.975	100.162	397.018	45.558	75.933	143.946	89.929	173.656	76.239	278.739
0.100	139.608	207.074	80.355	279.889	100.223	397.018	45.462	76.019	143.965	89.838	173.464	76.343	278.739
|Fo|	138.414	213.557	95.431	292.905	97.409	397.018	56.991	71.179	146.153	103.629	184.533	74.846	278.739

Table A.2.34. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2632, B=-0.31522, K=20.03156)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	139.769	211.514	81.078	280.220	99.416	396.298	46.751	74.686	143.863	91.578	174.564	75.644	277.753
0.001	139.771	211.467	81.075	280.212	99.422	396.298	46.742	74.695	143.864	91.569	174.545	75.654	277.753
0.002	139.772	211.420	81.072	280.203	99.428	396.298	46.732	74.704	143.866	91.560	174.525	75.665	277.753
0.003	139.774	211.373	81.069	280.195	99.434	396.298	46.722	74.712	143.868	91.550	174.506	75.675	277.753
0.004	139.776	211.326	81.066	280.186	99.440	396.298	46.713	74.721	143.870	91.541	174.487	75.686	277.753
0.005	139.778	211.279	81.063	280.177	99.446	396.298	46.703	74.730	143.872	91.532	174.468	75.696	277.753
0.006	139.779	211.232	81.060	280.169	99.453	396.298	46.694	74.738	143.874	91.523	174.449	75.707	277.753
0.007	139.781	211.185	81.057	280.160	99.459	396.298	46.684	74.747	143.876	91.514	174.429	75.717	277.753
0.008	139.783	211.138	81.054	280.152	99.465	396.298	46.675	74.756	143.877	91.505	174.410	75.728	277.753
0.009	139.785	211.090	81.052	280.143	99.471	396.298	46.665	74.764	143.879	91.496	174.391	75.738	277.753
0.010	139.786	211.043	81.049	280.134	99.477	396.298	46.655	74.773	143.881	91.487	174.372	75.748	277.753
0.020	139.804	210.573	81.020	280.048	99.538	396.298	46.560	74.859	143.900	91.395	174.180	75.853	277.753
0.030	139.821	210.103	80.991	279.962	99.599	396.298	46.464	74.945	143.919	91.304	173.988	75.958	277.753
0.040	139.839	209.632	80.962	279.876	99.660	396.298	46.368	75.032	143.937	91.213	173.796	76.063	277.753
0.050	139.856	209.162	80.933	279.790	99.721	396.298	46.273	75.118	143.956	91.121	173.604	76.167	277.753
0.060	139.873	208.691	80.904	279.704	99.782	396.298	46.177	75.204	143.975	91.030	173.411	76.272	277.753
0.070	139.891	208.221	80.875	279.618	99.843	396.298	46.081	75.291	143.993	90.939	173.219	76.377	277.753
0.080	139.908	207.750	80.846	279.532	99.904	396.298	45.986	75.377	144.012	90.847	173.027	76.482	277.753
0.090	139.926	207.280	80.817	279.446	99.965	396.298	45.890	75.463	144.030	90.756	172.835	76.586	277.753
0.100	139.943	206.810	80.788	279.360	100.026	396.298	45.794	75.550	144.049	90.665	172.643	76.691	277.753
IFoI	138.342	213.412	95.360	292.626	97.274	396.298	56.878	71.019	145.801	103.374	184.040	75.611	277.753

Table A.2.35. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2636, B=-0.29943, K=20.02962)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	140.114	211.247	81.525	279.675	99.214	395.557	47.077	74.204	143.958	92.426	173.725	75.997	276.742
0.001	140.116	211.200	81.522	279.667	99.220	395.557	47.068	74.213	143.960	92.417	173.706	76.007	276.742
0.002	140.118	211.153	81.519	279.658	99.226	395.557	47.058	74.222	143.962	92.408	173.687	76.018	276.742
0.003	140.119	211.106	81.516	279.649	99.232	395.557	47.049	74.230	143.964	92.399	173.668	76.028	276.742
0.004	140.121	211.059	81.513	279.641	99.238	395.557	47.039	74.239	143.965	92.389	173.648	76.039	276.742
0.005	140.123	211.012	81.510	279.632	99.245	395.557	47.030	74.247	143.967	92.380	173.629	76.049	276.742
0.006	140.125	210.965	81.508	279.624	99.251	395.557	47.020	74.256	143.969	92.371	173.610	76.060	276.742
0.007	140.126	210.918	81.505	279.615	99.257	395.557	47.010	74.265	143.971	92.362	173.591	76.070	276.742
0.008	140.128	210.871	81.502	279.606	99.263	395.557	47.001	74.273	143.973	92.353	173.572	76.081	276.742
0.009	140.130	210.824	81.499	279.598	99.269	395.557	46.991	74.282	143.975	92.344	173.552	76.091	276.742
0.010	140.132	210.777	81.496	279.589	99.275	395.557	46.982	74.291	143.977	92.335	173.533	76.102	276.742
0.020	140.149	210.307	81.467	279.503	99.336	395.557	46.886	74.377	143.995	92.243	173.341	76.206	276.742
0.030	140.166	209.836	81.438	279.417	99.397	395.557	46.790	74.463	144.014	92.152	173.149	76.311	276.742
0.040	140.184	209.366	81.409	279.331	99.458	395.557	46.695	74.550	144.033	92.061	172.957	76.416	276.742
0.050	140.201	208.895	81.380	279.245	99.519	395.557	46.599	74.636	144.051	91.969	172.765	76.521	276.742
0.060	140.219	208.425	81.351	279.159	99.580	395.557	46.503	74.722	144.070	91.878	172.573	76.625	276.742
0.070	140.236	207.954	81.322	279.073	99.641	395.557	46.407	74.809	144.089	91.787	172.381	76.730	276.742
0.080	140.253	207.484	81.294	278.987	99.702	395.557	46.312	74.895	144.107	91.695	172.189	76.835	276.742
0.090	140.271	207.014	81.265	278.901	99.763	395.557	46.216	74.981	144.126	91.604	171.997	76.940	276.742
0.100	140.288	206.543	81.236	278.815	99.824	395.557	46.120	75.068	144.145	91.513	171.805	77.044	276.742
|Fo|	138.268	213.261	95.288	292.339	97.135	395.557	56.762	70.855	145.439	103.112	183.532	75.369	276.742

Table A.2.36. Calculated and Observed Structure Factors For Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2640, B=-0.28310, K=20.02792)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	140.470	210.981	81.984	279.116	99.007	394.798	47.398	73.710	144.066	93.294	172.869	76.357	275.705
0.001	140.472	210.934	81.981	279.107	99.013	394.798	47.388	73.719	144.068	93.285	172.850	76.367	275.705
0.002	140.473	210.887	81.978	279.099	99.019	394.798	47.379	73.728	144.070	93.276	172.830	76.378	275.705
0.003	140.475	210.840	81.975	279.090	99.025	394.798	47.369	73.736	144.072	93.266	172.811	76.388	275.705
0.004	140.477	210.793	81.972	279.081	99.031	394.798	47.360	73.745	144.073	93.257	172.792	76.399	275.705
0.005	140.479	210.746	81.969	279.073	99.037	394.798	47.350	73.753	144.075	93.248	172.773	76.409	275.705
0.006	140.480	210.699	81.966	279.064	99.044	394.798	47.341	73.762	144.077	93.239	172.753	76.419	275.705
0.007	140.482	210.652	81.963	279.056	99.050	394.798	47.331	73.771	144.079	93.230	172.734	76.430	275.705
0.008	140.484	210.605	81.960	279.047	99.056	394.798	47.321	73.779	144.081	93.221	172.715	76.440	275.705
0.009	140.486	210.558	81.957	279.038	99.062	394.798	47.312	73.788	144.083	93.212	172.696	76.451	275.705
0.010	140.487	210.511	81.955	279.030	99.068	394.798	47.302	73.797	144.085	93.203	172.677	76.461	275.705
0.020	140.505	210.040	81.926	278.944	99.129	394.798	47.207	73.883	144.103	93.111	172.485	76.566	275.705
0.030	140.522	209.570	81.897	278.858	99.190	394.798	47.111	73.969	144.122	93.020	172.293	76.671	275.705
0.040	140.539	209.099	81.868	278.772	99.251	394.798	47.015	74.056	144.141	92.929	172.100	76.776	275.705
0.050	140.557	208.629	81.839	278.686	99.312	394.798	46.919	74.142	144.159	92.837	171.908	76.880	275.705
0.060	140.574	208.158	81.810	278.600	99.373	394.798	46.824	74.228	144.178	92.746	171.716	76.985	275.705
0.070	140.592	207.688	81.781	278.514	99.434	394.798	46.728	74.315	144.197	92.655	171.524	77.090	275.705
0.080	140.609	207.218	81.752	278.428	99.495	394.798	46.632	74.401	144.215	92.563	171.332	77.195	275.705
0.090	140.626	206.747	81.723	278.342	99.556	394.798	46.537	74.487	144.234	92.472	171.140	77.299	275.705
0.100	140.644	206.277	81.694	278.256	99.617	394.798	46.441	74.574	144.253	92.381	170.948	77.404	275.705
IFoI	138.193	213.109	95.214	292.046	96.993	394.798	56.644	70.686	145.069	102.844	183.012	75.121	275.705

Table A.2.37. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2644, B=-0.26633, K=20.02617)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	140.833	210.712	82.454	278.540	98.798	394.020	47.713	73.206	144.188	94.183	171.995	76.721	274.643
0.001	140.835	210.665	82.451	278.531	98.804	394.020	47.703	73.215	144.190	94.174	171.975	76.731	274.643
0.002	140.837	210.618	82.448	278.523	98.810	394.020	47.694	73.223	144.192	94.165	171.956	76.742	274.643
0.003	140.839	210.571	82.445	278.514	98.817	394.020	47.684	73.232	144.193	94.156	171.937	76.752	274.643
0.004	140.840	210.524	82.442	278.506	98.823	394.020	47.675	73.240	144.195	94.146	171.918	76.763	274.643
0.005	140.842	210.477	82.439	278.497	98.829	394.020	47.665	73.249	144.197	94.137	171.899	76.773	274.643
0.006	140.844	210.430	82.436	278.488	98.835	394.020	47.655	73.258	144.199	94.128	171.879	76.784	274.643
0.007	140.846	210.383	82.433	278.480	98.841	394.020	47.646	73.266	144.201	94.119	171.860	76.794	274.643
0.008	140.847	210.336	82.430	278.471	98.847	394.020	47.636	73.275	144.203	94.110	171.841	76.804	274.643
0.009	140.849	210.289	82.427	278.463	98.853	394.020	47.627	73.284	144.205	94.101	171.822	76.815	274.643
0.010	140.851	210.242	82.425	278.454	98.859	394.020	47.617	73.292	144.207	94.092	171.803	76.825	274.643
0.020	140.868	209.771	82.396	278.368	98.920	394.020	47.521	73.379	144.225	94.000	171.610	76.930	274.643
0.030	140.886	209.301	82.367	278.282	98.981	394.020	47.426	73.465	144.244	93.909	171.418	77.035	274.643
0.040	140.903	208.830	82.338	278.196	99.042	394.020	47.330	73.551	144.262	93.818	171.226	77.140	274.643
0.050	140.920	208.360	82.309	278.110	99.103	394.020	47.234	73.638	144.281	93.726	171.034	77.244	274.643
0.060	140.938	207.890	82.280	278.024	99.164	394.020	47.139	73.724	144.300	93.635	170.842	77.349	274.643
0.070	140.955	207.419	82.251	277.938	99.225	394.020	47.043	73.810	144.318	93.544	170.650	77.454	274.643
0.080	140.973	206.949	82.222	277.852	99.286	394.020	46.947	73.897	144.337	93.452	170.458	77.559	274.643
0.090	140.990	206.478	82.193	277.766	99.347	394.020	46.852	73.983	144.356	93.361	170.266	77.663	274.643
0.100	141.007	206.008	82.164	277.680	99.408	394.020	46.756	74.069	144.374	93.270	170.074	77.768	274.643
|Fo|	138.116	212.952	95.139	291.745	96.848	394.020	56.522	70.514	144.689	102.569	182.480	74.867	274.643

Table A.2.38. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2648, B=-0.24905, K=20.02468)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	141.207	210.441	82.937	277.948	98.584	393.226	48.024	72.691	144.321	95.092	171.103	77.089	273.557
0.001	141.209	210.394	82.934	277.939	98.590	393.226	48.014	72.700	144.323	95.083	171.084	77.100	273.557
0.002	141.211	210.347	82.931	277.931	98.597	393.226	48.004	72.708	144.325	95.073	171.064	77.110	273.557
0.003	141.212	210.300	82.928	277.922	98.603	393.226	47.995	72.717	144.327	95.064	171.045	77.120	273.557
0.004	141.214	210.253	82.926	277.913	98.609	393.226	47.985	72.726	144.328	95.055	171.026	77.131	273.557
0.005	141.216	210.206	82.923	277.905	98.615	393.226	47.976	72.734	144.330	95.046	171.007	77.141	273.557
0.006	141.218	210.159	82.920	277.896	98.621	393.226	47.966	72.743	144.332	95.037	170.987	77.152	273.557
0.007	141.219	210.112	82.917	277.888	98.627	393.226	47.957	72.751	144.334	95.028	170.968	77.162	273.557
0.008	141.221	210.065	82.914	277.879	98.633	393.226	47.947	72.760	144.336	95.019	170.949	77.173	273.557
0.009	141.223	210.018	82.911	277.870	98.639	393.226	47.937	72.769	144.338	95.010	170.930	77.183	273.557
0.010	141.225	209.971	82.908	277.862	98.645	393.226	47.928	72.777	144.340	95.000	170.911	77.194	273.557
0.020	141.242	209.500	82.879	277.776	98.706	393.226	47.832	72.864	144.358	94.909	170.719	77.299	273.557
0.030	141.259	209.030	82.850	277.690	98.767	393.226	47.737	72.950	144.377	94.818	170.527	77.403	273.557
0.040	141.277	208.559	82.821	277.604	98.828	393.226	47.641	73.036	144.396	94.726	170.334	77.508	273.557
0.050	141.294	208.089	82.793	277.518	98.889	393.226	47.545	73.123	144.414	94.635	170.142	77.613	273.557
0.060	141.312	207.618	82.764	277.432	98.950	393.226	47.449	73.209	144.433	94.544	169.950	77.718	273.557
0.070	141.329	207.148	82.735	277.346	99.011	393.226	47.354	73.295	144.452	94.452	169.758	77.822	273.557
0.080	141.346	206.678	82.706	277.260	99.073	393.226	47.258	73.382	144.470	94.361	169.566	77.927	273.557
0.090	141.364	206.207	82.677	277.174	99.134	393.226	47.162	73.468	144.489	94.270	169.374	78.032	273.557
0.100	141.381	205.737	82.648	277.088	99.195	393.226	47.067	73.554	144.508	94.178	169.182	78.137	273.557
|Fo|	138.038	212.794	95.062	291.440	96.700	393.226	56.398	70.338	144.301	102.287	181.935	74.607	273.557

Table A.2.39. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2652, B=-0.23131, K=20.02316)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	141.591	210.167	83.432	277.341	98.365	392.413	48.327	72.164	144.467	96.020	170.197	77.463	272.448
0.001	141.593	210.120	83.429	277.333	98.371	392.413	48.318	72.173	144.469	96.011	170.177	77.473	272.448
0.002	141.595	210.073	83.426	277.324	98.378	392.413	48.308	72.182	144.470	96.002	170.158	77.484	272.448
0.003	141.597	210.026	83.423	277.316	98.384	392.413	48.299	72.190	144.472	95.993	170.139	77.494	272.448
0.004	141.598	209.979	83.421	277.307	98.390	392.413	48.289	72.199	144.474	95.984	170.120	77.505	272.448
0.005	141.600	209.932	83.418	277.298	98.396	392.413	48.279	72.208	144.476	95.975	170.101	77.515	272.448
0.006	141.602	209.885	83.415	277.290	98.402	392.413	48.270	72.216	144.478	95.966	170.081	77.526	272.448
0.007	141.604	209.838	83.412	277.281	98.408	392.413	48.260	72.225	144.480	95.957	170.062	77.536	272.448
0.008	141.605	209.791	83.409	277.273	98.414	392.413	48.251	72.233	144.482	95.947	170.043	77.547	272.448
0.009	141.607	209.744	83.406	277.264	98.420	392.413	48.241	72.242	144.483	95.938	170.024	77.557	272.448
0.010	141.609	209.697	83.403	277.255	98.426	392.413	48.232	72.251	144.485	95.929	170.005	77.568	272.448
0.020	141.626	209.227	83.374	277.169	98.487	392.413	48.136	72.337	144.504	95.838	169.813	77.672	272.448
0.030	141.644	208.756	83.345	277.083	98.548	392.413	48.040	72.423	144.523	95.746	169.620	77.777	272.448
0.040	141.661	208.286	83.316	276.997	98.609	392.413	47.944	72.510	144.541	95.655	169.428	77.882	272.448
0.050	141.678	207.815	83.288	276.911	98.670	392.413	47.849	72.596	144.560	95.564	169.236	77.987	272.448
0.060	141.696	207.345	83.259	276.825	98.731	392.413	47.753	72.682	144.579	95.472	169.044	78.091	272.448
0.070	141.713	206.874	83.230	276.739	98.792	392.413	47.657	72.769	144.597	95.381	168.852	78.196	272.448
0.080	141.731	206.404	83.201	276.653	98.853	392.413	47.562	72.855	144.616	95.290	168.660	78.301	272.448
0.090	141.748	205.934	83.172	276.567	98.915	392.413	47.466	72.941	144.635	95.199	168.468	78.406	272.448
0.100	141.765	205.463	83.143	276.481	98.976	392.413	47.370	73.028	144.653	95.107	168.276	78.510	272.448
|Fo|	137.959	212.632	94.984	291.128	96.548	392.413	56.271	70.157	143.904	102.000	181.378	74.342	272.448

Table A.2.40. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2656, B=0.21306, K=20.02186)

	|Fcl												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	141.986	209.894	83.938	276.720	98.145	391.584	48.624	71.629	144.626	96.968	169.274	77.840	271.315
0.001	141.988	209.847	83.826	276.712	98.151	391.584	48.614	71.637	144.628	96.959	169.255	77.850	271.315
0.002	141.989	209.800	83.714	276.703	98.157	391.584	48.605	71.646	144.630	96.949	169.236	77.861	271.315
0.003	141.991	209.753	83.602	276.695	98.163	391.584	48.595	71.655	144.632	96.940	169.216	77.871	271.315
0.004	141.993	209.706	83.490	276.686	98.169	391.584	48.586	71.663	144.634	96.931	169.197	77.882	271.315
0.005	141.995	209.659	83.378	276.677	98.175	391.584	48.576	71.672	144.636	96.922	169.178	77.892	271.315
0.006	141.996	209.612	83.266	276.669	98.181	391.584	48.567	71.680	144.637	96.913	169.159	77.903	271.315
0.007	141.998	209.565	83.154	276.660	98.187	391.584	48.557	71.689	144.639	96.904	169.140	77.913	271.315
0.008	142.000	209.518	83.042	276.652	98.193	391.584	48.547	71.698	144.641	96.895	169.120	77.924	271.315
0.009	142.002	209.470	82.930	276.643	98.200	391.584	48.538	71.706	144.643	96.886	169.101	77.934	271.315
0.010	142.003	209.423	82.818	276.634	98.206	391.584	48.528	71.715	144.645	96.876	169.082	77.945	271.315
0.020	142.021	208.953	81.697	276.548	98.267	391.584	48.433	71.801	144.663	96.785	168.890	78.049	271.315
0.030	142.038	208.483	80.576	276.462	98.328	391.584	48.337	71.888	144.682	96.694	168.698	78.154	271.315
0.040	142.056	208.012	79.456	276.376	98.389	391.584	48.241	71.974	144.701	96.602	168.506	78.259	271.315
0.050	142.073	207.542	78.335	276.290	98.450	391.584	48.145	72.060	144.719	96.511	168.314	78.364	271.315
0.060	142.090	207.071	77.214	276.204	98.511	391.584	48.050	72.147	144.738	96.420	168.122	78.468	271.315
0.070	142.108	206.601	76.093	276.118	98.572	391.584	47.954	72.233	144.757	96.328	167.930	78.573	271.315
0.080	142.125	206.130	74.973	276.032	98.633	391.584	47.858	72.319	144.775	96.237	167.738	78.678	271.315
0.090	142.143	205.660	73.852	275.946	98.694	391.584	47.763	72.406	144.794	96.146	167.546	78.783	271.315
0.100	142.160	205.190	72.731	275.860	98.755	391.584	47.667	72.492	144.813	96.054	167.353	78.887	271.315
|Fol	137.879	212.469	94.905	290.810	96.393	391.584	56.141	69.973	143.499	101.706	180.809	74.070	271.315

Table A.2.41. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2660, B=-0.19431, K=20.02070)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	142.391	209.616	84.458	276.083	97.921	390.736	48.916	71.082	144.798	97.934	168.336	78.220	270.157
0.001	142.393	209.569	84.455	276.075	97.927	390.736	48.907	71.091	144.800	97.925	168.317	78.231	270.157
0.002	142.394	209.522	84.453	276.066	97.933	390.736	48.897	71.100	144.802	97.915	168.298	78.241	270.157
0.003	142.396	209.474	84.450	276.057	97.939	390.736	48.888	71.108	144.804	97.906	168.279	78.252	270.157
0.004	142.398	209.427	84.447	276.049	97.945	390.736	48.878	71.117	144.806	97.897	168.259	78.262	270.157
0.005	142.400	209.380	84.444	276.040	97.951	390.736	48.869	71.126	144.808	97.888	168.240	78.273	270.157
0.006	142.401	209.333	84.441	276.032	97.957	390.736	48.859	71.134	144.809	97.879	168.221	78.283	270.157
0.007	142.403	209.286	84.438	276.023	97.963	390.736	48.849	71.143	144.811	97.870	168.202	78.294	270.157
0.008	142.405	209.239	84.435	276.014	97.969	390.736	48.840	71.151	144.813	97.861	168.183	78.304	270.157
0.009	142.407	209.192	84.432	276.006	97.975	390.736	48.830	71.160	144.815	97.851	168.163	78.315	270.157
0.010	142.408	209.145	84.429	275.997	97.982	390.736	48.821	71.169	144.817	97.842	168.144	78.325	270.157
0.020	142.426	208.675	84.401	275.911	98.043	390.736	48.725	71.255	144.836	97.751	167.952	78.430	270.157
0.030	142.443	208.204	84.372	275.825	98.104	390.736	48.629	71.341	144.854	97.660	167.760	78.534	270.157
0.040	142.461	207.734	84.343	275.739	98.165	390.736	48.534	71.428	144.873	97.568	167.568	78.639	270.157
0.050	142.478	207.263	84.314	275.653	98.226	390.736	48.438	71.514	144.892	97.477	167.376	78.744	270.157
0.060	142.495	206.793	84.285	275.567	98.287	390.736	48.342	71.600	144.910	97.386	167.184	78.849	270.157
0.070	142.513	206.323	84.256	275.481	98.348	390.736	48.246	71.687	144.929	97.294	166.992	78.953	270.157
0.080	142.530	205.852	84.227	275.395	98.409	390.736	48.151	71.773	144.948	97.203	166.800	79.058	270.157
0.090	142.548	205.382	84.198	275.309	98.470	390.736	48.055	71.859	144.966	97.112	166.608	79.163	270.157
0.100	142.565	204.911	84.169	275.223	98.531	390.736	47.959	71.946	144.985	97.020	166.416	79.268	270.157
IFoI	137.799	212.303	94.824	290.487	96.235	390.736	56.009	69.784	143.084	101.406	180.228	73.793	270.157

Table A.2.42. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2664, B=-0.17510, K=20.01962)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	142.804	209.337	84.990	275.430	97.693	389.873	49.202	70.526	144.984	98.918	167.385	78.604	268.979
0.001	142.805	209.290	84.987	275.421	97.699	389.873	49.192	70.534	144.986	98.909	167.366	78.614	268.979
0.002	142.807	209.243	84.984	275.412	97.705	389.873	49.183	70.543	144.988	98.900	167.347	78.625	268.979
0.003	142.809	209.196	84.981	275.404	97.711	389.873	49.173	70.552	144.990	98.891	167.328	78.635	268.979
0.004	142.811	209.149	84.978	275.395	97.717	389.873	49.164	70.560	144.992	98.882	167.308	78.646	268.979
0.005	142.812	209.102	84.975	275.387	97.723	389.873	49.154	70.569	144.993	98.872	167.289	78.656	268.979
0.006	142.814	209.055	84.972	275.378	97.730	389.873	49.144	70.578	144.995	98.863	167.270	78.667	268.979
0.007	142.816	209.008	84.969	275.369	97.736	389.873	49.135	70.586	144.997	98.854	167.251	78.677	268.979
0.008	142.818	208.961	84.966	275.361	97.742	389.873	49.125	70.595	144.999	98.845	167.232	78.688	268.979
0.009	142.819	208.914	84.964	275.352	97.748	389.873	49.116	70.603	145.001	98.836	167.212	78.698	268.979
0.010	142.821	208.867	84.961	275.344	97.754	389.873	49.106	70.612	145.003	98.827	167.193	78.709	268.979
0.020	142.838	208.397	84.932	275.258	97.815	389.873	49.010	70.698	145.021	98.736	167.001	78.813	268.979
0.030	142.856	207.926	84.903	275.172	97.876	389.873	48.915	70.785	145.040	98.644	166.809	78.918	268.979
0.040	142.873	207.456	84.874	275.086	97.937	389.873	48.819	70.871	145.059	98.553	166.617	79.023	268.979
0.050	142.891	206.985	84.845	275.000	97.998	389.873	48.723	70.957	145.077	98.462	166.425	79.128	268.979
0.060	142.908	206.515	84.816	274.914	98.059	389.873	48.628	71.044	145.096	98.370	166.233	79.232	268.979
0.070	142.925	206.044	84.787	274.828	98.120	389.873	48.532	71.130	145.115	98.279	166.041	79.337	268.979
0.080	142.943	205.574	84.758	274.742	98.181	389.873	48.436	71.216	145.133	98.188	165.849	79.442	268.979
0.090	142.960	205.104	84.729	274.656	98.242	389.873	48.340	71.303	145.152	98.096	165.657	79.547	268.979
0.100	142.978	204.633	84.701	274.570	98.303	389.873	48.245	71.389	145.171	98.005	165.465	79.651	268.979
|Fo|	137.717	212.134	94.743	290.159	96.075	389.873	55.874	69.593	142.662	101.100	179.635	73.511	268.979

Table A.2.43. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2667, B=-0.16035, K=20.01899)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	143.120	209.127	85.396	274.930	97.520	389.215	49.411	70.102	145.132	99.668	166.662	78.893	268.080
0.001	143.122	209.080	85.393	274.921	97.526	389.215	49.402	70.111	145.134	99.659	166.643	78.904	268.080
0.002	143.124	209.033	85.390	274.912	97.532	389.215	49.392	70.120	145.136	99.650	166.624	78.914	268.080
0.003	143.126	208.986	85.387	274.904	97.538	389.215	49.383	70.128	145.138	99.641	166.605	78.924	268.080
0.004	143.127	208.939	85.384	274.895	97.545	389.215	49.373	70.137	145.140	99.632	166.585	78.935	268.080
0.005	143.129	208.892	85.382	274.887	97.551	389.215	49.364	70.146	145.142	99.623	166.566	78.945	268.080
0.006	143.131	208.845	85.379	274.878	97.557	389.215	49.354	70.154	145.144	99.614	166.547	78.956	268.080
0.007	143.133	208.798	85.376	274.869	97.563	389.215	49.344	70.163	145.145	99.604	166.528	78.966	268.080
0.008	143.134	208.751	85.373	274.861	97.569	389.215	49.335	70.171	145.147	99.595	166.509	78.977	268.080
0.009	143.136	208.704	85.370	274.852	97.575	389.215	49.325	70.180	145.149	99.586	166.489	78.987	268.080
0.010	143.138	208.657	85.367	274.844	97.581	389.215	49.316	70.189	145.151	99.577	166.470	78.998	268.080
0.020	143.155	208.187	85.338	274.758	97.642	389.215	49.220	70.275	145.170	99.486	166.278	79.103	268.080
0.030	143.173	207.716	85.309	274.672	97.703	389.215	49.124	70.361	145.188	99.394	166.086	79.207	268.080
0.040	143.190	207.246	85.280	274.586	97.764	389.215	49.029	70.448	145.207	99.303	165.894	79.312	268.080
0.050	143.207	206.775	85.251	274.500	97.825	389.215	48.933	70.534	145.226	99.212	165.702	79.417	268.080
0.060	143.225	206.305	85.223	274.414	97.886	389.215	48.837	70.620	145.244	99.120	165.510	79.522	268.080
0.070	143.242	205.835	85.194	274.328	97.947	389.215	48.741	70.707	145.263	99.029	165.318	79.626	268.080
0.080	143.260	205.364	85.165	274.242	98.008	389.215	48.646	70.793	145.282	98.938	165.126	79.731	268.080
0.090	143.277	204.894	85.136	274.156	98.069	389.215	48.550	70.879	145.300	98.846	164.934	79.836	268.080
0.100	143.294	204.423	85.107	274.070	98.130	389.215	48.454	70.966	145.319	98.755	164.742	79.941	268.080
IFoI	137.656	212.006	94.681	289.909	95.952	389.215	55.771	69.446	142.340	100.866	179.183	73.296	268.080

Table A.2.44. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2668, B=-0.15537, K=20.01880)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	143.227	209.057	85.532	274.762	97.462	388.993	49.480	69.960	145.184	99.920	166.419	78.989	267.777
0.001	143.229	209.010	85.529	274.753	97.468	388.993	49.471	69.969	145.186	99.911	166.400	79.000	267.777
0.002	143.230	208.963	85.526	274.744	97.474	388.993	49.461	69.977	145.188	99.902	166.381	79.010	267.777
0.003	143.232	208.916	85.524	274.736	97.480	388.993	49.452	69.986	145.189	99.893	166.361	79.021	267.777
0.004	143.234	208.869	85.521	274.727	97.486	388.993	49.442	69.994	145.191	99.883	166.342	79.031	267.777
0.005	143.236	208.822	85.518	274.719	97.492	388.993	49.432	70.003	145.193	99.874	166.323	79.042	267.777
0.006	143.237	208.774	85.515	274.710	97.499	388.993	49.423	70.012	145.195	99.865	166.304	79.052	267.777
0.007	143.239	208.727	85.512	274.701	97.505	388.993	49.413	70.020	145.197	99.856	166.284	79.063	267.777
0.008	143.241	208.680	85.509	274.693	97.511	388.993	49.404	70.029	145.199	99.847	166.265	79.073	267.777
0.009	143.242	208.633	85.506	274.684	97.517	388.993	49.394	70.038	145.201	99.838	166.246	79.084	267.777
0.010	143.244	208.586	85.503	274.676	97.523	388.993	49.385	70.046	145.202	99.829	166.227	79.094	267.777
0.020	143.262	208.116	85.474	274.590	97.584	388.993	49.289	70.133	145.221	99.737	166.035	79.199	267.777
0.030	143.279	207.645	85.446	274.504	97.645	388.993	49.193	70.219	145.240	99.646	165.843	79.304	267.777
0.040	143.296	207.175	85.417	274.418	97.706	388.993	49.097	70.305	145.258	99.555	165.651	79.409	267.777
0.050	143.314	206.705	85.388	274.332	97.767	388.993	49.002	70.392	145.277	99.463	165.459	79.513	267.777
0.060	143.331	206.234	85.359	274.246	97.828	388.993	48.906	70.478	145.296	99.372	165.267	79.618	267.777
0.070	143.349	205.764	85.330	274.160	97.889	388.993	48.810	70.564	145.314	99.281	165.074	79.723	267.777
0.080	143.366	205.293	85.301	274.074	97.950	388.993	48.715	70.651	145.333	99.189	164.882	79.828	267.777
0.090	143.383	204.823	85.272	273.988	98.011	388.993	48.619	70.737	145.352	99.098	164.690	79.932	267.777
0.100	143.401	204.352	85.243	273.902	98.072	388.993	48.523	70.823	145.370	99.007	164.498	80.037	267.777
IFoI	137.635	211.964	94.660	289.825	95.911	388.993	55.736	69.397	142.232	100.788	179.031	73.223	267.777

Table A.2.45. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2669, B=-0.15032, K=20.01877)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	143.333	208.986	85.671	274.594	97.404	388.772	49.549	69.817	145.235	100.174	166.176	79.087	267.473
0.001	143.335	208.939	85.668	274.585	97.410	388.772	49.540	69.826	145.237	100.165	166.156	79.097	267.473
0.002	143.337	208.892	85.665	274.576	97.416	388.772	49.530	69.835	145.239	100.156	166.137	79.108	267.473
0.003	143.338	208.845	85.662	274.568	97.422	388.772	49.520	69.843	145.241	100.147	166.118	79.118	267.473
0.004	143.340	208.798	85.659	274.559	97.428	388.772	49.511	69.852	145.243	100.138	166.099	79.129	267.473
0.005	143.342	208.751	85.656	274.551	97.434	388.772	49.501	69.861	145.245	100.129	166.080	79.139	267.473
0.006	143.344	208.704	85.653	274.542	97.440	388.772	49.492	69.869	145.247	100.119	166.060	79.150	267.473
0.007	143.345	208.657	85.651	274.533	97.446	388.772	49.482	69.878	145.248	100.110	166.041	79.160	267.473
0.008	143.347	208.610	85.648	274.525	97.453	388.772	49.473	69.887	145.250	100.101	166.022	79.171	267.473
0.009	143.349	208.563	85.645	274.516	97.459	388.772	49.463	69.895	145.252	100.092	166.003	79.181	267.473
0.010	143.351	208.516	85.642	274.508	97.465	388.772	49.453	69.904	145.254	100.083	165.984	79.192	267.473
0.020	143.368	208.045	85.613	274.422	97.526	388.772	49.358	69.990	145.273	99.992	165.791	79.297	267.473
0.030	143.385	207.575	85.584	274.336	97.587	388.772	49.262	70.076	145.291	99.900	165.599	79.401	267.473
0.040	143.403	207.104	85.555	274.250	97.648	388.772	49.166	70.163	145.310	99.809	165.407	79.506	267.473
0.050	143.420	206.634	85.526	274.164	97.709	388.772	49.071	70.249	145.329	99.718	165.215	79.611	267.473
0.060	143.438	206.163	85.497	274.078	97.770	388.772	48.975	70.335	145.347	99.626	165.023	79.716	267.473
0.070	143.455	205.693	85.468	273.992	97.831	388.772	48.879	70.422	145.366	99.535	164.831	79.820	267.473
0.080	143.472	205.223	85.439	273.906	97.892	388.772	48.783	70.508	145.385	99.444	164.639	79.925	267.473
0.090	143.490	204.752	85.411	273.820	97.953	388.772	48.688	70.594	145.403	99.352	164.447	80.030	267.473
0.100	143.507	204.282	85.382	273.734	98.014	388.772	48.592	70.681	145.422	99.261	164.255	80.135	267.473
IFoI	137.616	211.922	94.640	289.742	95.870	388.772	55.701	69.348	142.123	100.709	178.879	73.150	267.473

Table A.2.46. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2670, B=-0.14533, K=20.01846)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	143.442	208.915	85.809	274.421	97.344	388.548	49.618	69.674	145.288	100.428	165.932	79.183	267.169
0.001	143.444	208.868	85.806	274.413	97.350	388.548	49.608	69.682	145.290	100.419	165.913	79.194	267.169
0.002	143.446	208.821	85.803	274.404	97.356	388.548	49.599	69.691	145.292	100.410	165.894	79.204	267.169
0.003	143.447	208.774	85.801	274.396	97.362	388.548	49.589	69.700	145.294	100.401	165.875	79.215	267.169
0.004	143.449	208.727	85.798	274.387	97.368	388.548	49.580	69.708	145.296	100.392	165.855	79.225	267.169
0.005	143.451	208.680	85.795	274.378	97.374	388.548	49.570	69.717	145.297	100.383	165.836	79.236	267.169
0.006	143.453	208.633	85.792	274.370	97.381	388.548	49.561	69.726	145.299	100.374	165.817	79.246	267.169
0.007	143.454	208.586	85.789	274.361	97.387	388.548	49.551	69.734	145.301	100.364	165.798	79.257	267.169
0.008	143.456	208.539	85.786	274.353	97.393	388.548	49.541	69.743	145.303	100.355	165.779	79.267	267.169
0.009	143.458	208.492	85.783	274.344	97.399	388.548	49.532	69.751	145.305	100.346	165.759	79.278	267.169
0.010	143.460	208.445	85.780	274.335	97.405	388.548	49.522	69.760	145.307	100.337	165.740	79.288	267.169
0.020	143.477	207.974	85.751	274.249	97.466	388.548	49.427	69.846	145.325	100.246	165.548	79.393	267.169
0.030	143.494	207.504	85.723	274.163	97.527	388.548	49.331	69.933	145.344	100.154	165.356	79.498	267.169
0.040	143.512	207.034	85.694	274.077	97.588	388.548	49.235	70.019	145.363	100.063	165.164	79.602	267.169
0.050	143.529	206.563	85.665	273.991	97.649	388.548	49.139	70.105	145.381	99.972	164.972	79.707	267.169
0.060	143.547	206.093	85.636	273.905	97.710	388.548	49.044	70.192	145.400	99.880	164.780	79.812	267.169
0.070	143.564	205.622	85.607	273.819	97.771	388.548	48.948	70.278	145.419	99.789	164.588	79.917	267.169
0.080	143.581	205.152	85.578	273.733	97.832	388.548	48.852	70.364	145.437	99.698	164.396	80.021	267.169
0.090	143.599	204.681	85.549	273.647	97.893	388.548	48.757	70.451	145.456	99.606	164.204	80.126	267.169
0.100	143.616	204.211	85.520	273.561	97.954	388.548	48.661	70.537	145.475	99.515	164.012	80.231	267.169
|Fo|	137.594	211.878	94.618	289.657	95.828	388.548	55.666	69.298	142.014	100.63	178.725	73.077	267.169

Table A.2.47. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2671, B=-0.14026, K=20.01836)

	IFcI												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	143.551	208.845	85.948	274.251	97.286	388.323	49.686	69.530	145.342	100.684	165.687	79.281	266.862
0.001	143.553	208.797	85.836	274.243	97.292	388.323	49.676	69.539	145.344	100.675	165.667	79.291	266.862
0.002	143.555	208.750	85.724	274.234	97.298	388.323	49.666	69.547	145.346	100.666	165.648	79.302	266.862
0.003	143.557	208.703	85.612	274.226	97.304	388.323	49.657	69.556	145.348	100.656	165.629	79.312	266.862
0.004	143.558	208.656	85.499	274.217	97.310	388.323	49.647	69.565	145.350	100.647	165.610	79.323	266.862
0.005	143.560	208.609	85.387	274.208	97.316	388.323	49.638	69.573	145.351	100.638	165.591	79.333	266.862
0.006	143.562	208.562	85.275	274.200	97.322	388.323	49.628	69.582	145.353	100.629	165.571	79.344	266.862
0.007	143.563	208.515	85.163	274.191	97.328	388.323	49.619	69.590	145.355	100.620	165.552	79.354	266.862
0.008	143.565	208.468	85.051	274.183	97.335	388.323	49.609	69.599	145.357	100.611	165.533	79.365	266.862
0.009	143.567	208.421	84.939	274.174	97.341	388.323	49.599	69.608	145.359	100.602	165.514	79.375	266.862
0.010	143.569	208.374	84.827	274.165	97.347	388.323	49.590	69.616	145.361	100.592	165.494	79.386	266.862
0.020	143.586	207.904	83.706	274.079	97.408	388.323	49.494	69.703	145.379	100.501	165.302	79.490	266.862
0.030	143.604	207.433	82.586	273.993	97.469	388.323	49.398	69.789	145.398	100.410	165.110	79.595	266.862
0.040	143.621	206.963	81.465	273.907	97.530	388.323	49.303	69.875	145.417	100.318	164.918	79.700	266.862
0.050	143.638	206.492	80.344	273.821	97.591	388.323	49.207	69.962	145.435	100.227	164.726	79.805	266.862
0.060	143.656	206.022	79.223	273.735	97.652	388.323	49.111	70.048	145.454	100.136	164.534	79.909	266.862
0.070	143.673	205.552	78.103	273.649	97.713	388.323	49.016	70.134	145.473	100.045	164.342	80.014	266.862
0.080	143.691	205.081	76.982	273.563	97.774	388.323	48.920	70.221	145.491	99.953	164.150	80.119	266.862
0.090	143.708	204.611	75.861	273.477	97.835	388.323	48.824	70.307	145.510	99.862	163.958	80.224	266.862
0.100	143.725	204.140	74.741	273.391	97.896	388.323	48.728	70.393	145.529	99.771	163.766	80.328	266.862
IFoI	137.574	211.835	94.597	289.572	95.786	388.323	55.631	69.248	141.904	100.550	178.151	73.004	266.862

Table A.2.48. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2672, B=-0.13514, K=20.01824)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	143.660	208.774	86.086	274.079	97.228	388.099	49.753	69.385	145.396	100.940	165.441	79.378	266.555
0.001	143.662	208.727	86.083	274.071	97.234	388.099	49.743	69.394	145.398	100.931	165.422	79.389	266.555
0.002	143.664	208.680	86.080	274.062	97.240	388.099	49.734	69.402	145.400	100.922	165.402	79.399	266.555
0.003	143.666	208.633	86.078	274.053	97.246	388.099	49.724	69.411	145.402	100.913	165.383	79.410	266.555
0.004	143.667	208.586	86.075	274.045	97.252	388.099	49.715	69.419	145.404	100.904	165.364	79.420	266.555
0.005	143.669	208.539	86.072	274.036	97.258	388.099	49.705	69.428	145.405	100.895	165.345	79.431	266.555
0.006	143.671	208.492	86.069	274.028	97.264	388.099	49.696	69.437	145.407	100.886	165.326	79.441	266.555
0.007	143.673	208.444	86.066	274.019	97.270	388.099	49.686	69.445	145.409	100.877	165.306	79.452	266.555
0.008	143.674	208.397	86.063	274.010	97.276	388.099	49.676	69.454	145.411	100.867	165.287	79.462	266.555
0.009	143.676	208.350	86.060	274.002	97.282	388.099	49.667	69.463	145.413	100.858	165.268	79.473	266.555
0.010	143.678	208.303	86.057	273.993	97.289	388.099	49.657	69.471	145.415	100.849	165.249	79.483	266.555
0.020	143.695	207.833	86.028	273.907	97.350	388.099	49.562	69.558	145.433	100.758	165.057	79.588	266.555
0.030	143.713	207.362	86.000	273.821	97.411	388.099	49.466	69.644	145.452	100.666	164.865	79.693	266.555
0.040	143.730	206.892	85.971	273.735	97.472	388.099	49.370	69.730	145.471	100.575	164.673	79.797	266.555
0.050	143.747	206.422	85.942	273.649	97.533	388.099	49.274	69.817	145.489	100.484	164.481	79.902	266.555
0.060	143.765	205.951	85.913	273.563	97.594	388.099	49.179	69.903	145.508	100.392	164.288	80.007	266.555
0.070	143.782	205.481	85.884	273.477	97.655	388.099	49.083	69.989	145.527	100.301	164.096	80.112	266.555
0.080	143.800	205.010	85.855	273.391	97.716	388.099	48.987	70.076	145.545	100.210	163.904	80.216	266.555
0.090	143.817	204.540	85.826	273.305	97.777	388.099	48.892	70.162	145.564	100.119	163.712	80.321	266.555
0.100	143.834	204.070	85.797	273.219	97.838	388.099	48.796	70.248	145.583	100.027	163.520	80.426	266.555
|Fo|	137.553	211.792	94.577	289.488	95.745	388.099	55.596	69.198	141.794	100.470	178.417	72.930	266.555

Table A.2.49. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2676, B=-0.11440, K=20.01788)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	144.102	208.488	86.654	273.380	96.991	387.188	50.020	68.802	145.515	101.977	164.451	79.767	265.310
0.001	144.103	208.441	86.651	273.372	96.998	387.188	50.011	68.811	145.517	101.968	164.432	79.778	265.310
0.002	144.105	208.394	86.648	273.363	97.004	387.188	50.001	68.819	145.519	101.959	164.413	79.788	265.310
0.003	144.107	208.347	86.645	273.355	97.010	387.188	49.991	68.828	145.521	101.950	164.393	79.799	265.310
0.004	144.109	208.300	86.642	273.346	97.016	387.188	49.982	68.837	145.523	101.941	164.374	79.809	265.310
0.005	144.110	208.253	86.639	273.337	97.022	387.188	49.972	68.845	145.525	101.931	164.355	79.820	265.310
0.006	144.112	208.206	86.637	273.329	97.028	387.188	49.963	68.854	145.527	101.922	164.336	79.830	265.310
0.007	144.114	208.159	86.634	273.320	97.034	387.188	49.953	68.863	145.528	101.913	164.316	79.841	265.310
0.008	144.116	208.112	86.631	273.312	97.040	387.188	49.944	68.871	145.530	101.904	164.297	79.851	265.310
0.009	144.117	208.065	86.628	273.303	97.046	387.188	49.934	68.880	145.532	101.895	164.278	79.862	265.310
0.010	144.119	208.018	86.625	273.294	97.052	387.188	49.924	68.888	145.534	101.886	164.259	79.872	265.310
0.020	144.136	207.548	86.596	273.208	97.113	387.188	49.829	68.975	145.553	101.794	164.067	79.977	265.310
0.030	144.154	207.077	86.567	273.122	97.174	387.188	49.733	69.061	145.571	101.703	163.875	80.082	265.310
0.040	144.171	206.607	86.538	273.036	97.235	387.188	49.637	69.147	145.590	101.612	163.683	80.186	265.310
0.050	144.189	206.136	86.509	272.950	97.297	387.188	49.542	69.234	145.609	101.520	163.491	80.291	265.310
0.060	144.206	205.666	86.480	272.864	97.358	387.188	49.446	69.320	145.627	101.429	163.299	80.396	265.310
0.070	144.223	205.195	86.452	272.778	97.419	387.188	49.350	69.406	145.646	101.338	163.106	80.501	265.310
0.080	144.241	204.725	86.423	272.692	97.480	387.188	49.254	69.493	145.665	101.246	162.914	80.605	265.310
0.090	144.258	204.255	86.394	272.606	97.541	387.188	49.159	69.579	145.683	101.155	162.722	80.710	265.310
0.100	144.276	203.784	86.365	272.520	97.602	387.188	49.063	69.665	145.702	101.064	162.530	80.815	265.310
|Fo|	137.471	211.619	94.492	289.145	95.576	387.188	55.453	68.995	141.348	100.147	177.791	72.632	265.310

Table A.2.50. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2680, B=-0.09324, K=20.01752)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	144.553	208.203	87.231	272.667	96.752	386.261	50.280	68.209	145.276	103.030	163.448	80.159	264.046
0.001	144.555	208.156	87.228	272.659	96.758	386.261	50.271	68.218	145.277	103.021	163.429	80.169	264.046
0.002	144.557	208.109	87.225	272.650	96.764	386.261	50.261	68.226	145.279	103.011	163.410	80.180	264.046
0.003	144.559	208.062	87.222	272.642	96.770	386.261	50.252	68.235	145.281	103.002	163.390	80.190	264.046
0.004	144.560	208.015	87.219	272.633	96.776	386.261	50.242	68.243	145.283	102.993	163.371	80.200	264.046
0.005	144.562	207.968	87.216	272.624	96.782	386.261	50.232	68.252	145.285	102.984	163.352	80.211	264.046
0.006	144.564	207.921	87.213	272.616	96.789	386.261	50.223	68.261	145.287	102.975	163.333	80.221	264.046
0.007	144.566	207.874	87.210	272.607	96.795	386.261	50.213	68.269	145.289	102.966	163.314	80.232	264.046
0.008	144.567	207.827	87.207	272.599	96.801	386.261	50.204	68.278	145.290	102.957	163.294	80.242	264.046
0.009	144.569	207.780	87.205	272.590	96.807	386.261	50.194	68.287	145.292	102.948	163.275	80.253	264.046
0.010	144.571	207.733	87.202	272.581	96.813	386.261	50.185	68.295	145.294	102.938	163.256	80.263	264.046
0.020	144.588	207.262	87.173	272.495	96.874	386.261	50.089	68.382	145.313	102.847	163.064	80.368	264.046
0.030	144.606	206.792	87.144	272.409	96.935	386.261	49.993	68.468	145.331	102.756	162.872	80.473	264.046
0.040	144.623	206.321	87.115	272.323	96.996	386.261	49.897	68.554	145.350	102.664	162.680	80.578	264.046
0.050	144.640	205.851	87.086	272.237	97.057	386.261	49.802	68.641	145.369	102.573	162.488	80.682	264.046
0.060	144.658	205.381	87.057	272.151	97.118	386.261	49.706	68.727	145.387	102.482	162.296	80.787	264.046
0.070	144.675	204.910	87.028	272.065	97.179	386.261	49.610	68.813	145.406	102.390	162.104	80.892	264.046
0.080	144.693	204.440	86.999	271.979	97.240	386.261	49.515	68.899	145.425	102.299	161.912	80.997	264.046
0.090	144.710	203.969	86.970	271.893	97.301	386.261	49.419	68.986	145.443	102.208	161.719	81.101	264.046
0.100	144.727	203.499	86.941	271.807	97.362	386.261	49.323	69.072	145.462	102.116	161.527	81.206	264.046
|Fo|	137.387	211.442	94.406	288.797	95.404	386.261	55.308	68.789	140.894	99.818	177.154	72.329	264.046

Table A.2.51: Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2684, B=-0.07152, K=20.01761)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	145.013	207.913	87.821	271.940	96.511	385.321	50.533	67.608	145.021	104.100	162.436	80.550	262.760
0.001	145.015	207.866	87.818	271.931	96.517	385.321	50.524	67.616	145.022	104.091	162.416	80.560	262.760
0.002	145.016	207.819	87.815	271.923	96.523	385.321	50.514	67.625	145.024	104.082	162.397	80.571	262.760
0.003	145.018	207.772	87.812	271.914	96.529	385.321	50.505	67.634	145.026	104.072	162.378	80.581	262.760
0.004	145.020	207.725	87.809	271.906	96.535	385.321	50.495	67.642	145.028	104.063	162.359	80.592	262.760
0.005	145.022	207.678	87.806	271.897	96.541	385.321	50.485	67.651	145.030	104.054	162.340	80.602	262.760
0.006	145.023	207.631	87.804	271.888	96.547	385.321	50.476	67.660	145.032	104.045	162.320	80.613	262.760
0.007	145.025	207.584	87.801	271.880	96.553	385.321	50.466	67.668	145.034	104.036	162.301	80.623	262.760
0.008	145.027	207.537	87.798	271.871	96.559	385.321	50.457	67.677	145.035	104.027	162.282	80.634	262.760
0.009	145.028	207.490	87.795	271.863	96.566	385.321	50.447	67.685	145.037	104.018	162.263	80.644	262.760
0.010	145.030	207.443	87.792	271.854	96.572	385.321	50.438	67.694	145.039	104.008	162.244	80.654	262.760
0.020	145.048	206.972	87.763	271.768	96.633	385.321	50.342	67.780	145.058	103.917	162.052	80.759	262.760
0.030	145.065	206.502	87.734	271.682	96.694	385.321	50.246	67.867	145.077	103.826	161.859	80.864	262.760
0.040	145.082	206.031	87.705	271.596	96.755	385.321	50.151	67.953	145.095	103.734	161.667	80.969	262.760
0.050	145.100	205.561	87.676	271.510	96.816	385.321	50.055	68.039	145.114	103.643	161.475	81.073	262.760
0.060	145.117	205.091	87.647	271.424	96.877	385.321	49.959	68.126	145.133	103.552	161.283	81.178	262.760
0.070	145.135	204.620	87.619	271.338	96.938	385.321	49.863	68.212	145.151	103.460	161.091	81.283	262.760
0.080	145.152	204.150	87.590	271.252	96.999	385.321	49.768	68.298	145.170	103.369	160.899	81.388	262.760
0.090	145.169	203.679	87.561	271.166	97.060	385.321	49.672	68.385	145.188	103.278	160.707	81.492	262.760
0.100	145.187	203.209	87.532	271.080	97.121	385.321	49.576	68.471	145.207	103.187	160.515	81.597	262.760
|Fo|	137.304	211.266	94.320	288.446	95.230	385.321	55.161	68.580	140.433	99.484	176.507	72.021	262.760

Table A.2.52. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2688, B=-0.04933, K=20.01787)

	|Fcl												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	145.485	207.621	88.420	271.198	96.268	384.366	50.779	67.000	144.753	105.185	161.411	80.942	261.456
0.001	145.487	207.574	88.417	271.190	96.274	384.366	50.770	67.009	144.755	105.176	161.392	80.952	261.456
0.002	145.489	207.527	88.415	271.181	96.280	384.366	50.760	67.017	144.757	105.166	161.373	80.963	261.456
0.003	145.491	207.480	88.412	271.172	96.286	384.366	50.751	67.026	144.759	105.157	161.354	80.973	261.456
0.004	145.492	207.433	88.409	271.164	96.292	384.366	50.741	67.035	144.760	105.148	161.335	80.984	261.456
0.005	145.494	207.385	88.406	271.155	96.298	384.366	50.732	67.043	144.762	105.139	161.315	80.994	261.456
0.006	145.496	207.338	88.403	271.147	96.304	384.366	50.722	67.052	144.764	105.130	161.296	81.005	261.456
0.007	145.497	207.291	88.400	271.138	96.310	384.366	50.712	67.061	144.766	105.121	161.277	81.015	261.456
0.008	145.499	207.244	88.397	271.129	96.316	384.366	50.703	67.069	144.768	105.112	161.258	81.026	261.456
0.009	145.501	207.197	88.394	271.121	96.323	384.366	50.693	67.078	144.770	105.103	161.239	81.036	261.456
0.010	145.503	207.150	88.391	271.112	96.329	384.366	50.684	67.086	144.772	105.093	161.219	81.047	261.456
0.020	145.520	206.680	88.362	271.026	96.390	384.366	50.588	67.173	144.790	105.002	161.027	81.151	261.456
0.030	145.537	206.209	88.334	270.940	96.451	384.366	50.492	67.259	144.809	104.911	160.835	81.256	261.456
0.040	145.555	205.739	88.305	270.854	96.512	384.366	50.397	67.345	144.828	104.819	160.643	81.361	261.456
0.050	145.572	205.269	88.276	270.768	96.573	384.366	50.301	67.432	144.846	104.728	160.451	81.466	261.456
0.060	145.590	204.798	88.247	270.682	96.634	384.366	50.205	67.518	144.865	104.637	160.259	81.570	261.456
0.070	145.607	204.328	88.218	270.596	96.695	384.366	50.109	67.604	144.884	104.545	160.067	81.675	261.456
0.080	145.624	203.857	88.189	270.510	96.756	384.366	50.014	67.691	144.902	104.454	159.875	81.780	261.456
0.090	145.642	203.387	88.160	270.424	96.817	384.366	49.918	67.777	144.921	104.363	159.683	81.885	261.456
0.100	145.659	202.916	88.131	270.338	96.878	384.366	49.822	67.863	144.940	104.271	159.491	81.989	261.456
|Fol	137.220	211.088	94.234	288.090	95.053	384.366	55.011	68.367	139.965	99.145	175.850	71.708	261.456

Table A.2.53. Calculated and Observed Structure Factors for Manganese Chromite with respect to Degree of Disorder (x).
(u=0.2700, B=-0.02023, K=20.02028)

	|Fc|												
x	220	311	222	400	422	440	531	620	533	622	444	642	800
0.000	146.952	206.734	90.289	268.883	95.525	381.419	51.478	65.129	143.863	108.528	158.286	82.115	257.430
0.001	146.954	206.687	90.286	268.874	95.531	381.419	51.469	65.137	143.864	108.518	158.267	82.126	257.430
0.002	146.955	206.640	90.283	268.866	95.537	381.419	51.459	65.146	143.866	108.509	158.247	82.136	257.430
0.003	146.957	206.593	90.280	268.857	95.543	381.419	51.449	65.155	143.868	108.500	158.228	82.147	257.430
0.004	146.959	206.546	90.277	268.848	95.550	381.419	51.440	65.163	143.870	108.491	158.209	82.157	257.430
0.005	146.961	206.499	90.274	268.840	95.556	381.419	51.430	65.172	143.872	108.482	158.190	82.168	257.430
0.006	146.962	206.452	90.272	268.831	95.562	381.419	51.421	65.181	143.874	108.473	158.171	82.178	257.430
0.007	146.964	206.405	90.269	268.823	95.568	381.419	51.411	65.189	143.876	108.464	158.151	82.189	257.430
0.008	146.966	206.358	90.266	268.814	95.574	381.419	51.402	65.198	143.877	108.454	158.132	82.199	257.430
0.009	146.968	206.311	90.263	268.805	95.580	381.419	51.392	65.207	143.879	108.445	158.113	82.210	257.430
0.010	146.969	206.264	90.260	268.797	95.586	381.419	51.382	65.215	143.881	108.436	158.094	82.220	257.430
0.020	146.987	205.793	90.231	268.711	95.647	381.419	51.287	65.301	143.900	108.345	157.902	82.325	257.430
0.030	147.004	205.323	90.202	268.625	95.708	381.419	51.191	65.388	143.919	108.254	157.710	82.430	257.430
0.040	147.022	204.852	90.173	268.539	95.769	381.419	51.095	65.474	143.937	108.162	157.518	82.534	257.430
0.050	147.039	204.382	90.144	268.453	95.830	381.419	51.000	65.560	143.956	108.071	157.326	82.639	257.430
0.060	147.056	203.911	90.115	268.367	95.891	381.419	50.904	65.647	143.975	107.980	157.133	82.744	257.430
0.070	147.074	203.441	90.087	268.281	95.952	381.419	50.808	65.733	143.993	107.888	156.941	82.849	257.430
0.080	147.091	202.971	90.058	268.195	96.013	381.419	50.713	65.819	144.012	107.797	156.749	82.953	257.430
0.090	147.109	202.500	90.029	268.109	96.074	381.419	50.617	65.906	144.030	107.706	156.557	83.058	257.430
0.100	147.126	202.030	90.000	268.023	96.135	381.419	50.521	65.992	144.049	107.614	156.365	83.163	257.430
|Fo|	136.969	210.547	93.969	287.001	94.509	381.419	54.550	67.710	138.519	98.097	173.821	70.742	257.430

Table A.3. Residual parameter for $CoCr_2O_4$ with respect to u and x at 1573 K.

Degree of Disorder x	$R = \frac{\sum \left\|\|F_o\| - \|F_c\|\right\|}{\sum \|F_o\|}$					
	u=0.2500 B=–0.56087 K=19.75001	u=0.2504 B=–0.56066 K=19.74994	u=0.2508 B=–0.56003 K=19.74979	u=0.2512 B=–0.55904 K=19.74931	u=0.2516 B=–0.55757 K=19.74895	u=0.2520 B=–0.55574 K=19.74825
0.000	0.04548	0.04523	0.04495	0.04466	0.04430	0.04392
0.010	0.04513	0.04489	0.04461	0.04432	0.04396	0.04358
0.020	0.04479	0.04454	0.04427	0.04397	0.04361	0.04324
0.030	0.04444	0.04420	0.04392	0.04363	0.04328	0.04289
0.040	0.04410	0.04385	0.04358	0.04329	0.04292	0.04255
0.050	0.04376	0.04351	0.04323	0.04294	0.04258	0.04220
0.060	0.04341	0.04317	0.04289	0.04260	0.04224	0.04186
0.070	0.04307	0.04282	0.04255	0.04225	0.04193	0.04173
0.080	0.04273	0.04249	0.04241	0.04231	0.04214	0.04194
0.090	0.04270	0.04271	0.04263	0.04253	0.04235	0.04216
0.100	0.04344	0.04339	0.04330	0.04319	0.04299	0.04277
0.110	0.04430	0.04425	0.04416	0.04404	0.04385	0.04362
0.120	0.04515	0.04511	0.04502	0.04490	0.04470	0.04448
0.130	0.04601	0.04596	0.04587	0.04576	0.04556	0.04534
0.140	0.04687	0.04682	0.04673	0.04662	0.04642	0.04620
0.150	0.04772	0.04768	0.04759	0.04747	0.04728	0.04705
0.160	0.04879	0.04874	0.04863	0.04844	0.04824	0.04796
0.170	0.04995	0.04989	0.04979	0.04960	0.04940	0.04911
0.180	0.05111	0.05105	0.05094	0.05076	0.05055	0.05027
0.190	0.05226	0.05221	0.05210	0.05191	0.05171	0.05143
0.200	0.05342	0.05337	0.05326	0.05307	0.05287	0.05259

Table A.3. (continued)

Degree of Disorder x	$R = \frac{\sum \left\|\|F_o\| - \|F_c\|\right\|}{\sum \|F_o\|}$					
	u=0.2524 B=−0.55351 K=19.74742	u=0.2528 B=−0.55084 K=19.74651	u=0.2532 B=−0.54773 K=19.74560	u=0.2536 B=−0.54773 K=19.74560	u=0.2540 B=−0.54037 K=19.74306	u=0.2544 B=−0.53605 K=19.74170
0.000	0.04351	0.04307	0.04259	0.04208	0.04154	0.04096
0.010	0.04317	0.04273	0.04225	0.04174	0.04119	0.04062
0.020	0.04282	0.04238	0.04190	0.04139	0.04085	0.04027
0.030	0.04248	0.04204	0.04156	0.04105	0.04050	0.03993
0.040	0.04213	0.04169	0.04122	0.04070	0.04016	0.03958
0.050	0.04179	0.04135	0.04087	0.04036	0.03981	0.03934
0.060	0.04145	0.04101	0.04071	0.04036	0.03998	0.03956
0.070	0.04150	0.04123	0.04092	0.04057	0.04019	0.03977
0.080	0.04171	0.04144	0.04113	0.04079	0.04040	0.03998
0.090	0.04192	0.04165	0.04135	0.04100	0.04062	0.04020
0.100	0.04250	0.04219	0.04184	0.04144	0.04100	0.04054
0.110	0.04336	0.04305	0.04270	0.04230	0.04186	0.04137
0.120	0.04422	0.04391	0.04356	0.04316	0.04272	0.04223
0.130	0.04508	0.04477	0.04441	0.04402	0.04358	0.04309
0.140	0.04593	0.04562	0.04527	0.04488	0.04444	0.04395
0.150	0.04679	0.04648	0.04613	0.04573	0.04529	0.04481
0.160	0.04765	0.04734	0.04699	0.04659	0.04615	0.04567
0.170	0.04878	0.04838	0.04794	0.04745	0.04701	0.04653
0.180	0.04994	0.04954	0.04910	0.04859	0.04803	0.04741
0.190	0.05110	0.05070	0.05025	0.04975	0.04919	0.04857
0.200	0.05225	0.05186	0.05141	0.05091	0.05035	0.04973

Table A.3 . (continued)

Degree of Disorder x	$R = \frac{\sum \left\| F_o \right\| - \left\| F_c \right\|}{\sum \left\| F_o \right\|}$					
	u=0.2548 B=–0.53137 K=19.74002	u=0.2552 B=–0.52624 K=19.73835	u=0.2556 B=–0.52066 K=19.73670	u=0.2560 B=–0.51471 K=19.73481	u=0.2564 B=–0.50836 K=19.73275	u=0.2568 B=–0.50158 K=19.73065
0.000	0.04035	0.03970	0.03902	0.03831	0.03758	0.03699
0.010	0.04000	0.03936	0.03867	0.03796	0.03721	0.03643
0.020	0.03966	0.03901	0.03833	0.03762	0.03686	0.03608
0.030	0.03931	0.03866	0.03798	0.03727	0.03652	0.03573
0.040	0.03897	0.03832	0.03764	0.03706	0.03645	0.03579
0.050	0.03888	0.03838	0.03785	0.03727	0.03666	0.03601
0.060	0.03909	0.03859	0.03806	0.03749	0.03688	0.03622
0.070	0.03931	0.03881	0.03827	0.03770	0.03709	0.03644
0.080	0.03952	0.03902	0.03849	0.03792	0.03730	0.03665
0.090	0.03973	0.03924	0.03870	0.03813	0.03752	0.03688
0.100	0.04009	0.03960	0.03909	0.03853	0.03794	0.03730
0.110	0.04084	0.04027	0.03965	0.03899	0.03835	0.03772
0.120	0.04170	0.04113	0.04051	0.03985	0.03914	0.03839
0.130	0.04256	0.04199	0.04137	0.04071	0.04000	0.03925
0.140	0.04342	0.04290	0.04223	0.04157	0.04087	0.04011
0.150	0.04428	0.04371	0.04309	0.04243	0.04173	0.04098
0.160	0.04514	0.04457	0.04396	0.04330	0.04259	0.04184
0.170	0.04600	0.04543	0.04482	0.04416	0.04346	0.04271
0.180	0.04686	0.04629	0.04568	0.04502	0.04432	0.04357
0.190	0.04789	0.04716	0.04654	0.04588	0.04521	0.04458
0.200	0.04905	0.04832	0.04753	0.04683	0.04624	0.04561

Table A.3. (continued)

Degree of Disorder x	$R = \frac{\sum \lvert \lvert F_o \rvert - \lvert F_c \rvert \rvert}{\sum \lvert F_o \rvert}$					
	u=0.2572 B=–0.49440 K=19.72845	u=0.2576 B=–0.48677 K=19.72623	u=0.2580 B=–0.47879 K=19.72373	u=0.2584 B=–0.47033 K=19.72135	u=0.2588 B=–0.46148 K=19.71883	u=0.2592 B=–0.45221 K=19.71631
0.000	0.03638	0.03574	0.03508	0.03440	0.03369	0.03296
0.010	0.03578	0.03514	0.03448	0.03380	0.03309	0.03236
0.020	0.03526	0.03455	0.03388	0.03320	0.03249	0.03179
0.030	0.03491	0.03417	0.03352	0.03296	0.03237	0.03175
0.040	0.03511	0.03438	0.03362	0.03292	0.03233	0.03172
0.050	0.03532	0.03460	0.03383	0.03303	0.03230	0.03168
0.060	0.03554	0.03481	0.03405	0.03325	0.03241	0.03165
0.070	0.03575	0.03503	0.03426	0.03346	0.03262	0.03175
0.080	0.03597	0.03524	0.03448	0.03368	0.03284	0.03196
0.090	0.03622	0.03551	0.03477	0.03399	0.03317	0.03232
0.100	0.03663	0.03593	0.03519	0.03441	0.03359	0.03274
0.110	0.03705	0.03635	0.03561	0.03483	0.03401	0.03316
0.120	0.03759	0.03677	0.03602	0.03525	0.03443	0.03358
0.130	0.03845	0.03761	0.03673	0.03580	0.03485	0.03402
0.140	0.03932	0.03848	0.03759	0.03666	0.03571	0.03485
0.150	0.04018	0.03934	0.03846	0.03756	0.03675	0.03589
0.160	0.04105	0.04021	0.03938	0.03860	0.03778	0.03693
0.170	0.04191	0.04115	0.04041	0.03963	0.03882	0.03797
0.180	0.04289	0.04219	0.04145	0.04067	0.03986	0.03900
0.190	0.04392	0.04322	0.04248	0.04171	0.04089	0.04004
0.200	0.04495	0.04425	0.04351	0.04274	0.04193	0.04108

Table A.3. (continued)

Degree of Disorder x	$R = \frac{\sum \lvert \lvert F_o \rvert - \lvert F_c \rvert \rvert}{\sum \lvert F_o \rvert}$					
	u=0.2596 B=–0.44253 K=19.71366	u=0.2600 B=–0.43248 K=19.71083	u=0.2604 B=–0.42195 K=19.70816	u=0.2608 B=–0.41101 K=19.70538	u=0.2612 B=–0.39968 K=19.70258	u=0.2616 B=–0.38792 K=19.69976
0.000	0.03220	0.03143	0.03063	0.02981	0.02896	0.02873
0.010	0.03160	0.03083	0.03003	0.02920	0.02836	0.02809
0.020	0.03114	0.03048	0.02979	0.02907	0.02832	0.02792
0.030	0.03111	0.03044	0.02975	0.02903	0.02829	0.02775
0.040	0.03108	0.03041	0.02972	0.02900	0.02825	0.02766
0.050	0.03104	0.03038	0.02968	0.02896	0.02822	0.02762
0.060	0.03101	0.03034	0.02965	0.02893	0.02818	0.02759
0.070	0.03097	0.03031	0.02961	0.02889	0.02815	0.02755
0.080	0.03105	0.03027	0.02959	0.02889	0.02826	0.02761
0.090	0.03143	0.03050	0.02976	0.02912	0.02860	0.02789
0.100	0.03185	0.03092	0.03000	0.02946	0.02894	0.02823
0.110	0.03227	0.03137	0.03059	0.02980	0.02928	0.02857
0.120	0.03271	0.03196	0.03118	0.03037	0.02962	0.02891
0.130	0.03330	0.03255	0.03177	0.03096	0.03012	0.02925
0.140	0.03396	0.03314	0.03236	0.03155	0.03071	0.02968
0.150	0.03500	0.03406	0.03309	0.03214	0.03131	0.03027
0.160	0.03603	0.03510	0.03413	0.03312	0.03208	0.03086
0.170	0.03707	0.03614	0.03517	0.03417	0.03312	0.03187
0.180	0.03811	0.03718	0.03622	0.03521	0.03417	0.03291
0.190	0.03915	0.03822	0.03726	0.03625	0.03521	0.03396
0.200	0.04019	0.03926	0.03830	0.03730	0.03626	0.03501

Table A.3. (continued)

Degree of Disorder x	$R = \frac{\sum \|\|F_o\| - \|F_c\|\|}{\sum \|F_o\|}$					
	u=0.2620 B=−0.37575 K=19.69685	u=0.2624 B=−0.33667 K=19.68850	u=0.2628 B=−0.35014 K=19.69118	u=0.2632 B=−0.33667 K=19.68850	u=0.2636 B=−0.32284 K=19.68564	u=0.2640 B=−0.30854 K=19.68295
0.000	0.02819	0.02780	0.02763	0.02762	0.02765	0.02799
0.010	0.02764	0.02735	0.02725	0.02733	0.02761	0.02795
0.020	0.02747	0.02718	0.02704	0.02725	0.02757	0.02791
0.030	0.02729	0.02700	0.02691	0.02721	0.02754	0.02788
0.040	0.02712	0.02686	0.02687	0.02718	0.02750	0.02784
0.050	0.02695	0.02685	0.02683	0.02714	0.02746	0.02780
0.060	0.02692	0.02685	0.02679	0.02710	0.02742	0.02776
0.070	0.02692	0.02684	0.02676	0.02706	0.02740	0.02777
0.080	0.02716	0.02698	0.02693	0.02722	0.02757	0.02794
0.090	0.02750	0.02718	0.02713	0.02739	0.02774	0.02810
0.100	0.02784	0.02738	0.02733	0.02755	0.02791	0.02827
0.110	0.02818	0.02760	0.02753	0.02772	0.02807	0.02844
0.120	0.02852	0.02795	0.02774	0.02789	0.02824	0.02861
0.130	0.02886	0.02829	0.02794	0.02806	0.02841	0.02878
0.140	0.02920	0.02863	0.02814	0.02823	0.02858	0.02895
0.150	0.02955	0.02897	0.02838	0.02840	0.02875	0.02912
0.160	0.03014	0.02931	0.02872	0.02857	0.02892	0.02929
0.170	0.03091	0.02981	0.02906	0.02874	0.02909	0.02946
0.180	0.03196	0.03080	0.02960	0.02891	0.02926	0.02963
0.190	0.03301	0.03185	0.03065	0.02949	0.02951	0.02980
0.200	0.03406	0.03290	0.03171	0.03047	0.03014	0.03024

Table A.3. (continued)

Degree of Disorder x	$R = \frac{\sum \lvert \lvert F_o \rvert - \lvert F_c \rvert \rvert}{\sum \lvert F_o \rvert}$				
	u=0.2625 B=−0.35990 K=19.69344	u=0.2626 B=−0.35668 K=19.69266	u=0.2627 B=−0.35339 K=19.69202	u=0.2628 B=−0.35014 K=19.69118	u=0.2629 B=−0.34682 K=19.69047
0.000	0.027701	0.027643	0.027638	0.027633	0.027630
0.010	0.027278	0.027209	0.027228	0.027247	0.027267
0.020	0.027104	0.027029	0.027020	0.027038	0.027059
0.030	0.026930	0.026855	0.026831	0.026905	0.026980
0.040	0.026836	0.026815	0.026795	0.026867	0.026942
0.050	0.026832	0.026811	0.026792	0.026829	0.026904
0.060	0.026828	0.026807	0.026788	0.026791	0.026866
0.061	0.026827	0.026807	0.026787	0.026787	0.026863
0.062	0.026827	0.026807	0.026787	0.026783	0.026859
0.063	0.026827	0.026806	0.026786	0.026779	0.026855
0.064	0.026826	0.026806	0.026786	0.026776	0.026851
0.065	0.026826	0.026805	0.026786	0.026772	0.026847
0.066	0.026825	0.026805	0.026785	0.026768	0.026844
0.067	0.026825	0.026805	0.026785	0.026764	0.026840
0.068	0.026825	0.026804	0.026784	0.026763	0.026836
0.069	0.026824	0.026804	0.026784	0.026763	0.026832
0.070	0.026824	0.026803	0.026784	0.026763	0.026828
0.071	0.026823	0.026803	0.026783	0.026762	0.026825
0.072	0.026823	0.026803	0.026783	0.026763	0.026828
0.073	0.026825	0.026811	0.026797	0.026783	0.026845
0.074	0.026845	0.026831	0.026818	0.026804	0.026862

Table A.3. (continued)

Degree of Disorder x	$R = \frac{\sum \left\| \lvert F_o \rvert - \lvert F_c \rvert \right\|}{\sum \lvert F_o \rvert}$					
	u=0.2644 B=–0.29386 K=19.68017	u=0.2648 B=–0.27874 K=19.67758	u=0.2652 B=–0.26322 K=19.67492	u=0.2656 B=–0.24728 K=19.67240	u=0.2660 B=–0.23089 K=19.66997	u=0.2664 B=–0.21413 K=19.66757
0.000	0.02835	0.02872	0.02911	0.02951	0.02993	0.03104
0.010	0.02831	0.02868	0.02907	0.02947	0.02990	0.03116
0.020	0.02827	0.02864	0.02903	0.02944	0.02986	0.03129
0.030	0.02823	0.02860	0.02899	0.02940	0.02986	0.03142
0.040	0.02819	0.02857	0.02895	0.02936	0.02998	0.03154
0.050	0.02816	0.02853	0.02892	0.02932	0.03011	0.03167
0.060	0.02811	0.02849	0.02888	0.02928	0.03024	0.03180
0.070	0.02815	0.02855	0.02896	0.02939	0.03054	0.03213
0.080	0.02832	0.02872	0.02913	0.02957	0.03088	0.03246
0.090	0.02849	0.02889	0.02930	0.02974	0.03121	0.03280
0.100	0.02866	0.02906	0.02947	0.03000	0.03155	0.03314
0.110	0.02883	0.02923	0.02964	0.03033	0.03188	0.03348
0.120	0.02900	0.02940	0.02982	0.03067	0.03222	0.03381
0.130	0.02917	0.02957	0.02999	0.03101	0.03256	0.03415
0.140	0.02964	0.02974	0.03016	0.03134	0.03289	0.03449
0.150	0.02951	0.02991	0.03033	0.03168	0.03323	0.03482
0.160	0.02968	0.03008	0.03050	0.03201	0.03356	0.03516
0.170	0.02985	0.03025	0.03084	0.03235	0.03390	0.03550
0.180	0.03002	0.03042	0.03117	0.03268	0.03424	0.03583
0.190	0.03019	0.03059	0.03151	0.03302	0.03457	0.03617
0.200	0.03036	0.03076	0.03184	0.03335	0.03491	0.03651

Table A.3. (continued)

Degree of Disorder x	$R = \frac{\sum \lvert \lvert F_o \rvert - \lvert F_c \rvert \rvert}{\sum \lvert F_o \rvert}$					
	u=0.2668 B=–0.19691 K=19.66534	u=0.2672 B=–0.17927 K=19.66331	u=0.2676 B=–0.16119 K=19.66140	u=0.2680 B=–0.14275 K=19.65943	u=0.2688 B=–0.10454 K=19.65631	u=0.2700 B=–0.10454 K=19.65631
0.000	0.03264	0.03431	0.03592	0.03743	0.04054	0.04539
0.010	0.03277	0.03444	0.03605	0.03756	0.04067	0.04552
0.020	0.03289	0.03457	0.03618	0.03769	0.04079	0.04565
0.030	0.03302	0.03470	0.03630	0.03782	0.04092	0.04578
0.040	0.03315	0.03482	0.03643	0.03794	0.04105	0.04591
0.050	0.03328	0.03495	0.03656	0.03807	0.04118	0.04604
0.060	0.03342	0.03512	0.03676	0.03829	0.04145	0.04637
0.070	0.03376	0.03546	0.03710	0.03863	0.04179	0.04672
0.080	0.03410	0.03580	0.03744	0.03897	0.04213	0.04706
0.090	0.03443	0.03614	0.03777	0.03931	0.04247	0.04741
0.100	0.03477	0.03648	0.03811	0.03965	0.04282	0.04786
0.110	0.03511	0.03681	0.03845	0.03999	0.04316	0.04843
0.120	0.03545	0.03715	0.03879	0.04033	0.04350	0.04900
0.130	0.03578	0.03749	0.03913	0.04067	0.04384	0.04957
0.140	0.03612	0.03783	0.03947	0.04101	0.04432	0.05014
0.150	0.03646	0.03817	0.03981	0.04135	0.04489	0.05071
0.160	0.03680	0.03851	0.04015	0.04169	0.04545	0.05129
0.170	0.03713	0.03884	0.04049	0.04224	0.04602	0.05186
0.180	0.03747	0.03918	0.04095	0.04281	0.04659	0.05243
0.190	0.03781	0.03956	0.04152	0.04337	0.04716	0.05300
0.200	0.03815	0.04012	0.04208	0.04394	0.04772	0.05357

Table A.4. Residual Parameter for $MnCr_2O_4$ with respect to u and x at 1573 K.

Degree of Disorder x	$R = \frac{\sum \lvert \lvert F_c \rvert - \lvert F_o \rvert \rvert}{\sum \lvert F_o \rvert}$					
	u=0.2500 B=–0.57012 K=20.08096	u=0.2504 B=–0.56989 K=20.08090	u=0.2508 B=–0.56918 K=20.08079	u=0.2512 B=–0.56806 K=20.08033	u=0.2516 B=–0.56639 K=20.08004	u=0.2520 B=–0.56432 K=20.07941
0.000	0.05809	0.05783	0.05753	0.05720	0.05683	0.05641
0.001	0.05809	0.05788	0.05753	0.05720	0.05683	0.05642
0.002	0.05809	0.05793	0.05753	0.05720	0.05683	0.05642
0.003	0.05809	0.05798	0.05754	0.05720	0.05683	0.05642
0.004	0.05809	0.05803	0.05754	0.05720	0.05683	0.05642
0.005	0.05809	0.05808	0.05754	0.05720	0.05683	0.05642
0.006	0.05810	0.05813	0.05754	0.05720	0.05683	0.05643
0.007	0.05810	0.05818	0.05754	0.05721	0.05684	0.05643
0.008	0.05810	0.05823	0.05754	0.05721	0.05684	0.05643
0.009	0.05810	0.05828	0.05754	0.05721	0.05684	0.05643
0.010	0.05810	0.05833	0.05756	0.05721	0.05684	0.05643
0.020	0.05812	0.05884	0.05756	0.05722	0.05685	0.05644
0.030	0.05813	0.05935	0.05757	0.05724	0.05687	0.05646
0.040	0.05814	0.05985	0.05759	0.05725	0.05688	0.05647
0.050	0.05816	0.06036	0.05760	0.05726	0.05689	0.05648
0.060	0.05817	0.06086	0.05761	0.05728	0.05703	0.05682
0.070	0.05818	0.06137	0.05778	0.05764	0.05746	0.05725
0.080	0.05835	0.06224	0.05821	0.05808	0.05791	0.05769
0.090	0.05879	0.06317	0.05865	0.05852	0.05834	0.05813
0.100	0.05923	0.06410	0.05909	0.05896	0.05878	0.05857

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \lvert \lvert F_o \rvert - \lvert F_c \rvert \rvert}{\sum \lvert F_o \rvert}$					
	u=0.2524 B=−0.56179 K=20.07867	u=0.2528 B=−0.55877 K=20.07787	u=0.2532 B=−0.55524 K=20.07711	u=0.2536 B=−0.55132 K=20.07602	u=0.2540 B=−0.54689 K=20.07488	u=0.2544 B=−0.54200 K=20.07372
0.000	0.05597	0.05548	0.05496	0.05439	0.05379	0.05315
0.001	0.05597	0.05548	0.05496	0.05440	0.05379	0.05316
0.002	0.05597	0.05548	0.05496	0.05440	0.05380	0.05316
0.003	0.05597	0.05548	0.05496	0.05440	0.05380	0.05316
0.004	0.05597	0.05549	0.05496	0.05440	0.05380	0.05316
0.005	0.05597	0.05549	0.05496	0.05440	0.05380	0.05316
0.006	0.05597	0.05549	0.05497	0.05440	0.05380	0.05316
0.007	0.05598	0.05549	0.05497	0.05440	0.05380	0.05316
0.008	0.05598	0.05549	0.05497	0.05441	0.05380	0.05317
0.009	0.05598	0.05549	0.05497	0.05441	0.05381	0.05317
0.010	0.05598	0.05549	0.05497	0.05441	0.05381	0.05317
0.020	0.05599	0.05551	0.05498	0.05442	0.05382	0.05318
0.030	0.05601	0.05552	0.05500	0.05444	0.05383	0.05331
0.040	0.05602	0.05553	0.05503	0.05465	0.05422	0.05375
0.050	0.05611	0.05581	0.05547	0.05508	0.05466	0.05419
0.060	0.05655	0.05625	0.05591	0.05553	0.05510	0.05463
0.070	0.05699	0.05669	0.05635	0.05596	0.05553	0.05507
0.080	0.05743	0.05713	0.05679	0.05640	0.05597	0.05551
0.090	0.05787	0.05757	0.05723	0.05684	0.05641	0.05595
0.100	0.05830	0.05801	0.05765	0.05728	0.05685	0.05638

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \left\|\|F_o\| - \|F_c\|\right\|}{\sum \|F_o\|}$					
	u=0.2548 B=−0.53669 K=20.07224	u=0.2552 B=−0.53087 K=20.07080	u=0.2556 B=−0.52454 K=20.06942	u=0.2560 B=−0.51779 K=20.06780	u=0.2564 B=−0.51059 K=20.06603	u=0.2568 B=−0.50290 K=20.06425
0.000	0.05247	0.05176	0.05099	0.05021	0.04937	0.04850
0.001	0.05247	0.05176	0.05100	0.05021	0.04937	0.04850
0.002	0.05248	0.05176	0.05100	0.05021	0.04937	0.04850
0.003	0.05248	0.05176	0.05100	0.05021	0.04938	0.04850
0.004	0.05248	0.05176	0.05101	0.05021	0.04938	0.04850
0.005	0.05248	0.05177	0.05101	0.05021	0.04938	0.04850
0.006	0.05248	0.05177	0.05101	0.05022	0.04938	0.04852
0.007	0.05248	0.05177	0.05101	0.05022	0.04938	0.04857
0.008	0.05248	0.05177	0.05101	0.05022	0.04938	0.04861
0.009	0.05249	0.05177	0.05101	0.05022	0.04939	0.04866
0.010	0.05249	0.05177	0.05101	0.05022	0.04943	0.04870
0.020	0.05250	0.05180	0.05120	0.05056	0.04987	0.04914
0.030	0.05279	0.05224	0.05164	0.05099	0.05031	0.04958
0.040	0.05323	0.05268	0.05208	0.05144	0.05075	0.05003
0.050	0.05367	0.05312	0.05252	0.05188	0.05120	0.05047
0.060	0.05411	0.05356	0.05296	0.05232	0.05164	0.05091
0.070	0.05455	0.05400	0.05340	0.05276	0.05208	0.05135
0.080	0.05499	0.05444	0.05384	0.05320	0.05252	0.05179
0.090	0.05543	0.05488	0.05428	0.05364	0.05296	0.05223
0.100	0.05587	0.05532	0.05472	0.05408	0.05340	0.05268

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \left\| F_o \right\| - \left\| F_c \right\|}{\sum \left\| F_o \right\|}$					
	u=0.2572 B=–0.49474 K=20.06241	u=0.2576 B=–0.48608 K=20.06057	u=0.2580 B=–0.47702 K=20.05846	u=0.2584 B=–0.46741 K=20.05651	u=0.2588 B=–0.45735 K=20.05445	u=0.2592 B=–0.44681 K=20.05243
0.000	0.04758	0.04668	0.04582	0.04492	0.04398	0.04300
0.001	0.04758	0.04672	0.04586	0.04497	0.04403	0.04304
0.002	0.04759	0.04676	0.04591	0.04501	0.04407	0.04309
0.003	0.04762	0.04681	0.04595	0.04505	0.04411	0.04313
0.004	0.04767	0.04685	0.04599	0.04510	0.04416	0.04318
0.005	0.04771	0.04690	0.04604	0.04514	0.04420	0.04322
0.006	0.04775	0.04694	0.04608	0.04519	0.04425	0.04326
0.007	0.04780	0.04699	0.04613	0.04523	0.04429	0.04331
0.008	0.04784	0.04703	0.04617	0.04528	0.04434	0.04335
0.009	0.04789	0.04707	0.04622	0.04532	0.04438	0.04340
0.010	0.04793	0.04712	0.04626	0.04536	0.04443	0.04344
0.020	0.04837	0.04756	0.04670	0.04581	0.04487	0.04389
0.030	0.04881	0.04800	0.04714	0.04525	0.04531	0.04433
0.040	0.04926	0.04845	0.04759	0.04670	0.04576	0.04478
0.050	0.04970	0.04889	0.04803	0.04714	0.04620	0.04522
0.060	0.05014	0.04933	0.04848	0.04758	0.04665	0.04567
0.070	0.05058	0.04977	0.04892	0.04803	0.04709	0.04611
0.080	0.05103	0.05022	0.04936	0.04847	0.04753	0.04656
0.090	0.05147	0.05066	0.04981	0.04891	0.04798	0.04700
0.100	0.05191	0.05110	0.05025	0.04936	0.04842	0.04744

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \left\|\|F_o\| - \|F_c\|\right\|}{\sum \|F_o\|}$					
	u=0.2596 B=–0.43581 K=20.05031	u=0.2560 B=–0.42437 K=20.04802	u=0.2604 B=–0.41240 K=20.04595	u=0.2608 B=–0.39995 K=20.04380	u=0.2612 B=–0.38704 K=20.04166	u=0.2616 B=–0.37365 K=20.03955
0.000	0.04197	0.04090	0.03979	0.03864	0.03745	0.03621
0.001	0.04202	0.04095	0.03984	0.03869	0.03749	0.03626
0.002	0.04206	0.04099	0.03988	0.03873	0.03754	0.03630
0.003	0.04210	0.04104	0.03993	0.03878	0.03758	0.03635
0.004	0.04215	0.04108	0.03997	0.03882	0.03763	0.03639
0.005	0.04219	0.04113	0.04002	0.03887	0.03767	0.03644
0.006	0.04224	0.04117	0.04006	0.03891	0.03772	0.03648
0.007	0.04228	0.04122	0.04010	0.03896	0.03776	0.03653
0.008	0.04233	0.04126	0.04015	0.03900	0.03781	0.03657
0.009	0.04237	0.04130	0.04020	0.03905	0.03785	0.03662
0.010	0.04242	0.04135	0.04024	0.03909	0.03790	0.03666
0.020	0.04286	0.04180	0.04069	0.03954	0.03834	0.03711
0.030	0.04331	0.04224	0.04113	0.03999	0.03879	0.03756
0.040	0.04375	0.04269	0.04158	0.04043	0.03924	0.03801
0.050	0.04420	0.04313	0.04203	0.04088	0.03969	0.03846
0.060	0.04464	0.04358	0.04247	0.04133	0.04014	0.03891
0.070	0.04509	0.04403	0.04292	0.04177	0.04058	0.03935
0.080	0.045553	0.04447	0.04337	0.04222	0.04103	0.03981
0.090	0.04598	0.04492	0.04381	0.04267	0.04148	0.04027
0.100	0.04643	0.04536	0.04426	0.04312	0.04193	0.04074

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \lvert \lvert F_o \rvert - \lvert F_c \rvert \rvert}{\sum \lvert F_o \rvert}$					
	u=0.2620 B=–0.35979 K=20.03738	u=0.2624 B=–0.34542 K=20.03534	u=0.2628 B=–0.33058 K=20.03334	u=0.2632 B=–0.31522 K=20.03156	u=0.2636 B=–0.29943 K=20.02962	u=0.2640 B=–0.28310 K=20.02792
0.000	0.03516	0.03419	0.03320	0.03222	0.03172	0.03121
0.001	0.03520	0.03425	0.03325	0.03227	0.03178	0.03127
0.002	0.03525	0.03429	0.03330	0.03233	0.03184	0.03133
0.003	0.03529	0.03433	0.03334	0.03239	0.03189	0.03138
0.004	0.03534	0.03438	0.03339	0.03244	0.03195	0.03144
0.005	0.03539	0.03443	0.03344	0.03250	0.03201	0.03150
0.006	0.03543	0.03447	0.03348	0.03256	0.03206	0.03156
0.007	0.03548	0.03452	0.03353	0.03261	0.03212	0.03161
0.008	0.03553	0.03457	0.03358	00.03267	0.03218	0.03167
0.009	0.03557	0.03461	0.03362	0.03273	0.03223	0.03173
0.010	0.03562	0.03466	0.03367	0.03278	0.03229	0.03178
0.020	0.03609	0.03513	00.03414	0.03335	0.03286	0.03235
0.030	0.03655	0.03559	0.03460	0.03391	0.03342	0.03292
0.040	0.03702	0.03636	0.03507	0.03448	0.03399	0.03349
0.050	0.03748	0.03653	0.03554	0.03505	0.03456	0.03405
0.060	0.03795	0.03699	0.03608	0.03561	0.03512	0.03462
0.070	0.03842	0.03746	0.03664	0.03618	0.03569	0.03519
0.080	0.03888	0.03793	0.03721	0.03674	0.03626	0.03576
0.090	0.03935	0.03839	0.03777	0.03731	0.03683	0.03633
0.100	0.03981	0.03886	0.03834	0.03787	0.03739	0.03689

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \left\| F_o \right\| - \left\| F_c \right\|}{\sum \left\| F_o \right\|}$					
	u=0.2644 B=–0.26633 K=20.03617	u=0.2648 B=–0.24905 K=20.02468	u=0.2652 B=–0.23131 K=20.02316	u=0.2656 B=–0.21306 K=20.02186	u=0.2660 B=–0.19431 K=20.02070	u=0.2664 B=–0.17510 K=20.01962
0.000	0.03069	0.03017	0.03012	0.03009	0.03006	0.03003
0.001	0.03075	0.03023	0.03018	0.03020	0.03012	0.03009
0.002	0.03080	0.03029	0.03024	0.03031	0.03018	0.03015
0.003	0.03086	0.03035	0.03030	0.03042	0.03024	0.03021
0.004	0.03092	0.03041	0.03036	0.03053	0.03030	0.03027
0.005	0.03097	0.03046	0.03042	0.03064	0.03035	0.03033
0.006	0.03103	0.03052	0.03048	0.03075	0.03041	0.03039
0.007	0.03109	0.03058	0.03054	0.03086	0.03047	0.03045
0.008	0.03115	0.03064	0.03060	0.03097	0.03053	0.03051
0.009	0.03120	0.03070	0.03065	0.03108	0.03059	0.03057
0.010	0.03126	0.03076	0.03071	0.03119	0.03065	0.03063
0.020	0.03183	0.03135	0.03130	0.03230	0.03124	0.03122
0.030	0.03240	0.03193	0.03189	0.03340	0.03183	0.03181
0.040	0.03297	0.03252	0.03248	0.03451	0.03243	0.03241
0.050	0.03354	0.03311	0.03307	0.03561	0.03302	0.03300
0.060	0.03411	0.03370	0.03366	0.03672	0.03361	0.03359
0.070	0.03467	0.03429	0.03425	0.03782	0.03420	0.03419
0.080	0.03524	0.03487	0.03484	0.03893	0.03479	0.03478
0.090	0.03581	0.03546	0.03543	0.04003	0.03538	0.03537
0.100	0.03638	0.03605	0.03602	0.04114	0.03598	0.03597

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \left\| \lvert F_o \rvert - \lvert F_c \rvert \right\|}{\sum \lvert F_o \rvert}$				
	u=0.2667 B=–0.16035 K=20.01899	u=0.2668 B=–0.15537 K=20.01880	u=0.2669 B=–0.15032 K=20.01877	u=0.2670 B=–0.14533 K=20.01846	u=0.2671 B=–0.50290 K=20.06425
0.000	0.030022	0.030020	0.030017	0.030013	0.029862
0.001	0.030081	0.030079	0.030076	0.030073	0.029869
0.002	0.030141	0.030139	0.030136	0.030132	0.029876
0.003	0.030201	0.030198	0.030195	0.030192	0.029883
0.004	0.030260	0.030258	0.030255	0.030251	0.029889
0.005	0.030319	0.030317	0.030314	0.030311	0.029896
0.006	0.030379	0.030377	0.030374	0.030370	0.029902
0.007	0.030438	0.030436	0.030433	0.030430	0.029909
0.008	0.030498	0.030496	0.030493	0.030489	0.029916
0.009	0.030557	0.030555	0.030552	0.030549	0.029922
0.010	0.030616	0.030614	0.030611	0.030608	0.029929
0.020	0.031211	0.031209	0.031206	0.031203	0.029995
0.030	0.031805	0.031803	0.031801	0.031799	0.030061
0.040	0.032399	0.032398	0.032396	0.032394	0.030127
0.050	0.032993	0.032992	0.032991	0.032989	0.030193
0.060	0.033587	0.033587	0.033585	0.033584	0.030259
0.070	0.034181	0.034181	0.034180	0.034179	0.030325
0.080	0.034775	0.034776	0.034775	0.034774	0.030391
0.090	0.035369	0.035370	0.035370	0.035359	0.030472
0.100	0.035963	0.035964	0.035965	0.035964	0.030620

Table A.4. (continued)

Degree of Disorder x	$R = \frac{\sum \left\|\|F_o\| - \|F_c\|\right\|}{\sum \|F_o\|}$					
	u=0.2672 B=−0.13514 K=20.01824	u=0.2676 B=−0.11440 K=20.01788	u=0.2680 B=−0.09324 K=20.01752	u=0.2684 B=−0.07152 K=20.01761	u=0.2688 B=−0.04933 K=20.01787	u=0.2700 B=−0.02023 K=20.02028
0.000	0.03046	0.03189	0.03336	0.03486	0.03639	0.04113
0.001	0.03051	0.03193	0.03341	0.03490	0.03644	0.04117
0.002	0.03056	0.03198	0.03345	0.03495	0.03648	0.04122
0.003	0.03061	0.03202	0.03349	0.03499	0.03652	0.04126
0.004	0.03066	0.03206	0.03353	0.03503	0.03656	0.04130
0.005	0.03071	0.03210	0.03358	0.03508	0.03661	0.04135
0.006	0.03077	0.03215	0.03362	0.03512	0.03665	0.04139
0.007	0.03082	0.03219	0.03366	0.03516	0.03669	0.04143
0.008	0.03087	0.03223	0.03371	0.03521	0.03674	0.041148
0.009	0.03092	0.03228	0.03375	0.03525	0.03677	0.04152
0.010	0.03097	0.03232	0.03379	0.03529	0.03682	0.04157
0.020	0.03148	0.03275	0.03422	0.03572	0.03725	0.04200
0.030	0.03199	0.03324	0.03465	0.03615	0.03769	0.04243
0.040	0.03250	0.03375	0.03508	0.03658	0.03812	0.04287
0.050	0.03301	0.03426	0.03551	0.03701	0.03855	0.04330
0.060	0.03359	0.03477	0.03594	0.03744	0.03898	0.04374
0.070	0.03418	0.03528	0.03639	0.03787	0.03941	0.04417
0.080	0.03478	0.03578	0.03690	0.03830	0.03984	0.04461
0.090	0.03538	0.03630	0.03741	0.03873	0.04027	0.04504
0.100	0.03597	0.03681	0.03792	0.03916	0.04070	0.04548