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DeLuca et al.

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(54) **(20R,25S)-2-METHYLENE-19,26-DINOR-1α,25-DIHYDROXYVITAMIN D_3 IN CRYSTALLINE FORM**

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C07C 401/00 (2006.01)
A61K 31/59 (2006.01)

(52) **U.S. Cl.** **552/653**; 514/167

(58) **Field of Classification Search** 514/167; 552/653

See application file for complete search history.

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Primary Examiner — Sabiha N Qazi

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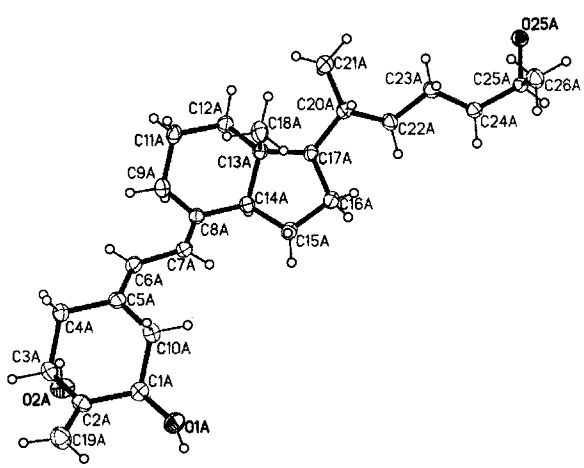
(57) **ABSTRACT**

A method of purifying (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 to obtain (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 in crystalline form. The method includes the steps of preparing a solvent of methanol and water, dissolving a product containing (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 to be purified in the solvent, cooling the solvent and dissolved product below ambient temperature for a sufficient amount of time to form a precipitate of (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 crystals, and recovering the (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 crystals.

16 Claims, 5 Drawing Sheets



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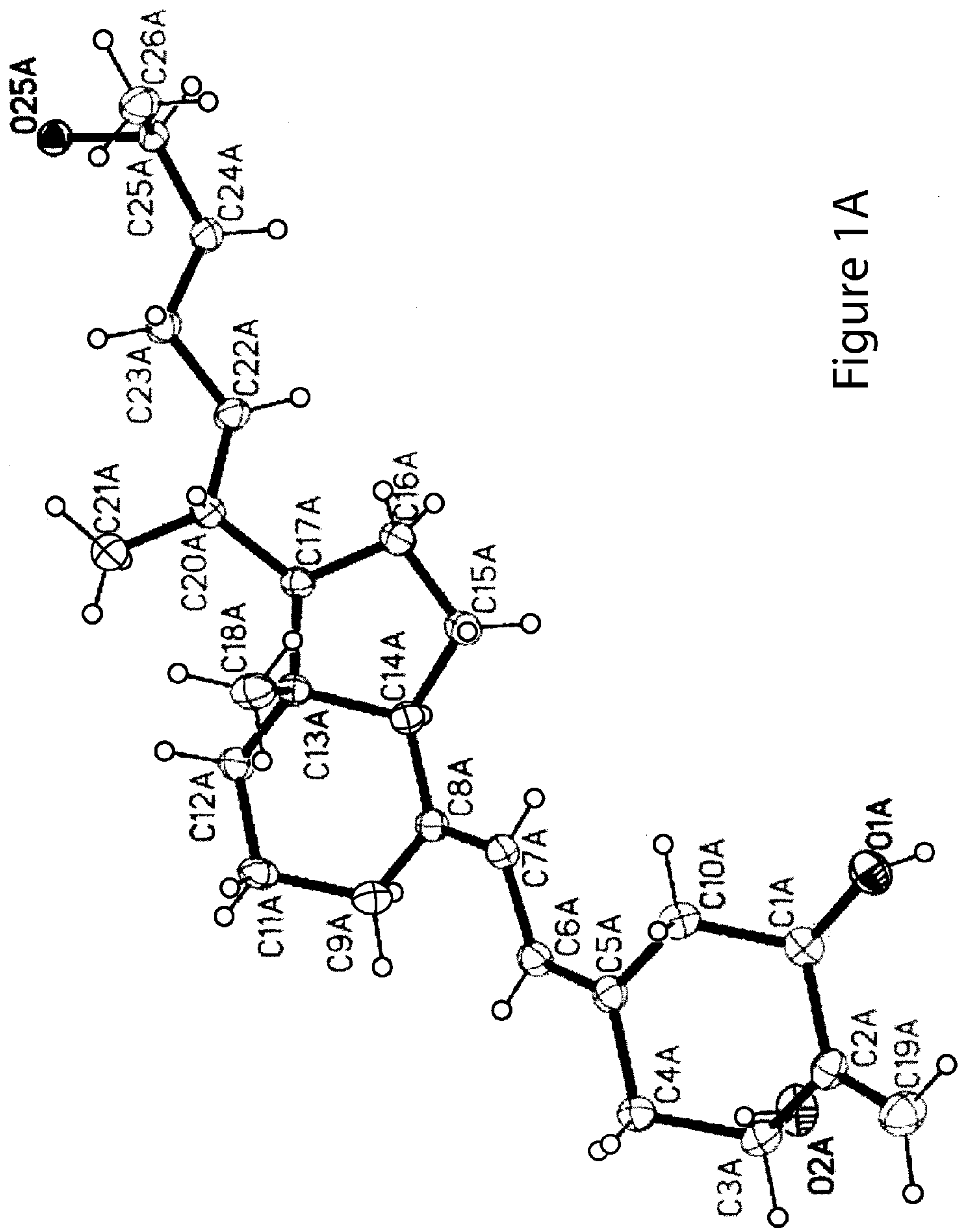
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C7A
C11A
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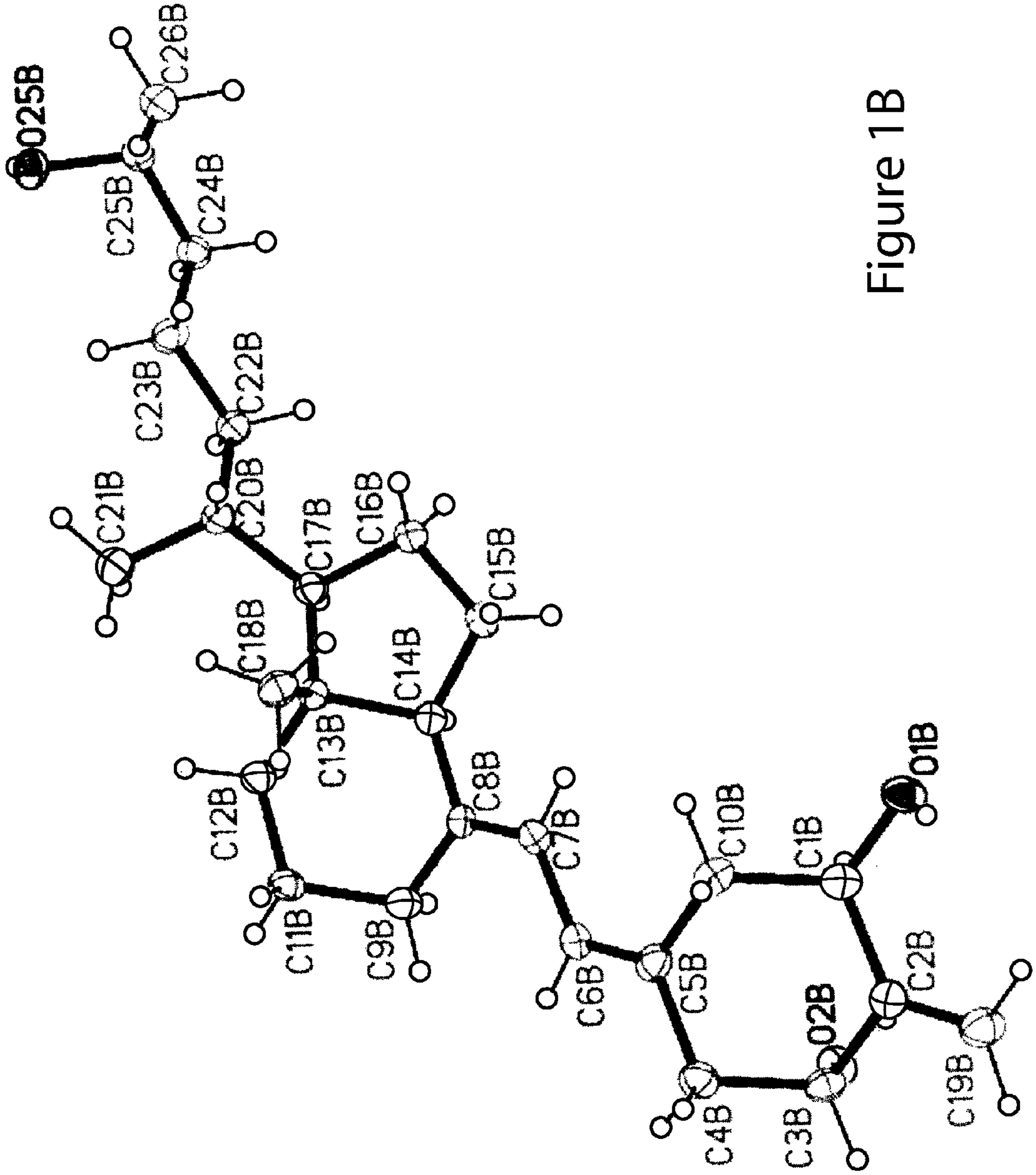
Figure 1A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C7B
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C3B
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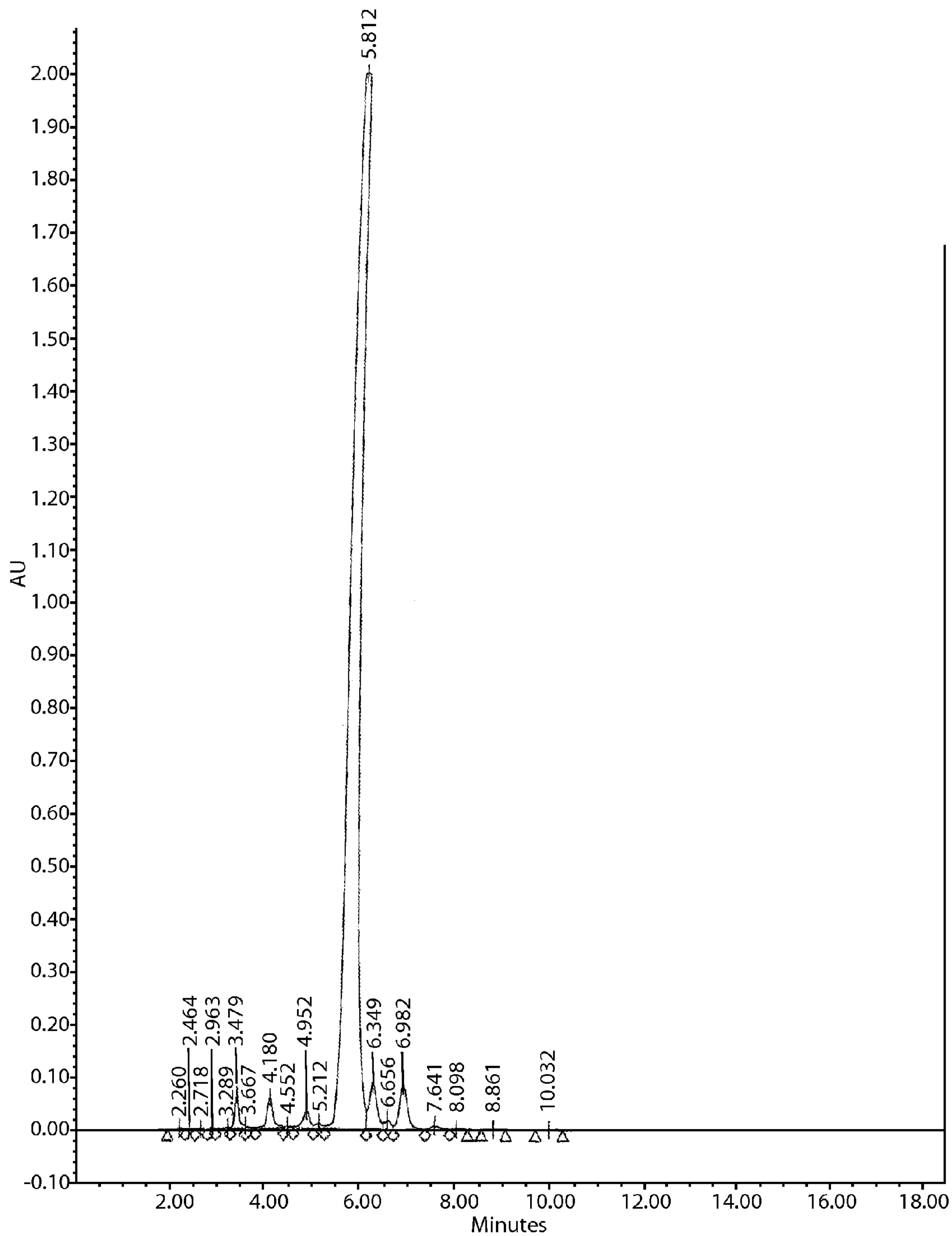
Figure 1B



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6.656
6.982
7.641
8.098
8.861
10.032
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1.60
1.50
1.40
1.30
1.20
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1.00
0.90
0.80
0.70
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0.50
0.40
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0.00
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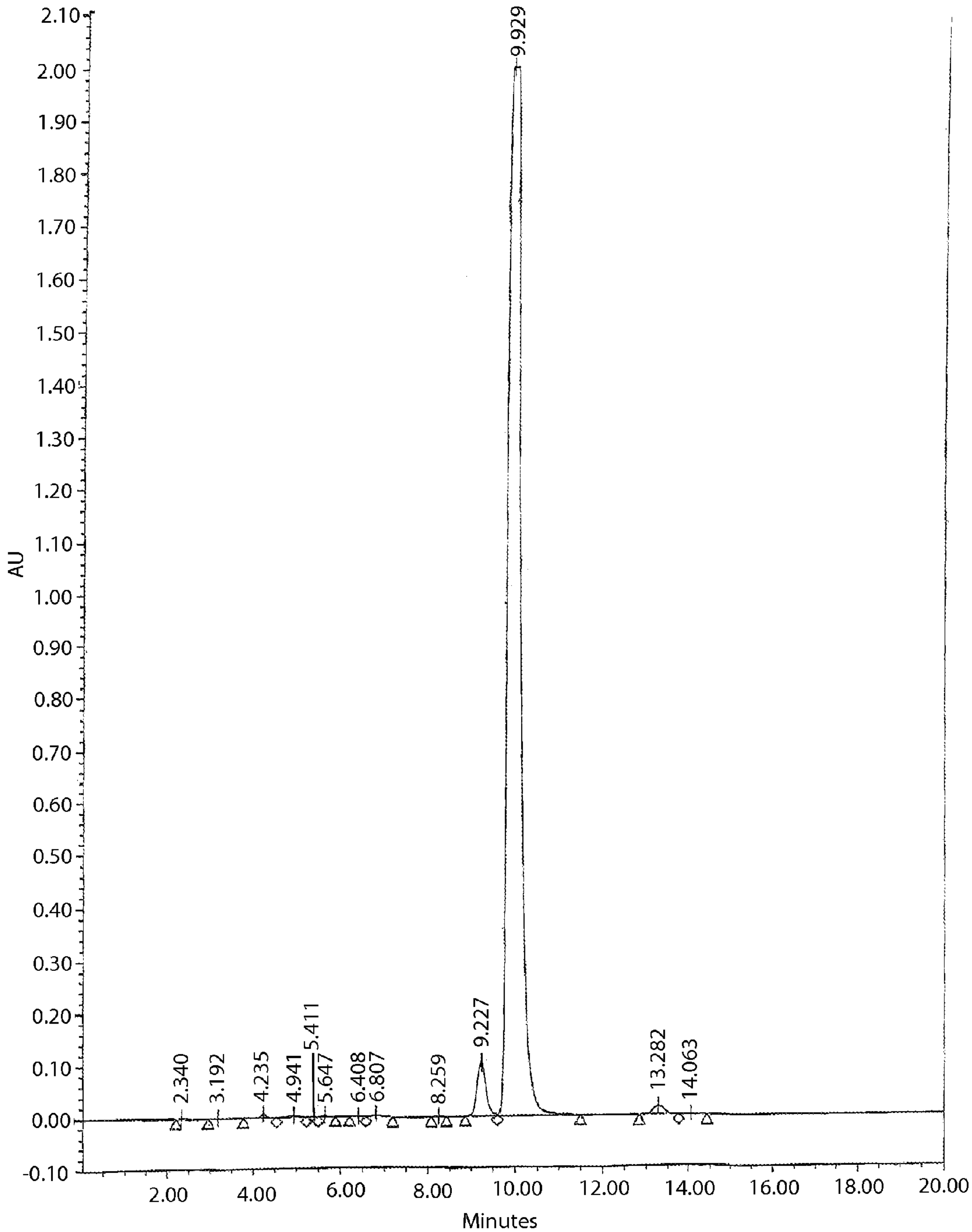
14.00
16.00
18.00
Minutes

Figure 2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0.50
0.40
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10.00
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18.00
20.00
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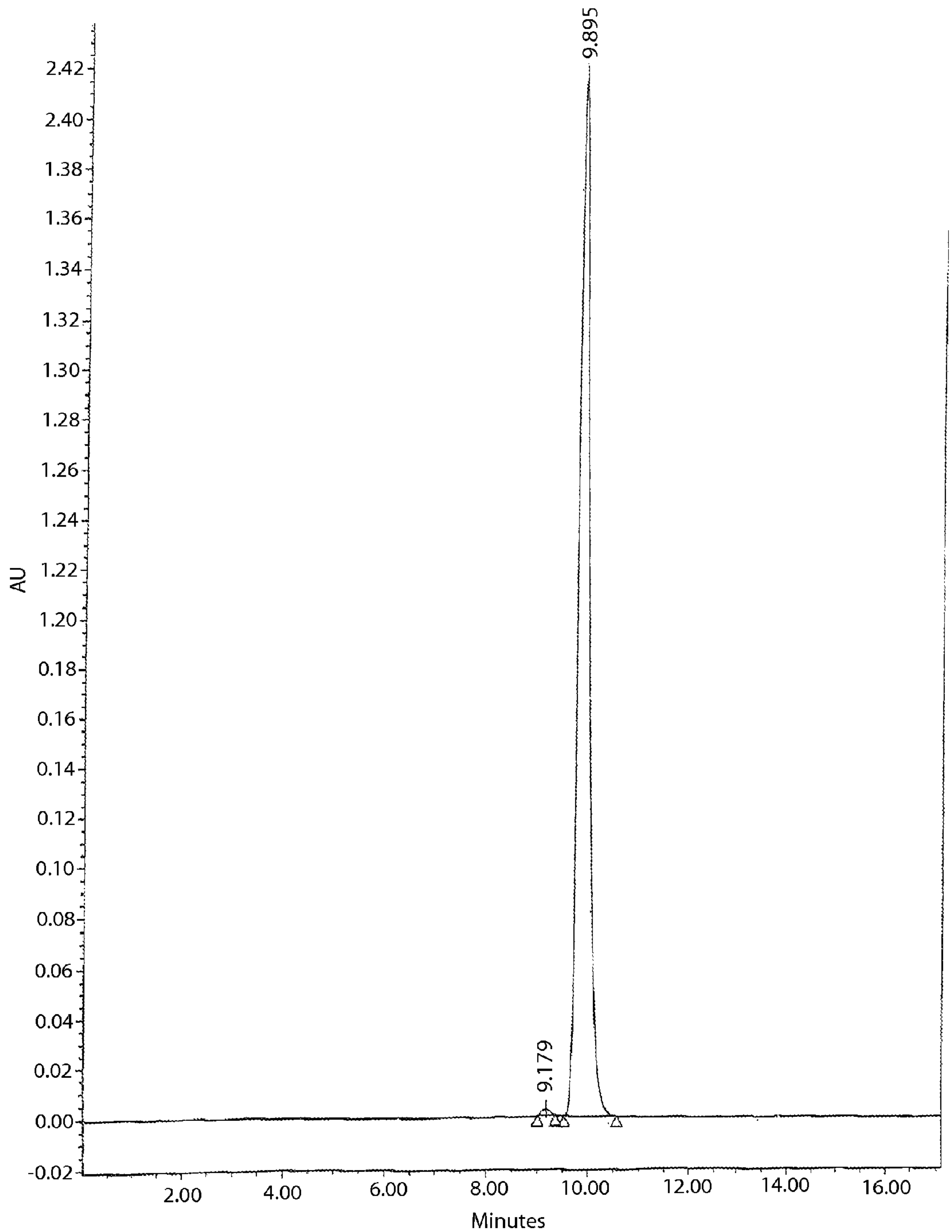
14.063

Figure 3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0.06
0.04
0.02
0.00
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4.00
6.00
8.00
10.00
12.00
14.00
16.00
Minutes

Figure 4

(20R,25S)-2-METHYLENE-19,26-DINOR-1α,25-DIHYDROXYVITAMIN D_3 IN CRYSTALLINE FORM

STATEMENT REGARDING FEDERALLY SPONSORED RESEARCH OR DEVELOPMENT

This invention was made with government support under DK047814 awarded by the National Institutes of Health. The government has certain rights in the invention.

BACKGROUND OF THE INVENTION

The present invention relates to purification of organic compounds, and more particularly to the purification of (20R,25S)-2-Methylene-19,26-Dinor-1α,25-Dihydroxyvitamin D_3 (referred to herein as "NEL") by preparing it in crystalline form.

Purification of organic compounds, especially those designated for pharmaceutical use, is of considerable importance for chemists synthesizing such compounds. Preparation of the compound usually requires many synthetic steps and, therefore, the final product can be contaminated not only with side-products derived from the last synthetic step of the procedure but also with compounds that were formed in previous steps. Even chromatographic purification, which is a very efficient but relatively time-consuming process, does not usually provide compounds which are sufficiently pure to be used as drugs.

Depending on the method used to synthesize 1α-hydroxyvitamin D compounds, different minor undesirable compounds can accompany the final product. Thus, for example, if direct C-1 hydroxylation of 5,6-trans geometric isomer of vitamin D is performed, followed by SeO^2/NMO oxidation and photochemical irradiation [see Andrews et al., *J. Org. Chem.* 51, 1635 (1986); Calverley et al., *Tetrahedron* 43, 4609 (1987); Choudry et al, *J. Org. Chem.* 58, 1496 (1993)], the final 1α-hydroxyvitamin D product can be contaminated with 1β-hydroxy- as well as 5,6-trans isomers. If the method consists of C-1 allylic oxidation of the 4-phenyl-1,2,4-triazoline-3,5-dione adduct of the previtamin D compound, followed by cycloreversion of the modified adduct under basic conditions [Nevinckx et al., *Tetrahedron* 47, 9419 (1991); Vanmaele et al, *Tetrahedron* 41, 141 (1985) and 40, 1179 (1994); Vanmaele et al., *Tetrahedron Lett.* 23. 995 (1982)], one can expect that the desired 1α-hydroxyvitamin can be contaminated with the previtamin 5(10), 6,8-triene and 1β-hydroxy isomer. One of the most useful C-1 hydroxylation methods, of very broad scope and numerous applications, is the experimentally simple procedure elaborated by Paaren et al. [see *J. Org. Chem.* 45, 3253 (1980) and *Proc. Natl. Acad. Sci. U.S.A.* 75, 2080 (1978)]. This method consists of allylic oxidation of 3,5-cyclovitamin D derivatives, readily obtained from the buffered solvolysis of vitamin D tosylates, with SeO_2/t-BuOOH and subsequent acid-catalyzed cycloreversion to the desired 1αhydroxy compounds. Taking into account this synthetic path it is reasonable to assume that the final product can be contaminated with 1α-hydroxy epimer, 5,6-trans isomer and the previtamin D form. 1α-hydroxyvitamin D_4 is another undesirable contaminant found in 1α-hydroxyvitamin D compounds synthesized from vitamin D_2 or from ergosterol. 1α-hydroxyvitamin D_4 results from C-1 oxidation of vitamin D_4, which in turn is derived from contamination of the commercial ergosterol material. Typically, the final product may contain up to about 1.5% by weight 1α-hydroxyvitamin D_4. Thus, a purification technique that would eliminate or substantially reduce the amount of 1α-hydroxyvitamin D_4 in the final product to less than about 0.1-0.2% would be highly desirable.

The vitamin D conjugated triene system is not only heat- and light-sensitive but it is also prone to oxidation, leading to the complex mixture of very polar compounds. Oxidation usually happens when a vitamin D compound has been stored for a prolonged time. Other types of processes that can lead to a partial decomposition of vitamin D compounds consist of some water-elimination reactions; their driving force is allylic (1α-) and homoallylic (3β-) position of the hydroxy groups. The presence of such above-mentioned oxidation and elimination products can be easily detected by thin-layer chromatography.

Usually, all 1α-hydroxylatation procedures require at least one chromatographic purification. However, even chromatographically purified 1αhydroxyvitamin D compounds, although showing consistent spectroscopic data, suggesting homogeneity, do not meet the purity criteria required for therapeutic agents that can be orally, parenterally or transdermally administered. Therefore, it was evident that a suitable method of purification of the 1αhydroxylated vitamin D compound NEL is required.

SUMMARY OF THE INVENTION

The present invention relates to a method of purifying NEL by means of crystallization to obtain NEL in crystalline form. The solvent plays a crucial role in the crystallization process, and is typically an individual liquid substance or a suitable mixture of different liquids. For crystallizing NEL, the most appropriate solvent and/or solvent system is characterized by the following factors:

(1) low toxicity;

(2) low boiling point;

(3) significant dependence of solubility properties with regard to temperature (condition necessary for providing satisfactory crystallization yield); and

(4) relatively low cost.

Interestingly, hexane, so frequently used for crystallization purposes, was found less suitable for crystallization of NEL. However, it was found that a mixture of two liquids, namely water and methanol, in amounts of from about 10% water with about 90% methanol to about 30% water with about 70% methanol, was most useful for the crystallization of NEL. In particular, it, was determined that a mixture of 20% water with 80% methanol (by volume) performed well. The water/methanol solvent mixture was also easy to remove by evaporation or other well known methods. In all cases the crystallization process occurred easily and efficiently; and the precipitated crystals were sufficiently large to assure their recovery by filtration or other means.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. **1**A is an illustration of the three dimensional structure of a first asymmetric molecular structure for NEL as defined by the atomic positional parameters discovered and set forth herein;

FIG. **1**B is, an illustration of the three dimensional structure of a second asymmetric molecular structure for NEL as defined by the atomic positional parameters discovered and set forth herein;

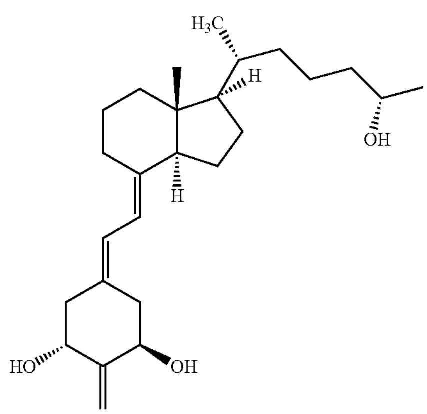
FIG. **2** is an HPLC (9.4 mm×25 cm Zorbax-Sil column, 15% 2-propanol in hexane; 6 mL/min; R_t=5.8 min.) profile of the solid material of NEL compound obtained after chemical synthesis; purity of the NEL compound before further HPLC purification was found to be 88.9%, checked by straight-phase HPLC;

FIG. **3** is an HPLC (9.4 mm×25 cm Zorbax RX-C18 column, 15% water in methanol; 3 mL/min; R_t=9.9 min.) profile of the NEL compound obtained after a first, straight-phase HPLC purification of the solid NEL material; purity of the NEL compound after this first HPLC purification was found to be 95.3%, checked by reversed-phase HPLC; and

FIG. **4** is an HPLC (9.4 mm×25 cm Zorbax RX-C18 column, 15% water in methanol; 3 ml/min; R_t=9.9 min.) profile of the NEL compound obtained after a second reversed-phase HPLC purification of the NEL compound obtained from the first HPLC purification; purity of the NEL compound after this second HPLC purification was found to be 99.5%, checked by reversed-phase HPLC. Crystals of the NEL compound were obtained after reversed-phase HPLC purification by single crystallization using a 20% water/80% methanol solvent system.

DETAILED DESCRIPTION OF THE INVENTION

The present invention provides (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 (NEL) in crystalline form, a pharmacologically important compound, characterized by the formula I shown below:



I

The present invention also provides a valuable method of purification of NEL. The purification technique involves obtaining the NEL product in crystalline form by utilizing a crystallization procedure wherein the NEL material to be purified is dissolved using as the solvent a mixture comprised of methanol and water in amounts of from about 10% water with about 90% methanol to about 30% water with about 70% methanol, by volume. Preferably the mixture comprises 80% methanol and 20% water (by volume). The solvent and dissolved product containing (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D3 (NEL) to be purified may then be cooled to about −20° C., or may in a first step be maintained at ambient temperature for a period of time (1 hour to 1 week) and then cooled in a second step to about −20° C. In either case, the solution is then maintained at about −20° C. for up to 7 weeks. Thereafter, the solvent can be removed by evaporation, with or without vacuum, or other means as is well known, or the resultant crystals may be filtered from the mother liquor. The technique can be used to purify a wide range of final products containing NEL obtained from any known synthesis thereof, and in varying concentrations, i.e. from microgram amounts to kilogram amounts. As is well known to those skilled in this art, the amount of solvent utilized should be minimized and/or adjusted according to the amount of NEL to be purified.

The usefulness and advantages of the present crystallization procedure is shown in the following specific Examples 1 and 2. After crystallization, the precipitated material was observed under a microscope to confirm its crystalline form. Additionally, the crystals were then analyzed to determine their initial purity (88.9%; FIG. **2**), and their significantly improved purity was confirmed after a first, straight-phase HPLC (95.3%, FIG. **3**), as well as a second, reversed-phase HPLC (99.5%; FIG. **4**). Yields of crystals were high and the obtained crystals showed a relatively sharp melting point of 154-155° C.

The described crystallization process of the synthetic NEL product represents a valuable purification method, which can remove most side products derived from the synthetic path. Such impurity is the result of the contamination of starting raw materials. The crystallization process occurred easily and efficiently; and the precipitated crystals were sufficiently large to assure their recovery by filtration, or other means.

EXAMPLE 1

Crystallization of (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 (NEL)

Crystals of the NEL analog were obtained from a solution of the compound in 20% water and 80% methanol (20% H_2O/80% MeOH) as follows:

14 mg of pure NEL compound was dissolved in 8 mL of water/methanol solvent mixture (water/methanol=2/8). The solution was kept at −20 degrees Celsius for 7 weeks. The precipitated crystals (M.p. 154-155° C.) were analyzed by straight phase HPLC (crystals: FIG. **2**) and found to be 99.5% pure.

EXAMPLE 2

Experimental

A colorless prism-shaped crystal of dimensions 0.47×0.12×0.18 mm was selected for structural analysis. Intensity data were collected using a Bruker AXS Platinum 135 CCD detector controlled with the PROTEUM software suite (Bruker AXS Inc., Madison, Wis.). The x-ray source was CuKα radiation (1.54178 Å) from a Rigaku RU200 x-ray generator equipped with Montel optics, operated at 50 kV and 80 mA. The x-ray data were processed with SAINT version 7.06A (Bruker AXS Inc) and, internally scaled with SADABS version 2005/1 (Bruker AXS Inc.). The sample was mounted on a glass fiber using vacuum grease and cooled to 100° K. The intensity data were measured as a series of phi and omega oscillation frames each of 1° for 10-15 sec/frame. The detector was operated in 1024/1024 mode and was positioned 4.5 cm from the sample. Cell parameters were determined from a non-linear least squares fit of 9999 peaks in the range of 3.0<theta<64.8°. The data were merged to form a set of 6791 independent data with R(int)=0.0326.

The triclinic space group P1 was determined by systematic absences and statistical tests and verified by subsequent refinement. The structure was solved by direct methods, and refined by full matrix least-squares methods on F^2, (a) G. M. Sheldrick (1994), SHELXTL Version 5 Reference Manual, Bruker AXS Inc.; (b) *International Tables for Crystallography, Vol, C*, Kluwer: Boston (1995). The asymmetric unit was comprised of two molecules of NEL, designated with A and B. Hydrogen atom positions were determined from difference peaks and ultimately refined by a riding model with idealized geometry. Non-hydrogen atoms were refined with anisotropic displacement parameters. A total of 523 parameters were refined against 3 restraints and 6781 data to give wR2=0.0943 and S=1.066 for weights of $w=1/[s^2(F^2)+(0.0613P)^2]$, where $P=[F^2+2F_c^2]/3$. The final R(F) was 0.0342 for the 6781 observed data. The largest shift/s.u. was 0.001 in the final refinement cycle and the final difference map had maxima and minima of 0.217 and −0.177 e/Å^3, respectively. The absolute structure was determined by refinement of the Flack parameter, H. D. Flack, *Acta Cryst. A*, vol. 39, 876-881 (1983).

The three dimensional structure of NEL as defined by the following physical data and atomic positional parameters described and calculated herein is illustrated in FIG. **1**A and FIG. **1**B.

TABLE 1

Crystal data and structure refinement for NEL.

Identification code	NEL
Empirical formula	C26H42O3
Formula weight	402.60
Temperature	100(1) K
Wavelength	1.54178 Å
Crystal system, space group	P1,
Unit cell dimensions	a = 6.3820(11) Å α = 110.920(5)°
	b = 12.594(2) Å β = 95.256(5)°
	c = 15.996(3)° Å γ = 90.609(5)°
Volume	1194.6(4) Å^3
Z, Calculated density	2, 1.119 Mg/m^3
Absorption coefficient	0.549 mm^{-1}
F(000)	444
Crystal size	0.47 × 0.12 × 0.18 mm
Theta range for data collection	2.97 to 64.82°
Limiting indices	−7 <= h <= 7, −14 <= k <= 14, −18 <= l <= 18
Reflections collected/unique	18206/6781 [R(int) = 0.0326]
Completeness to theta = 64.82	96.0%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	6781/3/523
Goodness-of-fit on F^2	1.066
Final R indices [I > 2σ(I)]	R1 = 0.0336, wR2 = 0.0943
R indices (all data)	R1 = 0.0342, wR2 = 0.0948
Absolute structure parameter	−0.04(13)
Largest diff. peak and hole	0.217 and −0.177 e/A^3

TABLE 2

Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (A^2 × 10^3) for NEL. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1B)	20004(2)	17550(1)	1623(1)	24(1)
O(25A)	17814(2)	15531(1)	1308(1)	22(1)
O(1A)	17343(2)	13368(1)	9956(1)	25(1)
O(2B)	26264(2)	18348(1)	1150(1)	24(1)
O(25B)	24669(2)	16177(1)	10298(1)	25(1)
O(2A)	23666(2)	12775(1)	10464(1)	30(1)
C(12B)	29763(3)	18997(2)	6571(1)	21(1)
C(3B)	24736(3)	19211(2)	1351(1)	21(1)
C(14A)	22676(3)	13599(2)	6215(1)	20(1)
C(1A)	19399(3)	12961(2)	9789(1)	22(1)
C(1B)	22059(3)	18070(2)	1796(1)	20(1)
C(7B)	26024(3)	18595(2)	4148(1)	23(1)
C(9B)	29674(3)	19090(2)	4995(1)	21(1)
C(7A)	22104(3)	12709(2)	7363(1)	22(1)
C(8A)	23258(3)	12850(2)	6750(1)	20(1)
C(18B)	25854(3)	19292(2)	6615(1)	23(1)

TABLE 2-continued

Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (A^2 × 10^3) for NEL. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(8B)	27529(3)	18497(2)	4760(1)	20(1)
C(4A)	22392(3)	11177(2)	9084(1)	22(1)
C(10B)	22526(3)	18874(2)	2783(1)	24(1)
C(13A)	22519(3)	12966(2)	5181(1)	21(1)
C(5A)	21554(3)	11878(2)	8545(1)	21(1)
C(13B)	27557(3)	18418(1)	6337(1)	18(1)
C(12A)	24663(3)	12455(2)	4951(1)	24(1)
C(4B)	25235(3)	19984(2)	2339(1)	23(1)
C(6B)	26236(3)	19238(2)	3562(1)	21(1)
C(5B)	24742(3)	19367(2)	2960(1)	22(1)
C(14B)	27268(3)	17751(2)	5300(1)	21(1)
C(10A)	19424(3)	12345(2)	8773(1)	24(1)
C(2B)	22531(3)	18696(2)	1180(1)	20(1)
C(11B)	30116(3)	19743(2)	6014(1)	22(1)
C(25A)	16921(3)	15954(2)	2170(1)	21(1)
C(11A)	25307(3)	11695(2)	5489(1)	26(1)
C(9A)	25341(3)	12322(2)	6512(1)	23(1)
C(2A)	20095(3)	12173(2)	10275(1)	22(1)
C(15B)	25289(4)	17009(2)	5155(1)	29(1)
C(19B)	21153(3)	18805(2)	546(1)	26(1)
C(22B)	26528(3)	16572(2)	7829(1)	24(1)
C(16A)	20397(3)	14647(2)	5542(1)	24(1)
C(19A)	18923(3)	11833(2)	10779(1)	29(1)
C(3A)	22290(3)	11784(2)	10098(1)	23(1)
C(6A)	22665(3)	12056(2)	7932(1)	22(1)
C(24A)	18538(3)	15914(2)	2914(1)	24(1)
C(15A)	20687(3)	14277(2)	6365(1)	28(1)
C(18A)	20768(3)	12036(2)	4871(1)	27(1)
C(20B)	26644(3)	17688(2)	7646(1)	22(1)
C(26B)	21533(3)	15634(2)	9292(1)	27(1)
C(25B)	23829(3)	15374(2)	9433(1)	21(1)
C(23B)	25282(3)	16605(2)	8603(1)	26(1)
C(16B)	25461(3)	16641(2)	5984(1)	26(1)
C(24B)	25149(3)	15444(2)	8706(1)	23(1)
C(23A)	19136(3)	14732(2)	2894(1)	26(1)
C(20A)	21004(3)	13700(2)	3878(1)	24(1)
C(17B)	27207(3)	17428(2)	6678(1)	20(1)
C(17A)	21928(3)	13962(1)	4855(1)	20(1)
C(22A)	20565(3)	14826(2)	3734(1)	24(1)
C(26A)	14899(3)	15287(2)	2077(1)	28(1)
C(21B)	28182(4)	18550(2)	8366(1)	33(1)
C(21A)	22416(4)	12988(2)	3186(1)	40(1)

TABLE 3

Bond lengths [Å] for NEL.

O(1B)—C(1B)	1.419(2)
O(1B)—H(1BA)	0.8200
O(25A)—C(25A)	1.461(2)
O(25A)—H(25A)	0.8200
O(1A)—C(1A)	1.427(2)
O(1A)—H(1AA)	0.8200
O(2B)—C(3B)	1.438(2)
O(2B)—H(2BA)	0.8200
O(25B)—C(25B)	1.441(2)
O(25B)—H(25B)	0.8200
O(2A)—C(3A)	1.426(2)
O(2A)—H(2AA)	0.8200
C(12B)—C(13B)	1.529(3)
C(12B)—C(11B)	1.536(3)
C(12B)—H(12A)	0.9700
C(12B)—H(12B)	0.9700
C(3B)—C(2B)	1.503(3)
C(3B)—C(4B)	1.533(2)
C(3B)—H(3BA)	0.9800
C(14A)—C(8A)	1.511(3)
C(14A)—C(15A)	1.527(3)
C(14A)—C(13A)	1.552(2)
C(14A)—H(14A)	0.9800

TABLE 3-continued

Bond lengths [Å] for NEL.	
C(1A)—C(2A)	1.511(3)
C(1A)—C(10A)	1.532(3)
C(1A)—H(1AB)	0.9800
C(1B)—C(2B)	1.513(3)
C(1B)—C(10B)	1.540(3)
C(1B)—H(1BB)	0.9800
C(7B)—C(8B)	1.346(3)
C(7B)—C(6B)	1.454(3)
C(7B)—H(7BA)	0.9300
C(9B)—C(8B)	1.502(3)
C(9B)—C(11B)	1.538(3)
C(9B)—H(9BA)	0.9700
C(9B)—H(9BB)	0.9700
C(7A)—C(8A)	1.338(3)
C(7A)—C(6A)	1.453(3)
C(7A)—H(7AA)	0.9300
C(8A)—C(9A)	1.512(3)
C(18B)—C(13B)	1.535(2)
C(18B)—H(18A)	0.9600
C(18B)—H(18B)	0.9600
C(18B)—H(18C)	0.9600
C(8B)—C(14B)	1.504(2)
C(4A)—C(5A)	1.508(3)
C(4A)—C(3A)	1.535(3)
C(4A)—H(4AA)	0.9700
C(4A)—H(4AB)	0.9700
C(10B)—C(5B)	1.499(3)
C(10B)—H(10A)	0.9700
C(10B)—H(10B)	0.9700
C(13A)—C(18A)	1.524(3)
C(13A)—C(12A)	1.538(2)
C(13A)—C(17A)	1.558(2)
C(5A)—C(6A)	1.342(3)
C(5A)—C(10A)	1.510(3)
C(13B)—C(17B)	1.551(2)
C(13B)—C(14B)	1.560(2)
C(12A)—C(11A)	1.536(3)
C(12A)—H(12C)	0.9700
C(12A)—H(12D)	0.9700
C(4B)—C(5B)	1.515(3)
C(4B)—H(4BA)	0.9700
C(4B)—H(4BB)	0.9700
C(6B)—C(5B)	1.345(3)
C(6B)—H(6BA)	0.9300
C(14B)—C(15B)	1.513(3)
C(14B)—H(14B)	0.9800
C(10A)—H(10C)	0.9700
C(10A)—H(10D)	0.9700
C(2B)—C(19B)	1.326(3)
C(11B)—H(11A)	0.9700
C(11B)—H(11B)	0.9700
C(25A)—C(26A)	1.499(3)
C(25A)—C(24A)	1.518(3)
C(25A)—H(25C)	0.9800
C(11A)—C(9A)	1.539(3)
C(11A)—H(11C)	0.9700
C(11A)—H(11D)	0.9700
C(9A)—H(9AA)	0.9700
C(9A)—H(9AB)	0.9700
C(2A)—C(19A)	1.320(3)
C(2A)—C(3A)	1.507(3)
C(15B)—C(16B)	1.548(3)
C(15B)—H(15A)	0.9700
C(15B)—H(15B)	0.9700
C(19B)—H(19A)	0.9300
C(19B)—H(19B)	0.9300
C(22B)—C(23B)	1.520(3)
C(22B)—C(20B)	1.537(2)
C(22B)—H(22A)	0.9700
C(22B)—H(22B)	0.9700
C(16A)—C(15A)	1.542(3)
C(16A)—C(17A)	1.563(2)
C(16A)—H(16A)	0.9700
C(16A)—H(16B)	0.9700
C(19A)—H(19C)	0.9300
C(19A)—H(19D)	0.9300
C(3A)—H(3AA)	0.9800
C(6A)—H(6AA)	0.9300

TABLE 3-continued

Bond lengths [Å] for NEL.	
C(24A)—C(23A)	1.531(3)
C(24A)—H(24A)	0.9700
C(24A)—H(24B)	0.9700
C(15A)—H(15C)	0.9700
C(15A)—H(15D)	0.9700
C(18A)—H(18D)	0.9600
C(18A)—H(18E)	0.9600
C(18A)—H(18F)	0.9600
C(20B)—C(21B)	1.532(3)
C(20B)—C(17B)	1.541(2)
C(20B)—H(20A)	0.9800
C(26B)—C(25B)	1.519(3)
C(26B)—H(26A)	0.9600
C(26B)—H(26B)	0.9600
C(26B)—H(26C)	0.9600
C(25B)—C(24B)	1.523(3)
C(25B)—H(25D)	0.9800
C(23B)—C(24B)	1.531(2)
C(23B)—H(23A)	0.9700
C(23B)—H(23B)	0.9700
C(16B)—C(17B)	1.556(3)
C(16B)—H(16C)	0.9700
C(16B)—H(16D)	0.9700
C(24B)—H(24B)	0.9700
C(24B)—H(24C)	0.9700
C(23A)—C(22A)	1.519(3)
C(23A)—H(23C)	0.9700
C(23A)—H(23D)	0.9700
C(20A)—C(21A)	1.527(3)
C(20A)—C(17A)	1.536(3)
C(20A)—C(22A)	1.541(2)
C(20A)—H(20B)	0.9800
C(17B)—H(17A)	0.9800
C(17A)—H(17B)	0.9800
C(22A)—H(22C)	0.9700
C(22A)—H(22D)	0.9700
C(26A)—H(26D)	0.9600
C(26A)—H(26E)	0.9600
C(26A)—H(26F)	0.9600
C(21B)—H(21A)	0.9600
C(21B)—H(21B)	0.9600
C(21B)—H(21C)	0.9600
C(21A)—H(21D)	0.9600
C(21A)—H(21E)	0.9600
C(21A)—H(21F)	0.9600

TABLE 4

Bond angles [°] for NEL.	
C(1B)—O(1B)—H(1BA)	109.5
C(25A)—O(25A)—H(25A)	109.5
C(1A)—O(1A)—H(1AA)	109.5
C(3B)—O(2B)—H(2BA)	109.5
C(25B)—O(25B)—H(25B)	109.5
C(3A)—O(2A)—H(2AA)	109.5
C(13B)—C(12B)—C(11B)	111.64(14)
C(13B)—C(12B)—H(12A)	109.3
C(11B)—C(12B)—H(12A)	109.3
C(13B)—C(12B)—H(12B)	109.3
C(11B)—C(12B)—H(12B)	109.3
H(12A)—C(12B)—H(12B)	108.0
O(2B)—C(3B)—C(2B)	111.37(14)
O(2B)—C(3B)—C(4B)	107.64(14)
C(2B)—C(3B)—C(4B)	110.89(15)
O(2B)—C(3B)—H(3BA)	109.0
C(2B)—C(3B)—H(3BA)	109.0
C(4B)—C(3B)—H(3BA)	109.0
C(8A)—C(14A)—C(15A)	120.67(16)
C(8A)—C(14A)—C(13A)	113.85(14)
C(15A)—C(14A)—C(13A)	104.06(14)
C(8A)—C(14A)—H(14A)	105.7
C(15A)—C(14A)—H(14A)	105.7
C(13A)—C(14A)—H(14A)	105.7
O(1A)—C(1A)—C(2A)	113.69(15)

TABLE 4-continued

Bond angles [°] for NEL.	
O(1A)—C(1A)—C(10A)	108.29(14)
C(2A)—C(1A)—C(10A)	109.59(14)
O(1A)—C(1A)—H(1AB)	108.4
C(2A)—C(1A)—H(1AB)	108.4
C(10A)—C(1A)—H(1AB)	108.4
O(1B)—C(1B)—C(2B)	114.49(15)
O(1B)—C(1B)—C(10B)	111.74(15)
C(2B)—C(1B)—C(10B)	109.51(15)
O(1B)—C(1B)—H(1BB)	106.9
C(2B)—C(1B)—H(1BB)	106.9
C(10B)—C(1B)—H(1BB)	106.9
C(8B)—C(7B)—C(6B)	125.92(18)
C(8B)—C(7B)—H(7BA)	117.0
C(6B)—C(7B)—H(7BA)	117.0
C(8B)—C(9B)—C(11B)	111.32(15)
C(8B)—C(9B)—H(9BA)	109.4
C(11B)—C(9B)—H(9BA)	109.4
C(8B)—C(9B)—H(9BB)	109.4
C(11B)—C(9B)—H(9BB)	109.4
H(9BA)—C(9B)—H(9BB)	108.0
C(8A)—C(7A)—C(6A)	126.04(17)
C(8A)—C(7A)—H(7AA)	117.0
C(6A)—C(7A)—H(7AA)	117.0
C(7A)—C(8A)—C(14A)	124.19(17)
C(7A)—C(8A)—C(9A)	125.42(16)
C(14A)—C(8A)—C(9A)	110.37(15)
C(13B)—C(18B)—H(18A)	109.5
C(13B)—C(18B)—H(18B)	109.5
H(18A)—C(18B)—H(18B)	109.5
C(13B)—C(18B)—H(18C)	109.5
H(18A)—C(18B)—H(18C)	109.5
H(18B)—C(18B)—H(18C)	109.5
C(7B)—C(8B)—C(9B)	125.88(17)
C(7B)—C(8B)—C(14B)	123.46(18)
C(9B)—C(8B)—C(14B)	110.66(15)
C(5A)—C(4A)—C(3A)	112.48(14)
C(5A)—C(4A)—H(4AA)	109.1
C(3A)—C(4A)—H(4AA)	109.1
C(5A)—C(4A)—H(4AB)	109.1
C(3A)—C(4A)—H(4AB)	109.1
H(4AA)—C(4A)—H(4AB)	107.8
C(5B)—C(10B)—C(1B)	110.68(15)
C(5B)—C(10B)—H(10A)	109.5
C(1B)—C(10B)—H(10A)	109.5
C(5B)—C(10B)—H(10B)	109.5
C(1B)—C(10B)—H(10B)	109.5
H(10A)—C(10B)—H(10B)	108.1
C(18A)—C(13A)—C(12A)	110.65(15)
C(18A)—C(13A)—C(14A)	111.01(15)
C(12A)—C(13A)—C(14A)	107.41(15)
C(18A)—C(13A)—C(17A)	110.89(15)
C(12A)—C(13A)—C(17A)	116.13(15)
C(14A)—C(13A)—C(17A)	100.21(13)
C(6A)—C(5A)—C(4A)	121.11(17)
C(6A)—C(5A)—C(10A)	124.93(17)
C(4A)—C(5A)—C(10A)	113.96(16)
C(12B)—C(13B)—C(18B)	111.30(15)
C(12B)—C(13B)—C(17B)	115.91(14)
C(18B)—C(13B)—C(17B)	110.94(15)
C(12B)—C(13B)—C(14B)	107.44(15)
C(18B)—C(13B)—C(14B)	110.58(14)
C(17B)—C(13B)—C(14B)	100.00(13)
C(11A)—C(12A)—C(13A)	111.24(15)
C(11A)—C(12A)—H(12C)	109.4
C(13A)—C(12A)—H(12C)	109.4
C(11A)—C(12A)—H(12D)	109.4
C(13A)—C(12A)—H(12D)	109.4
H(12C)—C(12A)—H(12D)	108.0
C(5B)—C(4B)—C(3B)	110.96(15)
C(5B)—C(4B)—H(4BA)	109.4
C(3B)—C(4B)—H(4BA)	109.4
C(5B)—C(4B)—H(4BB)	109.4
C(3B)—C(4B)—H(4BB)	109.4
H(4BA)—C(4B)—H(4BB)	108.0
C(5B)—C(6B)—C(7B)	126.94(18)
C(5B)—C(6B)—H(6BA)	116.5
C(7B)—C(6B)—H(6BA)	116.5
C(6B)—C(5B)—C(10B)	125.49(17)

TABLE 4-continued

Bond angles [°] for NEL.	
C(6B)—C(5B)—C(4B)	121.22(18)
C(10B)—C(5B)—C(4B)	113.17(15)
C(8B)—C(14B)—C(15B)	121.27(16)
C(8B)—C(14B)—C(13B)	113.18(14)
C(15B)—C(14B)—C(13B)	104.01(15)
C(8B)—C(14B)—H(14B)	105.7
C(15B)—C(14B)—H(14B)	105.7
C(13B)—C(14B)—H(14B)	105.7
C(5A)—C(10A)—C(1A)	111.36(15)
C(5A)—C(10A)—H(10C)	109.4
C(1A)—C(10A)—H(10C)	109.4
C(5A)—C(10A)—H(10D)	109.4
C(1A)—C(10A)—H(10D)	109.4
H(10C)—C(10A)—H(10D)	108.0
C(19B)—C(2B)—C(3B)	121.69(17)
C(19B)—C(2B)—C(1B)	124.35(18)
C(3B)—C(2B)—C(1B)	113.96(15)
C(12B)—C(11B)—C(9B)	112.84(15)
C(12B)—C(11B)—H(11A)	109.0
C(9B)—C(11B)—H(11A)	109.0
C(12B)—C(11B)—H(11B)	109.0
C(9B)—C(11B)—H(11B)	109.0
H(11A)—C(11B)—H(11B)	107.8
O(25A)—C(25A)—C(26A)	108.17(15)
O(25A)—C(25A)—C(24A)	109.76(15)
C(26A)—C(25A)—C(24A)	114.61(16)
O(25A)—C(25A)—H(25C)	108.0
C(26A)—C(25A)—H(25C)	108.0
C(24A)—C(25A)—H(25C)	108.0
C(12A)—C(11A)—C(9A)	112.71(15)
C(12A)—C(11A)—H(11C)	109.0
C(9A)—C(11A)—H(11C)	109.0
C(12A)—C(11A)—H(11D)	109.0
C(9A)—C(11A)—H(11D)	109.0
H(11C)—C(11A)—H(11D)	107.8
C(8A)—C(9A)—C(11A)	110.93(15)
C(8A)—C(9A)—H(9AA)	109.5
C(11A)—C(9A)—H(9AA)	109.5
C(8A)—C(9A)—H(9AB)	109.5
C(11A)—C(9A)—H(9AB)	109.5
H(9AA)—C(9A)—H(9AB)	108.0
C(19A)—C(2A)—C(3A)	123.23(17)
C(19A)—C(2A)—C(1A)	124.78(18)
C(3A)—C(2A)—C(1A)	111.96(16)
C(14B)—C(15B)—C(16B)	103.37(15)
C(14B)—C(15B)—H(15A)	111.1
C(16B)—C(15B)—H(15A)	111.1
C(14B)—C(15B)—H(15B)	111.1
C(16B)—C(15B)—H(15B)	111.1
H(15A)—C(15B)—H(15B)	109.1
C(2B)—C(19B)—H(19A)	120.0
C(2B)—C(19B)—H(19B)	120.0
H(19A)—C(19B)—H(19B)	120.0
C(23B)—C(22B)—C(20B)	115.28(16)
C(23B)—C(22B)—H(22A)	108.5
C(20B)—C(22B)—H(22A)	108.5
C(23B)—C(22B)—H(22B)	108.5
C(20B)—C(22B)—H(22B)	108.5
H(22A)—C(22B)—H(22B)	107.5
C(15A)—C(16A)—C(17A)	107.70(14)
C(15A)—C(16A)—H(16A)	110.2
C(17A)—C(16A)—H(16A)	110.2
C(15A)—C(16A)—H(16B)	110.2
C(17A)—C(16A)—H(16B)	110.2
H(16A)—C(16A)—H(16B)	108.5
C(2A)—C(19A)—H(19C)	120.0
C(2A)—C(19A)—H(19D)	120.0
H(19C)—C(19A)—H(19D)	120.0
O(2A)—C(3A)—C(2A)	106.68(15)
O(2A)—C(3A)—C(4A)	112.30(15)
C(2A)—C(3A)—C(4A)	109.87(15)
O(2A)—C(3A)—H(3AA)	109.3
C(2A)—C(3A)—H(3AA)	109.3
C(4A)—C(3A)—H(3AA)	109.3
C(5A)—C(6A)—C(7A)	128.24(17)
C(5A)—C(6A)—H(6AA)	115.9
C(7A)—C(6A)—H(6AA)	115.9
C(25A)—C(24A)—C(23A)	116.64(15)

TABLE 4-continued

Bond angles [°] for NEL.	
C(25A)—C(24A)—H(24A)	108.1
C(23A)—C(24A)—H(24A)	108.1
C(25A)—C(24A)—H(24B)	108.1
C(23A)—C(24A)—H(24B)	108.1
H(24A)—C(24A)—H(24B)	107.3
C(14A)—C(15A)—C(16A)	103.22(15)
C(14A)—C(15A)—H(15C)	111.1
C(16A)—C(15A)—H(15C)	111.1
C(14A)—C(15A)—H(15D)	111.1
C(16A)—C(15A)—H(15D)	111.1
H(15C)—C(15A)—H(15D)	109.1
C(13A)—C(18A)—H(18D)	109.5
C(13A)—C(18A)—H(18E)	109.5
H(18D)—C(18A)—H(18E)	109.5
C(13A)—C(18A)—H(18F)	109.5
H(18D)—C(18A)—H(18F)	109.5
H(18E)—C(18A)—H(18F)	109.5
C(21B)—C(20B)—C(22B)	109.89(15)
C(21B)—C(20B)—C(17B)	113.74(16)
C(22B)—C(20B)—C(17B)	109.14(14)
C(21B)—C(20B)—H(20A)	108.0
C(22B)—C(20B)—H(20A)	108.0
C(17B)—C(20B)—H(20A)	108.0
C(25B)—C(26B)—H(26A)	109.5
C(25B)—C(26B)—H(26B)	109.5
H(26A)—C(26B)—H(26B)	109.5
C(25B)—C(26B)—H(26C)	109.5
H(26A)—C(26B)—H(26C)	109.5
H(26B)—C(26B)—H(26C)	109.5
O(25B)—C(25B)—C(26B)	106.88(15)
O(25B)—C(25B)—C(24B)	109.97(15)
C(26B)—C(25B)—C(24B)	113.97(15)
O(25B)—C(25B)—H(25D)	108.6
C(26B)—C(25B)—H(25D)	108.6
C(24B)—C(25B)—H(25D)	108.6
C(22B)—C(23B)—C(24B)	111.82(15)
C(22B)—C(23B)—H(23A)	109.3
C(24B)—C(23B)—H(23A)	109.3
C(22B)—C(23B)—H(23B)	109.3
C(24B)—C(23B)—H(23B)	109.3
H(23A)—C(23B)—H(23B)	107.9
C(15B)—C(16B)—C(17B)	107.10(15)
C(15B)—C(16B)—H(16C)	110.3
C(17B)—C(16B)—H(16C)	110.3
C(15B)—C(16B)—H(16D)	110.3
C(17B)—C(16B)—H(16D)	110.3
H(16C)—C(16B)—H(16D)	108.6
C(25B)—C(24B)—C(23B)	115.78(15)
C(25B)—C(24B)—H(24B)	108.3
C(23B)—C(24B)—H(24B)	108.3
C(25B)—C(24B)—H(24C)	108.3
C(23B)—C(24B)—H(24C)	108.3
H(24B)—C(24B)—H(24C)	107.4
C(22A)—C(23A)—C(24A)	110.47(15)
C(22A)—C(23A)—H(23C)	109.6
C(24A)—C(23A)—H(23C)	109.6
C(22A)—C(23A)—H(23D)	109.6
C(24A)—C(23A)—H(23D)	109.6
H(23C)—C(23A)—H(23D)	108.1
C(21A)—C(20A)—C(17A)	113.40(17)
C(21A)—C(20A)—C(22A)	110.07(17)
C(17A)—C(20A)—C(22A)	109.15(14)
C(21A)—C(20A)—H(20B)	108.0
C(17A)—C(20A)—H(20B)	108.0
C(22A)—C(20A)—H(20B)	108.0
C(20B)—C(17B)—C(13B)	119.83(14)
C(20B)—C(17B)—C(16B)	110.64(15)
C(13B)—C(17B)—C(16B)	104.20(14)
C(20B)—C(17B)—H(17A)	107.2
C(13B)—C(17B)—H(17A)	107.2
C(16B)—C(17B)—H(17A)	107.2
C(20A)—C(17A)—C(13A)	119.67(14)
C(20A)—C(17A)—C(16A)	111.84(15)
C(13A)—C(17A)—C(16A)	103.18(14)
C(20A)—C(17A)—H(17B)	107.2
C(13A)—C(17A)—H(17B)	107.2
C(16A)—C(17A)—H(17B)	107.2
C(23A)—C(22A)—C(20A)	116.00(16)
C(23A)—C(22A)—H(22C)	108.3
C(20A)—C(22A)—H(22C)	108.3
C(23A)—C(22A)—H(22D)	108.3
C(20A)—C(22A)—H(22D)	108.3
H(22C)—C(22A)—H(22D)	107.4
C(25A)—C(26A)—H(26D)	109.5
C(25A)—C(26A)—H(26E)	109.5
H(26D)—C(26A)—H(26E)	109.5
C(25A)—C(26A)—H(26F)	109.5
H(26D)—C(26A)—B(26F)	109.5
H(26E)—C(26A)—H(26F)	109.5
C(20B)—C(21B)—H(21A)	109.5
C(20B)—C(21B)—H(21B)	109.5
H(21A)—C(21B)—H(21B)	109.5
C(20B)—C(21B)—H(21C)	109.5
H(21A)—C(21B)—H(21C)	109.5
H(21B)—C(21B)—H(21C)	109.5
C(20A)—C(21A)—H(21D)	109.5
C(20A)—C(21A)—H(21E)	109.5
H(21D)—C(21A)—H(21E)	109.5
C(20A)—C(21A)—H(21F)	109.5
H(21D)—C(21A)—H(21F)	109.5
H(21E)—C(21A)—H(21F)	109.5

TABLE 5

Anisotropic displacement parameters ($Å^2 \times 10^3$) for NEL. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \ldots + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1B)	17(1)	27(1)	31(1)	16(1)	0(1)	−2(1)
O(25A)	26(1)	23(1)	20(1)	9(1)	4(1)	1(1)
O(1A)	20(1)	26(1)	28(1)	8(1)	5(1)	3(1)
O(2B)	19(1)	24(1)	26(1)	6(1)	2(1)	2(1)
O(25B)	30(1)	24(1)	20(1)	9(1)	−2(1)	4(1)
O(2A)	21(1)	34(1)	29(1)	4(1)	2(1)	−6(1)
C(12B)	18(1)	24(1)	22(1)	11(1)	−3(1)	−4(1)
C(3B)	22(1)	22(1)	23(1)	13(1)	2(1)	4(1)
C(14A)	21(1)	19(1)	20(1)	7(1)	3(1)	1(1)
C(1A)	20(1)	20(1)	25(1)	7(1)	2(1)	−2(1)
C(1B)	18(1)	21(1)	24(1)	11(1)	3(1)	2(1)
C(7B)	23(1)	22(1)	20(1)	5(1)	1(1)	−5(1)
C(9B)	20(1)	22(1)	23(1)	11(1)	2(1)	0(1)
C(7A)	23(1)	20(1)	20(1)	5(1)	2(1)	3(1)
C(8A)	21(1)	18(1)	19(1)	5(1)	−1(1)	1(1)
C(18B)	24(1)	26(1)	24(1)	13(1)	3(1)	4(1)
C(8B)	25(1)	18(1)	15(1)	3(1)	2(1)	−1(1)
C(4A)	24(1)	21(1)	23(1)	10(1)	3(1)	2(1)
C(10B)	26(1)	27(1)	22(1)	13(1)	5(1)	3(1)
C(13A)	23(1)	19(1)	22(1)	9(1)	2(1)	1(1)
C(5A)	24(1)	17(1)	18(1)	4(1)	0(1)	−1(1)
C(13B)	20(1)	19(1)	17(1)	7(1)	0(1)	−1(1)
C(12A)	26(1)	26(1)	24(1)	12(1)	9(1)	7(1)
C(4B)	24(1)	20(1)	25(1)	9(1)	2(1)	1(1)
C(6B)	25(1)	19(1)	17(1)	4(1)	1(1)	−2(1)
C(5B)	27(1)	20(1)	18(1)	6(1)	5(1)	3(1)
C(14B)	24(1)	19(1)	18(1)	7(1)	1(1)	−2(1)
C(10A)	25(1)	25(1)	24(1)	13(1)	1(1)	1(1)
C(2B)	20(1)	19(1)	20(1)	6(1)	2(1)	3(1)
C(11B)	17(1)	24(1)	25(1)	12(1)	−2(1)	−4(1)
C(25A)	27(1)	21(1)	17(1)	8(1)	4(1)	5(1)
C(11A)	24(1)	29(1)	31(1)	17(1)	11(1)	11(1)
C(9A)	21(1)	26(1)	27(1)	14(1)	2(1)	2(1)
C(2A)	24(1)	23(1)	17(1)	6(1)	0(1)	−3(1)
C(15B)	35(1)	28(1)	22(1)	9(1)	−4(1)	−13(1)
C(19B)	22(1)	31(1)	29(1)	17(1)	2(1)	1(1)
C(22B)	26(1)	24(1)	22(1)	9(1)	0(1)	−2(1)
C(16A)	26(1)	23(1)	25(1)	10(1)	4(1)	5(1)
C(19A)	26(1)	37(1)	29(1)	17(1)	5(1)	2(1)
C(3A)	23(1)	24(1)	21(1)	11(1)	−2(1)	−1(1)
C(6A)	24(1)	18(1)	22(1)	6(1)	1(1)	2(1)
C(24A)	33(1)	19(1)	20(1)	6(1)	1(1)	3(1)
C(15A)	34(1)	27(1)	27(1)	13(1)	10(1)	12(1)

TABLE 5-continued

Anisotropic displacement parameters ($Å^2 \times 10^3$) for NEL. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
C(18A)	29(1)	22(1)	32(1)	13(1)	−4(1)	−3(1)
C(20B)	22(1)	24(1)	19(1)	9(1)	1(1)	−1(1)
C(26B)	26(1)	29(1)	26(1)	10(1)	1(1)	−4(1)
C(25B)	24(1)	19(1)	21(1)	8(1)	−1(1)	−1(1)
C(23B)	36(1)	23(1)	23(1)	11(1)	6(1)	1(1)
C(16B)	30(1)	26(1)	21(1)	10(1)	−1(1)	−7(1)
C(24B)	27(1)	20(1)	22(1)	8(1)	0(1)	−1(1)
C(23A)	35(1)	21(1)	21(1)	8(1)	−2(1)	2(1)
C(20A)	29(1)	19(1)	24(1)	6(1)	0(1)	3(1)
C(17B)	20(1)	20(1)	20(1)	8(1)	1(1)	0(1)
C(17A)	20(1)	17(1)	22(1)	7(1)	0(1)	0(1)
C(22A)	30(1)	21(1)	22(1)	9(1)	−1(1)	1(1)
C(26A)	30(1)	34(1)	25(1)	15(1)	3(1)	3(1)
C(21B)	43(1)	33(1)	22(1)	14(1)	−6(1)	−10(1)
C(21A)	59(2)	42(1)	23(1)	13(1)	8(1)	25(1)

TABLE 6

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for NEL.

	x	y	z	U(eq)
H(1BA)	19161	17964	1490	35
H(25A)	18570	16034	1263	33
H(1AA)	17440	14003	10350	38
H(2BA)	25660	17721	897	36
H(25B)	25582	15881	10525	37
H(2AA)	24659	12701	10160	45
H(12A)	30805	18420	6459	25
H(12B)	29951	19463	7205	25
H(3BA)	24872	19664	970	25
H(14A)	23849	14164	6358	24
N(1AB)	20405	13618	9985	26
H(1BB)	23051	17459	1699	24
H(7BA)	24730	18218	4096	27
H(9BA)	29766	19618	4680	25
H(9BB)	30734	18533	4798	25
H(7AA)	20824	13061	7432	26
H(18A)	26102	19896	6397	35
H(18B)	25900	19599	7259	35
H(18C)	24494	18928	6363	35
H(4AA)	23843	11012	8972	27
H(4AB)	21582	10459	8883	27
H(10A)	21552	19485	2912	29
H(10B)	22323	18458	3178	29
H(12C)	24585	12009	4312	29
H(12D)	25726	13065	5083	29
H(4BA)	26714	20228	2451	27
H(4BB)	24412	20656	2462	27
H(6BA)	27544	19598	3608	26
H(14B)	28424	17229	5174	25
H(10C)	18361	11726	8562	29

TABLE 6-continued

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for NEL.

	x	y	z	U(eq)
H(10D)	19077	12870	8467	29
H(11A)	31562	20046	6148	26
H(11B)	29205	20381	6189	26
H(25C)	16590	16751	2294	25
H(11C)	26696	11421	5353	31
H(11D)	24327	11039	5303	31
H(9AA)	25631	11790	6817	28
H(9AB)	26460	12912	6716	28
H(15A)	25251	16354	4601	35
H(15B)	24038	17434	5137	35
H(19A)	21542	19209	194	39
H(19B)	19798	18479	454	39
H(22A)	25901	15976	7287	28
H(22B)	27952	16366	7953	28
H(16A)	20720	15457	5724	29
H(16B)	18952	14489	5269	29
H(19C)	19444	11330	11045	44
H(19D)	17576	12098	10868	44
H(3AA)	22660	11257	10408	27
H(6AA)	23960	11720	7861	26
H(24A)	18004	16316	3486	29
H(24B)	19810	16327	2892	29
H(15C)	20875	14932	6921	33
H(15D)	19488	13807	6380	33
H(18D)	19443	12371	5020	41
H(18E)	21043	11501	5166	41
H(18F)	20715	11650	4232	41
H(20A)	25243	18002	7690	26
H(26A)	20801	15579	9775	41
H(26B)	20899	15098	8731	41
H(26C)	21447	16391	9283	41
H(25D)	23893	14605	9451	26
H(23A)	23870	16840	8498	32
H(23B)	25948	17163	9157	32
H(16C)	25832	15852	5811	31
H(16D)	24128	16721	6241	31
H(24B)	24572	14884	8135	28
H(24C)	26567	15235	8835	28
H(23C)	17871	14278	2858	31
H(23D)	19853	14353	2365	31
H(20B)	19657	13272	3783	29
H(17A)	28500	17005	6615	24
H(17B)	23208	14447	4956	23
H(22C)	19938	15328	4253	29
H(22D)	21902	15184	3712	29
H(26D)	13962	15360	1598	43
H(26E)	14256	15574	2630	43
H(26F)	15183	14500	1945	43
H(21A)	28248	19245	8248	49
H(21B)	29556	18246	8354	49
H(21C)	27705	18701	8948	49
H(21D)	22673	12286	3278	61
H(21E)	23730	13402	3253	61
H(21F)	21731	12827	2591	61

TABLE 7

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	2	−18	48	43	2	1	0	−16	58	59	1	1	0	−15	78	80	1	2	−4	−14	52	53	1	2	8	−14	65	70	1
1	2	−18	75	71	2	2	0	−16	67	68	1	2	0	−15	127	130	2	3	−4	−14	33	37	2	3	8	−14	140	139	2
0	3	−18	30	27	2	3	0	−16	44	45	1	3	0	−15	32	29	1	−1	−3	−14	60	62	2	4	8	−14	51	50	2
1	3	−18	35	36	1	−1	1	−16	44	45	2	4	0	−15	9	9	8	0	−3	−14	21	18	2	−3	9	−14	28	27	3
2	3	−18	26	28	2	0	1	−16	138	127	3	−1	1	−15	95	98	2	1	−3	−14	34	29	1	−2	9	−14	92	90	2
−1	4	−18	12	10	6	1	1	−16	110	118	1	0	1	−15	39	37	2	2	−3	−14	37	36	1	−1	9	−14	53	52	1
0	4	−18	55	56	2	2	1	−16	43	41	1	1	1	−15	70	68	1	3	−3	−14	48	43	1	0	9	−14	116	116	2
1	4	−18	38	40	1	3	1	−16	44	44	1	2	1	−15	96	95	1	−1	−2	−14	35	35	2	1	9	−14	28	26	1
2	4	−18	36	34	1	4	1	−16	38	41	1	3	1	−15	73	75	1	0	−2	−14	40	43	1	2	9	−14	34	27	2
−1	5	−18	25	23	3	−2	2	−16	24	23	3	4	1	−15	31	28	1	1	−2	−14	44	42	1	3	9	−14	71	66	2
0	5	−18	33	29	2	−1	2	−16	86	84	2	−2	2	−15	81	87	2	2	−2	−14	32	35	1	−3	10	−14	100	99	2
1	5	−18	68	65	1	0	2	−16	106	101	2	−1	2	−15	79	74	2	3	−2	−14	43	42	1	−2	10	−14	70	76	2
2	5	−18	41	37	2	1	2	−16	67	64	1	0	2	−15	47	46	2	4	−2	−14	91	85	1	−1	10	−14	64	61	1
−1	6	−18	12	14	5	2	2	−16	63	63	1	1	2	−15	86	83	2	−1	−1	−14	68	68	1	0	10	−14	26	25	2
0	6	−18	21	20	3	3	2	−16	105	102	1	2	2	−15	72	76	1	0	−1	−14	59	52	1	1	10	−14	58	51	1
1	6	−18	69	68	1	4	2	−16	31	29	1	3	2	−15	35	40	1	1	−1	−14	72	76	1	2	10	−14	73	74	2
2	6	−18	13	11	5	−2	3	−16	58	60	2	4	2	−15	59	55	1	2	−1	−14	112	117	1	3	10	−14	12	14	6
−1	7	−18	22	21	3	−1	3	−16	72	72	2	−2	3	−15	79	75	2	3	−1	−14	46	42	1	−2	11	−14	47	47	2
0	7	−18	19	22	2	0	3	−16	38	30	2	−1	3	−15	58	58	2	4	−1	−14	54	52	1	−1	11	−14	12	14	4
1	7	−18	109	102	2	1	3	−16	52	51	1	0	3	−15	13	10	3	−1	0	−14	63	63	2	0	11	−14	24	22	1
2	7	−18	90	92	2	2	3	−16	35	32	1	1	3	−15	200	198	3	0	0	−14	86	86	1	1	11	−14	60	62	1
1	8	−18	58	61	1	3	3	−16	14	15	3	2	3	−15	116	121	1	1	0	−14	43	45	1	2	11	−14	66	69	2
1	−1	−17	77	82	2	4	3	−16	71	71	1	3	3	−15	10	13	4	2	0	−14	101	102	2	−2	12	−14	20	23	3
0	0	−17	39	34	2	−2	4	−16	31	31	3	4	3	−15	54	53	1	3	0	−14	109	111	1	−1	12	−14	80	78	2
1	0	−17	111	105	3	−1	4	−16	45	43	2	5	3	−15	105	111	2	4	0	−14	69	66	1	0	12	−14	57	56	1
2	0	−17	16	18	2	0	4	−16	90	93	2	−2	4	−15	39	42	2	−2	1	−14	57	60	2	1	12	−14	13	19	3
−1	1	−17	87	83	2	1	4	−16	96	96	2	−1	4	−15	61	62	2	−1	1	−14	73	72	2	2	12	−14	14	12	4
0	1	−17	211	197	5	2	4	−16	21	22	1	0	4	−15	39	44	1	0	1	−14	50	51	1	0	13	−14	66	59	2
1	1	−17	38	33	1	3	4	−16	54	56	1	1	4	−15	86	87	1	1	1	−14	9	7	5	1	13	−14	50	53	2
2	1	−17	117	113	1	4	4	−16	26	26	1	2	4	−15	109	108	1	2	1	−14	99	102	1	0	−6	−13	41	37	2
3	1	−17	85	84	2	−2	5	−16	24	20	3	3	4	−15	67	73	1	3	1	−14	115	116	1	1	−6	−13	41	38	1
−1	2	−17	53	54	2	−1	5	−16	97	96	2	4	4	−15	44	43	1	4	1	−14	21	19	2	−1	−5	−13	92	84	2
0	2	−17	124	117	3	0	5	−16	69	69	1	5	4	−15	31	27	2	5	1	−14	23	23	2	0	−5	−13	44	43	1
1	2	−17	88	85	1	1	5	−16	46	47	1	−2	5	−15	27	25	3	−2	2	−14	100	108	3	1	−5	−13	110	106	2
2	2	−17	49	50	1	2	5	−16	58	56	1	−1	5	−15	177	181	3	−1	2	−14	92	92	3	2	−5	−13	39	41	1
3	2	−17	48	49	1	3	5	−16	87	87	1	0	5	−15	162	200	4	0	2	−14	226	229	2	3	−5	−13	52	55	1
−1	3	−17	42	35	2	4	5	−16	49	53	1	1	5	−15	108	106	2	1	2	−14	91	88	1	−2	−4	−13	32	31	2
0	3	−17	100	96	2	−2	6	−16	89	87	2	2	5	−15	72	72	1	2	2	−14	145	146	2	−1	−4	−13	83	86	2
1	3	−17	43	44	1	−1	6	−16	43	42	2	3	5	−15	122	120	2	3	2	−14	73	75	1	0	−4	−13	44	39	1
2	3	−17	11	7	4	0	6	−16	122	118	2	4	5	−15	86	85	1	4	2	−14	21	15	2	1	−4	−13	85	81	1
3	3	−17	34	34	1	1	6	−16	93	90	2	−3	6	−15	51	51	2	5	2	−14	21	21	2	2	−4	−13	26	24	2
−2	4	−17	51	52	2	2	6	−16	18	14	2	−2	6	−15	48	51	2	−2	3	−14	145	149	3	3	−4	−13	81	80	1
−1	4	−17	46	46	2	3	6	−16	36	34	1	−1	6	−15	68	68	2	−1	3	−14	221	227	3	4	−4	−13	13	14	2
0	4	−17	131	123	3	4	6	−16	57	62	2	0	6	−15	154	158	4	0	3	−14	237	243	4	−2	−3	−13	80	82	2
1	4	−17	18	16	3	−2	7	−16	18	25	3	1	6	−15	30	25	2	1	3	−14	121	125	1	−1	−3	−13	43	40	2
2	4	−17	51	50	1	−1	7	−16	64	61	2	2	6	−15	42	42	1	2	3	−14	75	80	1	0	−3	−13	55	53	1
3	4	−17	10	8	7	0	7	−16	32	33	2	3	6	−15	84	84	1	3	3	−14	194	197	3	1	−3	−13	54	60	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−2	5	−17	42	39	2	1	7	−16	104	106	1	4	6	−15	103	107	2	4	3	−14	61	55	1	2	−3	−13	11	10	4
−1	5	−17	37	36	2	2	7	−16	88	86	2	−3	7	−15	29	31	3	5	3	−14	17	15	4	3	−3	−13	52	53	1
0	5	−17	18	14	2	3	7	−16	38	35	1	−2	7	−15	127	126	3	−2	4	−14	67	64	2	4	−3	−13	33	33	1
1	5	−17	59	60	1	−2	8	−16	64	64	2	−1	7	−15	73	70	2	−1	4	−14	182	190	3	−3	−2	−13	74	76	2
2	5	−17	36	35	1	−1	8	−16	68	63	2	0	7	−15	51	54	1	0	4	−14	327	325	5	−1	−2	−13	43	40	1
3	5	−17	18	17	2	0	8	−16	60	56	1	1	7	−15	48	52	1	1	4	−14	129	138	2	0	−2	−13	24	24	2
−2	6	−17	83	78	2	1	8	−16	21	22	2	2	7	−15	56	58	1	2	4	−14	125	123	1	1	−2	−13	77	79	1
−1	6	−17	41	39	2	2	8	−16	59	61	2	3	7	−15	67	69	1	3	4	−14	184	206	3	2	−2	−13	34	38	1
0	6	−17	16	15	3	3	8	−16	52	45	2	4	7	−15	42	40	2	4	4	−14	65	65	1	3	−2	−13	108	109	1
1	6	−17	105	108	2	−2	9	−16	64	62	2	−3	8	−15	81	85	2	5	4	−14	51	49	2	4	−2	−13	108	107	1
2	6	−17	67	68	2	−1	9	−16	84	80	2	−2	8	−15	43	43	2	−2	5	−14	53	51	2	5	−2	−13	27	32	2
3	6	−17	21	20	2	0	9	−16	37	32	1	−1	8	−15	66	67	2	−1	5	−14	59	54	2	−3	−1	−13	30	26	2
−2	7	−17	103	101	2	1	9	−16	39	37	1	0	8	−15	123	121	2	0	5	−14	83	100	2	−1	−1	−13	31	26	2
−1	7	−17	42	41	2	2	9	−16	67	65	2	1	8	−15	29	27	1	1	5	−14	73	75	1	0	−1	−13	107	102	1
0	7	−17	54	51	1	3	9	−16	55	58	2	2	8	−15	80	78	2	2	5	−14	171	173	2	1	−1	−13	135	131	1
1	7	−17	16	18	2	−2	10	−16	47	44	2	3	8	−15	85	85	1	3	5	−14	74	69	1	2	−1	−13	13	8	2
2	7	−17	33	30	2	−1	10	−16	36	36	2	−3	9	−15	40	43	2	4	5	−14	63	63	1	3	−1	−13	110	108	1
3	7	−17	15	16	3	0	10	−16	16	17	2	−2	9	−15	38	37	2	5	5	−14	62	58	2	4	−1	−13	31	34	1
−2	8	−17	17	18	3	1	10	−16	114	117	2	−1	9	−15	43	44	1	−3	6	−14	44	45	2	5	−1	−13	31	32	1
−1	8	−17	86	83	2	2	10	−16	121	122	3	0	9	−15	65	60	1	−2	6	−14	34	29	2	−4	0	−13	19	17	3
0	8	−17	11	9	5	−1	11	−16	19	18	2	1	9	−15	53	56	1	−1	6	−14	9	4	9	−3	0	−13	73	72	2
1	8	−17	77	75	1	0	11	−16	17	14	2	2	9	−15	114	107	3	0	6	−14	207	203	5	−1	0	−13	28	30	2
2	8	−17	35	30	2	1	11	−16	44	44	2	3	9	−15	51	53	2	1	6	−14	47	47	1	0	0	−13	37	39	1
3	8	−17	13	18	4	1	−4	−15	46	47	1	−2	10	−15	60	61	2	2	6	−14	84	87	1	1	0	−13	161	153	2
−1	9	−17	25	25	2	0	−3	−15	108	106	2	−1	10	−15	78	74	1	3	6	−14	99	97	2	2	0	−13	15	20	2
0	9	−17	50	46	1	1	−3	−15	49	48	1	0	10	−15	56	56	1	4	6	−14	34	34	1	3	0	−13	68	75	1
1	9	−17	47	49	1	2	−3	−15	56	53	1	1	10	−15	47	45	1	5	6	−14	43	41	2	4	0	−13	9	10	2
2	9	−17	67	64	2	−1	−2	−15	57	61	1	2	10	−15	63	62	2	−3	7	−14	44	44	2	5	0	−13	88	90	1
0	10	−17	61	56	2	0	−2	−15	109	103	2	−2	11	−15	49	44	2	−2	7	−14	75	74	2	−4	1	−13	49	46	2
1	10	−17	19	19	3	1	−2	−15	51	52	1	−1	11	−15	47	42	1	−1	7	−14	158	171	2	−3	1	−13	152	156	3
0	−2	−16	40	37	1	2	−2	−15	30	31	1	0	11	−15	43	36	1	0	7	−14	140	143	3	−2	1	−13	94	97	3
1	−2	−16	27	34	2	3	−2	−15	51	51	1	1	11	−15	90	88	2	1	7	−14	161	165	2	−1	1	−13	70	78	2
2	−2	−16	26	27	2	−1	−1	−15	72	66	2	2	11	−15	30	27	2	2	7	−14	82	86	1	0	1	−13	48	45	1
−1	−1	−16	17	21	5	0	−1	−15	36	36	2	0	12	−15	64	60	1	3	7	−14	115	115	2	1	1	−13	147	154	1
0	−1	−16	61	59	1	1	−1	−15	33	37	2	1	12	−15	67	67	2	4	7	−14	62	63	1	2	1	−13	23	24	2
1	−1	−16	88	82	1	2	−1	−15	13	12	3	0	−5	−14	37	48	2	−3	8	−14	59	55	2	3	1	−13	80	82	1
2	−1	−16	40	44	1	3	−1	−15	37	37	1	1	−5	−14	13	10	3	−2	8	−14	24	26	3	4	1	−13	43	44	1
3	−1	−16	9	13	8	4	−1	−15	26	26	1	−1	−4	−14	19	12	3	−1	8	−14	69	76	1	5	1	−13	132	129	2
−1	0	−16	94	91	2	−1	0	−15	12	7	12	0	−4	−14	39	37	1	0	8	−14	84	83	1	−4	2	−13	54	52	2
0	0	−16	125	125	2	0	0	−15	25	25	2	1	−4	−14	82	82	1	1	8	−14	117	119	1	−3	2	−13	143	141	3
−2	2	−13	173	185	4	−1	13	−13	47	47	1	−3	3	−12	48	51	2	2	12	−12	69	67	2	5	1	−11	132	127	2
−1	2	−13	57	59	2	0	13	−13	5	9	4	−2	3	−12	98	102	2	−2	13	−12	73	73	1	−5	2	−11	31	24	2
0	2	−13	142	139	1	1	13	−13	52	51	2	−1	3	−12	89	95	1	−1	13	−12	81	83	1	−4	2	−11	83	82	2
1	2	−13	158	158	1	0	−7	−12	46	43	2	0	3	−12	122	127	1	0	13	−12	58	51	1	−3	2	−11	41	42	2
2	2	−13	55	56	1	1	−7	−12	21	24	2	1	3	−12	185	194	2	1	13	−12	30	30	1	−2	2	−11	54	56	1
3	2	−13	118	120	2	−1	−6	−12	44	45	2	2	3	−12	85	85	1	2	13	−12	34	38	2	−1	2	−11	136	136	2
4	2	−13	34	28	1	0	−6	−12	31	35	2	3	3	−12	28	29	1	−1	−7	−11	49	51	2	0	2	−11	193	194	2
5	2	−13	126	122	2	1	−6	−12	60	59	1	4	3	−12	202	204	5	0	−7	−11	60	61	2	1	2	−11	90	89	1
−4	3	−13	58	57	2	2	−6	−12	111	108	2	5	3	−12	115	117	1	1	−7	−11	35	37	1	2	2	−11	18	14	1

TABLE 7-continued

Observed and calculated structure factors for NEL																													
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−3	3	−13	119	120	3	3	−6	−12	75	76	2	−5	4	−12	95	97	2	2	−7	−11	79	80	2	3	2	−11	114	119	1
−2	3	−13	57	51	2	−2	−5	−12	44	43	2	−4	4	−12	32	26	2	3	−7	−11	47	49	2	4	2	−11	115	111	2
−1	3	−13	29	34	2	−1	−5	−12	28	24	3	−3	4	−12	103	107	2	−2	−6	−11	101	97	2	5	2	−11	94	93	1
0	3	−13	311	310	3	0	−5	−12	24	27	2	−2	4	−12	22	20	2	−1	−6	−11	55	54	2	6	2	−11	38	38	1
1	3	−13	23	20	1	1	−5	−12	88	88	1	−1	4	−12	132	131	2	0	−6	−11	95	88	2	−5	3	−11	37	36	2
2	3	−13	125	127	1	2	−5	−12	29	30	2	0	4	−12	42	41	1	1	−6	−11	42	38	1	−4	3	−11	143	144	3
3	3	−13	102	103	2	3	−5	−12	139	138	2	1	4	−12	180	179	2	2	−6	−11	68	67	1	−3	3	−11	84	87	2
4	3	−13	129	134	2	4	−5	−12	71	78	2	2	4	−12	94	96	1	3	−6	−11	37	37	1	−2	3	−11	93	97	1
5	3	−13	127	119	3	−3	−4	−12	72	74	2	3	4	−12	61	63	1	−3	−5	−11	112	115	3	−1	3	−11	127	134	1
−2	4	−13	138	137	3	−2	−4	−12	69	69	2	4	4	−12	30	28	1	−2	−5	−11	49	47	1	0	3	−11	458	460	4
−1	4	−13	131	130	2	−1	−4	−12	79	76	2	5	4	−12	158	161	1	−1	−5	−11	88	82	2	1	3	−11	58	63	1
0	4	−13	63	69	1	0	−4	−12	45	42	1	6	4	−12	38	37	1	0	−5	−11	24	26	2	2	3	−11	114	113	1
1	4	−13	13	14	2	1	−4	−12	85	92	2	−4	5	−12	99	99	2	1	−5	−11	79	78	1	3	3	−11	97	98	1
2	4	−13	80	82	1	2	−4	−12	70	65	1	−2	5	−12	55	53	2	2	−5	−11	51	53	1	4	3	−11	186	183	2
3	4	−13	26	30	1	3	−4	−12	67	66	1	−1	5	−12	220	225	2	3	−5	−11	57	54	1	5	3	−11	25	21	1
4	4	−13	27	22	2	4	−4	−12	27	28	1	0	5	−12	116	112	1	4	−5	−11	67	66	1	6	3	−11	90	93	1
5	4	−13	123	116	3	−3	−3	−12	22	22	3	1	5	−12	145	147	1	−4	−4	−11	53	50	2	−5	4	−11	40	35	2
−2	5	−13	104	103	3	−2	−3	−12	52	52	1	2	5	−12	110	114	1	−3	−4	−11	61	57	2	−4	4	−11	203	194	5
−1	5	−13	234	233	3	−1	−3	−12	79	82	1	3	5	−12	184	182	3	−2	−4	−11	82	79	1	−3	4	−11	66	63	2
0	5	−13	430	428	5	0	−3	−12	90	86	2	4	5	−12	144	145	1	−1	−4	−11	66	67	1	−2	4	−11	59	59	1
1	5	−13	199	204	2	1	−3	−12	124	121	2	5	5	−12	40	42	1	0	−4	−11	88	90	2	−1	4	−11	164	167	2
2	5	−13	48	49	1	2	−3	−12	41	47	1	6	5	−12	24	25	1	1	−4	−11	60	65	2	0	4	−11	108	105	1
3	5	−13	96	98	2	3	−3	−12	77	79	1	−3	6	−12	69	70	2	2	−4	−11	137	139	2	1	4	−11	16	19	1
4	5	−13	122	123	2	4	−3	−12	79	76	1	−2	6	−12	154	151	3	3	−4	−11	15	14	2	2	4	−11	80	81	1
5	5	−13	30	25	1	5	−3	−12	42	43	2	−1	6	−12	152	152	2	4	−4	−11	23	23	1	3	4	−11	62	61	1
−3	6	−13	55	53	2	−4	−2	−12	50	47	2	0	6	−12	121	117	1	5	−4	−11	22	21	3	4	4	−11	107	107	1
−2	6	−13	108	108	3	−3	−2	−12	121	120	3	1	6	−12	161	164	2	−4	−3	−11	16	13	4	5	4	−11	73	73	1
−1	6	−13	104	103	2	−2	−2	−12	67	65	1	2	6	−12	64	62	1	−3	−3	−11	104	103	2	6	4	−11	82	75	1
0	6	−13	285	317	12	−1	−2	−12	128	124	2	3	6	−12	153	157	2	−2	−3	−11	77	81	1	−5	5	−11	19	21	4
1	6	−13	156	148	2	0	−2	−12	234	230	3	4	6	−12	80	84	1	−1	−3	−11	79	74	1	−4	5	−11	85	85	2
2	6	−13	58	63	1	1	−2	−12	101	109	1	5	6	−12	30	30	1	0	−3	−11	41	29	1	−3	5	−11	109	110	2
3	6	−13	110	112	2	2	−2	−12	96	127	1	−3	7	−12	122	129	3	1	−3	−11	54	53	1	−2	5	−11	93	96	2
4	6	−13	103	105	1	3	−2	−12	160	159	2	−2	7	−12	70	66	2	2	−3	−11	87	89	1	−1	5	−11	85	86	1
5	6	−13	47	46	1	4	−2	−12	77	78	1	−1	7	−12	188	186	2	3	−3	−11	95	94	1	0	5	−11	109	110	1
−3	7	−13	98	103	3	5	−2	−12	71	72	2	0	7	−12	123	124	1	4	−3	−11	12	12	3	1	5	−11	124	125	1
−2	7	−13	93	93	2	−4	−1	−12	28	28	3	1	7	−12	159	158	2	5	−3	−11	40	38	2	2	5	−11	160	158	1
−1	7	−13	31	32	2	−3	−1	−12	78	78	2	2	7	−12	128	129	1	−4	−2	−11	39	34	2	3	5	−11	33	32	1
0	7	−13	172	160	4	−2	−1	−12	99	100	2	3	7	−12	115	117	1	−3	−2	−11	164	161	4	4	5	−11	148	147	1
1	7	−13	87	81	1	−1	−1	−12	37	33	2	4	7	−12	85	82	1	−2	−2	−11	131	130	2	5	5	−11	17	16	1
2	7	−13	156	166	2	0	−1	−12	241	249	2	5	7	−12	119	121	1	−1	−2	−11	98	96	1	6	5	−11	25	24	1
3	7	−13	26	24	2	1	−1	−12	81	83	1	−3	8	−12	107	106	3	0	−2	−11	75	71	1	−5	6	−11	37	38	2
4	7	−13	92	93	1	2	−1	−12	208	209	4	−2	8	−12	50	54	2	1	−2	−11	84	88	1	−4	6	−11	100	101	2
5	7	−13	51	51	1	3	−1	−12	57	60	1	−1	8	−12	219	223	4	2	−2	−11	74	72	1	−3	6	−11	93	96	2
−3	8	−13	21	16	4	4	−1	−12	44	43	1	0	8	−12	109	109	2	3	−2	−11	27	27	1	−2	6	−11	155	152	2
−2	8	−13	132	131	3	5	−1	−12	94	92	1	1	8	−12	196	208	3	4	−2	−11	121	121	1	−1	6	−11	140	145	2
−1	8	−13	98	104	2	−4	0	−12	45	41	2	2	8	−12	85	89	1	5	−2	−11	51	49	1	0	6	−11	121	112	1
0	8	−13	56	63	1	−3	0	−12	80	82	2	3	8	−12	157	153	2	−5	−1	−11	12	20	7	1	6	−11	203	207	2
1	8	−13	70	66	1	−2	0	−12	48	44	2	4	8	−12	87	89	1	−4	−1	−11	28	21	3	2	6	−11	113	108	1
2	8	−13	63	60	1	−1	0	−12	89	86	1	5	8	−12	45	44	1	−3	−1	−11	99	95	2	3	6	−11	140	140	1

TABLE 7-continued

Observed and calculated structure factors for NEL																													
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	8	−13	43	43	1	0	0	−12	88	88	1	−3	9	−12	64	69	2	−2	−1	−11	245	244	5	4	6	−11	131	129	1
4	8	−13	60	58	1	1	0	−12	120	119	1	−2	9	−12	55	55	2	−1	−1	−11	162	167	1	5	6	−11	106	108	1
5	8	−13	21	18	1	2	0	−12	67	71	1	−1	9	−12	56	54	1	0	−1	−11	87	85	1	−3	7	−11	35	31	2
−3	9	−13	108	109	3	3	0	−12	105	108	1	0	9	−12	70	75	1	1	−1	−11	238	237	2	−2	7	−11	259	264	6
−2	9	−13	147	145	3	4	0	−12	24	23	1	1	9	−12	118	122	2	2	−1	−11	158	157	1	−1	7	−11	53	52	1
−1	9	−13	24	25	2	5	0	−12	148	142	2	2	9	−12	63	65	2	3	−1	−11	136	135	1	0	7	−11	87	84	1
0	9	−13	102	99	2	−5	1	−12	90	87	2	3	9	−12	12	15	5	4	−1	−11	140	141	1	1	7	−11	80	83	1
1	9	−13	63	61	1	−4	1	−12	33	27	2	4	9	−12	48	52	1	5	−1	−11	40	40	1	2	7	−11	281	289	2
2	9	−13	127	141	3	−3	1	−12	182	179	4	5	9	−12	35	36	1	−5	0	−11	64	63	2	3	7	−11	38	36	1
3	9	−13	45	42	2	−2	1	−12	59	58	2	−3	10	−12	67	65	2	−4	0	−11	44	41	2	4	7	−11	37	33	1
4	9	−13	40	40	1	−1	1	−12	141	146	2	−2	10	−12	60	64	2	−3	0	−11	121	120	3	5	7	−11	35	31	1
−3	10	−13	26	26	3	0	1	−12	52	51	1	−1	10	−12	3	4	3	−2	0	−11	135	143	2	−3	8	−11	79	75	2
−2	10	−13	71	68	2	1	1	−12	257	259	2	0	10	−12	23	19	2	−1	0	−11	130	132	1	−2	8	−11	97	97	3
−1	10	−13	36	36	1	2	1	−12	113	112	1	1	10	−12	47	50	1	0	0	−11	225	221	2	−1	8	−11	59	63	1
0	10	−13	69	69	1	3	1	−12	88	93	2	2	10	−12	37	36	2	1	0	−11	155	148	1	0	8	−11	163	157	2
1	10	−13	39	37	1	4	1	−12	97	95	2	3	10	−12	30	28	2	2	0	−11	68	62	1	1	8	−11	215	214	2
2	10	−13	88	81	2	5	1	−12	90	88	1	4	10	−12	67	66	1	3	0	−11	89	89	1	2	8	−11	128	122	1
3	10	−13	61	62	2	−5	2	−12	95	91	2	−3	11	−12	53	56	2	4	0	−11	35	36	1	3	8	−11	34	31	1
−3	11	−13	21	25	3	−4	2	−12	45	40	2	−2	11	−12	10	1	10	5	0	−11	65	61	1	4	8	−11	87	83	1
−2	11	−13	52	51	2	−3	2	−12	41	41	2	−1	11	−12	84	84	1	−5	1	−11	54	54	2	5	8	−11	39	39	1
−1	11	−13	97	90	2	−2	2	−12	136	140	2	0	11	−12	26	25	2	−4	1	−11	42	40	2	−3	9	−11	50	49	2
0	11	−13	25	22	2	−1	2	−12	104	106	2	1	11	−12	41	45	1	−3	1	−11	76	72	2	−2	9	−11	118	117	3
1	11	−13	78	77	1	0	2	−12	48	45	1	2	11	−12	66	63	2	−2	1	−11	55	52	1	−1	9	−11	136	145	2
2	11	−13	124	121	3	1	2	−12	80	83	1	3	11	−12	68	67	2	−1	1	−11	154	165	1	0	9	−11	184	188	3
−2	12	−13	19	22	3	2	2	−12	33	29	1	−3	12	−12	29	31	2	0	1	−11	117	117	1	1	9	−11	47	51	1
−1	12	−13	17	12	2	3	2	−12	28	26	1	−2	12	−12	49	49	2	1	1	−11	18	12	1	2	9	−11	144	141	3
0	12	−13	66	62	1	4	2	−12	59	61	1	−1	12	−12	38	37	1	2	1	−11	176	164	1	3	9	−11	104	102	1
1	12	−13	85	80	1	5	2	−12	184	178	3	0	12	−12	62	61	1	3	1	−11	94	96	1	4	9	−11	52	48	1
2	12	−13	18	16	3	−4	3	−12	37	31	2	1	12	−12	12	15	1	4	1	−11	35	35	1	5	9	−11	45	48	1
−3	10	−11	16	20	4	6	−2	−10	20	27	2	1	6	−10	88	84	1	2	−6	−9	73	71	1	−3	2	−9	19	19	2
−2	10	−11	149	157	3	−5	−1	−10	71	70	2	2	6	−10	64	66	1	3	−6	−9	58	59	1	−2	2	−9	18	15	2
−1	10	−11	153	151	4	−4	−1	−10	65	69	2	3	6	−10	78	73	1	4	−6	−9	50	52	1	−1	2	−9	105	113	1
0	10	−11	42	44	1	−3	−1	−10	72	83	2	4	6	−10	50	50	1	5	−6	−9	18	18	4	0	2	−9	91	99	1
1	10	−11	169	173	3	−2	−1	−10	92	96	1	5	6	−10	89	88	1	−4	−5	−9	39	38	2	1	2	−9	192	194	2
2	10	−11	104	102	2	−1	−1	−10	86	86	1	−5	7	−10	77	82	2	−3	−5	−9	62	57	2	2	2	−9	99	104	1
3	10	−11	29	30	2	0	−1	−10	68	66	1	−4	7	−10	50	47	2	−2	−5	−9	106	103	3	3	2	−9	99	101	1
4	10	−11	59	58	1	1	−1	−10	72	69	1	−3	7	−10	120	124	3	−1	−5	−9	117	118	3	4	2	−9	106	106	1
−3	11	−11	14	10	4	2	−1	−10	116	115	1	−2	7	−10	244	241	4	0	−5	−9	9	6	4	5	2	−9	14	17	2
−2	11	−11	129	124	3	3	−1	−10	53	55	1	−1	7	−10	159	164	2	1	−5	−9	116	116	1	6	2	−9	30	23	1
−1	11	−11	46	46	1	4	−1	−10	79	78	1	0	7	−10	288	271	3	2	−5	−9	81	80	1	−6	3	−9	81	78	2
0	11	−11	72	73	1	5	−1	−10	39	41	1	1	7	−10	117	118	1	3	−5	−9	133	130	2	−5	3	−9	97	95	3
1	11	−11	103	99	1	−5	0	−10	151	149	3	2	7	−10	252	251	1	4	−5	−9	22	19	2	−4	3	−9	67	78	2
2	11	−11	147	145	3	−4	0	−10	37	47	2	3	7	−10	100	98	1	5	−5	−9	100	100	2	−3	3	−9	68	66	1
3	11	−11	29	32	2	−3	0	−10	153	162	4	4	7	−10	48	48	1	−5	−4	−9	24	23	3	−2	3	−9	109	106	1
4	11	−11	61	61	1	−2	0	−10	99	95	2	5	7	−10	75	74	1	−4	−4	−9	23	21	3	−1	3	−9	243	248	2
−3	12	−11	54	54	2	−1	0	−10	107	108	1	−3	8	−10	92	89	2	−2	−4	−9	120	123	3	0	3	−9	129	121	1
−2	12	−11	62	69	2	0	0	−10	36	31	1	−2	8	−10	29	30	2	−1	−4	−9	88	86	1	1	3	−9	21	15	1
−1	12	−11	64	62	1	1	0	−10	169	171	1	−1	8	−10	116	108	1	0	−4	−9	43	46	1	2	3	−9	170	172	1
0	12	−11	57	55	1	2	0	−10	105	105	1	0	8	−10	148	139	2	1	−4	−9	62	61	1	3	3	−9	119	122	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	12	−11	72	71	1	3	0	−10	44	41	1	1	8	−10	158	156	1	2	−4	−9	56	59	1	4	3	−9	74	76	1
2	12	−11	18	19	3	4	0	−10	158	158	1	2	8	−10	76	78	1	3	−4	−9	136	138	2	5	3	−9	98	94	1
−2	13	−11	13	17	3	5	0	−10	50	47	1	3	8	−10	139	140	1	4	−4	−9	134	126	1	6	3	−9	28	30	1
−1	13	−11	53	54	1	−5	1	−10	164	153	4	4	8	−10	60	60	1	5	−4	−9	85	84	2	−6	4	−9	40	38	2
0	13	−11	28	25	1	−4	1	−10	65	76	2	5	8	−10	22	17	1	−5	−3	−9	26	22	2	−5	4	−9	100	96	2
1	13	−11	58	55	1	−3	1	−10	158	167	2	−3	9	−10	60	57	2	−4	−3	−9	91	89	2	−3	4	−9	192	192	3
2	13	−11	19	18	3	−2	1	−10	154	147	2	−2	9	−10	97	92	3	−3	−3	−9	98	115	3	−2	4	−9	49	57	1
−1	14	−11	5	7	5	−1	1	−10	133	133	1	−1	9	−10	76	79	1	−2	−3	−9	45	46	1	−1	4	−9	60	64	1
0	14	−11	30	33	1	0	1	−10	84	87	1	0	9	−10	58	55	1	−1	−3	−9	142	141	2	0	4	−9	92	92	1
−1	−8	−10	61	60	2	1	1	−10	275	283	2	1	9	−10	59	66	1	0	−3	−9	31	30	1	1	4	−9	151	142	1
0	−8	−10	86	87	2	2	1	−10	117	114	1	2	9	−10	42	37	2	1	−3	−9	39	37	1	2	4	−9	62	61	1
1	−8	−10	29	29	2	3	1	−10	14	16	1	3	9	−10	31	29	1	2	−3	−9	115	114	1	3	4	−9	157	157	1
2	−8	−10	29	27	2	4	1	−10	193	189	2	4	9	−10	99	98	1	3	−3	−9	267	267	2	4	4	−9	143	143	1
−2	−7	−10	55	51	2	5	1	−10	116	117	1	5	9	−10	107	108	2	4	−3	−9	140	137	1	5	4	−9	221	216	2
−1	−7	−10	72	73	2	6	1	−10	75	75	1	−3	10	−10	57	57	2	5	−3	−9	47	42	1	−6	5	−9	18	18	3
0	−7	−10	69	65	2	−5	2	−10	154	155	3	−2	10	−10	62	64	2	6	−3	−9	76	75	2	−5	5	−9	57	57	2
1	−7	−10	62	61	1	−3	2	−10	73	79	1	−1	10	−10	136	142	2	−5	−2	−9	23	23	3	−4	5	−9	124	116	3
2	−7	−10	101	97	2	−2	2	−10	64	65	1	0	10	−10	125	120	2	−4	−2	−9	104	108	3	−3	5	−9	111	111	2
3	−7	−10	35	39	2	−1	2	−10	110	116	1	1	10	−10	107	104	1	−3	−2	−9	63	77	2	−2	5	−9	65	68	1
−3	−6	−10	97	97	1	0	2	−10	67	64	1	2	10	−10	149	148	2	−2	−2	−9	121	120	2	−1	5	−9	164	176	2
−2	−6	−10	75	76	1	1	2	−10	52	58	1	3	10	−10	13	13	2	−1	−2	−9	70	69	1	0	5	−9	91	93	1
−1	−6	−10	53	51	1	2	2	−10	42	44	1	4	10	−10	18	17	1	0	−2	−9	228	221	2	1	5	−9	249	260	2
0	−6	−10	64	62	1	3	2	−10	93	95	1	−4	11	−10	45	44	2	1	−2	−9	58	59	1	2	5	−9	50	42	1
1	−6	−10	68	68	1	4	2	−10	121	118	1	−3	11	−10	79	77	2	2	−2	−9	212	205	2	3	5	−9	138	144	1
2	−6	−10	70	68	1	5	2	−10	102	103	1	−2	11	−10	58	55	2	3	−2	−9	162	157	1	4	5	−9	141	148	1
3	−6	−10	53	52	1	6	2	−10	48	49	1	−1	11	−10	94	94	2	4	−2	−9	90	90	1	5	5	−9	146	146	2
4	−6	−10	64	63	1	−5	3	−10	233	224	5	0	11	−10	122	127	2	5	−2	−9	19	18	2	−5	6	−9	30	26	2
−4	−5	−10	29	28	2	−4	3	−10	173	184	4	1	11	−10	25	29	1	6	−2	−9	110	102	3	−4	6	−9	125	122	3
−3	−5	−10	126	122	2	−3	3	−10	60	56	1	2	11	−10	100	103	1	−5	−1	−9	44	47	2	−3	6	−9	78	74	1
−2	−5	−10	82	76	2	−2	3	−10	128	126	1	3	11	−10	33	34	2	−3	−1	−9	126	130	2	−2	6	−9	187	190	2
−1	−5	−10	142	145	2	−1	3	−10	24	25	1	4	11	−10	62	63	1	−2	−1	−9	116	121	2	−1	6	−9	126	127	1
0	−5	−10	20	23	2	0	3	−10	9	8	2	−3	12	−10	38	35	2	−1	−1	−9	133	129	1	0	6	−9	102	100	1
1	−5	−10	117	118	1	1	3	−10	198	209	2	−2	12	−10	44	42	2	0	−1	−9	93	85	1	1	6	−9	71	76	1
2	−5	−10	93	95	1	2	3	−10	85	84	1	−1	12	−10	42	46	1	1	−1	−9	36	33	1	2	6	−9	57	59	1
3	−5	−10	60	62	1	3	3	−10	31	26	1	0	12	−10	65	64	1	2	−1	−9	108	105	1	3	6	−9	94	91	1
4	−5	−10	49	51	1	4	3	−10	57	55	1	1	12	−10	44	43	1	3	−1	−9	213	213	2	4	6	−9	101	102	1
5	−5	−10	27	25	2	5	3	−10	53	51	1	2	12	−10	27	25	2	4	−1	−9	155	153	1	5	6	−9	105	112	2
−4	−4	−10	17	18	5	6	3	−10	12	12	2	−2	13	−10	48	44	1	5	−1	−9	30	28	1	−5	7	−9	14	7	5
−3	−4	−10	52	47	1	−5	4	−10	74	72	2	−1	13	−10	69	65	1	6	−1	−9	17	18	2	−4	7	−9	83	84	2
−2	−4	−10	80	79	2	−4	4	−10	17	16	4	0	13	−10	98	93	1	−6	0	−9	32	32	2	−3	7	−9	14	14	4
−1	−4	−10	46	44	1	−3	4	−10	102	103	2	1	13	−10	66	65	1	−5	0	−9	119	122	3	−2	7	−9	187	182	3
0	−4	−10	171	176	2	−2	4	−10	75	77	1	2	13	−10	21	15	3	−4	0	−9	22	22	3	−1	7	−9	135	131	2
1	−4	−10	29	31	1	−1	4	−10	73	66	1	−1	14	−10	101	101	1	−3	0	−9	15	13	3	0	7	−9	116	107	1
2	−4	−10	224	230	2	0	4	−10	126	124	1	0	14	−10	72	73	1	−2	0	−9	105	110	2	1	7	−9	154	152	1
3	−4	−10	109	107	2	1	4	−10	92	99	1	1	14	−10	58	59	2	−1	0	−9	327	333	3	2	7	−9	92	92	1
4	−4	−10	57	58	1	2	4	−10	98	100	1	0	−9	−9	32	31	2	0	0	−9	79	77	1	3	7	−9	85	75	1
5	−4	−10	86	85	2	3	4	−10	68	68	1	2	−9	−9	58	59	2	1	0	−9	236	243	2	4	7	−9	124	126	1
−4	−3	−10	51	51	2	4	4	−10	29	28	1	−2	−8	−9	89	81	2	2	0	−9	162	166	1	−4	8	−9	24	23	3
−3	−3	−10	33	35	2	5	4	−10	77	80	1	−1	−8	−9	27	28	2	3	0	−9	236	236	2	−3	8	−9	60	60	2

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−2	−3	−10	85	81	2	6	4	−10	114	108	1	0	−8	−9	44	42	2	4	0	−9	104	104	1	−2	8	−9	72	77	2
−1	−3	−10	78	82	1	−5	5	−10	92	92	2	1	−8	−9	30	29	2	5	0	−9	79	77	1	−1	8	−9	206	205	2
0	−3	−10	109	109	1	−4	5	−10	150	149	4	2	−8	−9	54	51	1	−6	1	−9	50	48	2	0	8	−9	156	149	2
1	−3	−10	157	164	1	−3	5	−10	82	87	1	3	−8	−9	73	74	2	−5	1	−9	90	88	2	1	8	−9	79	80	1
2	−3	−10	69	69	1	−2	5	−10	107	107	1	−3	−7	−9	40	38	1	−4	1	−9	23	21	3	2	8	−9	87	85	1
3	−3	−10	231	229	3	−1	5	−10	88	94	1	−2	−7	−9	89	90	2	−3	1	−9	42	42	1	3	8	−9	42	37	1
4	−3	−10	65	65	1	0	5	−10	74	72	1	−1	−7	−9	72	72	1	−2	1	−9	71	68	1	4	8	−9	164	165	1
5	−3	−10	17	18	3	1	5	−10	55	64	1	0	−7	−9	36	30	2	−1	1	−9	111	118	1	−3	9	−9	75	74	2
−5	−2	−10	27	23	2	2	5	−10	12	14	1	1	−7	−9	106	106	2	0	1	−9	26	24	1	−2	9	−9	105	99	3
−4	−2	−10	30	26	2	3	5	−10	211	214	2	2	−7	−9	92	91	2	1	1	−9	243	245	2	−1	9	−9	75	72	1
−3	−2	−10	17	15	3	4	5	−10	86	80	1	3	−7	−9	94	91	2	2	1	−9	86	83	1	0	9	−9	67	66	1
−1	−2	−10	62	65	1	5	5	−10	141	138	1	4	−7	−9	76	82	1	3	1	−9	136	140	1	1	9	−9	75	73	1
0	−2	−10	56	55	1	−5	6	−10	123	121	3	−4	−6	−9	68	71	2	4	1	−9	141	138	1	2	9	−9	99	97	2
1	−2	−10	98	97	1	−4	6	−10	60	58	2	−3	−6	−9	0	5	1	5	1	−9	175	170	1	3	9	−9	176	168	1
2	−2	−10	56	57	1	−3	6	−10	215	220	3	−2	−6	−9	116	115	3	6	1	−9	64	68	1	4	9	−9	75	74	1
3	−2	−10	93	96	1	−2	6	−10	72	68	1	−1	−6	−9	68	73	2	−6	2	−9	60	61	2	−3	10	−9	25	24	3
4	−2	−10	70	66	1	−1	6	−10	112	104	1	0	−6	−9	48	52	2	−5	2	−9	133	134	3	−2	10	−9	35	34	2
5	−2	−10	45	47	1	0	6	−10	137	132	1	1	−6	−9	130	128	2	−4	2	−9	96	118	2	−1	10	−9	115	115	2
0	10	−9	95	89	2	−5	−3	−8	72	71	2	4	3	−8	97	91	1	0	12	−8	82	74	1	−6	−2	−7	49	48	2
1	10	−9	97	97	1	−4	−3	−8	157	158	4	5	3	−8	47	45	1	1	12	−8	152	150	2	−5	−2	−7	41	40	2
2	10	−9	111	106	2	−3	−3	−8	193	219	5	6	3	−8	126	125	1	2	12	−8	116	112	3	−4	−2	−7	33	31	2
3	10	−9	63	63	1	−2	−3	−8	176	168	3	−6	4	−8	88	79	2	3	12	−8	51	61	1	−3	−2	−7	45	44	1
4	10	−9	79	80	1	−1	−3	−8	159	152	2	−5	4	−8	61	68	2	4	12	−8	12	12	2	−2	−2	−7	152	150	2
−4	11	−9	99	100	2	0	−3	−8	101	91	1	−4	4	−8	81	96	2	−3	13	−8	59	58	2	−1	−2	−7	57	50	1
−3	11	−9	78	80	2	1	−3	−8	173	171	1	−3	4	−8	142	138	2	−2	13	−8	166	164	2	0	−2	−7	83	86	1
−2	11	−9	123	124	2	2	−3	−8	95	95	1	−2	4	−8	45	45	1	−1	13	−8	96	88	1	1	−2	−7	110	110	1
−1	11	−9	107	102	3	3	−3	−8	68	64	1	−1	4	−8	54	53	1	0	13	−8	51	51	1	2	−2	−7	174	176	1
0	11	−9	75	72	1	4	−3	−8	231	235	2	0	4	−8	139	145	2	1	13	−8	143	142	2	3	−2	−7	181	177	1
1	11	−9	92	89	1	5	−3	−8	27	29	1	1	4	−8	168	163	2	2	13	−8	129	131	3	4	−2	−7	93	92	1
2	11	−9	39	37	1	6	−3	−8	32	31	1	2	4	−8	63	62	1	−2	14	−8	66	63	1	5	−2	−7	160	162	3
3	11	−9	60	61	2	−5	−2	−8	55	54	2	3	4	−8	117	123	1	−1	14	−8	91	88	1	6	−2	−7	48	47	1
4	11	−9	99	104	1	−4	−2	−8	35	32	2	4	4	−8	122	119	1	0	14	−8	101	95	1	−6	−1	−7	53	53	2
−3	12	−9	63	58	2	−3	−2	−8	142	141	2	5	4	−8	81	78	1	1	14	−8	50	51	2	−5	−1	−7	77	75	2
−2	12	−9	69	69	1	−2	−2	−8	112	103	2	−6	5	−8	36	37	2	−1	−10	−7	20	22	3	−4	−1	−7	89	91	2
−1	12	−9	40	43	1	−1	−2	−8	84	83	1	−5	5	−8	38	39	2	0	−10	−7	103	103	2	−3	−1	−7	272	274	4
0	12	−9	10	13	4	0	−2	−8	258	245	2	−4	5	−8	143	149	4	2	−10	−7	38	35	2	−2	−1	−7	65	54	1
1	12	−9	109	111	1	1	−2	−8	32	33	1	−3	5	−8	36	34	1	−2	−9	−7	71	71	2	−1	−1	−7	442	438	5
2	12	−9	44	45	2	2	−2	−8	42	38	1	−2	5	−8	101	97	1	−1	−9	−7	49	51	2	0	−1	−7	77	83	1
3	12	−9	10	7	5	3	−2	−8	189	188	2	−1	5	−8	166	162	1	0	−9	−7	0	6	1	1	−1	−7	230	225	4
−3	13	−9	120	118	3	4	−2	−8	201	199	2	0	5	−8	102	96	1	1	−9	−7	99	96	2	2	−1	−7	284	285	2
−2	13	−9	58	53	1	5	−2	−8	88	86	2	1	5	−8	81	85	1	2	−9	−7	31	26	2	3	−1	−7	153	156	1
−1	13	−9	35	32	1	6	−2	−8	60	57	1	2	5	−8	73	71	1	3	−9	−7	67	71	2	4	−1	−7	116	118	1
0	13	−9	58	59	1	−6	−1	−8	73	77	2	3	5	−8	170	168	1	−3	−8	−7	114	114	3	5	−1	−7	179	180	2
1	13	−9	55	56	1	−5	−1	−8	35	38	2	4	5	−8	84	86	1	−2	−8	−7	60	61	2	6	−1	−7	88	90	1
2	13	−9	46	42	2	−4	−1	−8	100	103	3	5	5	−8	11	14	7	−1	−8	−7	78	77	2	−6	0	−7	35	35	2
−1	14	−9	30	31	1	−3	−1	−8	77	75	1	−6	6	−8	9	9	9	0	−8	−7	37	36	2	−5	0	−7	61	59	2
0	14	−9	67	65	1	−2	−1	−8	64	65	1	−5	6	−8	68	66	2	1	−8	−7	118	112	2	−4	0	−7	158	162	2
1	14	−9	20	24	3	−1	−1	−8	98	92	1	−4	6	−8	111	109	3	2	−8	−7	65	65	1	−3	0	−7	125	123	2
−2	−9	−8	54	50	2	0	−1	−8	98	89	1	−3	6	−8	102	98	2	3	−8	−7	80	88	2	−2	0	−7	86	88	1

TABLE 7-continued

Observed and calculated structure factors for NEL																													
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−1	−9	−8	57	57	2	1	−1	−8	270	265	2	−2	6	−8	120	128	1	4	−8	−7	50	50	1	−1	0	−7	115	123	1
0	−9	−8	51	52	2	2	−1	−8	149	148	1	−1	6	−8	89	92	1	−4	−7	−7	68	62	2	0	0	−7	140	135	1
1	−9	−8	136	130	2	3	−1	−8	60	64	1	0	6	−8	423	414	6	−3	−7	−7	148	153	3	1	0	−7	332	332	4
2	−9	−8	25	22	3	4	−1	−8	295	296	2	1	6	−8	72	75	1	−2	−7	−7	48	58	2	2	0	−7	139	138	1
3	−9	−8	75	76	2	5	−1	−8	22	18	2	2	6	−8	179	184	1	0	−7	−7	83	80	2	3	0	−7	106	102	1
−3	−8	−8	91	90	2	6	−1	−8	57	54	1	3	6	−8	79	81	1	1	−7	−7	101	103	2	4	0	−7	65	68	1
−2	−8	−8	31	27	2	−6	0	−8	66	62	2	4	6	−8	245	244	4	2	−7	−7	86	84	1	5	0	−7	95	100	1
−1	−8	−8	117	122	3	−5	0	−8	47	50	2	5	6	−8	106	106	2	3	−7	−7	110	115	2	6	0	−7	68	65	1
0	−8	−8	22	22	3	−4	0	−8	139	139	3	−5	7	−8	85	84	2	4	−7	−7	27	27	1	7	0	−7	53	60	1
1	−8	−8	46	46	1	−3	0	−8	58	61	1	−4	7	−8	71	70	2	5	−7	−7	29	32	1	−6	1	−7	15	14	5
2	−8	−8	106	105	2	−2	0	−8	150	144	2	−3	7	−8	120	113	1	−4	−6	−7	57	55	2	−5	1	−7	109	114	3
3	−8	−8	167	165	4	−1	0	−8	138	135	1	−2	7	−8	42	40	1	−3	−6	−7	29	30	2	−4	1	−7	149	151	2
4	−8	−8	32	35	1	0	0	−8	420	414	5	−1	7	−8	70	63	1	−2	−6	−7	72	82	2	−3	1	−7	26	25	1
−4	−7	−8	65	71	2	1	0	−8	123	121	1	0	7	−8	109	104	1	−1	−6	−7	34	33	2	−2	1	−7	100	95	1
−3	−7	−8	48	47	2	2	0	−8	111	109	1	1	7	−8	46	45	1	0	−6	−7	164	161	2	−1	1	−7	495	499	5
−2	−7	−8	71	70	2	3	0	−8	69	68	1	2	7	−8	95	94	1	1	−6	−7	141	142	2	0	1	−7	11	10	1
−1	−7	−8	110	107	2	4	0	−8	170	173	1	3	7	−8	58	57	1	2	−6	−7	237	237	2	1	1	−7	175	166	2
0	−7	−8	161	158	3	5	0	−8	39	36	1	4	7	−8	275	275	5	3	−6	−7	67	71	1	2	1	−7	306	296	3
1	−7	−8	85	82	1	6	0	−8	73	73	1	−5	8	−8	43	42	2	4	−6	−7	75	80	1	3	1	−7	93	93	1
2	−7	−8	113	109	2	−6	1	−8	34	29	2	−4	8	−8	85	81	2	5	−6	−7	51	50	1	4	1	−7	116	113	1
3	−7	−8	33	38	1	−5	1	−8	60	60	2	−3	8	−8	133	135	3	−5	−5	−7	133	132	3	5	1	−7	180	179	1
4	−7	−8	70	69	1	−4	1	−8	126	122	3	−2	8	−8	90	92	2	−4	−5	−7	20	19	3	6	1	−7	53	52	1
5	−7	−8	25	28	3	−3	1	−8	162	159	2	−1	8	−8	76	79	1	−3	−5	−7	187	202	5	7	1	−7	12	9	2
−4	−6	−8	15	14	5	−2	1	−8	74	74	1	0	8	−8	130	124	1	−2	−5	−7	76	75	1	−6	2	−7	53	52	2
−3	−6	−8	70	70	2	−1	1	−8	242	246	2	1	8	−8	48	45	1	−1	−5	−7	105	107	2	−5	2	−7	123	119	3
−2	−6	−8	123	134	3	0	1	−8	95	86	1	2	8	−8	101	95	1	0	−5	−7	85	82	1	−4	2	−7	77	82	1
−1	−6	−8	113	108	2	1	1	−8	433	443	6	3	8	−8	202	194	1	1	−5	−7	81	85	1	−3	2	−7	34	40	1
0	−6	−8	94	91	2	2	1	−8	66	64	1	4	8	−8	13	11	1	2	−5	−7	60	58	1	−2	2	−7	179	172	2
1	−6	−8	7	3	7	3	1	−8	111	112	1	−3	9	−8	81	77	2	3	−5	−7	187	187	2	−1	2	−7	260	252	2
2	−6	−8	120	118	1	4	1	−8	27	26	1	−2	9	−8	244	251	4	4	−5	−7	106	107	1	0	2	−7	225	205	2
3	−6	−8	84	84	1	5	1	−8	15	12	1	−1	9	−8	93	96	1	5	−5	−7	135	136	1	1	2	−7	315	308	3
4	−6	−8	23	23	2	6	1	−8	34	33	1	0	9	−8	135	135	2	6	−5	−7	84	87	2	2	2	−7	77	76	1
5	−6	−8	14	18	2	−6	2	−8	138	138	3	1	9	−8	254	256	2	−5	−4	−7	50	47	2	3	2	−7	68	71	1
−5	−5	−8	24	24	3	−5	2	−8	35	37	2	2	9	−8	217	219	2	−4	−4	−7	148	141	3	4	2	−7	96	102	1
−4	−5	−8	47	46	2	−4	2	−8	101	105	2	3	9	−8	152	154	1	−3	−4	−7	236	230	5	5	2	−7	240	251	2
−3	−5	−8	31	36	2	−3	2	−8	73	66	1	4	9	−8	38	37	1	−2	−4	−7	91	82	1	6	2	−7	67	66	1
−2	−5	−8	84	106	2	−2	2	−8	184	188	2	−3	10	−8	63	61	2	−1	−4	−7	346	344	5	7	2	−7	42	44	1
−1	−5	−8	32	34	2	−1	2	−8	140	133	1	−2	10	−8	220	214	5	0	−4	−7	63	61	1	−6	3	−7	51	46	2
0	−5	−8	65	61	1	0	2	−8	34	34	1	−1	10	−8	98	100	1	1	−4	−7	208	207	2	−5	3	−7	99	104	3
1	−5	−8	39	43	1	1	2	−8	165	152	3	0	10	−8	43	42	1	2	−4	−7	54	50	1	−4	3	−7	43	41	1
2	−5	−8	75	79	1	2	2	−8	141	136	1	1	10	−8	190	199	2	3	−4	−7	118	111	1	−3	3	−7	119	123	2
3	−5	−8	110	110	1	3	2	−8	60	55	1	2	10	−8	153	149	2	4	−4	−7	23	26	1	−2	3	−7	93	91	1
4	−5	−8	21	20	2	4	2	−8	128	121	1	3	10	−8	114	112	1	5	−4	−7	146	149	2	−1	3	−7	86	88	1
5	−5	−8	19	20	1	5	2	−8	103	109	1	4	10	−8	129	129	1	6	−4	−7	78	79	1	0	3	−7	197	181	2
−5	−4	−8	21	15	3	6	2	−8	114	115	1	−4	11	−8	90	87	2	−5	−3	−7	82	81	2	1	3	−7	147	147	1
−4	−4	−8	40	39	2	7	2	−8	24	26	1	−3	11	−8	35	31	2	−4	−3	−7	85	84	2	2	3	−7	102	98	1
−3	−4	−8	66	68	2	−6	3	−8	108	107	3	−2	11	−8	41	47	2	−3	−3	−7	324	324	5	3	3	−7	94	93	1
−2	−4	−8	161	160	2	−5	3	−8	83	93	3	−1	11	−8	31	33	1	−2	−3	−7	108	103	2	4	3	−7	91	87	1
−1	−4	−8	223	226	3	−4	3	−8	77	80	2	0	11	−8	24	29	2	−1	−3	−7	99	87	1	5	3	−7	121	124	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	−4	−8	17	13	2	−3	3	−8	58	54	1	1	11	−8	48	47	1	0	−3	−7	48	54	1	−6	4	−7	88	82	2
1	−4	−8	239	242	2	−2	3	−8	120	119	1	2	11	−8	121	115	2	1	−3	−7	22	23	1	−5	4	−7	27	29	2
2	−4	−8	194	188	2	−1	3	−8	226	230	2	3	11	−8	64	61	1	2	−3	−7	193	186	1	−4	4	−7	121	123	2
3	−4	−8	106	111	1	0	3	−8	181	164	2	4	11	−8	57	57	1	3	−3	−7	116	122	1	−3	4	−7	59	58	1
4	−4	−8	85	83	1	1	3	−8	105	100	1	−3	12	−8	50	51	2	4	−3	−7	75	74	1	−2	4	−7	98	93	1
5	−4	−8	109	106	1	2	3	−8	83	74	1	−2	12	−8	171	172	3	5	−3	−7	132	135	2	−1	4	−7	112	115	1
6	−4	−8	33	39	1	3	3	−8	85	88	1	−1	12	−8	62	61	1	6	−3	−7	47	48	1	0	4	−7	96	105	1
1	4	−7	455	435	5	−2	14	−7	79	78	1	−6	−2	−6	43	39	2	1	4	−6	309	298	3	−2	14	−6	11	12	4
2	4	−7	51	49	1	−1	14	−7	53	59	1	−5	−2	−6	92	92	2	2	4	−6	205	206	2	−1	14	−6	82	85	1
3	4	−7	64	64	1	0	14	−7	85	82	1	−4	−2	−6	344	350	5	3	4	−6	69	68	2	0	14	−6	49	46	1
4	4	−7	98	91	2	1	14	−7	59	57	2	−3	−2	−6	28	23	1	4	4	−6	57	62	1	1	14	−6	76	74	2
5	4	−7	113	111	3	2	14	−7	36	43	2	−2	−2	−6	257	262	3	5	4	−6	97	92	2	2	14	−6	39	43	2
−6	5	−7	32	31	2	−2	−10	−6	16	79	2	−1	−2	−6	229	236	3	−6	5	−6	25	22	2	−1	−11	−5	73	72	2
−4	5	−7	128	137	2	−1	−10	−6	78	77	2	0	−2	−6	587	573	6	−5	5	−6	146	168	4	2	−11	−5	18	18	4
−3	5	−7	226	231	3	0	−10	−6	169	162	4	1	−2	−6	115	120	1	−4	5	−6	157	159	2	−3	−10	−5	39	39	2
−2	5	−7	88	84	1	2	−10	−6	107	110	3	2	−2	−6	187	182	2	−3	5	−6	179	170	3	−2	−10	−5	92	89	2
−1	5	−7	46	48	1	3	−10	−6	64	60	2	3	−2	−6	37	40	1	−2	5	−6	112	114	1	−1	−10	−5	107	108	3
0	5	−7	238	212	3	−3	−9	−6	0	9	1	4	−2	−6	203	209	1	−1	5	−6	392	368	5	0	−10	−5	50	45	2
1	5	−7	191	180	2	−2	−9	−6	75	77	2	5	−2	−6	202	199	5	0	5	−6	126	112	1	2	−10	−5	54	53	1
2	5	−7	99	103	1	−1	−9	−6	120	118	3	6	−2	−6	57	55	1	1	5	−6	358	343	4	3	−10	−5	21	20	3
3	5	−7	134	129	1	0	−9	−6	101	103	2	−6	−1	−6	46	45	2	2	5	−6	63	65	1	4	−10	−5	68	71	2
4	5	−7	176	177	4	1	−9	−6	108	107	2	−5	−1	−6	15	13	4	3	5	−6	139	139	2	−3	−9	−5	26	24	3
5	5	−7	168	173	4	2	−9	−6	191	192	3	−4	−1	−6	182	178	3	4	5	−6	168	174	4	−2	−9	−5	118	120	3
−6	6	−7	32	30	2	3	−9	−6	101	97	2	−3	−1	−6	51	55	1	−6	6	−6	35	34	2	−1	−9	−5	116	114	3
−5	6	−7	170	162	4	4	−9	−6	17	18	3	−2	−1	−6	147	139	2	−5	6	−6	113	125	3	0	−9	−5	105	100	2
−4	6	−7	43	45	2	−4	−8	−6	62	61	2	−1	−1	−6	24	17	1	−4	6	−6	153	157	2	1	−9	−5	66	64	1
−3	6	−7	93	89	1	−3	−8	−6	120	122	3	0	−1	−6	208	202	2	−3	6	−6	153	158	2	2	−9	−5	134	141	2
−2	6	−7	201	205	2	−2	−8	−6	103	111	3	1	−1	−6	71	71	1	−2	6	−6	149	151	1	3	−9	−5	108	107	2
−1	6	−7	34	27	1	−1	−8	−6	40	37	2	2	−1	−6	253	259	2	−1	6	−6	79	84	1	4	−9	−5	32	30	1
0	6	−7	41	40	1	0	−8	−6	140	139	3	3	−1	−6	115	114	1	0	6	−6	274	261	3	−4	−8	−5	40	40	2
1	6	−7	142	140	1	1	−8	−6	126	125	2	4	−1	−6	154	152	1	1	6	−6	263	271	2	−3	−8	−5	24	19	3
2	6	−7	103	99	1	2	−8	−6	151	154	2	5	−1	−6	79	81	1	2	6	−6	61	69	1	−2	−8	−5	67	78	2
3	6	−7	146	139	2	3	−8	−6	104	106	2	6	−1	−6	27	27	1	3	6	−6	253	253	3	0	−8	−5	106	104	2
4	6	−7	94	90	2	4	−8	−6	49	44	1	−6	0	−6	82	83	2	4	6	−6	53	57	2	1	−8	−5	111	113	1
−6	7	−7	129	129	3	5	−8	−6	26	25	1	−5	0	−6	132	131	3	−6	7	−6	50	45	2	2	−8	−5	28	23	2
−5	7	−7	123	118	3	−4	−7	−6	55	56	2	−4	0	−6	165	166	2	−5	7	−6	100	100	2	3	−8	−5	129	136	1
−4	7	−7	164	159	4	−3	−7	−6	33	35	2	−3	0	−6	77	74	1	−4	7	−6	67	64	2	4	−8	−5	65	59	1
−3	7	−7	56	51	1	−2	−7	−6	110	127	3	−2	0	−6	155	154	2	−3	7	−6	109	108	1	5	−8	−5	29	33	1
−2	7	−7	44	46	1	−1	−7	−6	57	57	2	−1	0	−6	106	108	1	−2	7	−6	47	54	1	−4	−7	−5	36	33	2
−1	7	−7	40	38	1	0	−7	−6	130	125	2	0	0	−6	379	387	3	−1	7	−6	330	331	3	−3	−7	−5	89	92	2
0	7	−7	224	214	2	1	−7	−6	151	153	2	1	0	−6	165	172	1	0	7	−6	169	163	1	−2	−7	−5	172	188	4
1	7	−7	193	188	1	2	−7	−6	174	172	2	2	0	−6	322	317	4	1	7	−6	176	180	1	−1	−7	−5	187	192	3
2	7	−7	41	35	1	3	−7	−6	130	134	1	3	0	−6	112	115	1	2	7	−6	163	168	1	0	−7	−5	122	127	2
3	7	−7	205	200	2	4	−7	−6	47	47	1	4	0	−6	200	201	1	3	7	−6	249	249	3	1	−7	−5	60	62	1
−5	8	−7	149	147	3	5	−7	−6	76	77	1	5	0	−6	47	52	1	−5	8	−6	140	135	3	2	−7	−5	250	254	2
−4	8	−7	80	78	2	−5	−6	−6	42	40	2	6	0	−6	127	128	1	−4	8	−6	22	25	3	3	−7	−5	159	163	2
−3	8	−7	88	84	2	−4	−6	−6	86	88	2	7	0	−6	39	41	1	−3	8	−6	264	270	3	4	−7	−5	43	44	1
−2	8	−7	152	155	2	−3	−6	−6	82	84	2	−6	1	−6	44	43	2	−2	8	−6	98	94	1	5	−7	−5	46	46	1
−1	8	−7	116	116	1	−2	−6	−6	317	328	8	−5	1	−6	209	209	4	−1	8	−6	134	132	1	−5	−6	−5	53	49	2

TABLE 7-continued

Observed and calculated structure factors for NEL																													
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	8	−7	136	134	1	−1	−6	−6	171	174	3	−4	1	−6	105	105	2	0	8	−6	65	61	1	−4	−6	−5	25	24	3
1	8	−7	76	71	1	0	−6	−6	13	5	3	−3	1	−6	108	105	1	1	8	−6	165	163	1	−3	−6	−5	20	15	3
2	8	−7	83	83	1	1	−6	−6	61	63	1	−2	1	−6	220	217	2	2	8	−6	119	117	1	−2	−6	−5	201	194	3
3	8	−7	230	219	2	2	−6	−6	328	333	3	−1	1	−6	345	343	4	3	8	−6	222	227	2	−1	−6	−5	144	136	2
4	8	−7	242	249	3	3	−6	−6	201	203	2	0	1	−6	280	279	2	4	8	−6	65	70	1	0	−6	−5	61	58	1
−3	9	−7	133	123	3	4	−6	−6	134	132	2	1	1	−6	332	335	3	−5	9	−6	67	70	2	1	−6	−5	111	111	1
−2	9	−7	316	319	5	5	−6	−6	65	67	1	2	1	−6	253	245	3	−3	9	−6	138	141	3	2	−6	−5	31	29	1
−1	9	−7	65	63	1	6	−6	−6	29	34	1	3	1	−6	113	110	1	−2	9	−6	21	16	4	3	−6	−5	143	145	1
0	9	−7	67	69	1	−5	−5	−6	23	25	3	4	1	−6	126	121	1	−1	9	−6	157	160	1	4	−6	−5	39	39	1
1	9	−7	77	75	1	−4	−5	−6	75	73	2	5	1	−6	131	134	1	0	9	−6	55	54	1	5	−6	−5	53	54	1
2	9	−7	226	235	1	−3	−5	−6	121	122	3	6	1	−6	70	76	1	1	9	−6	217	222	2	6	−6	−5	46	42	1
3	9	−7	176	169	1	−2	−5	−6	195	190	3	7	1	−6	37	42	1	2	9	−6	92	94	1	−5	−5	−5	112	122	3
4	9	−7	86	84	1	−1	−5	−6	37	38	1	−6	2	−6	61	63	2	3	9	−6	225	224	2	−4	−5	−5	102	107	3
−3	10	−7	10	11	10	0	−5	−6	72	76	1	−5	2	−6	45	46	2	4	9	−6	29	32	1	−3	−5	−5	267	266	4
−2	10	−7	128	123	3	1	−5	−6	52	51	1	−4	2	−6	49	41	1	−3	10	−6	149	150	3	−2	−5	−5	171	168	2
−1	10	−7	62	58	1	2	−5	−6	224	222	2	−3	2	−6	72	69	1	−2	10	−6	136	140	3	−1	−5	−5	170	164	2
0	10	−7	99	101	1	3	−5	−6	89	89	1	−2	2	−6	98	97	1	−1	10	−6	82	83	1	0	−5	−5	96	99	1
1	10	−7	54	54	1	4	−5	−6	100	100	1	−1	2	−6	139	136	1	0	10	−6	39	39	1	1	−5	−5	259	265	2
2	10	−7	18	12	2	5	−5	−6	105	102	1	0	2	−6	181	172	1	1	10	−6	146	143	1	2	−5	−5	86	84	1
3	10	−7	129	133	1	6	−5	−6	74	74	1	1	2	−6	414	421	4	2	10	−6	114	116	2	3	−5	−5	78	80	1
4	10	−7	20	27	1	−5	−4	−6	40	37	2	2	2	−6	185	180	2	3	10	−6	226	226	2	4	−5	−5	125	129	1
−4	11	−7	85	90	2	−4	−4	−6	190	187	4	3	2	−6	229	236	2	4	10	−6	87	86	1	5	−5	−5	107	116	1
−3	11	−7	43	43	2	−3	−4	−6	49	45	1	4	2	−6	150	154	1	−4	11	−6	33	31	3	6	−5	−5	11	12	5
−2	11	−7	174	180	2	−2	−4	−6	113	115	2	5	2	−6	85	91	1	−3	11	−6	180	183	4	−6	−4	−5	20	24	3
−1	11	−7	82	89	2	−1	−4	−6	106	96	2	6	2	−6	57	56	1	−2	11	−6	78	74	1	−5	−4	−5	207	209	5
0	11	−7	47	52	2	0	−4	−6	82	86	1	7	2	−6	38	44	1	−1	11	−6	25	24	1	−4	−4	−5	122	127	3
1	11	−7	46	46	1	1	−4	−6	129	130	1	−6	3	−6	95	92	2	0	11	−6	90	91	2	−3	−4	−5	142	140	2
2	11	−7	282	282	4	2	−4	−6	266	266	2	−5	3	−6	42	41	2	1	11	−6	181	186	2	−2	−4	−5	202	195	3
3	11	−7	108	107	1	3	−4	−6	109	108	1	−4	3	−6	21	19	2	2	11	−6	7	15	7	−1	−4	−5	293	304	3
4	11	−7	67	68	1	4	−4	−6	48	51	1	−3	3	−6	9	2	4	3	11	−6	120	120	1	0	−4	−5	159	159	1
−4	12	−7	17	18	4	5	−4	−6	36	38	1	−2	3	−6	121	111	2	4	11	−6	60	59	1	1	−4	−5	275	283	3
−3	12	−7	117	117	3	6	−4	−6	15	20	3	−1	3	−6	283	281	3	−3	12	−6	145	143	3	2	−4	−5	157	151	1
−2	12	−7	89	86	1	−6	−3	−6	72	70	2	0	3	−6	164	155	1	−2	12	−6	38	40	1	3	−4	−5	65	65	1
−1	12	−7	103	109	2	−5	−3	−6	25	14	2	1	3	−6	257	254	2	−1	12	−6	29	31	1	4	−4	−5	42	42	1
0	12	−7	15	11	2	−4	−3	−6	128	129	3	2	3	−6	271	263	3	0	12	−6	85	80	1	5	−4	−5	119	119	2
1	12	−7	81	80	1	−3	−3	−6	77	79	1	3	3	−6	83	82	1	1	12	−6	40	43	1	6	−4	−5	6	9	5
2	12	−7	108	106	3	−2	−3	−6	182	173	3	4	3	−6	99	98	1	2	12	−6	91	89	2	−6	−3	−5	17	24	4
3	12	−7	52	55	2	−1	−3	−6	97	102	1	5	3	−6	47	45	1	3	12	−6	90	99	2	−5	−3	−5	115	117	3
4	12	−7	73	77	1	0	−3	−6	59	55	1	−6	4	−6	31	29	2	4	12	−6	83	89	1	−4	−3	−5	52	50	1
−3	13	−7	11	12	8	1	−3	−6	121	115	1	−5	4	−6	163	192	4	−3	13	−6	30	27	2	−3	−3	−5	118	125	2
−2	13	−7	58	57	1	2	−3	−6	176	173	1	−4	4	−6	28	26	1	−2	13	−6	77	78	1	−2	−3	−5	235	226	3
−1	13	−7	88	84	1	3	−3	−6	206	215	2	−3	4	−6	91	88	1	−1	13	−6	64	67	1	−1	−3	−5	290	287	3
0	13	−7	126	134	1	4	−3	−6	101	102	1	−2	4	−6	63	57	1	0	13	−6	80	85	1	0	−3	−5	413	400	4
1	13	−7	22	28	1	5	−3	−6	88	96	1	−1	4	−6	343	332	3	1	13	−6	63	70	1	1	−3	−5	214	209	2
2	13	−7	80	80	2	6	−3	−6	71	68	1	0	4	−6	294	281	2	2	13	−6	79	77	2	2	−3	−5	144	147	1
3	−3	−5	135	130	1	−5	4	−5	76	79	2	−3	13	−5	116	113	3	3	−4	−4	166	165	1	−5	3	−4	103	98	2
4	−3	−5	60	58	1	−4	4	−5	52	49	1	−2	13	−5	48	45	1	4	−4	−4	55	53	1	−4	3	−4	29	27	1
5	−3	−5	66	73	1	−3	4	−5	143	143	2	−1	13	−5	37	39	1	5	−4	−4	66	72	1	−3	3	−4	116	119	2
6	−3	−5	31	33	2	−2	4	−5	183	188	3	0	13	−5	81	78	1	6	−4	−4	64	59	1	−2	3	−4	185	193	3

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	−3	−5	18	16	4	−1	4	−5	223	216	3	1	13	−5	49	52	1	−5	−3	−4	162	169	4	−1	3	−4	587	613	6
−6	−2	−5	36	35	2	0	4	−5	368	363	3	2	13	−5	40	39	2	−4	−3	−4	50	50	2	0	3	−4	129	136	1
−5	−2	−5	94	97	2	1	4	−5	271	265	2	−2	14	−5	71	70	1	−3	−3	−4	84	87	1	1	3	−4	386	384	4
−4	−2	−5	250	263	4	2	4	−5	144	141	3	−1	14	−5	45	44	1	−2	−3	−4	142	135	2	4	3	−4	148	144	2
−3	−2	−5	253	268	4	3	4	−5	79	81	1	0	14	−5	61	55	1	−1	−3	−4	332	336	4	5	3	−4	165	165	2
−2	−2	−5	164	162	2	4	4	−5	240	224	3	1	14	−5	37	38	2	0	−3	−4	322	314	3	6	3	−4	21	21	3
−1	−2	−5	178	174	2	5	4	−5	69	72	1	2	14	−5	57	63	2	1	−3	−4	330	324	3	−7	4	−4	89	90	2
0	−2	−5	69	69	1	−6	5	−5	67	65	2	−2	−11	−4	44	40	2	2	−3	−4	96	87	1	−6	4	−4	79	79	2
1	−2	−5	213	204	2	−5	5	−5	79	92	2	−1	−11	−4	130	127	3	3	−3	−4	99	90	1	−5	4	−4	146	146	3
2	−2	−5	93	91	1	−4	5	−5	243	241	4	0	−11	−4	89	88	2	4	−3	−4	53	55	1	−4	4	−4	112	116	2
3	−2	−5	208	213	1	−3	5	−5	85	86	1	1	−11	−4	72	68	2	5	−3	−4	33	34	1	−3	4	−4	56	57	1
4	−2	−5	140	143	1	−2	5	−5	52	48	1	2	−11	−4	35	36	2	6	−3	−4	47	50	1	−2	4	−4	165	166	3
5	−2	−5	107	108	1	−1	5	−5	338	331	5	3	−11	−4	92	92	2	7	−3	−4	46	46	2	−1	4	−4	287	295	3
6	−2	−5	78	76	1	0	5	−5	608	595	6	−3	−10	−4	120	117	3	−6	−2	−4	83	85	2	0	4	−4	221	221	2
−6	−1	−5	39	40	2	1	5	−5	46	38	1	−2	−10	−4	48	49	2	−5	−2	−4	185	189	4	1	4	−4	157	160	1
−5	−1	−5	130	127	3	2	5	−5	104	88	2	−1	−10	−4	58	57	2	−4	−2	−4	125	122	3	3	4	−4	148	158	2
−4	−1	−5	101	101	2	3	5	−5	35	24	2	0	−10	−4	223	211	5	−3	−2	−4	68	69	1	4	4	−4	82	81	1
−3	−1	−5	263	266	4	4	5	−5	149	142	2	1	−10	−4	73	68	3	−2	−2	−4	151	151	2	5	4	−4	32	30	2
−2	−1	−5	176	184	2	−6	6	−5	71	67	2	2	−10	−4	30	27	2	−1	−2	−4	162	159	2	6	4	−4	73	78	2
−1	−1	−5	199	206	2	−5	6	−5	58	69	2	3	−10	−4	59	57	1	0	−2	−4	300	292	3	−6	5	−4	29	30	2
0	−1	−5	315	324	3	−4	6	−5	242	235	4	4	−10	−4	103	102	2	1	−2	−4	32	23	1	−5	5	−4	70	83	2
1	−1	−5	332	325	3	−3	6	−5	204	203	2	−3	−9	−4	61	62	2	2	−2	−4	248	247	2	−4	5	−4	8	13	7
2	−1	−5	96	95	1	−2	6	−5	111	119	1	−2	−9	−4	111	117	3	3	−2	−4	149	152	1	−3	5	−4	156	154	2
3	−1	−5	101	104	1	−1	6	−5	286	278	3	−1	−9	−4	75	87	2	4	−2	−4	28	29	1	−2	5	−4	90	93	1
4	−1	−5	119	119	1	0	6	−5	514	492	6	0	−9	−4	29	29	3	5	−2	−4	147	144	1	−1	5	−4	159	153	3
5	−1	−5	111	113	1	1	6	−5	75	76	1	1	−9	−4	74	70	1	6	−2	−4	55	52	1	0	5	−4	230	230	2
6	−1	−5	113	115	1	2	6	−5	78	82	1	2	−9	−4	133	133	2	7	−2	−4	97	98	2	1	5	−4	278	284	3
7	−1	−5	68	63	1	3	6	−5	33	24	2	3	−9	−4	80	80	2	−6	−1	−4	25	21	3	3	5	−4	14	17	2
−6	0	−5	37	38	2	−5	7	−5	101	102	3	4	−9	−4	32	34	1	−5	−1	−4	130	135	3	4	5	−4	57	56	1
−5	0	−5	124	123	3	−4	7	−5	275	265	6	5	−9	−4	52	55	2	−4	−1	−4	188	195	3	5	5	−4	90	92	2
−4	0	−5	42	39	1	−3	7	−5	182	187	2	−4	−8	−4	78	78	2	−3	−1	−4	183	196	4	−6	6	−4	10	13	10
−3	0	−5	96	101	1	−2	7	−5	129	136	1	−3	−8	−4	76	76	2	−2	−1	−4	48	46	1	−5	6	−4	70	79	2
−2	0	−5	314	302	3	−1	7	−5	131	130	1	−1	−8	−4	80	89	2	−1	−1	−4	166	166	2	−4	6	−4	144	138	2
−1	0	−5	113	115	1	0	7	−5	179	166	1	0	−8	−4	38	31	1	0	−1	−4	399	409	3	−3	6	−4	146	146	2
0	0	−5	307	311	2	1	7	−5	135	135	1	1	−8	−4	78	82	1	1	−1	−4	133	135	1	−2	6	−4	72	79	1
1	0	−5	36	42	1	2	7	−5	25	27	1	2	−8	−4	100	103	1	2	−1	−4	229	223	2	−1	6	−4	166	170	2
2	0	−5	21	23	1	3	7	−5	51	57	1	3	−8	−4	86	86	1	3	−1	−4	145	147	1	0	6	−4	398	389	5
3	0	−5	288	285	3	−6	8	−5	78	79	2	4	−8	−4	98	100	1	4	−1	−4	87	92	1	1	6	−4	10	9	2
4	0	−5	84	79	1	−5	8	−5	24	20	3	5	−8	−4	62	62	1	5	−1	−4	143	138	1	2	6	−4	75	78	1
5	0	−5	138	138	1	−4	8	−5	285	281	7	−5	−7	−4	58	62	2	6	−1	−4	37	34	1	−5	7	−4	88	88	2
6	0	−5	40	43	1	−3	8	−5	43	37	1	−4	−7	−4	57	56	2	7	−1	−4	68	71	1	−4	7	−4	71	73	2
7	0	−5	48	45	1	−2	8	−5	185	188	2	−3	−7	−4	92	89	2	−6	0	−4	66	65	2	−3	7	−4	300	302	3
−6	1	−5	110	111	3	−1	8	−5	69	67	1	−2	−7	−4	122	122	2	−5	0	−4	168	169	4	−2	7	−4	85	82	1
−5	1	−5	129	128	3	0	8	−5	173	164	2	−1	−7	−4	24	19	2	−4	0	−4	192	194	3	−1	7	−4	359	355	4
−4	1	−5	160	164	2	1	8	−5	134	130	1	0	−7	−4	128	129	2	−3	0	−4	63	56	1	0	7	−4	344	333	3
−3	1	−5	116	114	1	2	8	−5	193	202	1	1	−7	−4	89	85	1	−2	0	−4	83	87	1	1	7	−4	172	171	1
−2	1	−5	109	105	1	3	8	−5	46	46	1	2	−7	−4	83	80	1	−1	0	−4	97	102	1	2	7	−4	102	101	1
−1	1	−5	222	228	2	4	8	−5	88	88	1	3	−7	−4	29	29	1	0	0	−4	189	195	1	3	7	−4	201	204	2
0	1	−5	190	186	1	−5	9	−5	26	27	3	4	−7	−4	50	53	1	1	0	−4	127	128	1	−6	8	−4	30	29	2

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	1	−5	247	254	2	−4	9	−5	49	49	2	5	−7	−4	66	66	1	2	0	−4	243	243	2	−5	8	−4	82	76	2
2	1	−5	87	86	1	−3	9	−5	291	296	7	6	−7	−4	80	78	2	3	0	−4	141	144	1	−4	8	−4	123	122	3
3	1	−5	92	87	1	−2	9	−5	257	258	4	−5	−6	−4	21	20	3	4	0	−4	210	206	1	−3	8	−4	229	231	2
4	1	−5	168	172	1	−1	9	−5	66	67	1	−4	−6	−4	33	33	2	5	0	−4	90	90	1	−2	8	−4	179	184	2
5	1	−5	163	160	1	0	9	−5	45	43	1	−3	−6	−4	142	144	2	6	0	−4	71	69	1	−1	8	−4	264	257	3
6	1	−5	127	126	1	1	9	−5	83	88	1	−2	−6	−4	60	53	1	7	0	−4	36	38	1	0	8	−4	108	98	1
7	1	−5	52	58	1	2	9	−5	321	321	2	−1	−6	−4	114	112	2	−6	1	−4	124	121	3	1	8	−4	308	306	2
−6	2	−5	28	30	2	3	9	−5	73	77	1	0	−6	−4	49	48	1	−5	1	−4	187	192	3	2	8	−4	122	119	1
−5	2	−5	117	117	3	4	9	−5	68	68	1	1	−6	−4	166	170	2	−4	1	−4	150	144	2	3	8	−4	139	145	1
−4	2	−5	21	24	2	−3	10	−5	159	160	4	2	−6	−4	210	207	2	−3	1	−4	77	77	1	4	8	−4	18	19	1
−3	2	−5	85	88	1	−2	10	−5	141	144	2	3	−6	−4	43	40	1	−2	1	−4	67	72	1	−5	9	−4	61	65	2
−2	2	−5	157	157	2	−1	10	−5	49	52	1	4	−6	−4	79	81	1	−1	1	−4	264	272	3	−4	9	−4	110	110	3
−1	2	−5	212	209	2	0	10	−5	79	79	1	5	−6	−4	73	74	1	0	1	−4	239	249	1	−3	9	−4	264	260	6
0	2	−5	113	106	1	1	10	−5	96	100	1	6	−6	−4	41	43	1	1	1	−4	339	346	3	−2	9	−4	89	81	1
1	2	−5	325	328	3	2	10	−5	151	152	2	−5	−5	−4	94	98	2	2	1	−4	32	31	1	−1	9	−4	136	132	1
2	2	−5	302	291	4	3	10	−5	24	28	1	−4	−5	−4	77	79	2	4	1	−4	206	218	2	0	9	−4	43	45	1
4	2	−5	82	83	1	4	10	−5	80	98	1	−3	−5	−4	46	47	1	5	1	−4	87	75	1	1	9	−4	186	179	1
5	2	−5	173	177	2	5	10	−5	76	76	1	−2	−5	−4	136	132	2	6	1	−4	64	65	1	2	9	−4	175	172	1
6	2	−5	80	82	1	−3	11	−5	85	86	2	−1	−5	−4	142	142	2	7	1	−4	72	77	1	3	9	−4	139	140	1
7	2	−5	55	54	1	−2	11	−5	121	124	2	0	−5	−4	110	111	1	−7	2	−4	35	32	2	4	9	−4	81	80	1
−6	3	−5	198	190	4	−1	11	−5	90	95	2	1	−5	−4	173	178	2	−6	2	−4	14	14	5	−3	10	−4	78	76	2
−5	3	−5	35	36	2	0	11	−5	70	73	1	2	−5	−4	135	138	1	−5	2	−4	167	163	2	−2	10	−4	68	63	1
−4	3	−5	95	89	1	1	11	−5	54	56	1	3	−5	−4	56	57	1	−4	2	−4	95	96	1	−1	10	−4	47	46	1
−3	3	−5	118	117	1	2	11	−5	96	95	1	4	−5	−4	36	36	1	−3	2	−4	252	258	3	0	10	−4	95	90	1
−2	3	−5	237	231	3	3	11	−5	82	85	1	5	−5	−4	37	35	1	−2	2	−4	329	324	4	1	10	−4	43	41	1
−1	3	−5	496	510	4	4	11	−5	37	36	1	6	−5	−4	51	47	1	−1	2	−4	130	133	1	2	10	−4	114	114	1
0	3	−5	219	210	1	−3	12	−5	51	52	2	−5	−4	−4	19	20	4	0	2	−4	315	325	2	3	10	−4	93	94	1
1	3	−5	175	176	1	−2	12	−5	100	100	2	−4	−4	−4	62	64	2	1	2	−4	560	572	5	4	10	−4	82	81	1
2	3	−5	224	220	3	−1	12	−5	59	61	1	−3	−4	−4	89	92	1	2	2	−4	143	152	2	5	10	−4	27	27	1
3	3	−5	59	56	1	0	12	−5	62	60	1	−2	−4	−4	48	43	1	4	2	−4	164	154	2	−3	11	−4	137	135	3
4	3	−5	74	71	1	1	12	−5	27	26	1	−1	−4	−4	129	131	1	5	2	−4	177	178	2	−2	11	−4	25	26	2
5	3	−5	53	53	1	2	12	−5	137	136	3	0	−4	−4	325	314	4	6	2	−4	76	85	2	−1	11	−4	93	90	2
6	3	−5	69	81	2	3	12	−5	49	53	2	1	−4	−4	140	136	1	−7	3	−4	37	36	2	0	11	−4	58	72	2
−6	4	−5	68	62	2	4	12	−5	45	46	2	2	−4	−4	58	50	1	−6	3	−4	45	45	2	1	11	−4	196	199	2
2	11	−4	145	145	2	3	−5	−3	121	118	1	6	2	−3	87	107	2	3	10	−3	15	16	2	2	−6	−2	174	179	1
3	11	−4	52	49	2	4	−5	−3	70	76	1	7	3	−3	0	8	1	4	10	−3	75	72	1	3	−6	−2	96	89	1
4	11	−4	29	32	1	5	−5	−3	43	46	1	−6	3	−3	50	49	2	5	10	−3	59	59	1	4	−6	−2	141	148	1
−3	12	−4	16	14	5	6	−5	−3	26	25	2	−5	3	−3	55	57	1	−3	11	−3	71	71	2	5	−6	−2	40	47	1
−2	12	−4	91	90	2	−3	−4	−3	19	22	3	−4	3	−3	127	124	2	−2	11	−3	85	82	1	6	−6	−2	60	56	1
−1	12	−4	48	47	1	−2	−4	−3	183	168	2	−3	3	−3	84	75	2	−1	11	−3	52	55	1	−2	−5	−2	99	92	1
0	12	−4	57	59	1	−1	−4	−3	136	145	1	−2	3	−3	89	84	2	0	11	−3	77	79	1	−1	−5	−2	277	268	4
1	12	−4	43	44	1	0	−4	−3	127	123	2	−1	3	−3	279	295	3	1	11	−3	81	78	1	0	−5	−2	94	96	1
2	12	−4	101	100	1	1	−4	−3	208	213	2	0	3	−3	320	320	3	2	11	−3	116	113	2	1	−5	−2	31	27	1
3	12	−4	160	164	4	2	−4	−3	351	355	5	1	3	−3	259	259	2	3	11	−3	175	179	4	2	−5	−2	237	239	2
−3	13	−4	55	55	2	3	−4	−3	73	72	1	3	3	−3	44	38	2	4	11	−3	24	23	1	3	−5	−2	45	48	1
−2	13	−4	90	89	1	4	−4	−3	125	122	1	4	3	−3	58	59	1	−4	12	−3	53	52	2	4	−5	−2	143	147	1
−1	13	−4	77	79	1	5	−4	−3	52	58	1	5	3	−3	176	181	4	−3	12	−3	21	24	4	5	−5	−2	112	120	1
0	13	−4	58	56	1	6	−4	−3	68	70	1	6	3	−3	154	171	3	−2	12	−3	93	94	2	6	−5	−2	29	26	2
1	13	−4	55	55	1	7	−4	−3	50	52	2	−7	4	−3	33	33	2	−1	12	−3	60	62	1	−2	−4	−2	338	315	5

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	13	−4	47	48	2	−3	−3	−3	181	177	4	−6	4	−3	53	48	2	0	12	−3	42	47	1	−1	−4	−2	221	222	2
−2	14	−4	46	49	1	−2	−3	−3	175	171	2	−5	4	−3	28	29	2	1	12	−3	55	53	1	0	−4	−2	174	176	2
−1	14	−4	41	39	1	−1	−3	−3	84	78	1	−4	4	−3	197	191	3	2	12	−3	71	70	1	1	−4	−2	103	101	1
0	14	−4	11	10	2	0	−3	−3	533	535	6	−3	4	−3	106	101	1	3	12	−3	104	109	2	2	−4	−2	230	210	4
1	14	−4	56	57	2	1	−3	−3	101	99	1	−2	4	−3	142	145	3	−3	13	−3	72	71	2	3	−4	−2	147	148	1
−2	−12	−3	71	68	2	2	−3	−3	242	237	3	−1	4	−3	111	117	1	−2	13	−3	49	45	1	4	−4	−2	83	81	1
−1	−12	−3	85	83	2	3	−3	−3	280	275	2	0	4	−3	134	139	1	−1	13	−3	3	12	2	5	−4	−2	65	66	1
1	−12	−3	39	38	3	4	−3	−3	19	22	1	1	4	−3	178	170	1	0	13	−3	20	22	1	6	−4	−2	76	75	1
−3	−11	−3	24	22	2	5	−3	−3	124	122	1	3	4	−3	91	89	1	1	13	−3	17	18	1	7	−4	−2	114	113	3
−2	−11	−3	38	34	2	6	−3	−3	79	81	1	4	4	−3	39	42	1	2	13	−3	64	61	2	−3	−3	−2	82	78	2
−1	−11	−3	60	60	2	7	−3	−3	138	125	3	5	4	−3	246	241	5	−2	14	−3	63	62	2	−2	−3	−2	311	313	6
0	−11	−3	29	26	2	−3	−2	−3	196	202	3	6	4	−3	123	112	3	−1	14	−3	33	34	1	−1	−3	−2	309	295	3
1	−11	−3	67	68	3	−2	−2	−3	322	335	5	−7	5	−3	27	22	2	0	14	−3	34	30	1	0	−3	−2	116	120	1
2	−11	−3	121	118	2	−1	−2	−3	126	119	1	−6	5	−3	148	140	3	1	14	−3	91	93	2	1	−3	−2	190	186	1
3	−11	−3	25	18	2	0	−2	−3	706	721	7	−5	5	−3	103	126	3	−2	−12	−2	54	53	2	2	−3	−2	40	39	1
4	−11	−3	34	40	2	1	−2	−3	101	104	1	−4	5	−3	119	113	2	−1	−12	−2	68	65	2	3	−3	−2	209	203	2
−4	−10	−3	71	70	2	2	−2	−3	443	435	4	−3	5	−3	45	43	1	0	−12	−2	70	71	1	4	−3	−2	126	123	1
−3	−10	−3	43	38	2	3	−2	−3	153	145	1	−2	5	−3	169	171	2	1	−12	−2	49	48	3	5	−3	−2	47	44	1
−2	−10	−3	22	19	3	4	−2	−3	198	203	1	−1	5	−3	206	201	4	2	−12	−2	43	41	2	6	−3	−2	67	67	1
−1	−10	−3	63	65	2	5	−2	−3	61	60	1	0	5	−3	92	91	1	3	−12	−2	39	37	1	7	−3	−2	55	55	2
0	−10	−3	45	38	2	6	−2	−3	21	20	1	1	5	−3	385	374	4	−3	−11	−2	28	27	2	−3	−2	−2	314	315	6
1	−10	−3	28	23	4	−3	−1	−3	121	124	2	3	5	−3	205	195	3	−2	−11	−2	85	81	2	−2	−2	−2	399	379	6
2	−10	−3	123	119	2	−2	−1	−3	229	233	2	4	5	−3	43	39	2	−1	−11	−2	135	133	3	−1	−2	−2	430	439	5
3	−10	−3	94	95	2	−1	−1	−3	248	259	3	5	5	−3	161	157	3	0	−11	−2	56	53	2	0	−2	−2	168	169	2
4	−10	−3	22	22	2	0	−1	−3	538	566	5	−6	6	−3	44	42	2	1	−11	−2	57	56	3	1	−2	−2	624	638	5
−4	−9	−3	83	80	2	1	−1	−3	385	400	3	−5	6	−3	32	37	2	2	−11	−2	50	48	1	2	−2	−2	291	284	2
−3	−9	−3	58	59	2	2	−1	−3	259	257	2	−4	6	−3	186	186	3	3	−11	−2	67	66	1	3	−2	−2	143	142	1
−2	−9	−3	82	83	2	3	−1	−3	366	349	4	−3	6	−3	80	78	1	4	−11	−2	27	26	2	4	−2	−2	95	96	1
−1	−9	−3	89	116	2	4	−1	−3	47	52	1	−2	6	−3	48	50	1	−4	−10	−2	98	102	2	5	−2	−2	188	185	1
0	−9	−3	50	48	2	5	−1	−3	35	33	1	−1	6	−3	391	391	5	−3	−10	−2	79	83	2	6	−2	−2	17	17	1
1	−9	−3	74	77	1	6	−1	−3	141	144	1	0	6	−3	176	170	2	−2	−10	−2	59	59	2	7	−2	−2	20	18	3
2	−9	−3	96	101	2	7	−1	−3	42	40	1	1	6	−3	315	315	3	−1	−10	−2	54	63	2	−3	−1	−2	158	165	4
3	−9	−3	67	66	1	−7	0	3	17	22	4	2	6	−3	160	156	1	0	−10	−2	12	12	6	−2	−1	−2	288	287	4
4	−9	−3	38	37	1	−6	0	−3	16	7	4	3	6	−3	96	104	1	1	−10	−2	61	62	2	−1	−1	−2	422	425	6
5	−9	−3	30	37	1	−4	0	−3	151	151	3	4	6	−3	135	137	3	2	−10	−2	105	102	2	0	−1	−2	605	633	7
−5	−8	−3	28	31	2	−3	0	−3	179	173	2	−6	7	−3	13	12	5	3	−10	−2	91	91	2	1	−1	−2	474	489	4
−4	−8	−3	56	54	2	−2	0	−3	205	208	2	−5	7	−3	40	43	2	4	−10	−2	40	40	1	2	−1	−2	110	105	1
−3	−8	−3	99	103	2	−1	0	−3	179	189	2	−4	7	−3	135	133	2	5	−10	−2	27	26	3	3	−1	−2	121	115	1
−2	−8	−3	76	76	2	0	0	−3	181	191	1	−3	7	−3	128	127	1	−4	−9	−2	75	80	2	4	−1	−2	147	142	1
0	−8	−3	21	14	2	1	0	−3	90	91	1	−2	7	−3	149	152	1	−3	−9	−2	91	96	2	5	−1	−2	36	34	1
1	−8	−3	61	63	1	2	0	−3	98	91	1	−1	7	−3	190	193	2	−1	−9	−2	149	155	4	6	−1	−2	98	102	1
2	−8	−3	96	96	1	3	0	−3	229	225	2	0	7	−3	214	209	2	1	−9	−2	172	178	2	7	−1	−2	14	9	2
3	−8	−3	42	50	1	4	0	−3	209	208	2	1	7	−3	183	192	1	2	−9	−2	61	60	2	−3	0	−2	327	320	5
4	−8	−3	151	183	3	5	0	−3	113	113	1	2	7	−3	80	70	1	3	−9	−2	189	193	3	−2	0	−2	194	195	2
5	−8	−3	63	62	1	6	0	−3	180	178	1	3	7	−3	68	63	1	4	−9	−2	63	62	1	−1	0	−2	283	295	4
−5	−7	−3	22	21	3	7	0	−3	113	111	1	−5	8	−3	38	33	2	5	−9	−2	9	10	5	0	0	−2	448	469	4
−4	−7	−3	43	40	2	−7	1	−3	58	58	2	−4	8	−3	39	39	2	−4	−8	−2	67	72	2	1	0	−2	255	264	2
−3	−7	−3	133	135	3	−6	1	−3	108	101	2	−3	8	−3	139	141	1	−3	−8	−2	41	47	2	2	0	−2	197	198	2
−1	−7	−3	153	152	2	−5	1	−3	138	128	3	−2	8	−3	195	197	2	−2	−8	−2	84	84	1	3	0	−2	53	62	1

TABLE 7-continued

Observed and calculated structure factors for NEL																													
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	−7	−3	136	138	1	−4	1	−3	167	166	2	−1	8	−3	76	80	1	−1	−8	−2	184	182	3	4	0	−2	200	199	2
2	−7	−3	145	144	1	−3	1	−3	119	108	2	0	8	−3	141	129	1	0	−8	−2	57	56	1	5	0	−2	126	125	1
3	−7	−3	79	82	1	−2	1	−3	136	140	1	1	8	−3	52	54	1	1	−8	−2	23	23	1	6	0	−2	49	48	1
4	−7	−3	127	146	2	−1	1	−3	156	169	2	2	8	−3	84	79	1	2	−8	−2	123	120	1	7	0	−2	39	35	1
5	−7	−3	42	47	1	0	1	−3	193	195	1	3	8	−3	168	165	1	3	−8	−2	78	79	1	−7	1	−2	33	37	2
6	−7	−3	58	59	1	1	1	−3	93	95	1	4	8	−3	86	92	1	4	−8	−2	65	72	1	−6	1	−2	65	62	2
−4	−6	−3	178	174	4	2	1	−3	131	133	1	−5	9	−3	72	73	2	5	−8	−2	102	102	1	−5	1	−2	41	42	2
−3	−6	−3	162	164	2	4	1	−3	229	226	2	−4	9	−3	67	71	2	6	−8	−2	78	77	2	−4	1	−2	149	149	3
−2	−6	−3	200	196	3	5	1	−3	98	97	1	−3	9	−3	145	145	3	−4	−7	−2	103	105	2	−3	1	−2	179	168	2
−1	−6	−3	163	164	2	6	1	−3	135	136	1	−2	9	−3	101	100	1	−2	−7	−2	119	122	2	−2	1	−2	97	101	1
0	−6	−3	174	169	1	7	1	−3	56	51	1	−1	9	−3	120	113	1	−1	−7	−2	91	88	1	−1	1	−2	299	306	4
1	−6	−3	111	114	1	−7	2	−3	68	70	2	0	9	−3	255	256	2	0	−7	−2	92	92	1	0	1	−2	381	397	3
2	−6	−3	83	81	1	−6	2	−3	135	129	3	1	9	−3	46	43	1	1	−7	−2	91	86	1	1	1	−2	226	235	2
3	−6	−3	69	71	1	−5	2	−3	154	154	2	2	9	−3	74	74	1	2	−7	−2	29	27	1	2	1	−2	361	374	8
4	−6	−3	41	46	1	−4	2	−3	49	51	1	3	9	−3	42	41	1	3	−7	−2	107	113	1	3	1	−2	69	65	2
5	−6	−3	74	79	1	−3	2	−3	4	4	4	4	9	−3	75	74	1	4	−7	−2	45	48	1	4	1	−2	180	184	1
6	−6	−3	56	55	1	−2	2	−3	160	156	2	5	9	−3	35	36	1	5	−7	−2	78	75	1	5	1	−2	172	172	2
−3	−5	−3	61	60	1	−1	2	−3	458	468	6	−3	10	−3	61	64	2	6	−7	−2	39	39	1	6	1	−2	37	33	1
−2	−5	−3	230	233	3	0	2	−3	143	147	1	−2	10	−3	218	213	3	−3	−6	−2	143	146	3	7	1	−2	64	64	1
−1	−5	−3	115	118	1	1	2	−3	177	183	1	−1	10	−3	139	142	1	−2	−6	−2	133	131	2	−7	2	−2	25	28	3
0	−5	−3	251	244	3	3	2	−3	133	128	3	0	10	−3	29	30	1	−1	−6	−2	19	19	1	−6	2	−2	120	119	3
1	−5	−3	206	202	2	4	2	−3	158	159	2	1	10	−3	230	240	2	0	−6	−2	129	131	1	−5	2	−2	109	99	2
2	−5	−3	231	236	2	5	2	−3	233	227	3	2	10	−3	140	138	2	1	−6	−2	75	74	1	−4	2	−2	53	50	1
−3	2	−2	115	119	2	−4	9	−2	32	35	2	−1	−7	−1	61	62	1	4	1	−1	94	96	1	−5	8	−1	55	54	2
−2	2	−2	228	229	3	−3	9	−2	65	64	1	0	−7	−1	83	86	1	5	1	−1	177	182	2	−4	8	−1	121	116	3
−1	2	−2	436	445	6	−2	9	−2	74	75	1	1	−7	−1	99	100	1	6	1	−1	76	79	1	−3	8	−1	80	77	1
0	2	−2	578	596	5	−1	9	−2	133	129	1	2	−7	−1	109	109	1	7	1	−1	49	44	1	−2	8	−1	61	62	1
1	2	−2	378	390	3	0	9	−2	29	32	1	3	−7	−1	132	134	1	−7	2	−1	94	93	2	−1	8	−1	150	149	1
2	2	−2	191	219	4	1	9	−2	147	145	1	4	−7	−1	130	136	1	−6	2	−1	43	40	2	0	8	−1	108	109	1
3	2	−2	163	164	4	2	9	−2	53	52	1	5	−7	−1	12	13	3	−5	2	−1	218	218	5	1	8	−1	70	73	1
4	2	−2	136	132	1	3	9	−2	80	77	1	6	−7	−1	54	55	1	−4	2	−1	69	71	1	2	8	−1	150	149	1
5	2	−2	32	36	2	4	9	−2	14	9	2	−2	−6	−1	133	142	3	−3	2	−1	237	242	5	3	8	−1	91	95	1
6	2	−2	49	56	2	5	9	−2	80	79	1	−1	−6	−1	70	66	2	−2	2	−1	222	217	2	4	8	−1	126	116	1
7	2	−2	18	13	1	−3	10	−2	65	59	2	0	−6	−1	64	62	1	−1	2	−1	665	679	7	5	8	−1	45	40	1
−7	3	−2	62	59	2	−2	10	−2	182	182	3	1	−6	−1	180	175	2	0	2	−1	273	281	2	−5	9	−1	0	8	1
−6	3	−2	31	30	2	−1	10	−2	88	89	1	2	−6	−1	55	51	1	1	2	−1	600	624	5	−4	9	−1	51	50	2
−5	3	−2	26	23	2	0	10	−2	24	28	1	3	−6	−1	162	158	1	2	2	−1	213	253	5	−3	9	−1	46	47	2
−4	3	−2	154	155	2	1	10	−2	58	60	1	4	−6	−1	117	111	1	3	2	−1	913	392	9	−2	9	−1	98	96	1
−3	3	−2	111	110	2	2	10	−2	96	97	1	5	−6	−1	21	23	1	4	2	−1	133	137	1	−1	9	−1	13	8	2
−2	3	−2	182	183	2	3	10	−2	98	95	1	6	−6	−1	77	71	1	5	2	−1	197	189	4	0	9	−1	149	147	1
−1	3	−2	77	75	1	4	10	−2	32	33	1	−2	−5	−1	153	147	2	6	2	−1	19	19	1	1	9	−1	123	117	1
0	3	−2	68	70	1	5	10	−2	61	55	1	−1	−5	−1	131	137	2	7	2	−1	37	27	1	2	9	−1	188	192	1
1	3	−2	293	307	2	−3	11	−2	92	90	2	0	−5	−1	160	162	2	−7	3	−1	57	54	2	3	9	−1	127	125	1
3	3	−2	194	193	4	−2	11	−2	111	112	2	1	−5	−1	76	77	1	−6	3	−1	62	63	2	4	9	−1	42	45	1
4	3	−2	46	50	1	−1	11	−2	158	163	2	2	−5	−1	164	157	2	−5	3	−1	277	279	4	5	9	−1	70	65	1
5	3	−2	53	55	2	0	11	−2	105	103	2	3	−5	−1	189	173	2	−4	3	−1	76	71	1	−3	10	−1	41	46	3
6	3	−2	52	45	2	1	11	−2	107	109	1	4	−5	−1	127	123	1	−3	3	−1	221	210	4	−2	10	−1	44	38	1
−7	4	−2	30	26	2	2	11	−2	104	104	2	5	−5	−1	35	32	1	−2	3	−1	377	386	4	−1	10	−1	88	91	1
−6	4	−2	130	127	3	3	11	−2	75	75	2	6	−5	−1	134	133	2	−1	3	−1	145	148	1	0	10	−1	20	19	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−5	4	−2	111	116	2	−3	12	−2	69	65	2	−3	−4	−1	25	31	2	0	3	−1	292	296	2	1	10	−1	117	121	1
−4	4	−2	195	194	3	−2	12	−2	102	105	2	−2	−4	−1	213	190	3	1	3	−1	296	295	2	2	10	−1	100	94	1
−3	4	−2	147	150	2	−1	12	−2	43	40	1	−1	−4	−1	155	152	2	2	3	−1	188	198	4	3	10	−1	91	90	2
−2	4	−2	320	304	6	0	12	−2	80	81	1	0	−4	−1	341	354	5	3	3	−1	497	472	11	4	10	−1	18	10	2
−1	4	−2	55	52	1	1	12	−2	39	34	1	1	−4	−1	31	32	1	4	3	−1	65	66	1	−3	11	−1	95	98	3
0	4	−2	208	208	1	2	12	−2	93	96	1	2	−4	−1	476	461	5	5	3	−1	117	116	2	−2	11	−1	59	59	1
1	4	−2	181	186	2	3	12	−2	23	25	2	3	−4	−1	150	148	1	6	3	−1	28	27	2	−1	11	−1	57	60	1
3	4	−2	210	212	3	−3	13	−2	53	54	2	4	−4	−1	57	57	1	7	3	−1	62	61	2	0	11	−1	35	36	1
4	4	−2	33	30	1	−2	13	−2	72	73	1	5	−4	−1	179	179	1	−7	4	−1	26	30	2	1	11	−1	65	68	1
5	4	−2	90	85	2	−1	13	−2	38	42	1	6	−4	−1	87	81	2	−6	4	−1	37	34	2	2	11	−1	90	89	1
6	4	−2	199	197	4	0	13	−2	67	64	1	−3	−3	−1	338	340	7	−5	4	−1	145	147	2	3	11	−1	75	77	2
−7	5	−2	25	28	2	1	13	−2	14	14	1	−2	−3	−1	72	72	1	−4	4	−1	140	142	2	−3	12	−1	55	52	2
−6	5	−2	118	116	3	2	13	−2	96	97	2	−1	−3	−1	421	421	5	−3	4	−1	213	211	3	−2	12	−1	56	59	1
−5	5	−2	86	98	2	−1	14	−2	28	30	1	0	−3	−1	376	382	4	−2	4	−1	226	220	4	−1	12	−1	82	84	1
−4	5	−2	49	50	1	0	14	−2	44	45	1	1	−3	−1	398	401	3	−1	4	−1	58	58	1	0	12	−1	43	45	1
−3	5	−2	103	97	1	1	14	−2	82	83	2	2	−3	−1	63	56	1	0	4	−1	462	464	4	1	12	−1	53	54	1
−2	5	−2	65	61	1	−1	−13	−1	42	42	2	3	−3	−1	339	317	4	1	4	−1	152	147	1	2	12	−1	80	78	2
−1	5	−2	350	355	7	0	−13	−1	101	101	3	4	−3	−1	118	118	1	2	4	−1	160	146	2	3	12	−1	34	35	2
0	5	−2	106	113	1	1	−13	−1	64	64	2	5	−3	−1	130	132	1	3	4	−1	81	77	2	−3	13	−1	51	51	2
1	5	−2	227	219	2	−3	−12	−1	34	37	2	6	−3	−1	70	74	1	4	4	−1	58	53	1	−2	13	−1	23	20	2
2	5	−2	321	322	5	−2	−12	−1	89	88	2	−3	−2	−1	272	260	5	5	4	−1	200	201	4	−1	13	−1	51	51	1
3	5	−2	211	206	3	−1	−12	−1	48	46	2	−2	−2	−1	123	120	2	6	4	−1	18	16	4	0	13	−1	35	35	1
4	5	−2	109	107	2	0	−12	−1	32	29	2	−1	−2	−1	659	682	10	−7	5	−1	10	10	9	1	13	−1	86	83	1
5	5	−2	25	27	2	1	−12	−1	132	130	3	0	−2	−1	808	843	10	−6	5	−1	94	96	2	2	13	−1	167	170	4
6	5	−2	122	113	2	2	−12	−1	164	162	3	1	−2	−1	784	818	6	−5	5	−1	127	132	3	0	14	−1	12	10	2
−6	6	−2	34	33	2	3	−12	−1	42	45	1	2	−2	−1	412	405	3	−4	5	−1	37	37	1	−2	−13	0	83	79	2
−5	6	−2	73	82	2	−3	−11	−1	46	45	2	3	−2	−1	380	360	4	−3	5	−1	287	275	4	−1	−13	0	138	143	3
−4	6	−2	147	148	2	−2	−11	−1	128	130	3	4	−2	−1	133	130	1	−2	5	−1	39	45	1	0	−13	0	77	75	1
−3	6	−2	152	151	2	−1	−11	−1	73	78	2	5	−2	−1	117	112	1	−1	5	−1	137	134	2	1	−13	0	109	110	3
−2	6	−2	105	93	1	0	−11	−1	74	72	2	6	−2	−1	72	72	1	0	5	−1	130	138	1	2	−13	0	105	103	3
−1	6	−2	338	327	5	2	−11	−1	152	153	2	7	−2	−1	7	12	6	1	5	−1	178	179	1	−3	−12	0	29	25	2
0	6	−2	232	232	2	3	−11	−1	114	113	2	−3	−1	−1	151	147	3	2	5	−1	152	141	1	−2	−12	0	47	42	2
1	6	−2	97	96	1	4	−11	−1	11	9	5	−2	−1	−1	121	114	2	3	5	−1	211	205	2	−1	−12	0	255	240	6
2	6	−2	265	270	2	−4	−10	−1	73	77	2	−1	−1	−1	608	629	12	4	5	−1	97	98	2	0	−12	0	64	64	2
3	6	−2	120	115	1	−3	−10	−1	6	8	6	0	−1	−1	146	147	2	5	5	−1	36	26	2	1	−12	0	100	97	3
4	6	−2	98	91	2	1	−10	−1	35	35	2	1	−1	−1	821	845	7	6	5	−1	68	68	2	2	−12	0	121	121	2
5	6	−2	63	63	2	2	−10	−1	57	51	1	2	−1	−1	215	215	1	−6	6	−1	70	72	2	3	−12	0	36	37	1
−6	7	−2	23	18	3	3	−10	−1	21	22	2	3	−1	−1	426	407	4	−5	6	−1	62	67	2	−4	−11	0	44	44	2
−5	7	−2	48	52	2	4	−10	−1	42	43	2	4	−1	−1	48	51	1	−4	6	−1	72	72	1	−3	−11	0	34	31	2
−4	7	−2	135	142	2	5	−10	−1	28	34	2	5	−1	−1	195	195	1	−3	6	−1	174	160	2	1	−11	0	74	74	2
−3	7	−2	81	79	1	−4	−9	−1	79	85	2	6	−1	−1	63	65	1	−2	6	−1	230	224	3	2	−11	0	77	81	2
−2	7	−2	117	116	1	−2	−9	−1	124	122	3	7	−1	−1	11	3	3	−1	6	−1	177	175	2	3	−11	0	95	93	2
−1	7	−2	138	141	1	−1	−9	−1	79	77	1	−3	0	−1	90	92	1	0	6	−1	95	88	1	4	−11	0	21	22	2
0	7	−2	155	152	1	0	−9	−1	146	151	2	−1	0	−1	120	127	2	1	6	−1	26	25	1	−4	−10	0	19	17	3
1	7	−2	49	53	1	1	−9	−1	42	35	2	0	0	−1	76	82	1	2	6	−1	86	81	1	−2	−10	0	57	56	2
2	7	−2	90	96	1	2	−9	−1	178	178	2	1	0	−1	53	54	1	3	6	−1	52	48	1	0	−10	0	76	77	2
3	7	−2	221	221	2	3	−9	−1	28	32	2	2	0	−1	406	401	3	4	6	−1	115	97	1	1	−10	0	241	243	5
4	7	−2	12	12	6	4	−9	−1	129	136	2	3	0	−1	101	98	1	5	6	−1	88	91	2	2	−10	0	104	102	3
−6	8	−2	20	20	3	5	−9	−1	98	97	1	4	0	−1	219	221	2	−6	7	−1	58	52	2	3	−10	0	94	93	2

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−5	8	−2	34	34	2	−3	−8	−1	65	67	2	5	0	−1	136	137	1	−5	7	−1	34	40	2	4	−10	0	92	88	2
−4	8	−2	86	87	2	−2	−8	−1	182	181	3	6	0	−1	38	32	1	−4	7	−1	114	117	2	5	−10	0	24	24	1
−3	8	−2	167	167	2	−1	−8	−1	140	141	2	7	0	−1	20	21	1	−3	7	−1	176	173	3	−3	−9	0	69	70	2
−2	8	−2	84	84	1	0	−8	−1	53	53	1	−7	1	−1	84	79	2	−2	7	−1	107	102	1	−2	−9	0	120	114	3
−1	8	−2	58	60	1	1	−8	−1	61	62	1	−4	1	−1	173	167	4	−1	7	−1	155	159	1	−1	−9	0	76	76	2
0	8	−2	39	41	1	2	−8	−1	131	131	2	−3	1	−1	127	118	2	0	7	−1	139	138	1	0	−9	0	97	95	2
1	8	−2	126	123	1	3	−8	−1	142	143	1	−2	1	−1	458	459	7	1	7	−1	134	136	1	1	−9	0	33	35	1
2	8	−2	181	183	1	4	−8	−1	106	102	2	−1	1	−1	566	583	8	2	7	−1	72	75	1	2	−9	0	52	52	2
3	8	−2	25	21	1	5	−8	−1	86	87	1	0	1	−1	368	385	3	3	7	−1	226	218	2	3	−9	0	45	48	1
4	8	−2	113	114	1	6	−8	−1	65	65	1	1	1	−1	930	924	21	4	7	−1	63	65	1	4	−9	0	87	92	1
5	8	−2	43	38	1	−3	−7	−1	64	74	2	2	1	−1	280	280	6	5	7	−1	25	27	4	5	−9	0	24	19	1
−5	9	−2	29	27	2	−2	−7	−1	91	91	2	3	1	−1	227	201	5	−6	8	−1	35	37	2	−3	−8	0	126	129	3
−2	−8	0	23	24	2	0	1	0	140	148	1	5	7	0	115	114	1	4	−9	1	51	50	1	0	1	1	144	147	1
−1	−8	0	138	136	3	1	1	0	828	873	7	6	7	0	12	6	3	5	−9	1	12	8	3	1	1	1	601	629	5
0	−8	0	47	43	1	2	1	0	225	227	3	−6	8	0	64	66	2	−2	−8	1	148	148	3	2	1	1	125	114	1
1	−8	0	215	216	2	3	1	0	264	260	6	−5	8	0	76	75	2	−1	−8	1	72	74	2	3	1	1	153	146	1
2	−8	0	38	36	1	4	1	0	68	67	1	−4	8	0	13	9	8	0	−8	1	111	109	2	4	1	1	107	111	1
3	−8	0	61	64	1	5	1	0	104	103	1	−3	8	0	61	64	1	1	−8	1	150	150	1	5	1	1	183	181	1
4	−8	0	7	9	6	6	1	0	165	171	1	−2	8	0	41	36	1	2	−8	1	60	62	1	6	1	1	84	81	1
5	−8	0	76	75	1	7	1	0	72	70	1	−1	8	0	215	216	2	3	−8	1	80	76	1	7	1	1	39	37	1
6	−8	0	66	65	1	−7	2	0	66	63	2	0	8	0	47	43	1	4	−8	1	120	117	1	−7	2	1	16	12	4
−2	−7	0	178	176	4	−6	2	0	182	183	4	1	8	0	137	137	1	5	−8	1	53	54	1	−6	2	1	70	72	2
−1	−7	0	224	222	5	−5	2	0	121	119	3	2	8	0	25	24	1	6	−8	1	35	37	1	−5	2	1	112	111	3
0	−7	0	71	74	1	−4	2	0	142	138	2	3	8	0	130	129	1	−2	−7	1	71	76	2	−4	2	1	130	130	3
1	−7	0	164	168	2	−3	2	0	412	403	9	4	8	0	127	125	1	−1	−7	1	136	136	1	−3	2	1	377	360	8
2	−7	0	195	195	2	−2	2	0	270	259	3	5	8	0	66	62	1	0	−7	1	141	138	1	−2	2	1	414	405	5
3	−7	0	125	116	1	−1	2	0	243	250	3	−5	9	0	22	20	3	1	−7	1	157	158	2	−1	2	1	795	818	9
4	−7	0	70	70	1	0	2	0	597	604	5	−4	9	0	89	92	2	2	−7	1	106	102	1	0	2	1	808	842	7
5	−7	0	100	94	1	1	2	0	350	368	3	−3	9	0	46	49	2	3	−7	1	176	173	1	1	2	1	660	682	5
6	−7	0	73	71	1	3	2	0	142	144	3	−2	9	0	54	52	1	4	−7	1	112	117	1	2	2	1	127	120	1
−2	−6	0	143	137	3	4	2	0	80	76	1	−1	9	0	33	35	1	5	−7	1	41	40	1	3	2	1	274	259	6
−1	−6	0	50	52	1	5	2	0	34	30	1	0	9	0	99	95	1	6	−7	1	58	52	1	4	2	1	167	167	2
0	−6	0	65	66	1	6	2	0	76	80	1	1	9	0	77	76	1	−2	−6	1	88	81	1	5	2	1	132	128	1
1	−6	0	111	108	1	7	2	0	60	59	1	2	9	0	114	113	1	−1	−6	1	25	25	1	6	2	1	31	31	1
2	−6	0	142	135	1	−7	3	0	77	74	2	3	9	0	73	70	2	0	−6	1	91	87	1	7	2	1	90	89	1
3	−6	0	69	68	1	−6	3	0	171	167	4	4	9	0	108	105	1	1	−6	1	175	174	2	−7	3	1	67	65	2
4	−6	0	108	106	1	−5	3	0	47	48	1	5	9	0	55	58	1	2	−6	1	229	224	2	−6	3	1	68	74	2
5	−6	0	91	92	1	−4	3	0	44	39	1	−3	10	0	90	93	2	3	−6	1	170	160	1	−5	3	1	126	132	2
6	−6	0	138	136	2	−3	3	0	229	213	5	−2	10	0	107	103	2	4	−6	1	74	72	1	−4	3	1	116	118	2
−2	−5	0	177	166	2	−2	3	0	201	196	2	−1	10	0	239	243	4	5	−6	1	68	67	1	−3	3	1	345	318	7
−1	−5	0	133	132	1	−1	3	0	411	416	5	0	10	0	80	78	1	6	−6	1	67	72	1	−2	3	1	63	56	1
0	−5	0	26	26	1	0	3	0	882	918	7	1	10	0	134	157	2	−2	−5	1	149	140	3	−1	3	1	394	401	4
1	−5	0	161	165	1	1	3	0	295	292	2	2	10	0	58	56	1	−1	−5	1	177	179	2	0	3	1	375	381	3
2	−5	0	94	85	1	2	3	0	201	201	2	3	10	0	102	104	2	0	−5	1	129	138	2	1	3	1	426	422	3
3	−5	0	191	183	2	3	3	0	108	109	3	−3	11	0	95	93	2	1	−5	1	134	133	1	2	3	1	73	71	1
4	−5	0	61	55	1	4	3	0	50	48	1	−2	11	0	80	80	1	3	−5	1	282	276	2	3	3	1	338	340	5
5	−5	0	15	17	2	5	3	0	110	103	2	−1	11	0	72	75	1	4	−5	1	39	38	1	4	3	1	35	30	1
6	−5	0	100	98	2	6	3	0	43	47	1	0	11	0	166	165	3	5	−5	1	131	132	1	5	3	1	146	142	1
−2	−4	0	647	625	10	7	3	0	20	19	1	1	11	0	115	119	1	6	−5	1	94	95	2	6	3	1	38	31	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−1	−4	0	121	120	1	−7	4	0	52	53	2	2	11	0	73	72	1	−2	−4	1	160	147	2	7	3	1	105	102	1
0	−4	0	63	66	1	−6	4	0	133	131	3	3	11	0	35	32	2	−1	−4	1	154	147	1	−7	4	1	71	73	2
1	−4	0	131	134	1	−5	4	0	106	104	2	−3	12	0	35	36	2	0	−4	1	456	464	5	−6	4	1	87	82	2
2	−4	0	348	337	4	−4	4	0	27	29	1	−2	12	0	121	122	2	1	−4	1	57	58	1	−5	4	1	175	179	3
3	−4	0	219	217	2	−3	4	0	220	216	3	−1	12	0	99	98	1	2	−4	1	218	219	2	−4	4	1	57	57	1
4	−4	0	27	29	1	−2	4	0	352	337	7	0	12	0	66	65	1	3	−4	1	207	210	2	−3	4	1	149	147	2
5	−4	0	105	104	1	−1	4	0	130	134	1	1	12	0	247	240	3	4	−4	1	140	142	1	−2	4	1	477	461	10
6	−4	0	134	130	2	0	4	0	65	67	1	2	12	0	44	41	2	5	−4	1	145	147	1	−1	4	1	28	32	1
−2	−3	0	202	200	3	1	4	0	120	120	1	3	12	0	25	25	2	6	−4	1	36	33	1	0	4	1	344	355	2
−1	−3	0	292	291	3	2	4	0	658	625	8	−2	13	0	105	104	2	−2	−3	1	199	197	4	1	4	1	156	151	1
0	−3	0	888	919	9	3	4	0	100	94	2	−1	13	0	110	109	1	−1	−3	1	296	296	3	2	4	1	215	191	2
1	−3	0	407	416	3	4	4	0	101	95	2	0	13	0	78	75	1	0	−3	1	298	297	4	3	4	1	28	31	1
2	−3	0	206	198	2	5	4	0	38	40	1	1	13	0	138	143	2	1	−3	1	142	148	1	4	4	1	146	140	1
3	−3	0	224	213	2	6	4	0	110	116	1	2	13	0	78	79	2	2	−3	1	384	387	3	5	4	1	111	119	1
4	−3	0	45	39	1	−7	5	0	113	103	3	0	−14	1	13	11	8	3	−3	1	215	210	2	6	4	1	19	17	1
5	−3	0	45	48	1	−6	5	0	96	97	2	1	−14	1	57	62	2	4	−3	1	77	71	1	−7	5	1	67	69	2
6	−3	0	172	167	2	−5	5	0	11	18	7	−2	−13	1	172	170	4	5	−3	1	277	280	2	−6	5	1	133	133	3
7	−3	0	74	74	2	−4	5	0	59	55	1	−1	−13	1	89	83	2	6	−3	1	60	63	1	−5	5	1	33	32	2
0	−2	0	599	604	7	−3	5	0	195	183	3	0	−13	1	36	35	2	7	−3	1	58	54	2	−4	5	1	126	123	2
1	−2	0	242	250	2	−2	5	0	91	84	2	1	−13	1	54	51	3	−1	−2	1	590	624	14	−3	5	1	193	173	3
2	−2	0	271	260	2	−1	5	0	167	166	2	2	−13	1	19	20	5	0	−2	1	−281	281	3	−2	5	1	165	157	2
3	−2	0	413	402	4	0	5	0	26	26	1	3	−13	1	48	50	2	1	−2	1	642	679	6	−1	5	1	77	78	1
4	−2	0	146	138	1	1	5	0	135	133	1	−3	−12	1	35	35	2	2	−2	1	220	217	2	0	5	1	159	161	1
5	−2	0	124	119	1	2	5	0	178	166	2	−1	−12	1	53	54	2	3	−2	1	239	241	2	1	5	1	133	138	1
6	−2	0	185	184	1	3	5	0	90	79	1	2	−12	1	57	59	1	4	−2	1	69	72	1	2	5	1	153	147	1
7	−2	0	63	63	2	4	5	0	106	107	1	3	−12	1	55	53	1	5	−2	1	220	218	2	3	5	1	19	13	1
−3	−1	0	263	260	3	5	5	0	58	58	1	4	−12	1	53	51	1	6	−2	1	40	39	1	4	5	1	119	123	1
−2	−1	0	224	227	4	6	5	0	48	56	1	−4	−11	1	18	22	3	7	−2	1	92	94	2	5	5	1	54	54	1
−1	−1	0	761	873	18	−6	6	0	143	136	3	−2	−11	1	91	89	2	0	−1	1	377	385	8	6	5	1	54	52	1
0	−1	0	138	148	1	−4	6	0	106	105	2	−1	−11	1	57	68	2	1	−1	1	556	583	5	−6	6	1	81	72	2
1	−1	0	787	821	7	−3	6	0	68	68	1	0	−11	1	37	36	2	2	−1	1	458	459	4	−5	6	1	15	23	4
2	−1	0	307	298	2	−2	6	0	142	135	2	2	−11	1	57	60	2	3	−1	1	126	118	1	−4	6	1	116	111	2
3	−1	0	219	217	2	−1	6	0	113	108	1	3	−11	1	98	98	2	4	−1	1	176	167	1	−3	6	1	163	158	2
4	−1	0	62	60	1	0	6	0	67	65	1	4	−11	1	59	56	1	5	−1	1	243	241	2	−2	6	1	57	52	1
5	−1	0	108	105	1	1	6	0	51	52	1	−4	−10	1	12	10	9	6	−1	1	126	121	1	−1	6	1	182	175	2
6	−1	0	44	45	1	2	6	0	142	136	1	−3	−10	1	89	90	2	7	−1	1	86	80	2	0	6	1	66	63	1
7	−1	0	38	43	1	3	6	0	180	177	1	−2	−10	1	101	94	2	−3	0	1	98	98	2	1	6	1	71	66	1
−3	0	0	118	117	2	4	6	0	125	133	1	−1	−10	1	116	121	3	−2	0	1	411	402	8	2	6	1	138	143	1
−2	0	0	348	341	7	5	6	0	28	33	1	0	−10	1	17	18	3	−1	0	1	52	55	1	3	6	1	23	19	1
−1	0	0	126	133	2	6	6	0	28	18	1	1	−10	1	87	92	1	0	0	1	76	82	1	4	6	1	115	120	1
1	0	0	127	132	1	−6	7	0	71	71	2	2	−10	1	44	38	2	1	0	1	123	127	1	5	6	1	6	8	6
2	0	0	344	341	3	−4	7	0	69	71	2	3	−10	1	47	46	1	2	0	1	195	197	2	6	6	1	27	27	1
3	0	0	119	117	1	−3	7	0	125	117	2	4	−10	1	106	103	2	3	0	1	92	93	1	−6	7	1	53	55	2
4	0	0	307	302	3	−2	7	0	196	196	2	5	−10	1	6	5	6	4	0	1	146	146	1	−5	7	1	0	14	1
5	0	0	12	8	2	−1	7	0	165	168	1	−3	−9	1	124	125	3	5	0	1	74	78	1	−4	7	1	130	135	3
6	0	0	45	38	1	0	7	0	71	74	1	−1	−9	1	123	117	3	6	0	1	94	91	1	−3	7	1	135	134	2
7	0	0	64	63	1	1	7	0	219	222	2	0	−9	1	143	147	2	7	0	1	96	91	1	−2	7	1	110	110	1
−3	1	0	214	218	5	2	7	0	184	177	1	1	−9	1	14	8	3	−3	1	1	420	408	9	−1	7	1	99	101	1
−2	1	0	304	297	3	3	7	0	88	88	1	2	−9	1	97	95	2	−2	1	1	212	214	2	0	7	1	83	86	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−1	1	0	792	821	9	4	7	0	68	72	1	3	−9	1	47	46	1	−1	1	1	814	844	9	1	7	1	61	62	1
2	7	1	92	91	1	2	−9	2	73	75	1	7	0	2	60	64	1	0	7	2	90	92	1	2	−9	3	99	100	2
3	7	1	68	74	1	3	−9	2	69	64	1	−3	1	2	117	115	2	1	7	2	91	88	1	3	−9	3	146	144	2
4	7	1	71	74	1	4	−9	2	37	36	1	−2	1	2	110	105	1	2	7	2	120	121	1	4	−9	3	69	70	1
5	7	1	63	60	1	5	−9	2	29	27	1	−1	1	2	479	489	5	3	7	2	101	103	1	5	−9	3	73	74	1
6	7	1	66	69	1	−2	−8	2	179	183	3	0	1	2	604	633	5	4	7	2	103	105	1	−2	−8	3	80	78	1
−5	8	1	83	87	2	−1	−8	2	123	123	2	1	1	2	417	426	3	5	7	2	63	65	1	−1	−8	3	53	55	1
−4	8	1	107	101	3	0	−8	2	38	41	1	2	1	2	295	287	3	−5	8	2	101	102	2	0	−8	3	142	129	2
−3	8	1	140	142	2	1	−8	2	59	61	1	3	1	2	167	165	1	−4	8	2	75	72	2	1	−8	3	74	80	1
−2	8	1	130	131	1	2	−8	2	86	84	1	4	1	2	182	181	1	−3	8	2	80	80	1	2	−8	3	194	196	2
−1	8	1	60	62	1	3	−8	2	170	167	1	5	1	2	31	30	1	−2	8	2	124	120	1	3	−8	3	142	142	1
0	8	1	52	53	1	4	−8	2	85	88	1	6	1	2	112	107	1	−1	8	2	20	23	1	4	−8	3	37	39	1
1	8	1	137	141	1	5	−8	2	33	33	1	7	1	2	51	52	1	0	8	2	57	56	1	5	−8	3	37	33	1
2	8	1	181	181	1	6	−8	2	25	20	2	−7	2	2	25	18	3	1	8	2	184	182	2	6	−8	3	48	61	1
3	8	1	67	67	1	−2	−7	2	93	95	2	−6	2	2	17	17	4	2	8	2	83	83	1	−1	−7	3	188	192	4
4	8	1	152	162	1	−1	−7	2	46	52	2	−5	2	2	185	186	4	3	8	2	41	46	1	0	−7	3	215	209	3
5	8	1	4	4	3	0	−7	2	154	152	2	−4	2	2	93	96	1	4	8	2	69	72	2	1	−7	3	192	194	2
−5	9	1	95	97	2	1	−7	2	139	142	1	−3	2	2	140	142	3	5	8	2	81	82	1	2	−7	3	148	151	1
−4	9	1	133	135	3	2	−7	2	116	116	1	−2	2	2	292	283	3	−5	9	2	3	10	3	3	−7	3	128	128	1
−3	9	1	33	33	2	3	−7	2	82	79	1	−1	2	2	630	638	7	−4	9	2	62	62	2	4	−7	3	137	133	1
−2	9	1	178	179	2	4	−7	2	140	142	1	0	2	2	169	169	1	−3	9	2	190	193	4	5	−7	3	43	43	1
−1	9	1	36	34	1	5	−7	2	55	52	1	1	2	2	430	439	3	−2	9	2	60	60	1	6	−7	3	10	11	2
0	9	1	150	151	1	6	−7	2	11	17	1	2	2	2	403	380	4	−1	9	2	175	177	2	−1	−6	3	320	315	7
1	9	1	80	78	1	−1	−6	2	97	96	2	3	2	2	324	316	4	0	9	2	65	64	1	0	−6	3	170	171	2
2	9	1	120	122	1	0	−6	2	232	231	3	4	2	2	44	46	1	1	9	2	153	155	2	1	−6	3	383	392	4
3	9	1	85	90	2	1	−6	2	333	327	4	5	2	2	60	57	1	2	9	2	64	65	1	2	−6	3	47	51	1
5	9	1	75	77	1	2	−6	2	106	94	1	6	2	2	119	119	1	3	9	2	90	96	1	3	−6	3	79	78	1
−3	10	1	26	23	3	3	−6	2	151	151	1	7	2	2	59	55	1	−3	10	2	89	91	2	4	−6	3	186	185	2
−2	10	1	58	51	1	4	−6	2	150	148	1	−7	3	2	54	55	2	−2	10	2	104	102	2	5	−6	3	35	37	1
−1	10	1	29	35	1	5	−6	2	81	82	1	−6	3	2	65	67	2	−1	10	2	59	62	1	6	−6	3	43	42	2
0	10	1	100	121	2	6	−6	2	35	33	2	−5	3	2	47	44	1	0	10	2	14	12	3	−1	−5	3	381	374	8
1	10	1	119	124	1	−1	−5	2	225	220	3	−4	3	2	126	123	2	1	10	2	62	63	1	0	−5	3	90	91	1
2	10	1	55	53	1	0	−5	2	107	113	1	−3	3	2	213	202	4	2	10	2	61	59	1	1	−5	3	202	201	3
3	10	1	8	8	7	1	−5	2	363	354	5	−2	3	2	40	40	1	3	10	2	81	84	2	2	−5	3	175	171	2
−3	11	1	114	114	3	2	−5	2	68	61	1	−1	3	2	191	186	2	−3	11	2	66	66	2	3	−5	3	43	43	1
−2	11	1	152	153	2	3	−5	2	101	97	1	0	3	2	115	119	1	−2	11	2	51	48	1	4	−5	3	119	114	1
−1	11	1	168	164	3	4	−5	2	51	50	1	1	3	2	307	295	2	−1	11	2	56	57	1	5	−5	3	115	126	2
0	11	1	72	72	1	5	−5	2	99	98	1	2	3	2	317	314	3	0	11	2	56	53	1	6	−5	3	144	140	2
1	11	1	82	78	1	6	−5	2	116	115	2	3	3	2	84	78	1	1	11	2	133	133	1	−3	−4	3	89	89	2
2	11	1	124	130	2	−3	−4	2	210	211	5	4	3	2	26	24	1	2	11	2	83	81	1	−2	−4	3	283	270	6
3	11	1	44	46	2	−2	−4	2	232	232	5	5	3	2	57	55	1	3	11	2	25	27	2	−1	−4	3	177	170	2
−3	12	1	47	45	2	−1	−4	2	178	186	2	6	3	2	68	68	1	−3	12	2	42	37	2	0	−4	3	138	139	2
−2	12	1	164	162	2	0	−4	2	211	208	3	−7	4	2	114	113	3	−2	12	2	47	41	1	1	−4	3	109	118	1
−1	12	1	131	129	2	1	−4	2	53	52	1	−6	4	2	76	75	2	−1	12	2	50	49	1	2	−4	3	141	146	1
0	12	1	28	29	1	2	−4	2	314	304	3	−5	4	2	67	66	2	0	12	2	76	72	1	3	−4	3	105	101	1
1	12	1	47	46	1	3	−4	2	149	150	1	−4	4	2	81	82	1	1	12	2	70	65	1	4	−4	3	194	190	2
2	12	1	90	89	2	4	−4	2	195	194	2	−3	4	2	145	147	2	2	12	2	55	54	2	5	−4	3	28	30	1
−2	13	1	105	105	2	5	−4	2	113	117	1	−2	4	2	230	210	5	−1	13	2	76	76	2	6	−4	3	52	48	1
−1	13	1	66	64	1	6	−4	2	131	127	2	−1	4	2	102	101	1	0	13	2	108	109	2	7	−4	3	29	32	2

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	13	1	102	102	1	7	−4	2	28	26	2	0	4	2	176	176	1	−1	−14	3	94	93	2	−3	−3	3	38	38	2
1	13	1	41	43	2	−3	−3	2	197	194	4	1	4	2	222	221	2	0	−14	3	34	30	2	−2	−3	3	99	93	2
−1	−14	2	85	83	2	−1	−3	2	296	307	4	2	4	2	338	315	3	1	−14	3	35	34	2	−1	−3	3	251	259	4
0	−14	2	45	45	2	0	−3	2	69	70	1	3	4	2	96	94	1	2	−14	3	60	62	2	0	−3	3	320	319	5
1	−14	2	29	30	3	1	−3	2	73	74	1	4	4	2	79	77	1	−3	−13	3	31	32	2	1	−3	3	285	295	3
−2	−13	2	99	97	2	2	−3	2	188	184	1	5	4	2	91	92	1	−2	−13	3	65	61	2	2	−3	3	88	84	1
0	−13	2	68	64	2	3	−3	2	107	111	1	6	4	2	69	63	1	−1	−13	3	20	18	3	3	−3	3	78	75	1
1	−13	2	41	42	3	4	−3	2	154	154	1	−6	5	2	29	26	2	0	−13	3	19	22	3	4	−3	3	124	124	1
2	−13	2	73	73	2	5	−3	2	27	23	1	−5	5	2	105	120	3	2	−13	3	44	45	3	5	−3	3	55	57	1
3	−13	2	54	54	1	6	−3	2	35	29	1	−4	5	2	142	147	2	3	−13	3	73	72	1	6	−3	3	51	48	1
−3	−12	2	26	25	2	7	−3	2	58	59	2	−3	5	2	45	47	1	−3	−12	3	106	108	2	7	−3	3	8	8	6
−2	−12	2	97	96	2	−1	−2	2	365	390	9	−2	5	2	240	239	3	−2	−12	3	73	71	2	−2	−2	3	207	210	5
−1	−12	2	38	35	2	0	−2	2	596	596	8	−1	5	2	29	26	1	−1	−12	3	50	53	2	−1	−2	3	174	183	2
0	−12	2	83	81	2	1	−2	2	430	446	4	0	5	2	92	96	1	0	−12	3	45	47	2	0	−2	3	144	147	2
2	−12	2	103	105	2	2	−2	2	224	227	2	1	5	2	275	268	2	1	−12	3	63	62	2	1	−2	3	446	467	4
3	−12	2	65	64	1	3	−2	2	112	118	1	2	5	2	100	92	1	2	−12	3	92	93	2	2	−2	3	156	155	1
4	−12	2	53	52	1	4	−2	2	53	50	1	3	5	2	57	56	1	3	−12	3	26	25	2	3	−2	3	6	4	3
−4	−11	2	53	54	2	5	−2	2	106	99	1	4	5	2	90	86	1	4	−12	3	56	52	2	4	−2	3	48	52	1
−3	−11	2	74	75	2	6	−2	2	115	119	2	5	5	2	78	83	1	−3	−11	3	172	179	4	5	−2	3	154	154	2
−2	−11	2	106	104	2	7	−2	2	29	28	2	6	5	2	30	29	1	−2	−11	3	116	113	3	6	−2	3	128	129	2
−1	−11	2	93	109	3	−1	−1	2	223	236	4	−6	6	2	58	57	2	−1	−11	3	73	77	2	7	−2	3	66	70	2
0	−11	2	95	104	3	0	−1	2	377	397	4	−5	6	2	35	47	2	0	−11	3	68	78	2	−2	−1	3	136	133	2
1	−11	2	156	163	4	1	−1	2	295	306	2	−4	6	2	139	148	2	1	−11	3	54	55	2	−1	−1	3	90	94	1
2	−11	2	110	112	3	2	−1	2	96	100	1	−3	6	2	100	90	1	2	−11	3	89	82	2	0	−1	3	190	195	2
3	−11	2	95	91	2	3	−1	2	179	168	1	−2	6	2	176	178	2	3	−11	3	73	71	2	1	−1	3	158	169	1
4	−11	2	52	53	1	4	−1	2	149	149	1	−1	6	2	75	74	1	4	−11	3	9	5	9	2	−1	3	132	139	1
−3	−10	2	97	96	2	5	−1	2	44	43	1	0	6	2	129	131	1	−3	−10	3	13	16	6	3	−1	3	120	108	1
−2	−10	2	94	97	2	6	−1	2	64	62	1	1	6	2	18	19	1	−2	−10	3	140	138	3	4	−1	3	168	166	1
−1	−10	2	57	60	2	7	−1	2	38	37	2	2	6	2	133	130	1	−1	−10	3	235	240	5	5	−1	3	136	128	1
0	−10	2	25	28	2	−3	0	2	52	61	1	3	6	2	145	146	1	0	−10	3	27	30	2	6	−1	3	101	101	2
1	−10	2	89	90	1	−2	0	2	191	198	4	4	6	2	56	57	1	1	−10	3	140	142	2	7	−1	3	61	58	2
2	−10	2	182	182	4	−1	0	2	253	265	3	5	6	2	12	11	3	2	−10	3	216	213	5	−2	0	3	96	91	1
3	−10	2	61	59	1	0	0	2	450	469	4	6	6	2	57	56	1	3	−10	3	65	64	1	−1	0	3	90	92	1
4	−10	2	84	80	2	1	0	2	284	295	3	−6	7	2	35	39	2	4	−10	3	40	38	2	0	0	3	182	191	1
5	−10	2	57	55	1	2	0	2	195	195	1	−5	7	2	78	75	2	5	−10	3	37	38	1	1	0	3	178	189	1
−2	−9	2	52	52	1	3	0	2	326	319	3	−4	7	2	48	48	2	−2	−9	3	74	74	1	2	0	3	207	207	1
−1	−9	2	147	145	2	4	0	2	173	165	1	−3	7	2	110	113	2	−1	−9	3	48	43	1	3	0	3	179	173	2
0	−9	2	28	31	2	5	0	2	90	83	1	−2	7	2	28	28	1	0	−9	3	251	256	4	4	0	3	154	150	1
1	−9	2	132	129	3	6	0	2	114	115	1	−1	7	2	89	85	1	1	−9	3	120	114	3	5	0	3	100	101	1
6	0	3	11	7	2	1	7	3	151	152	1	5	−8	4	81	76	1	6	1	4	24	21	1	−1	9	4	73	70	1
7	0	3	23	21	3	2	7	3	100	95	1	6	−8	4	26	29	1	−7	2	4	94	98	2	0	9	4	26	29	1
−3	1	3	357	349	8	3	7	3	135	135	2	−1	−7	4	176	171	4	−6	2	4	54	52	2	1	9	4	82	87	2
−2	1	3	258	256	3	4	7	3	44	41	2	0	−7	4	349	334	4	−5	2	4	146	145	3	2	9	4	118	117	1
−1	1	3	391	401	4	5	7	3	28	21	1	1	−7	4	357	355	4	−4	2	4	28	29	1	3	9	4	59	62	1
0	1	3	544	566	4	−5	8	3	60	62	2	2	−7	4	84	82	1	−3	2	4	151	152	3	4	9	4	46	57	1
1	1	3	244	258	2	−4	8	3	180	184	3	3	−7	4	300	302	3	−2	2	4	248	247	3	−3	10	4	59	58	2
2	1	3	230	232	2	−3	8	3	46	50	1	4	−7	4	72	73	1	−1	2	4	31	23	1	−2	10	4	29	28	2
3	1	3	123	123	1	−2	8	3	95	95	1	5	−7	4	87	88	2	0	2	4	290	292	2	−1	10	4	70	68	1
4	1	3	26	20	1	−1	8	3	63	63	1	6	−7	4	105	115	2	1	2	4	165	159	1	0	10	4	218	211	3

TABLE 7-continued

Observed and calculated structure factors for NEL																													
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	1	3	94	94	1	0	8	3	19	14	1	−1	−6	4	7	10	7	2	2	4	155	152	1	1	10	4	59	57	1
6	1	3	73	72	1	1	8	3	184	190	2	0	−6	4	398	389	6	3	2	4	69	70	1	2	10	4	47	49	1
7	1	3	23	23	2	2	8	3	74	76	1	1	−6	4	165	170	2	4	2	4	130	122	1	3	10	4	119	117	3
−7	2	3	49	55	2	3	8	3	100	103	1	2	−6	4	71	79	1	5	2	4	186	190	1	−3	11	4	90	92	2
−6	2	3	14	20	5	4	8	3	57	54	2	3	−6	4	147	146	1	6	2	4	83	85	1	−2	11	4	39	36	1
−5	2	3	62	61	2	−3	9	3	69	66	2	4	−6	4	146	138	1	−7	3	4	48	46	2	−1	11	4	72	69	1
−4	2	3	197	203	3	−2	9	3	97	101	2	5	−6	4	82	79	1	−6	3	4	47	50	2	0	11	4	93	87	1
−3	2	3	153	145	3	−1	9	3	77	77	1	6	−6	4	10	13	7	−5	3	4	36	35	2	1	11	4	129	126	1
−2	2	3	443	434	5	0	9	3	44	48	1	−1	−5	4	284	283	6	−4	3	4	54	55	1	2	11	4	41	40	2
−1	2	3	101	103	1	1	9	3	94	116	2	0	−5	4	231	230	5	−3	3	4	96	89	1	−2	12	4	56	59	2
0	2	3	692	721	5	2	9	3	88	84	1	1	−5	4	153	153	2	−2	3	4	94	87	1	−1	12	4	66	64	1
1	2	3	127	119	1	3	9	3	54	59	1	2	−5	4	90	93	1	−1	3	4	333	325	4	0	12	4	36	36	1
2	2	3	331	334	3	−3	10	3	94	96	2	3	−5	4	154	154	1	0	3	4	312	314	3	1	12	4	61	66	2
3	2	3	199	202	1	−2	10	3	123	119	2	4	−5	4	15	13	2	1	3	4	345	337	4	−2	−14	5	66	63	1
4	2	3	131	131	1	−1	10	3	23	23	1	5	−5	4	78	83	1	2	3	4	140	135	1	−1	−14	5	37	38	2
5	2	3	89	88	1	0	10	3	43	38	1	6	−5	4	31	31	2	3	3	4	84	87	1	0	−14	5	58	55	2
6	2	3	38	38	1	1	10	3	69	65	1	−3	−4	4	146	158	3	4	3	4	51	50	1	1	−14	5	42	44	2
−7	3	3	136	125	3	2	10	3	20	19	1	−2	−4	4	115	111	3	5	3	4	167	170	1	2	−14	5	72	70	2
−6	3	3	76	81	2	3	10	3	43	38	2	−1	−4	4	151	159	2	6	3	4	30	30	1	−3	−13	5	85	87	2
−5	3	3	122	123	2	−3	11	3	24	18	3	0	−4	4	223	221	3	−6	4	4	58	59	2	−2	−13	5	38	39	2
−4	3	3	21	22	2	−2	11	3	122	118	2	1	−4	4	287	295	3	−5	4	4	71	72	2	−1	−13	5	51	52	2
−3	3	3	280	276	4	−1	11	3	68	67	1	2	−4	4	163	166	2	−4	4	4	52	52	1	0	−13	5	80	78	2
−2	3	3	237	237	3	0	11	3	29	26	1	3	−4	4	55	57	1	−3	4	4	169	166	2	1	−13	5	38	39	2
−1	3	3	99	99	1	1	11	3	59	59	1	4	−4	4	110	115	1	−2	4	4	58	51	1	2	−13	5	44	45	3
0	3	3	524	535	4	2	11	3	37	33	1	5	−4	4	144	146	2	−1	4	4	139	136	2	3	−13	5	115	113	3
1	3	3	84	77	1	3	11	3	22	22	3	6	−4	4	77	79	1	0	4	4	315	314	3	−3	−12	5	52	54	2
2	3	3	179	172	1	−2	12	3	125	121	3	−3	−3	4	105	109	2	1	4	4	128	131	1	−2	−12	5	136	136	3
3	3	3	178	177	1	−1	12	3	42	37	1	−2	−3	4	67	55	2	2	4	4	51	43	1	−1	−12	5	29	26	2
4	3	3	102	103	1	0	12	3	39	35	1	−1	−3	4	390	384	6	3	4	4	89	92	1	0	−12	5	60	60	2
5	3	3	90	91	1	1	12	3	81	82	1	0	−3	4	130	136	2	4	4	4	64	64	1	1	−12	5	64	61	2
6	3	3	87	86	1	−2	−14	4	25	25	2	1	−3	4	594	613	9	5	4	4	20	21	1	2	−12	5	100	100	2
−7	4	3	54	53	2	0	−14	4	14	10	4	2	−3	4	190	193	2	6	4	4	68	76	1	3	−12	5	52	52	1
−6	4	3	70	70	2	1	−14	4	40	39	2	3	−3	4	113	120	1	−6	5	4	53	47	2	4	−12	5	92	89	2
−5	4	3	53	58	2	−2	−13	4	48	48	2	4	−3	4	29	27	1	−5	5	4	36	36	2	−3	−11	5	81	85	2
−4	4	3	123	122	2	−1	−13	4	57	55	2	5	−3	4	100	98	1	−4	5	4	35	36	1	−2	−11	5	96	95	2
−3	4	3	75	71	1	0	−13	4	58	56	2	6	−3	4	46	45	1	−3	5	4	58	57	1	−1	−11	5	50	56	2
−2	4	3	358	355	7	2	−13	4	89	89	3	7	−3	4	41	37	2	−2	5	4	138	138	1	0	−11	5	61	73	2
−1	4	3	207	214	3	3	−13	4	52	55	1	−3	−2	4	129	139	3	−1	5	4	172	178	1	1	−11	5	95	95	2
0	4	3	123	123	1	−3	−12	4	165	164	4	−2	−2	4	147	153	3	0	5	4	106	111	1	2	−11	5	122	124	3
1	4	3	136	145	1	−2	−12	4	102	100	2	−1	−2	4	550	572	7	1	5	4	142	142	1	3	−11	5	88	86	2
2	4	3	176	168	1	−1	−12	4	41	44	2	0	−2	4	317	325	4	2	5	4	133	132	1	4	−11	5	89	84	2
3	4	3	21	22	1	0	−12	4	57	59	2	1	−2	4	130	133	1	3	5	4	45	46	1	−2	−10	5	145	152	2
4	4	3	81	82	1	1	−12	4	51	47	2	2	−2	4	328	323	4	4	5	4	78	79	1	−1	−10	5	96	99	2
5	4	3	53	55	1	2	−12	4	92	90	2	3	−2	4	253	258	2	5	5	4	96	97	1	0	−10	5	78	79	1
6	4	3	87	82	1	3	−12	4	18	14	3	4	−2	4	93	96	1	6	5	4	67	83	2	1	−10	5	51	52	1
−6	5	3	27	25	3	4	−12	4	156	154	4	5	−2	4	163	162	2	−6	6	4	42	43	2	2	−10	5	137	144	2
−5	5	3	43	46	2	−3	−11	4	51	50	2	6	−2	4	16	14	3	−5	6	4	68	74	2	3	−10	5	159	160	2
−4	5	3	69	75	1	−2	−11	4	144	145	3	7	−2	4	35	33	2	−3	6	4	44	40	1	4	−10	5	130	130	3
−3	5	3	121	119	2	0	−11	4	57	72	2	−2	−1	4	31	31	1	−2	6	4	209	207	2	5	−10	5	69	67	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−2	5	3	232	236	3	1	−11	4	92	90	2	−1	−1	4	328	346	3	−1	6	4	164	170	1	−2	−9	5	316	321	5
−1	5	3	206	202	3	2	−11	4	25	26	3	0	−1	4	237	248	2	0	6	4	49	48	1	−1	−9	5	86	88	1
0	5	3	247	244	3	3	−11	4	139	135	2	1	−1	4	258	272	2	1	6	4	112	112	1	0	−9	5	54	43	1
1	5	3	114	117	1	4	−11	4	13	10	5	2	−1	4	67	72	1	2	6	4	57	53	1	1	−9	5	65	67	1
2	5	3	225	233	1	−3	−10	4	90	94	2	3	−1	4	77	77	1	3	6	4	142	144	1	2	−9	5	252	257	4
3	5	3	62	60	1	−2	−10	4	119	114	3	4	−1	4	147	144	1	4	6	4	34	33	2	3	−9	5	293	295	4
4	5	3	137	136	1	−1	−10	4	43	41	1	6	−1	4	123	122	2	−5	7	4	67	66	2	4	−9	5	45	49	1
5	5	3	48	41	1	0	−10	4	94	91	2	7	−1	4	69	66	2	−4	7	4	55	53	2	5	−9	5	26	27	2
6	5	3	13	13	3	1	−10	4	49	47	1	−3	0	4	138	144	3	−3	7	4	29	30	2	−1	−8	5	136	131	2
−6	6	3	58	55	2	2	−10	4	63	63	2	−2	0	4	236	243	3	−2	7	4	82	80	1	0	−8	5	176	165	2
−5	6	3	65	79	2	3	−10	4	77	76	1	−1	0	4	125	127	1	−1	7	4	90	84	1	1	−8	5	71	67	1
−4	6	3	36	47	2	4	−10	4	86	87	2	0	0	4	192	195	1	0	7	4	128	129	1	2	−8	5	184	189	2
−3	6	3	67	70	1	5	−10	4	21	19	2	1	0	4	96	101	1	1	7	4	22	19	1	3	−8	5	43	36	1
−2	6	3	83	82	1	−2	−9	4	171	173	3	2	0	4	80	87	1	2	7	4	123	123	1	4	−8	5	283	281	4
−1	6	3	110	115	1	−1	−9	4	187	179	3	3	0	4	63	56	1	3	7	4	89	89	1	5	−8	5	23	20	2
0	6	3	169	168	1	0	−9	4	44	44	1	4	0	4	189	194	1	4	7	4	55	56	2	6	−8	5	78	79	2
1	6	3	164	164	1	1	−9	4	136	132	2	5	0	4	165	168	1	−5	8	4	68	63	2	−1	−7	5	140	135	3
2	6	3	201	196	1	2	−9	4	87	81	2	6	0	4	65	64	1	−4	8	4	99	99	2	0	−7	5	177	165	2
3	6	3	165	165	1	3	−9	4	260	261	3	7	0	4	15	18	3	−3	8	4	89	86	1	1	−7	5	132	130	1
4	6	3	178	174	1	4	−9	4	111	109	2	−3	1	4	143	148	3	−2	8	4	97	103	2	2	−7	5	130	135	1
5	6	3	69	71	1	5	−9	4	63	64	1	−2	1	4	229	223	2	−1	8	4	78	82	1	3	−7	5	184	187	2
−6	7	3	59	59	2	−2	−8	4	121	119	3	−1	1	4	132	135	1	0	8	4	35	31	1	4	−7	5	272	265	4
−5	7	3	45	47	2	−1	−8	4	310	306	5	0	1	4	401	409	3	1	8	4	89	88	1	5	−7	5	102	102	2
−4	7	3	146	145	3	0	−8	4	109	98	2	1	1	4	169	165	1	2	8	4	148	151	2	6	−7	5	34	48	1
−3	7	3	77	81	1	1	−8	4	263	257	3	2	1	4	49	47	1	3	8	4	74	76	1	−1	−6	5	77	76	2
−2	7	3	144	144	1	2	−8	4	178	184	1	3	1	4	185	196	1	4	8	4	77	78	2	0	−6	5	508	492	8
−1	7	3	138	139	1	3	−8	4	231	231	2	4	1	4	199	195	1	−3	9	4	80	79	2	1	−6	5	281	278	4
0	7	3	92	84	1	4	−8	4	122	123	2	5	1	4	135	135	1	−2	9	4	133	133	2	2	−6	5	111	119	1
3	−6	5	205	204	2	−6	3	5	29	32	2	−1	−13	6	68	70	2	−2	−2	6	181	179	3	4	5	6	72	73	1
4	−6	5	241	234	2	−5	3	5	71	73	2	0	−13	6	81	85	2	−1	−2	6	417	421	5	5	5	6	26	25	2
5	−6	5	69	69	1	−4	3	5	63	57	1	1	−13	6	59	67	2	0	−2	6	173	172	2	−6	6	6	29	34	2
6	−6	5	65	67	1	−3	3	5	137	130	2	2	−13	6	78	78	2	1	−2	6	146	136	2	−5	6	6	65	67	2
−1	−5	5	48	39	1	−2	3	5	146	147	2	3	−13	6	24	28	3	2	−2	6	98	97	2	−4	6	6	134	132	3
0	−5	5	609	595	9	−1	3	5	215	208	2	−3	−12	6	99	99	2	3	−2	6	69	69	1	−3	6	6	201	203	3
1	−5	5	342	331	4	0	3	5	413	400	4	−2	−12	6	91	89	2	4	−2	6	47	41	1	−2	6	6	327	333	3
2	−5	5	53	48	1	1	3	5	295	288	3	−1	−12	6	36	43	2	5	−2	6	48	46	1	−1	6	6	64	63	1
3	−5	5	86	86	1	2	3	5	233	226	2	0	−12	6	84	80	2	6	−2	6	60	63	2	0	6	6	6	5	6
4	−5	5	243	241	2	3	3	5	117	125	1	1	−12	6	32	31	2	−2	−1	6	250	246	4	1	6	6	173	174	1
5	−5	5	87	92	1	4	3	5	52	50	1	2	−12	6	42	40	2	−1	−1	6	331	335	3	2	6	6	325	327	4
6	−5	5	65	64	1	5	3	5	115	118	2	3	−12	6	145	143	3	0	−1	6	278	279	3	3	6	6	83	84	1
−2	−4	5	146	142	3	−6	4	5	2	9	2	4	−12	6	71	71	2	1	−1	6	334	342	4	4	6	6	85	87	2
−1	−4	5	263	265	4	−5	4	5	118	119	3	−3	−11	6	119	120	3	2	−1	6	217	217	3	−5	7	6	77	77	2
0	−4	5	366	363	5	−4	4	5	42	41	1	−2	−11	6	17	15	4	3	−1	6	106	105	1	−4	7	6	48	47	2
1	−4	5	221	217	2	−3	4	5	65	65	1	−1	−11	6	182	186	4	4	−1	6	105	106	1	−3	7	6	134	135	3
2	−4	5	180	188	2	−2	4	5	158	150	2	0	−11	6	81	91	2	5	−1	6	194	209	5	−2	7	6	174	172	3
3	−4	5	140	143	1	−1	4	5	283	283	4	1	−11	6	28	24	3	6	−1	6	43	42	1	−1	7	6	151	153	1
4	−4	5	52	49	1	0	4	5	157	159	1	2	−11	6	80	74	2	−3	0	6	113	115	2	0	7	6	134	125	1
5	−4	5	83	79	1	1	4	5	296	305	2	3	−11	6	185	184	3	−2	0	6	325	316	5	1	7	6	56	57	1
6	−4	5	66	62	2	2	4	5	205	196	1	4	−11	6	31	31	3	−1	0	6	166	172	2	2	7	6	109	127	2

TABLE 7-continued

Observed and calculated structure factors for NEL																													
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−3	−3	5	57	56	2	3	4	5	143	140	1	−2	−10	6	114	116	3	0	0	6	387	387	4	3	7	6	31	35	1
−2	−3	5	220	220	5	4	4	5	124	127	2	−1	−10	6	150	144	2	1	0	6	105	109	1	4	7	6	53	56	2
−1	−3	5	174	176	2	−6	5	5	14	12	5	0	−10	6	39	40	1	2	0	6	150	155	2	−2	8	6	150	154	4
0	−3	5	218	210	3	−5	5	5	102	117	3	1	−10	6	86	83	1	3	0	6	79	74	1	−1	8	6	126	125	2
1	−3	5	497	511	5	−4	5	5	120	128	3	2	−10	6	137	140	3	4	0	6	163	166	1	0	8	6	143	140	2
2	−3	5	236	232	2	−3	5	5	78	80	1	3	−10	6	148	150	2	5	0	6	132	131	3	1	8	6	38	37	1
3	−3	5	116	116	1	−2	5	5	86	84	1	4	−10	6	85	85	2	6	0	6	85	83	1	2	8	6	107	111	1
4	−3	5	93	89	1	−1	5	5	259	264	2	5	−10	6	90	95	1	−6	1	6	25	26	3	3	8	6	118	121	2
5	−3	5	35	36	1	0	5	5	92	98	1	−2	−9	6	90	93	1	−5	1	6	78	80	2	4	8	6	51	61	2
6	−3	5	191	189	5	1	5	5	169	164	1	−1	−9	6	221	221	3	−4	1	6	153	152	2	−3	9	6	101	97	3
−3	−2	5	107	104	3	2	5	5	169	169	1	0	−9	6	53	53	1	−3	1	6	113	114	2	−2	9	6	195	192	4
−2	−2	5	295	291	4	3	5	5	262	266	2	1	−9	6	159	160	2	−2	1	6	254	259	3	−1	9	6	112	108	2
−1	−2	5	328	328	4	4	5	5	105	107	2	2	−9	6	18	15	3	−1	1	6	73	71	1	0	9	6	103	103	1
0	−2	5	114	106	1	−6	6	5	46	42	2	3	−9	6	140	141	2	0	1	6	206	201	2	1	9	6	120	118	1
1	−2	5	209	209	2	−5	6	5	55	53	2	4	−9	6	63	78	2	1	1	6	24	16	1	2	9	6	71	77	1
2	−2	5	160	157	2	−4	6	5	31	39	2	5	−9	6	71	71	1	2	1	6	151	139	1	3	9	6	0	8	1
3	−2	5	85	88	1	−3	6	5	142	144	2	−1	−8	6	166	163	2	3	1	6	49	54	1	−2	10	6	113	110	3
4	−2	5	23	24	1	−2	6	5	31	29	1	0	−8	6	65	62	1	4	1	6	180	178	1	−1	10	6	157	147	2
5	−2	5	114	118	2	−1	6	5	113	112	1	1	−8	6	134	131	2	5	1	6	8	13	7	0	10	6	167	161	2
6	−2	5	30	30	1	0	6	5	61	59	1	2	−8	6	95	94	1	6	1	6	49	45	1	1	10	6	79	77	1
7	−2	5	58	60	2	1	6	5	144	137	1	3	−8	6	268	269	3	−6	2	6	58	54	2	2	10	6	77	79	1
−3	−1	5	91	88	2	2	6	5	203	195	2	4	−8	6	20	25	2	−5	2	6	197	199	5	−2	11	6	7	9	6
−2	−1	5	86	86	1	3	6	5	21	16	1	5	−8	6	138	134	2	−4	2	6	206	209	3	−1	11	6	61	61	1
−1	−1	5	247	254	2	4	6	5	29	24	3	6	−8	6	52	50	2	−3	2	6	35	41	1	0	11	6	95	91	1
0	−1	5	191	186	2	−5	7	5	50	46	2	−1	−7	6	173	180	3	−2	2	6	187	181	2	1	11	6	78	92	2
1	−1	5	217	228	2	−4	7	5	43	44	2	0	−7	6	169	163	2	−1	2	6	121	120	1	−1	−14	7	60	57	2
2	−1	5	110	105	1	−3	7	5	160	162	4	1	−7	6	331	332	4	0	2	6	591	573	7	0	−14	7	85	83	2
3	−1	5	116	113	1	−2	7	5	245	254	3	2	−7	6	47	54	1	1	2	6	230	236	3	1	−14	7	53	59	2
4	−1	5	158	165	1	−1	7	5	59	62	1	3	−7	6	110	108	1	2	2	6	259	262	2	−3	−13	7	54	58	2
5	−1	5	125	129	3	0	7	5	123	128	1	4	−7	6	63	63	1	3	2	6	28	23	1	−2	−13	7	81	80	2
6	−1	5	108	111	2	1	7	5	190	192	2	5	−7	6	100	99	2	4	2	6	347	350	3	−1	−13	7	27	28	3
−3	0	5	283	285	6	2	7	5	183	188	2	6	−7	6	48	44	2	5	2	6	91	92	1	0	−13	7	127	134	3
−2	0	5	23	23	1	3	7	5	89	92	1	−1	−6	6	274	271	5	6	2	6	41	39	2	1	−13	7	85	83	2
−1	0	5	36	41	1	4	7	5	35	33	2	0	−6	6	270	261	4	−6	3	6	69	68	2	2	−13	7	54	56	2
0	0	5	306	311	2	−4	8	5	64	58	2	1	−6	6	82	84	1	−5	3	6	94	96	2	3	−13	7	9	13	8
1	0	5	109	116	1	−2	8	5	30	24	2	2	−6	6	148	150	1	−4	3	6	102	102	2	−3	−12	7	57	55	2
2	0	5	308	302	3	−1	8	5	110	113	1	3	−6	6	151	157	1	−3	3	6	205	215	3	−2	−12	7	107	106	3
3	0	5	99	101	1	0	8	5	103	104	1	4	−6	6	157	157	1	−2	3	6	179	173	2	−1	−12	7	74	80	2
4	0	5	43	40	1	1	8	5	194	198	3	5	−6	6	127	125	2	−1	3	6	122	115	2	0	−12	7	18	11	4
5	0	5	125	123	3	2	8	5	79	78	1	6	−6	6	32	34	1	0	3	6	59	54	1	1	−12	7	100	109	3
6	0	5	38	37	1	3	8	5	22	19	2	−1	−5	6	362	344	8	1	3	6	97	103	1	2	−12	7	89	86	2
−4	1	5	116	119	3	4	8	5	35	40	2	0	−5	6	124	113	2	2	3	6	180	172	1	3	−12	7	118	117	3
−3	1	5	101	103	2	−3	9	5	110	107	3	1	−5	6	387	368	5	3	3	6	77	79	1	4	−12	7	24	18	2
−2	1	5	94	94	1	−2	9	5	137	141	3	2	−5	6	111	113	1	4	3	6	127	128	2	−3	−11	7	109	107	3
−1	1	5	332	325	4	−1	9	5	67	63	1	3	−5	6	176	169	2	5	3	6	15	13	5	−2	−11	7	288	282	6
0	1	5	315	324	2	0	9	5	103	100	2	4	−5	6	158	159	2	−6	4	6	18	19	4	−1	−11	7	44	45	2
1	1	5	199	206	2	1	9	5	117	114	2	5	−5	6	163	168	2	−5	4	6	36	39	2	0	−11	7	45	52	2
2	1	5	182	184	1	2	9	5	119	119	1	6	−5	6	22	22	3	−4	4	6	49	51	1	1	−11	7	88	89	2
3	1	5	264	266	1	3	9	5	32	24	2	−2	−4	6	207	206	5	−3	4	6	108	109	2	2	−11	7	177	179	3

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	1	5	100	101	1	−3	10	5	23	20	3	−1	−4	6	305	297	7	−2	4	6	266	265	3	3	−11	7	44	43	2
5	1	5	129	127	3	−2	10	5	54	52	2	0	−4	6	296	280	6	−1	4	6	127	130	1	4	−11	7	94	89	2
6	1	5	43	40	1	−1	10	5	49	47	1	1	−4	6	339	333	5	0	4	6	82	86	1	−2	−10	7	21	11	3
−7	2	5	51	48	2	0	10	5	51	46	1	2	−4	6	64	57	1	1	4	6	106	97	1	−1	−10	7	52	55	1
−6	2	5	77	76	2	1	10	5	107	108	1	3	−4	6	88	88	1	2	4	6	113	115	1	0	−10	7	99	100	2
−5	2	5	106	109	2	2	10	5	90	89	1	4	−4	6	29	26	2	3	4	6	46	45	1	1	−10	7	63	58	1
−4	2	5	139	143	2	−2	11	5	21	19	2	5	−4	6	186	192	3	4	4	6	187	187	3	2	−10	7	125	123	3
−3	2	5	210	213	3	−1	11	5	98	94	1	6	−4	6	34	30	2	5	4	6	37	36	2	3	−10	7	19	10	3
−2	2	5	89	90	1	0	11	5	71	67	1	−2	−3	6	263	262	4	−6	5	6	75	74	2	4	−10	7	68	67	2
−1	2	5	213	204	2	1	11	5	73	71	1	−1	−3	6	255	254	4	−5	5	6	102	101	3	5	−10	7	137	139	3
0	2	5	68	69	1	−2	−14	6	45	42	1	0	−3	6	168	155	3	−3	5	6	89	88	1	−2	−9	7	229	235	3
1	2	5	178	174	2	−1	−14	6	78	74	2	1	−3	6	286	281	3	−2	5	6	224	221	2	−1	−9	7	79	76	1
2	2	5	165	162	1	0	−14	6	47	46	2	2	−3	6	124	112	1	−1	5	6	51	51	1	0	−9	7	67	69	1
3	2	5	262	268	1	1	−14	6	84	85	2	3	−3	6	8	2	3	0	5	6	71	76	1	1	−9	7	66	62	1
4	2	5	256	263	1	2	−14	6	9	12	9	4	−3	6	21	19	2	1	5	6	36	38	1	2	−9	7	315	319	5
5	2	5	98	97	1	−3	−13	6	166	168	4	5	−3	6	42	41	1	2	5	6	196	190	2	3	−9	7	131	122	2
6	2	5	39	36	2	−2	−13	6	80	78	2	6	−3	6	93	92	2	3	5	6	116	121	1	4	−9	7	50	50	1
5	−9	7	44	41	1	1	1	7	435	439	6	−1	−14	8	52	51	2	2	−3	8	117	119	1	−2	5	8	74	80	1
−1	−8	7	77	71	1	2	1	7	61	53	1	0	−14	8	99	95	2	3	−3	8	58	54	1	−1	5	8	39	43	1
0	−8	7	139	135	2	3	1	7	275	274	2	−3	−13	8	60	62	2	4	−3	8	81	80	1	0	5	8	68	61	1
1	−8	7	117	116	1	4	1	7	88	91	1	−2	−13	8	134	131	3	5	−3	8	95	93	1	1	5	8	31	34	1
2	−8	7	155	155	2	5	1	7	78	75	2	−1	−13	8	146	142	3	6	−3	8	113	107	3	2	5	8	89	106	2
3	−8	7	92	85	1	6	1	7	54	54	1	0	−13	8	50	51	2	−3	−2	8	62	56	2	3	5	8	38	37	1
4	−8	7	77	79	1	−6	2	7	50	47	2	3	−13	8	56	58	2	−2	−2	8	142	136	3	4	5	8	44	46	2
5	−8	7	145	147	2	−5	2	7	162	162	4	−3	−12	8	59	60	2	−1	−2	8	159	151	2	−5	6	8	13	18	6
−1	−7	7	194	188	3	−4	2	7	95	93	1	−2	−12	8	112	112	3	0	−2	8	36	34	2	−4	6	8	24	23	3
0	−7	7	224	213	3	−3	2	7	181	177	3	−1	−12	8	143	150	4	1	−2	8	140	134	1	−3	6	8	86	84	2
1	−7	7	42	39	1	−2	2	7	178	176	2	0	−12	8	82	73	2	2	−2	8	184	188	1	−2	6	8	120	118	3
2	−7	7	43	46	1	−1	2	7	111	110	1	1	−12	8	61	61	2	3	−2	8	74	66	1	−1	6	8	6	3	6
3	−7	7	59	51	1	0	2	7	84	85	1	2	−12	8	168	172	4	4	−2	8	103	105	2	0	6	8	95	91	1
4	−7	7	160	159	2	1	2	7	56	50	1	3	−12	8	48	51	2	5	−2	8	36	38	1	1	6	8	107	108	1
5	−7	7	121	118	2	2	2	7	149	149	1	4	−12	8	18	20	3	6	−2	8	138	138	2	2	6	8	131	133	2
6	−7	7	128	128	3	3	2	7	48	44	1	−3	−11	8	64	62	2	−3	−1	8	111	112	2	3	6	8	69	70	1
−1	−6	7	143	140	3	4	2	7	32	31	1	−2	−11	8	122	115	3	−2	−1	8	69	63	1	4	6	8	19	14	3
0	−6	7	40	41	1	5	2	7	44	41	1	−1	−11	8	46	47	2	−1	−1	8	446	443	6	−2	7	8	114	109	3
1	−6	7	35	28	1	−6	3	7	48	48	2	0	−11	8	24	29	3	0	−1	8	96	86	1	−1	7	8	83	82	2
2	−6	7	204	204	2	−5	3	7	136	135	3	1	−11	8	39	33	2	1	−1	8	244	247	3	0	7	8	157	158	2
3	−6	7	93	89	1	−4	3	7	75	74	1	2	−11	8	46	47	2	2	−1	8	76	75	1	1	7	8	102	107	1
4	−6	7	42	44	1	−3	3	7	114	122	2	3	−11	8	36	31	2	3	−1	8	163	160	1	2	7	8	70	70	1
5	−6	7	164	162	2	−2	3	7	192	186	3	4	−11	8	93	87	2	4	−1	8	123	120	2	3	7	8	47	47	1
6	−6	7	31	31	1	−1	3	7	23	24	1	−2	−10	8	155	148	3	5	−1	8	59	59	1	−2	8	8	105	105	3
−2	−5	7	98	103	2	0	3	7	48	54	1	−1	−10	8	195	199	3	6	−1	8	33	29	1	−1	8	8	46	46	1
−1	−5	7	189	179	4	1	3	7	99	88	1	0	−10	8	45	42	1	−5	0	8	38	35	2	0	8	8	19	22	2
0	−5	7	238	212	5	2	3	7	108	103	1	1	−10	8	105	100	2	−4	0	8	167	173	3	1	8	8	122	121	1
1	−5	7	47	48	1	3	3	7	322	324	3	2	−10	8	219	214	5	−3	0	8	68	68	1	2	8	8	31	27	1
2	−5	7	89	84	1	4	3	7	83	84	1	3	−10	8	61	62	2	−2	0	8	115	110	2	3	8	8	90	91	2
3	−5	7	224	230	2	5	3	7	80	81	2	4	−10	8	87	80	2	−1	0	8	123	121	1	−2	9	8	27	22	3
4	−5	7	133	137	1	−6	4	7	79	80	2	5	−10	8	54	52	2	0	0	8	427	414	5	−1	9	8	136	130	2
5	−5	7	108	112	1	−5	4	7	145	149	3	−2	−9	8	214	219	3	1	0	8	138	135	1	0	9	8	52	52	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
6	−5	7	32	31	2	−4	4	7	22	26	3	−1	−9	8	261	256	4	2	0	8	149	143	1	1	9	8	58	57	1
−2	−4	7	50	49	1	−3	4	7	118	110	2	0	−9	8	135	135	2	3	0	8	58	60	1	−1	10	8	14	6	3
−1	−4	7	462	435	10	−2	4	7	54	50	1	1	−9	8	94	96	2	4	0	8	145	139	2	0	10	8	33	36	1
0	−4	7	97	106	2	−1	4	7	204	206	2	2	−9	8	248	252	6	5	0	8	49	50	2	−2	−14	9	10	9	8
1	−4	7	111	115	1	0	4	7	63	62	1	3	−9	8	83	78	2	6	0	8	68	62	1	−1	−14	9	23	23	3
2	−4	7	98	94	1	1	4	7	347	344	3	4	−9	8	105	107	2	−6	1	8	56	54	2	0	−14	9	66	65	2
3	−4	7	59	58	1	2	4	7	89	81	1	5	−9	8	95	94	2	−5	1	8	22	19	3	−3	−13	9	17	17	3
4	−4	7	121	124	1	3	4	7	231	230	3	−2	−8	8	100	96	2	−4	1	8	292	296	4	−2	−13	9	45	42	2
5	−4	7	31	29	1	4	4	7	142	141	2	−1	−8	8	49	45	1	−3	1	8	63	64	1	−1	−13	9	58	56	2
6	−4	7	84	82	2	5	4	7	54	48	2	0	−8	8	130	123	2	−2	1	8	150	148	2	0	−13	9	61	59	2
−2	−3	7	99	97	1	−6	5	7	85	87	2	1	−8	8	76	79	1	−1	1	8	269	265	3	−3	−12	9	0	6	1
−1	−3	7	145	147	2	−5	5	7	138	137	3	2	−8	8	89	92	2	0	1	8	99	90	1	−2	−12	9	49	45	2
0	−3	7	198	182	4	−3	5	7	189	187	4	3	−8	8	136	135	2	1	1	8	99	93	1	−1	−12	9	105	111	3
1	−3	7	87	87	1	−2	5	7	61	59	1	4	−8	8	78	81	2	2	1	8	66	65	1	0	−12	9	0	13	1
2	−3	7	92	92	1	−1	5	7	80	85	1	5	−8	8	44	42	1	3	1	8	76	75	1	1	−12	9	44	44	2
3	−3	7	118	123	1	0	5	7	86	81	1	−2	−7	8	97	95	2	4	1	8	105	103	1	3	−12	9	60	57	2
4	−3	7	46	41	1	1	5	7	103	107	1	−1	−7	8	43	45	1	5	1	8	37	37	2	−3	−11	9	60	60	2
5	−3	7	106	104	1	2	5	7	77	74	1	0	−7	8	107	104	2	−6	2	8	60	57	2	−2	−11	9	43	38	2
6	−3	7	52	46	2	3	5	7	207	203	2	1	−7	8	70	63	1	−5	2	8	88	87	2	−1	−11	9	90	90	2
−2	−2	7	76	75	1	4	5	7	22	19	2	2	−7	8	41	40	1	−4	2	8	200	199	3	0	−11	9	63	71	2
−1	−2	7	309	308	4	−5	6	7	50	49	2	3	−7	8	120	113	1	−3	2	8	187	188	3	1	−11	9	104	102	3
0	−2	7	216	205	3	−4	6	7	81	80	2	4	−7	8	70	70	2	−2	2	8	42	38	1	2	−11	9	126	124	3
1	−2	7	260	252	3	−3	6	7	72	72	2	5	−7	8	83	83	1	−1	2	8	33	33	1	3	−11	9	77	80	2
2	−2	7	177	173	2	−2	6	7	237	238	3	6	−7	8	10	8	10	0	2	8	254	246	2	4	−11	9	101	100	2
3	−2	7	33	40	1	−1	6	7	141	142	1	−2	−6	8	180	184	4	1	2	8	83	84	1	−3	−10	9	63	63	2
4	−2	7	77	82	1	0	6	7	167	161	1	−1	−6	8	71	75	1	2	2	8	113	104	1	−2	−10	9	118	107	3
5	−2	7	124	118	2	1	6	7	34	33	1	0	−6	8	416	414	5	3	2	8	139	141	1	−1	−10	9	99	96	2
6	−2	7	54	52	2	2	6	7	70	81	1	1	−6	8	91	92	1	4	2	8	33	33	1	1	−10	9	113	115	3
−3	−1	7	94	92	2	3	6	7	32	30	1	2	−6	8	120	127	1	5	2	8	55	54	2	2	−10	9	36	33	3
−2	−1	7	302	296	5	4	6	7	56	55	2	3	−6	8	101	99	1	−6	3	8	32	31	2	3	−10	9	23	24	3
−1	−1	7	177	166	2	−4	7	7	24	28	3	4	−6	8	107	109	2	−4	3	8	205	235	6	4	−10	9	16	11	5
0	−1	7	12	10	1	−3	7	7	113	115	2	5	−6	8	65	65	1	−3	3	8	67	64	1	−2	−9	9	95	97	2
1	−1	7	494	499	7	−2	7	7	84	85	2	6	−6	8	6	9	6	−2	3	8	94	94	1	−1	−9	9	73	73	1
2	−1	7	99	95	1	−1	7	7	101	103	2	−2	−5	8	77	72	2	−1	3	8	169	171	1	0	−9	9	67	66	1
3	−1	7	27	25	1	0	7	7	81	79	1	−1	−5	8	83	85	2	0	3	8	100	91	1	1	−9	9	73	72	1
4	−1	7	149	152	1	1	7	7	26	28	1	0	−5	8	95	96	1	1	3	8	158	151	1	2	−9	9	108	100	3
5	−1	7	109	114	2	2	7	7	58	58	1	1	−5	8	168	161	2	2	3	8	176	168	1	3	−9	9	73	74	2
6	−1	7	11	14	4	3	7	7	150	153	2	2	−5	8	102	97	1	3	3	8	215	220	2	4	−9	9	36	35	3
−3	0	7	105	102	1	4	7	7	64	62	2	3	−5	8	36	34	1	4	3	8	159	157	2	5	−9	9	58	57	1
−2	0	7	137	137	2	−2	8	7	67	66	2	4	−5	8	151	149	2	5	3	8	71	72	2	−2	−8	9	89	85	1
−1	0	7	333	332	4	−1	8	7	115	112	2	5	−5	8	36	39	1	−6	4	8	38	39	2	−1	−8	9	81	80	1
0	0	7	139	135	1	0	8	7	33	36	1	6	−5	8	33	37	2	−5	4	8	109	107	3	0	−8	9	151	150	2
1	0	7	115	123	2	1	8	7	76	76	1	−2	−4	8	64	62	1	−4	4	8	75	83	2	1	−8	9	201	205	3
2	0	7	85	87	1	2	8	7	59	60	1	−1	−4	8	173	164	3	−3	4	8	105	111	1	2	−8	9	74	78	2
3	0	7	124	123	1	3	8	7	111	115	2	0	−4	8	136	144	2	−2	4	8	192	188	2	3	−8	9	65	60	2
4	0	7	158	162	1	−2	9	7	33	26	2	1	−4	8	55	53	1	−1	4	8	235	242	2	4	−8	9	21	23	2
5	0	7	59	60	2	−1	9	7	99	96	2	2	−4	8	44	45	1	0	4	8	16	14	1	5	−8	9	64	63	1
6	0	7	36	35	1	0	9	7	5	5	5	3	−4	8	138	138	1	1	4	8	223	225	2	−2	−7	9	90	92	1
−6	1	7	89	91	2	1	9	7	50	50	1	4	−4	8	91	96	1	2	4	8	164	160	1	−1	−7	9	154	152	2

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−5	1	7	177	180	4	2	9	7	73	70	1	5	−4	8	69	68	1	3	4	8	68	68	1	0	−7	9	113	108	2
−4	1	7	117	119	2	−2	10	7	43	35	2	6	−4	8	85	79	2	4	4	8	40	38	1	1	−7	9	135	131	1
−3	1	7	149	156	2	−1	10	7	45	40	1	−2	−3	8	83	74	2	5	4	8	16	14	4	2	−7	9	185	182	2
−2	1	7	284	285	3	0	10	7	103	104	1	−1	−3	8	104	101	1	−5	5	8	21	21	3	3	−7	9	13	14	4
−1	1	7	241	225	2	1	10	7	22	22	1	0	−3	8	189	164	4	−4	5	8	21	20	3	4	−7	9	84	84	2
0	1	7	78	83	1	−2	−14	8	89	92	2	1	−3	8	230	230	2	−3	5	8	114	110	3	5	−7	9	8	7	8
−2	−6	9	56	59	1	0	2	9	227	221	2	−2	−9	10	41	37	2	3	0	10	155	162	2	3	−11	11	7	10	7
−1	−6	9	71	75	1	1	2	9	70	70	1	−1	−9	10	60	66	1	4	0	10	44	47	1	4	−11	11	44	45	2
0	−6	9	99	100	2	2	2	9	121	120	1	0	−9	10	55	55	1	5	0	10	151	148	4	−3	−10	11	30	30	2
1	−6	9	124	127	1	3	2	9	66	77	1	1	−9	10	75	80	1	−6	1	10	40	39	2	−2	−10	11	99	102	3
2	−6	9	186	190	2	4	2	9	106	107	1	2	−9	10	98	91	3	−5	1	10	41	42	2	−1	−10	11	152	174	4
3	−6	9	78	74	1	5	2	9	24	23	3	3	−9	10	58	58	2	−4	1	10	78	78	2	0	−10	11	37	43	2
4	−6	9	121	122	2	−6	3	9	81	75	2	4	−9	10	50	48	2	−3	1	10	53	55	1	1	−10	11	148	151	4
5	−6	9	29	27	1	−5	3	9	46	42	2	5	−9	10	33	35	2	−2	1	10	112	115	1	2	−10	11	148	156	4
6	−6	9	34	33	2	−4	3	9	126	137	3	−2	−8	10	74	78	1	−1	1	10	71	68	1	3	−10	11	17	20	4
−2	−5	9	49	42	1	−3	3	9	262	267	3	−1	−8	10	157	156	2	0	1	10	68	67	1	4	−10	11	58	57	2
−1	−5	9	249	259	4	−2	3	9	115	114	1	0	−8	10	143	139	2	1	1	10	86	86	1	−3	−9	11	103	102	3
0	−5	9	89	93	1	−1	3	9	40	37	1	1	−8	10	114	109	2	2	1	10	95	96	1	−2	−9	11	148	141	3
1	−5	9	163	176	2	0	3	9	34	30	1	2	−8	10	30	31	2	3	1	10	81	83	3	−1	−9	11	48	51	2
2	−5	9	63	68	1	1	3	9	141	142	1	3	−8	10	89	88	2	4	1	10	70	69	1	1	−9	11	135	145	3
3	−5	9	110	112	1	2	3	9	45	45	1	4	−8	10	42	40	1	5	1	10	71	71	2	2	−9	11	116	117	3
4	−5	9	118	116	2	3	3	9	101	115	2	5	−8	10	26	24	2	−6	2	10	26	27	2	3	−9	11	50	49	2
5	−5	9	54	56	1	4	3	9	89	89	1	−2	−7	10	252	251	4	−5	2	10	45	47	2	4	−9	11	22	21	4
6	−5	9	21	18	3	5	3	9	24	22	3	−1	−7	10	114	118	2	−4	2	10	66	66	2	−3	−8	11	34	31	2
−2	−4	9	61	61	1	−5	4	9	87	84	2	0	−7	10	275	271	4	−3	2	10	88	97	2	−2	−8	11	121	121	2
−1	−4	9	150	142	2	−3	4	9	138	137	3	1	−7	10	158	164	2	−2	2	10	54	57	1	−1	−8	11	207	213	3
0	−4	9	94	92	1	−2	4	9	57	58	1	2	−7	10	237	241	4	−1	2	10	96	97	1	0	−8	11	160	157	2
1	−4	9	58	64	1	−1	4	9	57	61	1	3	−7	10	117	125	2	0	2	10	56	55	1	1	−8	11	56	64	1
2	−4	9	50	57	1	0	4	9	44	46	1	4	−7	10	46	47	2	1	2	10	63	64	1	2	−8	11	101	97	3
3	−4	9	188	192	2	1	4	9	88	86	1	5	−7	10	82	82	1	2	2	10	56	59	1	3	−8	11	76	76	2
4	−4	9	155	166	2	2	4	9	114	123	1	−2	−6	10	67	66	1	3	2	10	14	14	3	4	−8	11	92	90	2
5	−4	9	96	96	1	3	4	9	84	84	1	−1	−6	10	90	85	1	4	2	10	31	27	1	−3	−7	11	38	35	2
6	−4	9	37	38	2	4	4	9	23	21	3	0	−6	10	139	132	2	5	2	10	24	23	3	−2	−7	11	279	288	4
−2	−3	9	171	172	2	−5	5	9	103	101	2	1	−6	10	110	103	1	−5	3	10	20	18	3	−1	−7	11	78	83	1
−1	−3	9	21	15	1	−4	5	9	20	19	4	2	−6	10	71	67	1	−4	3	10	58	65	2	0	−7	11	86	84	1
0	−3	9	127	121	1	−3	5	9	138	130	3	3	−6	10	211	219	2	−2	3	10	67	70	1	1	−7	11	50	51	1
1	−3	9	241	247	2	−2	5	9	82	80	1	4	−6	10	56	58	2	−1	3	10	155	164	1	2	−7	11	248	264	4
2	−3	9	107	107	1	−1	5	9	113	116	2	5	−6	10	120	121	2	0	3	10	110	110	1	3	−7	11	31	30	2
3	−3	9	67	66	1	0	5	9	11	6	5	−2	−5	10	13	14	3	1	3	10	79	82	1	4	−7	11	113	116	2
4	−3	9	81	78	1	1	5	9	114	118	1	−1	−5	10	55	64	1	2	3	10	79	82	1	5	−7	11	78	78	1
5	−3	9	100	95	1	2	5	9	106	102	2	0	−5	10	75	72	1	3	3	10	36	35	1	−3	−6	11	138	141	3
6	−3	9	81	78	2	3	5	9	63	57	1	1	−5	10	90	95	1	4	3	10	53	50	2	−2	−6	11	117	108	2
−3	−2	9	97	100	1	4	5	9	38	38	2	2	−5	10	110	107	1	−5	4	10	85	84	2	−1	−6	11	204	206	3
−2	−2	9	98	104	1	−5	6	9	18	18	3	3	−5	10	82	87	1	−4	4	10	60	58	2	0	−6	11	123	112	2
−1	−2	9	193	194	2	−4	6	9	51	52	2	4	−5	10	151	149	4	−3	4	10	110	107	3	1	−6	11	140	145	1
0	−2	9	92	99	1	−3	6	9	59	59	2	5	−5	10	92	92	1	−2	4	10	219	231	3	2	−6	11	150	152	2
1	−2	9	106	113	1	−2	6	9	75	71	2	−2	−4	10	97	99	1	−1	4	10	29	31	2	3	−6	11	93	96	1
2	−2	9	18	14	1	−1	6	9	126	128	2	−1	−4	10	95	99	1	0	4	10	177	176	3	4	−6	11	100	101	2
3	−2	9	17	19	2	0	6	9	48	52	1	0	−4	10	125	124	1	1	4	10	46	44	1	5	−6	11	40	38	1

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	−2	9	99	117	3	1	6	9	70	73	1	1	−4	10	71	66	1	2	4	10	79	79	1	−3	−5	11	33	33	2
5	−2	9	138	134	2	2	6	9	114	115	1	2	−4	10	75	77	1	3	4	10	50	47	1	−2	−5	11	159	158	2
6	−2	9	59	60	1	3	6	9	7	5	7	3	−4	10	98	103	1	4	4	10	23	18	3	−1	−5	11	125	125	2
−4	−1	9	137	138	3	4	6	9	64	71	2	4	−4	10	19	16	2	−5	5	10	22	25	3	0	−5	11	111	110	2
−3	−1	9	134	139	2	−2	7	9	92	91	2	5	−4	10	75	72	1	−4	5	10	51	52	2	1	−5	11	86	86	1
−2	−1	9	85	83	1	−1	7	9	106	106	2	−3	−3	10	29	27	1	−3	5	10	61	61	2	2	−5	11	93	96	1
−1	−1	9	245	244	2	0	7	9	34	30	1	−2	−3	10	86	83	1	−2	5	10	91	95	2	3	−5	11	103	110	1
0	−1	9	26	24	1	1	7	9	73	72	1	−1	−3	10	201	209	3	−1	5	10	120	118	3	4	−5	11	85	85	2
1	−1	9	113	118	1	2	7	9	91	89	1	0	−3	10	14	8	2	0	5	10	22	23	2	5	−5	11	22	21	2
2	−1	9	72	68	1	3	7	9	39	38	2	1	−3	10	23	25	1	1	5	10	148	145	2	−3	−4	11	60	61	1
3	−1	9	44	42	1	−2	8	9	57	51	2	2	−3	10	129	125	1	2	5	10	76	76	1	−2	−4	11	81	81	1
4	−1	9	25	20	2	−1	8	9	29	29	2	3	−3	10	57	57	1	3	5	10	128	122	1	−1	−4	11	15	19	3
5	−1	9	87	89	1	0	8	9	43	42	1	4	−3	10	179	184	3	4	5	10	30	29	2	0	−4	11	106	105	1
6	−1	9	48	48	1	1	8	9	27	27	1	5	−3	10	231	224	3	−2	6	10	67	68	2	1	−4	11	164	167	2
−6	0	9	58	53	2	2	8	9	86	81	1	−4	−2	10	118	119	3	−1	6	10	68	69	2	2	−4	11	60	60	2
−5	0	9	78	77	2	−1	9	9	66	68	1	−3	−2	10	94	95	1	0	6	10	65	62	1	3	−4	11	64	63	1
−4	0	9	103	104	2	0	9	9	32	31	1	−2	−2	10	41	44	1	1	6	10	55	52	1	4	−4	11	203	194	3
−3	0	9	235	237	4	1	9	9	63	62	2	−1	−2	10	50	58	1	2	6	10	79	77	1	5	−4	11	39	36	1
−2	0	9	163	167	2	−1	−14	10	62	59	2	0	−2	10	70	64	1	3	6	10	101	96	1	−4	−3	11	183	184	4
−1	0	9	237	243	2	−3	−13	10	44	49	2	1	−2	10	110	115	1	−2	7	10	100	98	3	−3	−3	11	94	99	1
0	0	9	79	77	1	−2	−13	10	19	15	3	2	−2	10	67	66	1	−1	7	10	62	61	1	−2	−3	11	114	114	2
1	0	9	330	332	3	−1	−13	10	69	65	2	3	−2	10	77	79	1	0	7	10	69	65	1	−1	−3	11	60	62	1
2	0	9	107	110	1	0	−13	10	100	93	2	4	−2	10	129	131	2	1	7	10	72	72	1	0	−3	11	462	460	5
3	0	9	7	14	6	−3	−12	10	20	20	3	5	−2	10	152	155	3	2	7	10	53	51	1	1	−3	11	128	134	1
4	0	9	23	22	2	−2	−12	10	25	25	3	−5	−1	10	112	116	3	−2	8	10	29	27	2	2	−3	11	97	98	1
5	0	9	116	122	3	−1	−12	10	44	43	2	−4	−1	10	192	190	4	−1	8	10	29	28	2	3	−3	11	87	88	2
−6	1	9	18	19	3	0	−12	10	67	64	2	−3	−1	10	18	16	2	0	8	10	86	87	1	4	−3	11	143	145	2
−5	1	9	31	27	2	1	−12	10	41	45	2	−2	−1	10	116	115	1	1	8	10	62	60	1	5	−3	11	36	36	1
−4	1	9	156	153	4	3	−12	10	33	36	2	−1	−1	10	277	282	3	−1	−14	11	98	98	2	−5	−2	11	92	94	2
−3	1	9	213	213	3	−3	−11	10	33	34	2	0	−1	10	84	86	1	−2	−13	11	25	18	2	−4	−2	11	118	112	3
−2	1	9	111	106	1	−2	−11	10	103	102	2	1	−1	10	135	133	1	−1	−13	11	58	55	2	−3	−2	11	115	119	2
−1	1	9	35	32	1	−1	−11	10	26	29	2	2	−1	10	155	147	1	0	−13	11	27	25	3	−2	−2	11	19	14	2
0	1	9	94	85	1	0	−11	10	110	128	3	3	−1	10	161	166	1	−3	−12	11	88	85	2	−1	−2	11	91	89	1
1	1	9	137	129	1	1	−11	10	92	94	2	4	−1	10	77	77	1	−2	−12	11	21	19	3	0	−2	11	196	194	2
2	1	9	117	121	1	2	−11	10	56	56	2	5	−1	10	164	153	4	−1	−12	11	68	71	2	1	−2	11	139	136	1
3	1	9	127	130	1	3	−11	10	81	77	2	−6	0	10	80	76	2	0	−12	11	58	55	2	2	−2	11	57	57	1
4	1	9	147	150	2	4	−11	10	47	43	2	−5	0	10	47	47	2	1	−12	11	62	62	2	3	−2	11	39	41	2
5	1	9	50	47	2	−3	−10	10	14	13	6	−4	0	10	163	158	4	3	−12	11	53	54	2	4	−2	11	84	83	1
−6	2	9	111	103	3	−2	−10	10	152	148	3	−3	0	10	45	41	1	−3	−11	11	34	33	2	5	−2	11	21	24	1
−5	2	9	15	19	5	−1	−10	10	95	104	3	−2	0	10	102	104	1	−2	−11	11	141	145	3	−6	−1	11	86	82	2
−4	2	9	88	90	2	1	−10	10	135	142	3	−1	0	10	171	171	2	−1	−11	11	91	99	3	−5	−1	11	126	127	3
−3	2	9	159	157	2	2	−10	10	64	64	2	0	0	10	33	31	1	0	−11	11	67	73	2	−4	−1	11	39	36	2
−2	2	9	207	205	2	3	−10	10	59	57	2	1	0	10	111	108	1	1	−11	11	50	46	2	−3	−1	11	93	97	1
−1	2	9	58	60	1	4	−10	10	85	82	2	2	0	10	100	96	1	2	−11	11	123	124	3	−2	−1	11	174	164	3
−1	−1	11	13	11	3	0	−11	12	25	25	3	−4	−1	12	97	95	2	3	−9	13	108	109	3	−5	1	13	31	32	2
0	−1	11	117	117	1	1	−11	12	81	84	2	−3	−1	12	90	93	2	4	−9	13	63	60	2	−4	1	13	33	34	2
1	−1	11	160	166	1	2	−11	12	0	1	1	−2	−1	12	110	112	2	−3	−8	13	42	42	2	−3	1	13	106	108	3

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	−1	11	58	52	1	3	−11	12	48	56	2	−1	−1	12	260	259	4	−2	−8	13	66	60	2	−2	1	13	11	9	9
3	−1	11	72	72	1	−3	−10	12	32	28	2	0	−1	12	53	52	1	−1	−8	13	64	67	2	−1	1	13	137	130	3
4	−1	11	42	40	1	−2	−10	12	39	36	2	1	−1	12	144	145	1	0	−8	13	62	63	2	0	1	13	108	103	3
5	−1	11	53	54	2	−1	−10	12	44	50	2	2	−1	12	57	57	1	1	−8	13	102	104	2	1	1	13	32	26	1
−6	0	11	84	86	2	0	−10	12	25	19	3	3	−1	12	178	178	3	2	−8	13	128	131	3	2	1	13	161	170	2
−5	0	11	62	62	2	1	−10	12	8	4	8	4	−1	12	33	27	1	3	−8	13	18	16	5	3	1	13	26	26	2
−4	0	11	35	36	2	2	−10	12	60	63	2	−5	0	12	147	142	3	4	−8	13	88	89	2	4	1	13	23	24	2
−3	0	11	88	89	1	3	−10	12	63	65	2	−4	0	12	22	23	3	−4	−7	13	91	93	2	−5	2	13	31	32	2
−2	0	11	66	61	1	4	−10	12	38	36	2	−3	0	12	98	108	3	−3	−7	13	26	24	3	−4	2	13	111	108	2
−1	0	11	154	149	2	−3	−9	12	13	15	6	−2	0	12	65	70	1	−2	−7	13	161	166	4	−3	2	13	110	110	2
0	0	11	218	221	2	−2	−9	12	66	65	2	−1	0	12	120	119	2	−1	−7	13	74	81	2	−2	2	13	43	38	2
1	0	11	134	133	1	−1	−9	12	99	122	3	0	0	12	87	88	1	0	−7	13	171	159	4	−1	2	13	82	79	2
2	0	11	136	143	1	0	−9	12	68	75	2	1	0	12	90	85	1	1	−7	13	35	32	1	0	2	13	26	24	3
3	0	11	115	120	2	1	−9	12	54	54	2	2	0	12	46	44	1	2	−7	13	89	93	3	1	2	13	44	41	1
4	0	11	43	41	1	2	−9	12	57	54	2	3	0	12	80	82	1	3	−7	13	100	103	3	2	2	13	51	51	1
5	0	11	61	62	2	3	−9	12	67	69	2	4	0	12	45	41	1	4	−7	13	88	82	2	3	2	13	77	76	1
−6	1	11	52	50	2	4	−9	12	39	32	2	−5	1	12	93	92	2	−4	−6	13	103	105	2	−4	3	13	37	32	2
−5	1	11	39	40	2	−3	−8	12	153	153	4	−4	1	12	42	43	2	−3	−6	13	113	111	3	−3	3	13	54	53	2
−4	1	11	140	141	3	−2	−8	12	87	89	2	−2	1	12	201	209	3	−2	−6	13	60	64	2	−1	3	13	52	60	2
−3	1	11	118	135	2	−1	−8	12	198	208	4	−1	1	12	81	82	1	−1	−6	13	143	148	4	0	3	13	53	52	1
−2	1	11	154	157	2	0	−8	12	106	109	3	0	1	12	234	249	4	0	−6	13	312	317	4	1	3	13	43	40	1
−1	1	11	236	238	2	1	−8	12	218	222	5	1	1	12	37	33	1	1	−6	13	105	102	2	2	3	13	86	82	1
0	1	11	87	85	1	2	−8	12	44	54	3	2	1	12	99	101	1	2	−6	13	105	109	3	3	3	13	64	64	1
1	1	11	167	167	1	3	−8	12	109	105	3	3	1	12	78	78	1	3	−6	13	52	53	2	−1	4	13	81	81	2
2	1	11	239	244	3	4	−8	12	54	53	2	4	1	12	27	28	1	4	−6	13	79	78	1	0	4	13	43	40	1
3	1	11	100	95	2	−3	−7	12	115	117	3	−5	2	12	71	72	2	−4	−5	13	124	122	3	1	4	13	87	85	1
4	1	11	24	21	1	−2	−7	12	135	129	3	−4	2	12	79	78	2	−3	−5	13	99	98	2	2	4	13	33	31	1
5	1	11	15	20	4	−1	−7	12	160	158	2	−3	2	12	157	158	4	−2	−5	13	50	49	2	−1	5	13	109	106	3
−5	2	11	52	49	2	0	−7	12	127	124	2	−1	2	12	104	109	2	−1	−5	13	193	204	3	0	5	13	42	42	1
−4	2	11	117	121	3	1	−7	12	186	186	2	0	2	12	233	230	4	0	−5	13	427	428	7	1	5	13	89	84	1
−3	2	11	20	28	3	2	−7	12	69	65	2	1	2	12	125	124	1	1	−5	13	226	232	5	−1	6	13	37	38	2
−2	2	11	75	72	1	3	−7	12	123	130	3	2	2	12	68	65	1	2	−5	13	101	103	2	0	6	13	39	37	2
−1	2	11	83	88	1	4	−7	12	80	81	1	3	2	12	120	119	1	3	−5	13	100	101	3	−2	−12	14	8	12	7
0	2	11	76	71	1	−3	−6	12	154	157	3	4	2	12	51	47	2	4	−5	13	112	112	2	−1	−12	14	17	20	4
1	2	11	98	97	1	−2	−6	12	66	61	1	−5	3	12	45	43	2	−5	−4	13	121	117	3	0	−12	14	57	55	2
2	2	11	126	129	2	−1	−6	12	160	164	2	−4	3	12	81	75	2	−4	−4	13	28	22	3	−3	−11	14	32	36	2
3	2	11	160	161	2	0	−6	12	121	117	2	−3	3	12	76	79	2	−3	−4	13	31	31	2	−2	−11	14	65	68	2
4	2	11	31	33	1	1	−6	12	147	153	2	−1	3	12	126	121	3	−2	−4	13	82	83	2	−1	−11	14	60	61	2
−5	3	11	39	38	2	2	−6	12	147	152	2	0	3	12	91	85	1	−1	−4	13	16	14	2	0	−11	14	22	22	3
−4	3	11	15	13	5	3	−6	12	67	69	2	1	3	12	73	83	1	0	−4	13	65	69	1	−3	−10	14	14	14	5
−3	3	11	96	94	2	4	−6	12	75	73	1	2	3	12	54	52	1	1	−4	13	129	131	2	−2	−10	14	73	73	2
−2	3	11	88	89	2	5	−6	12	56	59	1	3	3	12	25	22	1	2	−4	13	137	138	2	−1	−10	14	55	50	2
−1	3	11	55	53	1	−3	−5	12	184	183	4	−4	4	12	32	27	2	3	−4	13	93	101	2	0	−10	14	26	24	3
0	3	11	37	29	1	−2	−5	12	111	113	2	−3	4	12	63	66	2	4	−4	13	69	62	2	2	−10	14	67	76	2
1	3	11	77	73	1	−1	−5	12	145	147	2	−1	4	12	89	92	2	−5	−3	13	124	118	3	3	−10	14	102	100	2
2	3	11	75	81	1	0	−5	12	122	113	2	0	4	12	47	43	1	−4	−3	13	132	134	3	−4	−9	14	63	64	2

TABLE 7-continued

Observed and calculated structure factors for NEL

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	3	11	104	102	1	1	−5	12	217	225	3	1	4	12	81	76	1	−3	−3	13	105	103	2	−3	−9	14	70	67	2
4	3	11	18	12	3	2	−5	12	54	53	2	2	4	12	69	69	1	−2	−3	13	122	127	3	−2	−9	14	33	27	2
−5	4	11	21	20	3	3	−5	12	129	133	2	3	4	12	76	74	1	−1	−3	13	23	21	2	−1	−9	14	26	26	2
−4	4	11	23	23	3	4	−5	12	100	99	2	−1	5	12	86	88	2	0	−3	13	308	309	4	0	−9	14	115	115	3
−3	4	11	11	14	10	5	−5	12	110	110	1	0	5	12	27	28	2	1	−3	13	33	35	2	2	−9	14	92	89	2
−2	4	11	142	139	3	−4	−4	12	29	27	2	1	5	12	26	24	2	2	−3	13	54	52	2	3	−9	14	28	28	3
−1	4	11	62	64	2	−3	−4	12	60	62	2	2	5	12	48	44	1	3	−3	13	117	119	2	−4	−8	14	49	50	2
0	4	11	93	91	1	−2	−4	12	92	95	1	−1	6	12	57	58	2	4	−3	13	57	57	1	−3	−8	14	142	139	3
1	4	11	65	67	1	−1	−4	12	181	178	3	0	6	12	34	35	1	−5	−2	13	125	122	3	−2	−8	14	70	70	2
2	4	11	82	80	1	0	−4	12	40	42	1	1	6	12	48	46	1	−4	−2	13	34	27	2	−1	−8	14	102	120	3
3	4	11	58	57	1	1	−4	12	130	131	1	2	6	12	77	77	2	−3	−2	13	117	121	3	0	−8	14	88	84	2
4	4	11	49	50	2	2	−4	12	18	19	6	−1	7	12	23	24	3	−2	−2	13	52	56	2	2	−8	14	29	27	3
−3	5	11	56	55	2	3	−4	12	101	107	2	0	7	12	43	43	2	−1	−2	13	161	158	2	3	−8	14	60	55	2
−1	5	11	83	77	2	4	−4	12	30	27	3	−2	−13	13	70	74	2	0	−2	13	143	139	2	4	−8	14	28	32	2
0	5	11	26	25	2	5	−4	12	97	98	1	−1	−13	13	54	51	2	1	−2	13	59	58	1	−4	−7	14	69	64	2
1	5	11	86	83	1	−5	−3	12	115	117	3	0	−13	13	0	9	1	2	−2	13	175	185	2	−3	−7	14	116	115	3
2	5	11	51	47	1	−4	−3	12	200	204	5	−3	−12	13	38	40	2	3	−2	13	141	141	2	−2	−7	14	85	87	2
3	5	11	113	114	1	−3	−3	12	27	29	3	−2	−12	13	22	16	3	4	−2	13	56	52	1	0	−7	14	140	143	3
−2	6	11	66	67	2	−2	−3	12	86	84	1	−1	−12	13	86	80	2	−5	−1	13	134	129	3	1	−7	14	164	171	4
−1	6	11	39	38	2	−1	−3	12	190	194	3	0	−12	13	64	61	2	−4	−1	13	44	44	2	2	−7	14	79	74	2
0	6	11	92	87	2	0	−3	12	124	127	1	−3	−11	13	56	53	2	−3	−1	13	73	83	2	3	−7	14	47	44	2
1	6	11	59	55	1	1	−3	12	90	95	1	−2	−11	13	124	121	3	−2	−1	13	20	24	3	4	−7	14	33	30	2
2	6	11	100	97	1	2	−3	12	98	102	1	−1	−11	13	77	77	2	−1	−1	13	149	155	3	−4	−6	14	34	34	2
−2	7	11	78	80	2	3	−3	12	46	51	1	0	−11	13	27	22	3	0	−1	13	49	46	1	−3	−6	14	99	97	2
−1	7	11	36	37	2	4	−3	12	37	31	2	3	−11	13	21	25	3	1	−1	13	74	78	1	−2	−6	14	81	87	2
0	7	11	61	61	1	5	−3	12	81	96	1	−3	−10	13	60	63	2	2	−1	13	98	97	1	−1	−6	14	41	47	2
1	7	11	53	50	1	−5	−2	12	179	178	4	−2	−10	13	87	81	2	3	−1	13	153	156	2	0	−6	14	209	203	5
−1	8	11	65	67	2	−4	−2	12	64	62	2	−1	−10	13	36	36	2	4	−1	13	48	46	1	1	−6	14	14	5	9
−2	−13	12	39	38	2	−3	−2	12	29	26	2	0	−10	13	67	69	2	−5	0	13	89	90	2	2	−6	14	36	29	3
−1	−13	12	33	31	2	−2	−2	12	33	29	1	1	−10	13	35	37	2	−4	0	13	10	10	10	3	−6	14	46	45	2
0	−13	12	59	52	2	−1	−2	12	81	83	1	2	−10	13	65	68	2	−3	0	13	60	75	2	4	−6	14	119	115	3
−3	−12	12	27	24	2	0	−2	12	47	46	1	3	−10	13	26	26	3	−2	0	13	14	20	5	−4	−5	14	63	63	2
−2	−12	12	67	66	2	1	−2	12	104	105	1	−3	−9	13	45	43	2	−1	0	13	159	153	4	−3	−5	14	76	69	2
−1	−12	12	17	15	4	2	−2	12	139	140	1	−2	−9	13	138	141	3	0	0	13	37	39	3	−2	−5	14	154	173	4
0	−12	12	62	61	2	3	−2	12	37	41	1	−1	−9	13	55	62	2	1	0	13	28	30	2	1	−5	14	60	54	3
−3	−11	12	72	67	2	4	−2	12	42	40	1	0	−9	13	98	99	3	2	0	13	116	121	1	2	−5	14	46	51	3
−2	−11	12	60	63	2	5	−2	12	95	91	2	1	−9	13	31	26	2	3	0	13	75	72	1	3	−5	14	98	100	3
−1	−11	12	40	46	2	−5	−1	12	88	88	2	2	−9	13	139	144	4	4	0	13	21	18	1	4	−5	14	25	24	2
−5	−4	14	49	49	2	3	1	14	8	8	8	3	−6	15	52	50	2	0	3	15	113	106	3	−3	−2	16	108	102	2
−4	−4	14	64	65	2	−4	2	14	92	85	2	−4	−5	15	86	85	2	1	3	15	65	58	2	−2	−2	16	66	63	2
−2	−4	14	110	123	3	−3	2	14	44	41	2	−3	−5	15	125	120	3	−2	−11	16	85	85	2	−1	−2	16	65	64	2
−1	−4	14	126	138	3	−2	2	14	30	35	2	−1	−5	15	107	107	3	−1	−11	16	45	44	2	0	−2	16	99	101	3
0	−4	14	331	325	8	−1	2	14	42	41	3	1	−5	15	179	181	4	−2	−10	16	123	121	3	1	−2	16	87	83	2
1	−4	14	186	190	4	0	2	14	38	43	3	2	−5	15	23	25	4	−1	−10	16	124	116	2	2	−2	16	26	23	3
2	−4	14	69	63	2	1	2	14	35	35	2	3	−5	15	39	39	2	0	−10	16	21	17	3	3	−2	16	34	35	2

TABLE 7-continued

Observed and calculated structure factors for NEL

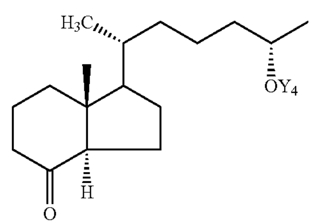
h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	−4	14	41	40	2	2	2	14	38	37	1	−4	−4	15	46	43	2	−3	−9	16	55	58	2	−3	−1	16	44	44	2
4	−4	14	80	77	1	−1	3	14	34	29	3	−3	−4	15	71	73	2	−2	−9	16	69	65	2	−2	−1	16	39	40	2
−5	−3	14	10	15	10	0	3	14	22	18	3	−1	−4	15	87	87	2	−1	−9	16	42	37	2	0	−1	16	130	127	3
−4	−3	14	58	56	2	1	3	14	64	61	1	0	−4	15	46	44	2	0	−9	16	36	31	2	1	−1	16	49	45	2
−3	−3	14	196	197	4	2	3	14	61	54	1	2	−4	15	41	42	2	−3	−8	16	53	44	2	2	−1	16	73	69	2
−1	−3	14	121	125	3	−1	4	14	80	82	2	3	−4	15	57	54	2	−2	−8	16	62	61	2	0	0	16	128	125	3
0	−3	14	238	244	5	0	4	14	41	38	1	−4	−3	15	54	53	2	−1	−8	16	20	22	3	1	0	16	94	91	2
1	−3	14	228	227	5	1	4	14	16	12	3	−3	−3	15	9	13	8	0	−8	16	61	57	2	0	1	16	59	59	2
2	−3	14	145	149	6	0	5	14	39	49	2	−2	−3	15	106	121	3	2	−8	16	67	64	2	1	1	16	17	21	3
3	−3	14	19	18	3	−1	−12	15	74	67	2	−1	−3	15	199	198	5	−4	−7	16	59	59	2	0	2	16	38	37	2
4	−3	14	69	67	2	−2	−11	15	30	27	2	1	−3	15	62	58	2	−3	−7	16	38	35	2	−1	−10	17	26	20	2
−5	−2	14	22	21	3	−1	−11	15	95	87	2	2	−3	15	83	75	2	−2	−7	16	93	86	2	−2	−9	17	68	64	2
−4	−2	14	20	16	3	0	−11	15	41	37	2	3	−3	15	84	81	2	−1	−7	16	107	106	2	−1	−9	17	49	49	2
−3	−2	14	69	76	2	−3	−10	15	105	100	2	−4	−2	15	59	55	2	0	−7	16	30	33	2	−3	−8	17	18	18	3
−1	−2	14	91	88	2	−2	−10	15	61	62	2	−3	−2	15	39	39	2	2	−7	16	23	25	3	−2	−8	17	30	30	2
0	−2	14	226	229	4	−1	−10	15	49	46	2	−2	−2	15	72	75	2	3	−7	16	74	76	2	−1	−8	17	76	75	2
1	−2	14	95	93	2	0	−10	15	57	56	2	−1	−2	15	87	83	2	−4	−6	16	58	62	2	−3	−7	17	14	16	4
2	−2	14	103	108	1	2	−10	15	60	60	2	0	−2	15	51	47	2	−3	−6	16	34	34	2	−2	−7	17	29	30	2
3	−2	14	46	44	1	−3	−9	15	54	52	2	1	−2	15	76	74	2	−2	−6	16	18	14	3	−1	−7	17	17	17	3
4	−2	14	43	46	1	−2	−9	15	112	107	3	3	−2	15	56	54	2	−1	−6	16	92	90	2	−3	−6	17	24	19	2
−5	−1	14	25	24	2	−1	−9	15	55	56	2	−4	−1	15	29	28	2	0	−6	16	120	118	3	−2	−6	17	69	68	2
−4	−1	14	11	19	10	0	−9	15	65	60	2	−3	−1	15	73	75	2	1	−6	16	42	42	3	−1	−6	17	104	108	2
−3	−1	14	109	116	3	2	−9	15	34	37	3	−2	−1	15	96	96	2	2	−6	16	89	87	2	2	−6	17	78	78	2
−2	−1	14	95	101	2	3	−9	15	43	43	2	−1	−1	15	71	69	2	3	−6	16	42	41	2	−3	−5	17	19	17	3
−1	−1	14	7	7	6	−4	−8	15	107	102	2	0	−1	15	40	38	3	−4	−5	16	52	53	2	−2	−5	17	37	34	2
0	−1	14	50	51	3	−3	−8	15	91	86	2	1	−1	15	92	98	2	−3	−5	16	87	88	2	−1	−5	17	59	60	2
1	−1	14	69	72	1	−2	−8	15	82	78	2	2	−1	15	64	64	1	−2	−5	16	57	56	2	1	−5	17	37	36	3
2	−1	14	57	60	1	−1	−8	15	33	27	2	3	−1	15	34	33	2	−1	−5	16	46	46	2	2	−5	17	43	39	2
3	−1	14	26	24	2	0	−8	15	122	122	3	−4	0	15	0	9	1	1	−5	16	96	96	3	−3	−4	17	10	9	9
4	−1	14	20	27	2	2	−8	15	42	44	2	−3	0	15	32	28	2	2	−5	16	26	20	3	−2	−4	17	52	51	2
−5	0	14	74	67	2	3	−8	15	89	85	2	−2	0	15	127	131	3	3	−5	16	40	35	2	−1	−4	17	17	16	4
−4	0	14	68	66	2	−4	−7	15	40	40	2	0	0	15	26	26	3	−4	−4	16	23	26	3	1	−4	17	48	46	2
−3	0	14	111	111	3	−3	−7	15	67	69	2	1	0	15	10	7	9	−3	−4	16	56	56	2	2	−4	17	50	51	2
−2	0	14	98	101	2	−2	−7	15	58	58	2	2	0	15	55	56	1	−2	−4	16	21	22	3	−3	−3	17	32	34	2
−1	0	14	46	46	2	−1	−7	15	50	52	2	3	0	15	34	40	2	−1	−4	16	98	96	2	−2	−3	17	13	7	6
0	0	14	87	86	2	0	−7	15	55	54	2	−4	1	15	23	27	3	1	−4	16	46	43	2	1	−3	17	40	35	2
1	0	14	64	63	1	2	−7	15	128	127	3	−2	1	15	7	11	6	2	−4	16	37	31	2	2	−3	17	49	48	2
2	0	14	125	128	2	3	−7	15	35	31	2	0	1	15	37	36	3	3	−4	16	0	10	1	−2	−2	17	50	49	2
3	0	14	11	10	6	−4	−6	15	110	107	2	1	1	15	72	65	1	−4	−3	16	72	71	2	2	−2	17	63	61	2
−4	1	14	57	52	2	−3	−6	15	86	84	2	2	1	15	45	47	1	−3	−3	16	15	14	5	0	0	17	30	35	3
−3	1	14	43	42	2	−2	−6	15	38	42	2	−1	2	15	50	51	2	−2	−3	16	35	32	2	−2	−6	18	12	11	6
−2	1	14	114	117	3	−1	−6	15	27	24	2	0	2	15	110	103	3	−1	−3	16	51	51	2						
0	1	14	55	53	2	0	−6	15	158	158	4	1	2	15	58	60	1	2	−3	16	59	60	2						
1	1	14	69	69	1	1	−6	15	66	68	2	2	2	15	21	21	2	3	−3	16	26	29	3						
2	1	14	85	82	1	2	−6	15	46	52	2	−1	3	15	48	48	2	−4	−2	16	28	28	2						

EXAMPLE 3

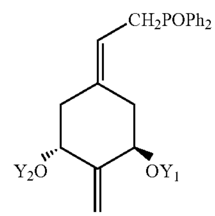
Synthesis of NEL

The preparation of NEL having the basic structure I can be accomplished by a common general method, i.e. the condensation of a bicyclic Windaus-Grundmann type ketone II with the allylic phosphine oxide III to the corresponding 2-methylene-19-nor-vitamin D analog IV followed by deprotection at C-1, C-3 and C-25 in the latter compound IV to obtain compound I, i.e. NEL.

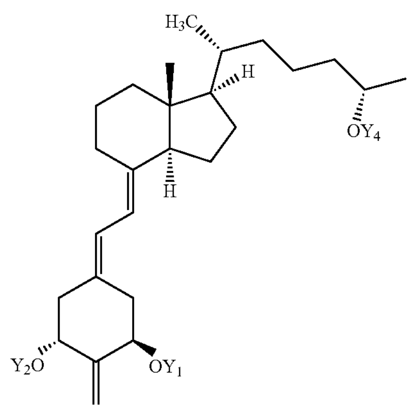
II



III



IV



In ketone II, Y_4 is preferably a hydroxy-protecting group such as a silyl protecting group. The t-butyldimethyl-silyl (TBDMS) group is an example of a particularly useful hydroxy-protecting group. In phosphine oxide III, Y_1 and Y_2 are preferably hydroxy-protecting groups such as silyl protecting groups. The t-butyldimethylsilyl (TMDMS) group is an example of a particularly useful hydroxy-protecting group. The process described above represents an application of the convergent synthesis concept, which has been applied effectively to the preparation of numerous vitamin D compounds (see Lythgoe et al., *J. Chem. Soc. Perkin Trans. I,* 590 (1978); Lythgoe, *Chem. Soc. Rev.* 9, 449 (1983); Toh et al., *J. Org. Chem.* 48, 1414 (1983); Baggiolini et al., *J. Org. Chem.* 51, 3098 (1986); Sardina et al., *J. Org. Chem.* 51, 1264 (1986); *J. Org. Chem.* 51, 1269 (1986); DeLuca et al., U.S. Pat. No. 5,086,191; DeLuca et al., U.S. Pat. No. 5,536,713; and DeLuca et al, U.S. Pat. No. 5,843,928 all of which are hereby incorporated by reference in their entirety and for all purposes as if fully set forth herein.

Phosphine oxide III is a convenient reagent that can be used to prepare a large number of 19-nor-vitamin D compounds and is prepared according to the procedures described by Sicinski et al., *J. Med. Chem.,* 41, 4662 (1998), DeLuca et al., U.S. Pat. No. 5,843,928; Perlman et al., *Tetrahedron Lett.* 32, 7663 (1991); and DeLuca et al., U.S. Pat. No. 5,086,191 which, are hereby incorporated by reference in their entirety as if fully set forth herein.

The overall process of the synthesis of compound I is illustrated and described more completely in U.S. Pat. No. 5,843,928 entitled "2-Alkylidene-19-Nor-Vitamin D Compounds" and in U.S. Pat. No. 7,528,122 entitled "Vitamin D Analog—NEL, Methods and Uses Thereof," the specifications of which are specifically incorporated herein by reference.

We claim:

1. (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 in crystalline form.

2. The crystalline form of (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 having molecular packing arrangement defined by space group P1 and unit cell dimensions a=6.4 Å, b=12.6 Å, c=16.0 Å, α=110.9°, β=95.3° and γ=90.6°.

3. A three dimensional structure for (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 as defined by the molecular packing arrangement set forth in claim **2**.

4. A method of purifying (20R,25S)-2-methylene-19,26-dinor, 1α,25-dihydroxyvitamin D_3, comprising the steps of:

(a) preparing a solvent comprising water and methanol;

(b) dissolving a product containing (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 to be purified in said solvent;

(c) cooling said solvent and dissolved product below ambient temperature for a sufficient amount of time to form a precipitate of (20R,25S)-2-methylene-19,26-dinor-1α, 25-dihydroxyvitamin D_3 crystals; and

(d) separating the (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 crystals from the solvent.

5. The method of claim **4** including the further step of maintaining said solvent and dissolved product at ambient temperature for a period of time prior to cooling below ambient temperature.

6. The method of claim **4** wherein said solvent comprises 20% water and 80% methanol, by volume.

7. The method of claim **4** wherein said solvent and dissolved product are cooled to about −20° C.

8. The method of claim **4** wherein the step of separating comprises filtering the solvent and precipitate to obtain the crystals.

9. The method of claim **4** including a further step (e) comprising repeating steps (a) through (d) using the recovered crystals from step (d) as the product of step (b).

10. The method of claim **7** wherein said solvent and dissolved product are maintained at −20° C. for up to 7 weeks.

11. A method of purifying (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3, comprising the steps of

(a) preparing a solvent comprising 80% methanol and 20% water, by volume;

(b) dissolving a product containing (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 to be purified in said solvent;

(c) cooling said solvent and dissolved product below ambient temperature for a sufficient amount of time to form a precipitate of (20R,25S)-2-methylene-19,26-dinor-1α, 25-dihydroxyvitamin D_3 crystals; and

(d) recovering the (20R,25S)-2-methylene-19,26-dinor-1α,25-dihydroxyvitamin D_3 crystals having a molecular packing arrangement defined by space group P1 and unit cell dimensions a=6.4 Å, b=12.6 Å c=16.0 Å, α=110.9°, β=95.3° and γ=90.6°, or any other space group that yields substantially the same crystalline packing arrangement.

12. The method of claim **11** wherein said solvent and dissolved product is maintained at ambient temperature for a period of time prior to cooling below ambient temperature.

13. The method of claim **11** wherein said solvent and dissolved product are cooled to about −20° C.

14. The method of claim **13** wherein said solvent and dissolved product are maintained at about −20° C. for up to 7 weeks.

15. The method of claim **11** wherein the step of recovering comprises filtering.

16. The method of claim **11** further including the step of (e) repeating steps (a) through (d) using the recovered crystals from step (d) as the product of step (b).

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