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DeLuca et al.

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(54) **CRYSTALLIZATION OF (20R) AND (20S) ANALOGS OF 2-METHYLENE-19-NOR-24-DIMETHYL-1α,25-DIHYDROXYVITAMIN D_3**

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C07C 401/00 (2006.01)

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CPC ***C07C 401/00*** (2013.01); *C07B 2200/13* (2013.01)
USPC **552/653**

(58) **Field of Classification Search**
USPC 552/653
See application file for complete search history.

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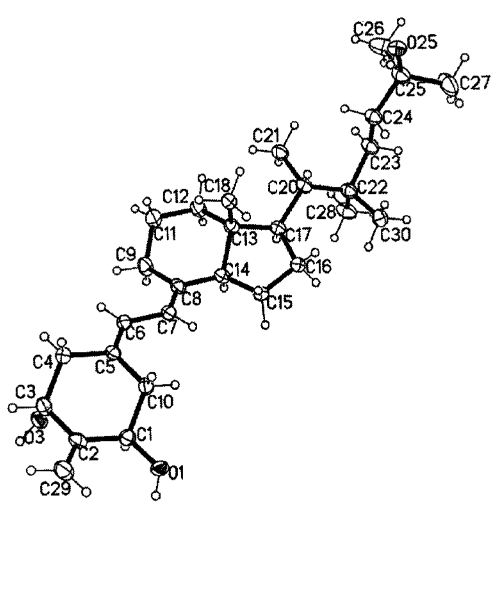
(57) **ABSTRACT**

Disclosed are methods of purifying (20R) and (20S) analogs of 2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 to obtain the (20R) and (20S) analogs in crystalline form. The method includes the steps of preparing a solvent of either diethyl ether or a mixture of 2-propanol and hexane, dissolving a product containing the (20R) and (20S) analog 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 crystals, and recovering the crystals.

17 Claims, 2 Drawing Sheets



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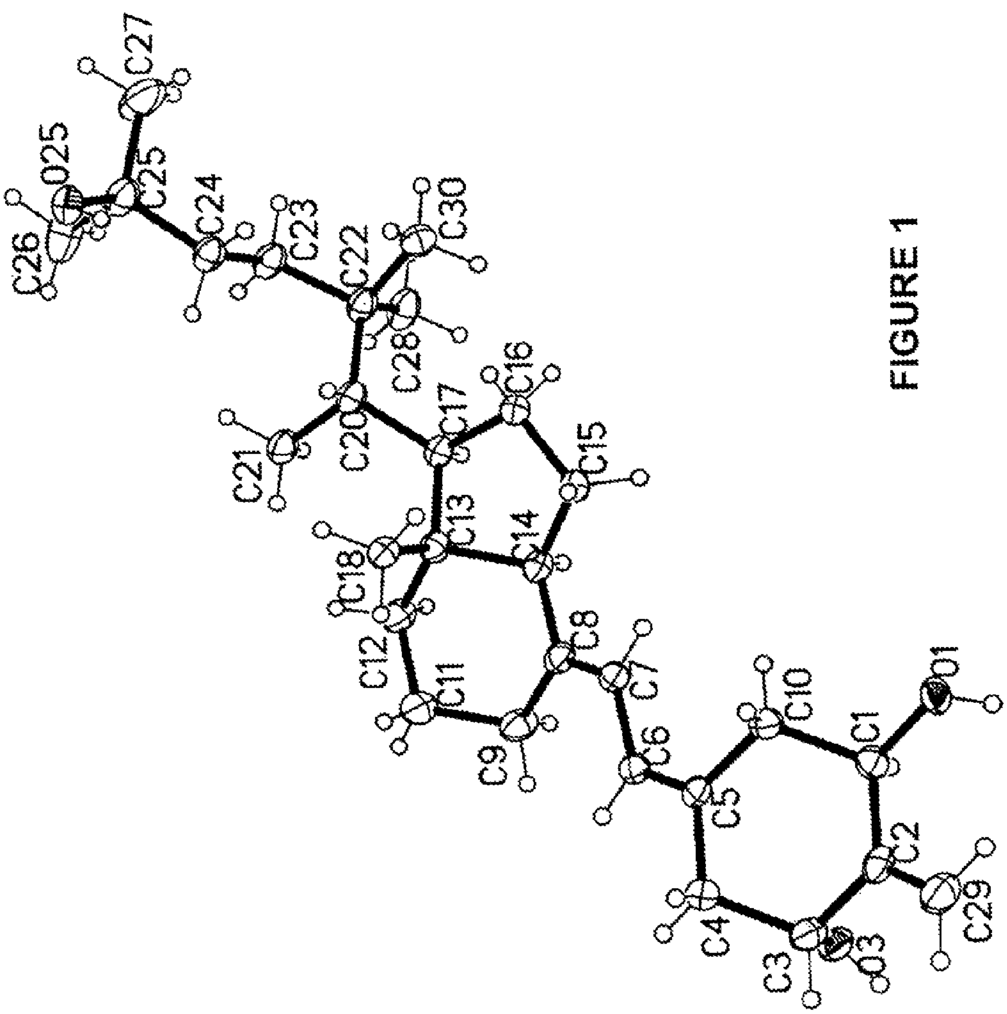
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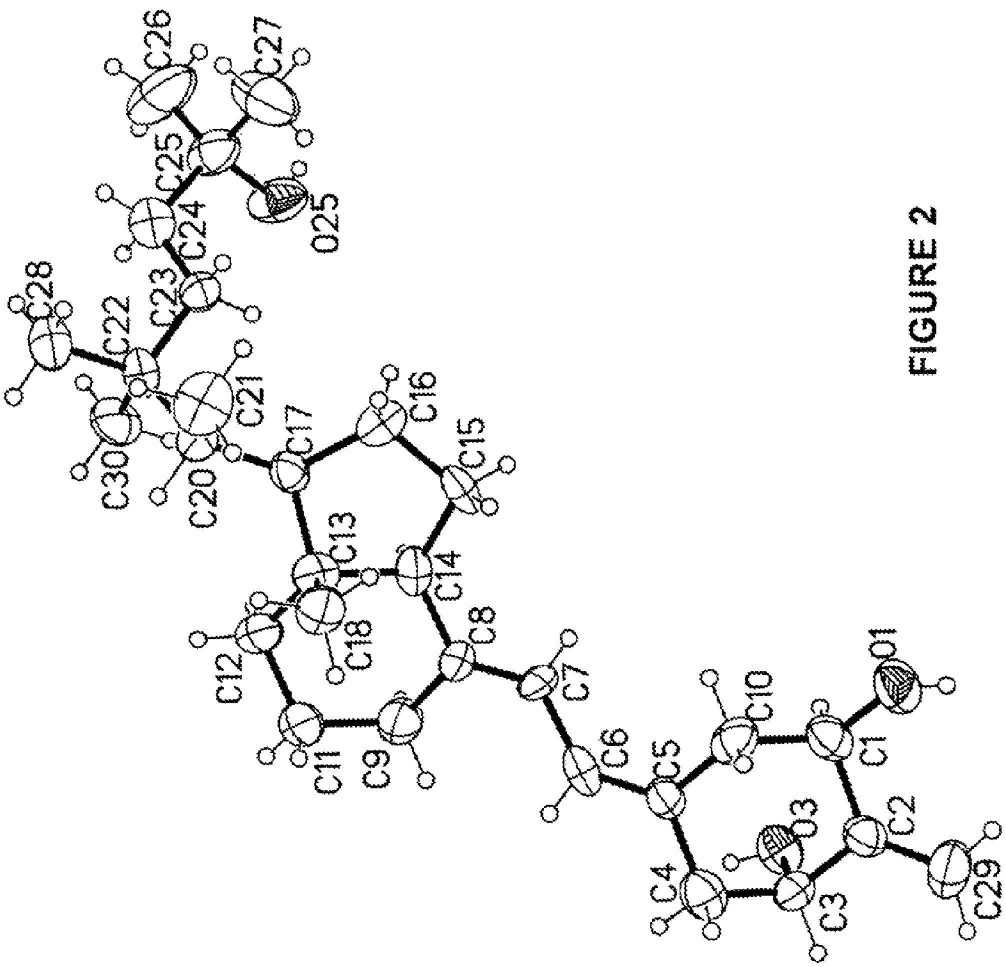
FIGURE 1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C6
C5
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O3
C2
C4
C3
C29

FIGURE 2

CRYSTALLIZATION OF (20R) AND (20S) ANALOGS OF 2-METHYLENE-19-NOR-24-DIMETHYL-1α,25-DIHYDROXYVITAMIN D_3

CROSS-REFERENCE TO RELATED PATENT APPLICATIONS

The present application claims the benefit under 35 U.S.C. §119(e) to U.S. Provisional Patent Application No. 61/652,965, filed on May 30, 2012, the content of which is incorporated herein by reference in its entirety.

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

The field of the present invention relates to purification of organic compounds, and more particularly to the purification of (20S) and (20R) analogs of 2-Methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 (referred to herein as "MET-1" and "MET-2" respectively) by preparing them 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 the 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 pre-vitamin D compound, followed by cycloreversion of the modified adduct under basic conditions, (see 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 pre-vitamin 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., *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 1α-hydroxy 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. The driving force for these reactions is the 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 1α-hydroxyvitamin D compounds, although showing consistent spectroscopic data that suggests homogeneity, do not meet the purity criteria required for therapeutic agents that can be orally, parenterally or transdermally administered. Therefore, it is evident that a suitable method of purification of the 1α-hydroxylated vitamin D compounds MET-1 and MET-2 is required.

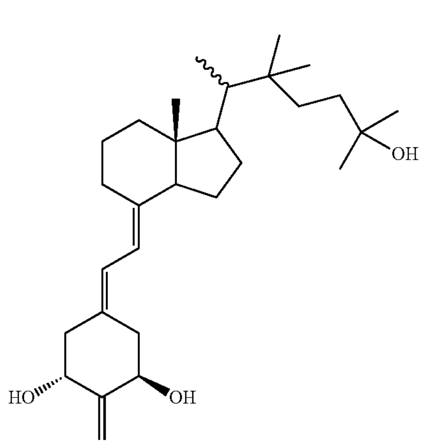
SUMMARY

Disclosed are methods of purifying MET-1 and MET-2 by means of crystallization to obtain MET-1 and MET-2 in crystalline form. The solvent plays an important role in the crystallization process, and is typically an individual liquid substance or a suitable mixture of different liquids. For crystallizing MET-1 and MET-2, 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 as the sole solvent for crystallization of MET-1 and MET-2. However, it was found that diethyl ether (Et_2O) was most useful for the crystallization of MET-1, and a mixture of 2-propanol and hexane, was most useful for the crystallization of MET-2. In particular, it was determined that a mixture of about 10% to about 20% 2-propanol with about 90% to about 80% hexane by volume, (preferably 15% 2-propanol with about 85% hexane by volume) performed well. The diethyl ether solvent and the 2-propanol/hexane solvent mixture both were easy to remove by evaporation or other well-known methods. In all cases the crystallization process occurred easily and efficiently. The precipitated crystals were sufficiently large to assure their recovery by filtration or other means, and thus were suitable for x-ray analysis.

Accordingly, disclosed is a compound having the formula:



in crystalline form, where the wavy line at carbon 20 indicates the methyl group attached to carbon 20 may be in its R or S orientation. More specifically, disclosed are (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 in crystalline form (otherwise referred to as "MET-1"), and (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 in crystalline form, (otherwise referred to as "MET-2").

BRIEF DESCRIPTION OF THE DRAWINGS

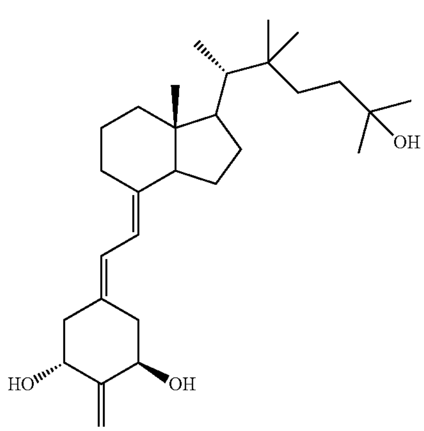
FIG. **1** is an illustration of the three dimensional molecular structure for MET-1 as defined by the atomic positional parameters discovered and set forth herein.

FIG. **2** is an illustration of the three dimensional molecular structure for MET-2 as defined by the atomic positional parameters discovered and set forth herein.

DETAILED DESCRIPTION

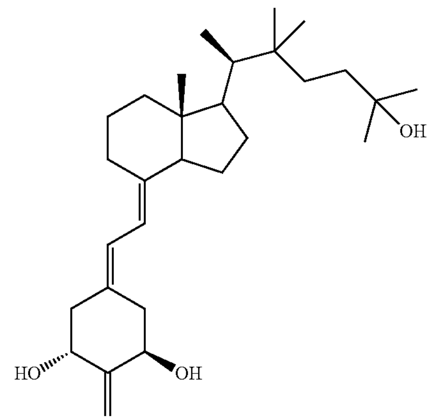
Disclosed herein is (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D3 (MET-1) in crystalline form, which is a pharmacologically important compound characterized by the formula I shown below:

I



Also disclosed herein is (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D3 (MET-2) in crystalline form, which also is a pharmacologically important compound characterized by the formula II shown below:

II



Also disclosed herein are methods of purifying MET-1 and MET-2. The purification technique typically involves obtaining the MET-1 and MET-2 products in crystalline form by utilizing a crystallization procedure wherein the material to be purified is dissolved using as the solvent either diethyl ether (Et_2O) as the sole solvent to obtain MET-1, or a mixture comprised of 2-propanol and hexane to obtain MET-2. In particular, it was determined that a mixture of about 10% to about 20% 2-propanol (v/v) with about 90% to about 80% hexane (v/v) performed well. Preferably the mixture comprises about 15% 2-propanol (v/v) and about 85% hexane (v/v). Thereafter, the solvent can be removed by evaporation, with or without vacuum, or other means as is well-known in the art. Alternatively, the resultant crystals may be filtered from the mother liquor. The technique can be used to purify a wide range of final products containing MET-1 and MET-2 obtained from any known synthesis thereof, and in varying concentrations, which may range from microgram amounts to kilogram amounts. As is well known to those skilled in this art, the amount of solvent utilized should be modulated according to the amount of MET-1 and MET-2 to be purified.

EXAMPLES

The following examples are illustrative and should not be interpreted as limiting the claimed subject matter.

The usefulness and advantages of the present crystallization procedure is shown in the following specific Examples. After crystallization, the precipitated material was observed under a microscope to confirm its crystalline form. Yields of crystals were relatively high and the obtained crystals showed a relatively sharp melting point of 99° C. (MET-1) and 154° C. (MET-2).

The described crystallization process of the synthetic MET-1 and MET-2 products represents a valuable purification method, which can remove most side products derived from the synthetic path. Such impurity may result from contamination of starting raw materials. The crystallization process occurred easily and efficiently. The precipitated crystals were sufficiently large to assure their recovery by filtration, or other means, and thus were suitable for x-ray analysis.

Example 1

Crystallization of (20S)-2-methylene-19-nor-22-dimethyl-1α,25 dihydroxyvitamin D_3 (MET-1)

Crystallization from Diethyl Ether.

(20 S2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 (MET-1) (14.3 mg), was dissolved in boiling

diethyl ether (3 mL) and left at room temperature for about 1 hour, then it was kept in a refrigerator for about 48 hours. The precipitated crystals were filtered off, washed with a small volume of a cold (0° C.) diethyl ether, and dried to give crystalline material.

Experimental.

A colorless prism-shaped crystal of dimensions 0.25×0.34×0.55 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 CuK radiation (1.54178 Å) from a Rigaku RU200 x-ray generator equipped with Montel optics, operated at 50 kV and 90 mA. The x-ray data were processed with SAINT version 7.06A (Broker AXS Inc.) and internally scaled with SADABS version 2005/1 (Broker 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 10-25 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 3265 peaks in the range of 4.0<theta<55°. The data were merged to form a set of 4624 independent data with R(int)=0.0287.

The monoclinic space group P2(1) 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, Broker AXS Inc.; (b) *International Tables for Crystallography, Vol. C*, Kluwer: Boston (1995). 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. In addition to the molecule of MET-1, one molecule of diethyl ether was present in the asymmetric unit of the crystalline lattice. A total of 334 parameters were refined against 1 restraint and 4624 data to give wR2=0.0995 and S=1.040 for weights of $w=1/[s^2(F^2)\ (0.0675P)^2]$, where $P=[F_o^2+2F_c^2]/3$. The final R(F) was 0.0332 for the 4624 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 0.238 and −0.201 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 MET-1 as defined by the following physical data and atomic positional parameters described and calculated herein (Tables 1-8) is illustrated in FIG. **1**.

Example 2

Crystallization of (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 (MET-2)

Crystallization from 2-propanol/hexane.

(20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 (22.7 mg), was suspended in hexane (4 mL) and then 2-propanol was added dropwise to the suspension. The mixture was heated in a water bath to dissolve the vitamin, then was left at room temperature for about 1 hour, and finally was kept in a refrigerator for about 48 hours. The precipitated crystals were filtered off, washed with a small volume of a cold (0° C.) 2-propanol/hexane (3:1) mixture, and dried to give crystalline material. It should be noted that an excess of 2-propanol should be avoided to get the point of saturation, i.e. only about 1 mole or less of 2-propanol should be added.

Experimental.

A colorless prism-shaped crystal of dimensions 0.36×0.17×0.03 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 CuK radiation (1.54178 Å) from a Rigaku RU200 x-ray generator equipped with Montel optics, operated at 50 kV and 90 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 in a quartz capillary tube and data collected at 298 K. The intensity data were measured as a series of phi and omega oscillation frames each of 1° for 20-40 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 2.51<theta<58.69°. The data were merged to form a set of 3985 independent data with R(int)=0.0473.

The monoclinic space group C2 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). 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. In addition to the molecule of MET-2, one molecule of isopropanol was present in the asymmetric unit of the crystalline lattice. A total of 325 parameters were refined against 1 restraint and 3985 data to give wR2=0.1600 and S=1.073 for weights of $w=1/[s^2(F^2)+(0.1033P)^2]$, where $P=[F_o^2+2F_c^2]/3$. The final R(F) was 0.0844 for the 3985 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 0.140 and −0.190 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 MET-2 as defined by the following physical data and atomic positional parameters described and calculated herein (Tables 9-16) is illustrated in FIG. **2**.

TABLE 1

Crystal data and structure refinement for MET-1.

Empirical formula	C33H58O4	
Formula weight	518.79	
Temperature	100(1) K	
Wavelength	1.54178 Å	
Crystal system, space group	Monoclinic, P2(1)	
Unit cell dimensions	a = 7.5780(15)Å	α = 90°
	b = 14.792(3) Å	β = 102.22(3)°
	c = 14.481(3) Å	γ = 90°
Volume	1586.5(6) Å^3	
Z	2	
Calculated density	1.086 Mg/m^3	
Absorption coefficient	0.532 mm^{-1}	
F(000)	576	
Crystal size	0.25 × 0.34 × 0.55 mm	
Theta range for data collection	3.12 to 63.06°	
Limiting indices	−8 <= h <= 8, −17 <= k <= 16, 0 <= l <= 16	

TABLE 1-continued

Crystal data and structure refinement for MET-1.	
Reflections collected/unique	7564/4624 [R(int) = 0.0287]
Data/restraints/parameters	4624/1/334
Goodness-of-fit on F^2	1.040
Final R indices [I > 2□(I)]	R1 = 0.0330, wR2 = 0.0955
R indices (all data)	R1 = 0.0332, wR2 = 0.0959
Absolute structure parameter	−0.01(15)
Largest diff. peak and hole	0.238 and −0.201 e/Å^3

TABLE 2

Atomic coordinates (Å^2 × 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for MET-1 U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(3)	−1435(2)	3847(1)	11389(1)	26(1)
O(100)	−1576(2)	5643(1)	10959(1)	32(1)
O(25)	−4404(2)	−6333(1)	12194(1)	27(1)
O(1)	3382(2)	2361(1)	11284(1)	28(1)
C(5)	−1471(2)	1831(1)	11117(1)	22(1)
C(13)	−3621(2)	−1411(1)	13186(1)	22(1)
C(6)	−2465(2)	1391(1)	11638(1)	23(1)
C(20)	−3217(2)	−3144(1)	13759(1)	23(1)
C(14)	−2234(2)	−617(1)	13380(1)	23(1)
C(2)	716(2)	3237(1)	10539(1)	24(1)
C(22)	−2071(2)	−3839(1)	14466(1)	27(1)
C(7)	−1882(2)	618(1)	12255(1)	23(1)
C(4)	−2313(2)	2542(1)	10414(1)	24(1)
C(8)	−2850(2)	217(1)	12818(1)	24(1)
C(23)	−2980(2)	−4791(1)	14332(1)	28(1)
C(3)	−1246(2)	3423(1)	10520(1)	25(1)
C(21)	−5206(2)	−3181(1)	13826(1)	30(1)
C(24)	−3359(2)	−5161(1)	13320(1)	27(1)
C(1)	1560(2)	2561(1)	11290(1)	23(1)
C(10)	502(2)	1670(1)	11152(1)	22(1)
C(15)	−456(2)	−1058(1)	13319(1)	26(1)
C(12)	−5392(2)	−1054(1)	13413(1)	28(1)
C(9)	−4631(2)	555(1)	12982(1)	29(1)
C(17)	−2546(2)	−2145(1)	13863(1)	22(1)
C(101)	−280(3)	6264(1)	11455(1)	40(1)
C(29)	1591(3)	3619(1)	9940(1)	31(1)
C(30)	−125(2)	−3978(1)	14326(1)	31(1)
C(16)	−580(2)	−2012(1)	13723(1)	25(1)
C(18)	−3930(2)	−1723(1)	12152(1)	24(1)
C(11)	−6056(2)	−197(1)	12851(1)	29(1)
C(25)	−3972(3)	−6149(1)	13189(1)	31(1)
C(201)	−3380(3)	6000(1)	10736(1)	38(1)
C(27)	−2516(4)	−6804(2)	13656(2)	65(1)
C(28)	−1941(3)	−3553(1)	15498(1)	35(1)
C(202)	−4591(3)	5306(2)	10178(2)	48(1)
C(26)	−5726(3)	−6301(2)	13518(1)	50(1)
C(102)	1535(3)	5832(2)	11596(2)	54(1)

TABLE 3

Bond lengths [Å] for MET-1.

O(3)—C(3)	1.440(2)	O(100)—C(101)	1.423(2)
O(100)—C(201)	1.437(2)	O(25)—C(25)	1.435(2)
O(1)—C(1)	1.4140(19)	C(5)—C(6)	1.342(2)
C(5)—C(10)	1.504(2)	C(5)—C(4)	1.508(2)
C(13)—C(18)	1.537(2)	C(13)—C(12)	1.542(2)
C(13)—C(14)	1.561(2)	C(13)—C(17)	1.570(2)
C(6)—C(7)	1.461(2)	C(20)—C(21)	1.532(2)
C(20)—C(17)	1.559(2)	C(20)—C(22)	1.575(2)
C(14)—C(8)	1.497(2)	C(14)—C(15)	1.516(2)
C(2)—C(29)	1.325(2)	C(2)—C(3)	1.506(2)
C(2)—C(1)	1.516(2)	C(22)—C(28)	1.536(2)
C(22)—C(30)	1.544(2)	C(22)—C(23)	1.562(2)
C(7)—C(8)	1.345(2)	C(4)—C(3)	1.524(2)
C(8)—C(9)	1.505(2)	C(23)—C(24)	1.533(2)
C(24)—C(25)	1.532(2)	C(1)—C(10)	1.533(2)

TABLE 3-continued

Bond lengths [Å] for MET-1.

C(15)—C(16)	1.539(2)	C(12)—C(11)	1.532(2)
C(9)—C(11)	1.534(2)	C(17)—C(16)	1.558(2)
C(101)—C(102)	1.491(3)	C(25)—C(27)	1.516(3)
C(25)—C(26)	1.521(3)	C(201)—C(202)	1.495(3)

TABLE 4

Bond angles [°] for MET-1.

C(101)—O(100)—C(201)	113.47(15)
C(6)—C(5)—C(10)	125.17(14)
C(6)—C(5)—C(4)	120.68(15)
C(10)—C(5)—C(4)	114.14(13)
C(18)—C(13)—C(12)	110.52(13)
C(18)—C(13)—C(14)	111.04(12)
C(12)—C(13)—C(14)	106.64(13)
C(18)—C(13)—C(17)	110.70(13)
C(12)—C(13)—C(17)	117.67(13)
C(14)—C(13)—C(17)	99.63(12)
C(5)—C(6)—C(7)	126.18(15)
C(21)—C(20)—C(17)	109.44(13)
C(21)—C(20)—C(22)	110.45(13)
C(17)—C(20)—C(22)	115.60(13)
C(8)—C(14)—C(15)	120.05(14)
C(8)—C(14)—C(13)	113.68(13)
C(15)—C(14)—C(13)	103.82(13)
C(29)—C(2)—C(3)	122.61(16)
C(29)—C(2)—C(1)	123.89(16)
C(3)—C(2)—C(1)	113.49(13)
C(28)—C(22)—C(30)	107.31(14)
C(28)—C(22)—C(23)	107.77(13)
C(30)—C(22)—C(23)	105.76(14)
C(28)—C(22)—C(20)	111.43(14)
C(30)—C(22)—C(20)	114.34(13)
C(23)—C(22)—C(20)	109.89(13)
C(8)—C(7)—C(6)	125.67(15)
C(5)—C(4)—C(3)	112.89(14)
C(7)—C(8)—C(14)	123.11(15)
C(7)—C(8)—C(9)	124.84(15)
C(14)—C(8)—C(9)	112.04(14)
C(24)—C(23)—C(22)	115.43(13)
O(3)—C(3)—C(2)	110.16(13)
O(3)—C(3)—C(4)	108.15(12)
C(2)—C(3)—C(4)	110.21(13)
C(25)—C(24)—C(23)	116.71(14)
O(1)—C(1)—C(2)	113.40(13)
O(1)—C(1)—C(10)	107.71(12)
C(2)—C(1)—C(10)	110.12(13)
C(5)—C(10)—C(1)	110.88(13)
C(14)—C(15)—C(16)	104.17(13)
C(11)—C(12)—C(13)	111.93(13)
C(8)—C(9)—C(11)	111.72(14)
C(20)—C(17)—C(16)	114.06(13)
C(20)—C(17)—C(13)	118.64(13)
C(16)—C(17)—C(13)	102.46(12)
O(100)—C(101)—C(102)	108.10(16)
C(15)—C(16)—C(17)	107.60(13)
C(12)—C(11)—C(9)	113.01(14)
O(25)—C(25)—C(27)	108.39(16)
O(25)—C(25)—C(26)	104.95(14)
C(27)—C(25)—C(26)	111.5(2)
O(25)—C(25)—C(24)	107.75(13)
C(27)—C(25)—C(24)	112.43(16)
C(26)—C(25)—C(24)	111.40(16)
O(100)—C(201)—C(202)	108.38(16)

TABLE 5

Anisotropic displacement parameters ($Å^2 \times 10^3$) for MET-1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(3)	26(1)	17(1)	37(1)	0(1)	10(1)	1(1)
O(100)	40(1)	19(1)	37(1)	2(1)	9(1)	3(1)
O(25)	28(1)	28(1)	26(1)	−2(1)	6(1)	−7(1)
O(1)	17(1)	23(1)	44(1)	−6(1)	8(1)	−2(1)
C(5)	21(1)	16(1)	27(1)	−4(1)	4(1)	−2(1)
C(13)	23(1)	21(1)	24(1)	0(1)	8(1)	−2(1)
C(6)	19(1)	18(1)	32(1)	−2(1)	6(1)	0(1)
C(20)	28(1)	20(1)	23(1)	1(1)	8(1)	−5(1)
C(14)	25(1)	20(1)	25(1)	−2(1)	6(1)	−3(1)
C(2)	27(1)	17(1)	29(1)	−5(1)	7(1)	−4(1)
C(22)	33(1)	22(1)	24(1)	3(1)	4(1)	−6(1)
C(7)	19(1)	18(1)	30(1)	−2(1)	6(1)	−1(1)
C(4)	21(1)	21(1)	30(1)	1(1)	3(1)	1(1)
C(8)	25(1)	18(1)	29(1)	−3(1)	6(1)	−1(1)
C(23)	38(1)	21(1)	25(1)	3(1)	6(1)	−5(1)
C(3)	29(1)	20(1)	28(1)	4(1)	7(1)	2(1)
C(21)	29(1)	23(1)	39(1)	2(1)	11(1)	−6(1)
C(24)	34(1)	22(1)	24(1)	2(1)	6(1)	−4(1)
C(1)	20(1)	22(1)	29(1)	−2(1)	8(1)	0(1)
C(10)	21(1)	20(1)	27(1)	2(1)	7(1)	2(1)
C(15)	20(1)	23(1)	33(1)	3(1)	4(1)	−3(1)
C(12)	29(1)	24(1)	34(1)	1(1)	14(1)	−2(1)
C(9)	30(1)	24(1)	38(1)	2(1)	16(1)	4(1)
C(17)	25(1)	20(1)	20(1)	0(1)	6(1)	−4(1)
C(101)	65(1)	25(1)	29(1)	−1(1)	10(1)	−9(1)
C(29)	33(1)	24(1)	39(1)	3(1)	13(1)	−2(1)
C(30)	33(1)	23(1)	36(1)	9(1)	1(1)	−1(1)
C(16)	22(1)	21(1)	29(1)	2(1)	1(1)	−2(1)
C(18)	25(1)	20(1)	26(1)	0(1)	4(1)	−1(1)
C(11)	25(1)	28(1)	39(1)	3(1)	16(1)	3(1)
C(25)	42(1)	23(1)	25(1)	2(1)	1(1)	−6(1)
C(201)	48(1)	28(1)	44(1)	11(1)	22(1)	15(1)
C(27)	93(2)	25(1)	55(1)	0(1)	−32(1)	8(1)
C(28)	49(1)	29(1)	26(1)	2(1)	4(1)	−12(1)
C(202)	35(1)	46(1)	58(1)	14(1)	2(1)	13(1)
C(26)	75(2)	50(1)	31(1)	−7(1)	23(1)	−34(1)
C(102)	54(1)	41(1)	57(1)	2(1)	−10(1)	−14(1)

TABLE 6

Hydrogen coordinates ($Å^2 \times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for MET-1.

H(3A)	−1246	4391	11360	40
H(25A)	−3854	−5981	11920	41
H(1A)	4033	2763	11559	41
H(6A)	−3636	1598	11604	27
H(20F)	−3157	−3339	13120	28
H(14A)	−2129	−451	14045	28
H(7A)	−743	383	12258	27
H(4A)	−3529	2665	10495	29
H(4B)	−2398	2310	9780	29
H(23A)	−2206	−5217	14739	34
H(23B)	−4112	−4761	14542	34
H(3B)	−1735	3823	9988	30
H(21A)	−5886	−2755	13392	45
H(21B)	−5311	−3033	14458	45
H(21C)	−5668	−3779	13671	45
H(24A)	−4282	−4787	12936	40
H(24B)	−2270	−5094	13075	40
H(1B)	1502	2809	11910	28
H(10F)	646	1386	10569	27
H(10G)	983	1262	11669	27
H(15A)	554	−727	13690	31
H(15B)	−316	−1087	12669	31
H(12A)	−6313	−1518	13267	33
H(12B)	−5200	−923	14084	33
H(9A)	−5058	1043	12544	35
H(9B)	−4464	795	13618	35
H(17A)	−2559	−1957	14511	26
H(10A)	−557	6412	12061	48

TABLE 6-continued

Hydrogen coordinates ($Å^2 \times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for MET-1.

H(10B)	−298	6817	11094	48
H(29A)	994	4020	9485	37
H(29B)	2803	3486	9975	37
H(30A)	485	−4408	14780	47
H(30B)	509	−3412	14411	47
H(30C)	−160	−4201	13700	47
H(16A)	271	−2075	14322	30
H(16B)	−299	−2463	13290	30
H(18A)	−4591	−1267	11750	35
H(18B)	−4607	−2276	12077	35
H(18C)	−2787	−1820	11983	35
H(11A)	−7122	26	13048	35
H(11B)	−6400	−349	12186	35
H(20A)	−3409	6551	10371	46
H(20B)	−3782	6139	11313	46
H(27A)	−1429	−6689	13435	97
H(27B)	−2910	−7412	13498	97
H(27C)	−2288	−6726	14328	97
H(28A)	−1234	−3988	15910	53
H(28B)	−3130	−3522	15627	53
H(28C)	−1377	−2970	15600	53
H(20C)	−5804	5534	10022	71
H(20D)	−4560	4764	10546	71
H(20E)	−4187	5175	9607	71
H(26A)	−6077	−6924	13425	75
H(26B)	−6654	−5923	13161	75
H(26C)	−5554	−6154	14177	75
H(10C)	2433	6241	11927	81
H(10D)	1798	5688	10993	81
H(10E)	1544	5288	11958	

TABLE 7

Torsion angles [deg] for MET-1.

C(10)—C(5)—C(6)—C(7)	−6.9(3)
C(4)—C(5)—C(6)—C(7)	172.04(14)
C(18)—C(13)—C(14)—C(8)	62.64(17)
C(12)—C(13)—C(14)—C(8)	−57.81(17)
C(17)—C(13)—C(14)—C(8)	179.34(12)
C(18)—C(13)—C(14)—C(15)	−69.49(16)
C(12)—C(13)—C(14)—C(15)	170.05(13)
C(17)—C(13)—C(14)—C(15)	47.21(14)
C(21)—C(20)—C(22)—C(28)	−68.60(17)
C(17)—C(20)—C(22)—C(28)	56.32(18)
C(21)—C(20)—C(22)—C(30)	169.50(14)
C(17)—C(20)—C(22)—C(30)	−65.58(18)
C(21)—C(20)—C(22)—C(23)	50.77(17)
C(17)—C(20)—C(22)—C(23)	175.69(13)
C(5)—C(6)—C(7)—C(8)	175.69(16)
C(6)—C(5)—C(4)—C(3)	129.93(16)
C(10)—C(5)—C(4)—C(3)	−50.98(18)
C(6)—C(7)—C(8)—C(14)	175.28(14)
C(6)—C(7)—C(8)—C(9)	−6.4(3)
C(15)—C(14)—C(8)—C(7)	−0.9(2)
C(13)—C(14)—C(8)—C(7)	−124.65(17)
C(15)—C(14)—C(8)—C(9)	−179.41(15)
C(13)—C(14)—C(8)—C(9)	56.87(17)
C(28)—C(22)—C(23)—C(24)	175.53(15)
C(30)—C(22)—C(23)—C(24)	−69.94(18)
C(20)—C(22)—C(23)—C(24)	53.94(19)
C(29)—C(2)—C(3)—O(3)	−116.79(17)
C(1)—C(2)—C(3)—O(3)	64.38(16)
C(29)—C(2)—C(3)—C(4)	123.95(17)
C(1)—C(2)—C(3)—C(4)	−54.88(17)
C(5)—C(4)—C(3)—O(3)	−69.91(16)
C(5)—C(4)—C(3)—C(2)	50.56(17)
C(22)—C(23)—C(24)—C(25)	170.72(15)
C(29)—C(2)—C(1)—O(1)	−1.0(2)
C(3)—C(2)—C(1)—O(1)	177.82(12)
C(29)—C(2)—C(1)—C(10)	−121.76(17)
C(3)—C(2)—C(1)—C(10)	57.05(16)
C(6)—C(5)—C(10)—C(1)	−128.78(16)
C(4)—C(5)—C(10)—C(1)	52.18(17)

TABLE 7-continued

Torsion angles [deg] for MET-1.	
O(1)—C(1)—C(10)—C(5)	−178.02(11)
C(2)—C(1)—C(10)—C(5)	−53.90(16)
C(8)—C(14)—C(15)—C(16)	−163.10(13)
C(13)—C(14)—C(15)—C(16)	−34.78(16)
C(18)—C(13)—C(12)—C(11)	−65.07(17)
C(14)—C(13)—C(12)—C(11)	55.72(17)
C(17)—C(13)—C(12)—C(11)	166.45(14)
C(7)—C(8)—C(9)—C(11)	130.33(18)
C(14)—C(8)—C(9)—C(11)	−51.22(17)
C(21)—C(20)—C(17)—C(16)	−175.23(13)
C(22)—C(20)—C(17)—C(16)	59.33(17)
C(21)—C(20)—C(17)—C(13)	−54.36(17)
C(22)—C(20)—C(17)—C(13)	−179.80(12)
C(18)—C(13)—C(17)—C(20)	−50.06(18)

TABLE 7-continued

Torsion angles [deg] for MET-1.	
C(12)—C(13)—C(17)—C(20)	78.34(18)
C(14)—C(13)—C(17)—C(20)	−167.02(12)
C(18)—C(13)—C(17)—C(16)	76.56(15)
C(12)—C(13)—C(17)—C(16)	−155.04(14)
C(14)—C(13)—C(17)—C(16)	−40.40(14)
C(201)—O(100)—C(101)—C(102)	−177.01(16)
C(14)—C(15)—C(16)—C(17)	8.55(16)
C(20)—C(17)—C(16)—C(15)	150.05(13)
C(13)—C(17)—C(16)—C(15)	20.53(16)
C(13)—C(12)—C(11)—C(9)	−54.82(19)
C(8)—C(9)—C(11)—C(12)	50.78(18)
C(23)—C(24)—C(25)—O(25)	175.01(14)
C(23)—C(24)—C(25)—C(27)	−65.6(2)
C(23)—C(24)—C(25)—C(26)	60.4(2)
C(101)—O(100)—C(201)—C(202)	177.20(15)

TABLE 8

Observed and calculated structure factors for MET-1.

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	−16	0	150	149	2	1	2	0	479	489	5	2	15	0	41	44	1	3	−9	1	37	37	1	4	1	1	139	136	2
1	−16	0	52	52	1	2	2	0	217	210	2	3	15	0	34	36	1	4	−9	1	188	187	3	5	1	1	75	72	1
2	−16	0	77	74	1	3	2	0	118	120	1	4	15	0	95	95	1	5	−9	1	192	181	3	6	1	1	131	124	2
3	−16	0	134	137	2	4	2	0	253	245	3	2	16	0	76	74	1	6	−9	1	3	6	3	7	1	1	154	157	2
1	−15	0	106	109	1	5	2	0	56	51	1	0	−17	1	74	72	1	−6	−8	1	25	23	1	8	1	1	21	20	1
2	−15	0	44	45	1	6	2	0	195	199	3	−3	−16	1	41	39	1	−5	−8	1	142	141	2	−8	2	1	47	49	1
3	−15	0	34	36	1	7	2	0	79	74	1	−2	−16	1	75	77	1	−4	−8	1	24	21	1	−7	2	1	143	145	2
4	−15	0	91	94	1	8	2	0	50	49	1	−1	−16	1	5	5	4	−3	−8	1	44	43	1	−6	2	1	40	38	1
0	−14	0	137	148	1	1	3	0	141	142	1	0	−16	1	51	50	1	−2	−8	1	66	64	1	−5	2	1	46	49	1
1	−14	0	18	16	1	2	3	0	272	281	3	1	−16	1	167	170	1	−1	−8	1	103	98	1	−4	2	1	59	51	1
2	−14	0	98	96	1	3	3	0	252	247	3	2	−16	1	4	6	4	0	−8	1	149	161	3	−3	2	1	448	429	5
3	−14	0	110	106	1	4	3	0	55	60	1	−4	−15	1	112	113	2	1	−8	1	187	189	2	−2	2	1	146	146	1
4	−14	0	22	21	1	5	3	0	70	68	1	−3	−15	1	114	109	1	2	−8	1	160	151	1	−1	2	1	328	333	3
1	−13	0	104	107	1	6	3	0	151	145	2	−2	−15	1	105	99	1	3	−8	1	88	80	1	0	2	1	275	279	4
2	−13	0	74	72	1	7	3	0	72	70	1	−1	−15	1	63	66	1	4	−8	1	203	198	3	1	2	1	372	371	4
3	−13	0	102	95	1	8	3	0	30	33	1	0	−15	1	57	53	1	5	−8	1	115	116	2	2	2	1	189	195	2
4	−13	0	123	117	2	0	4	0	924	916	22	1	−15	1	39	39	1	6	−8	1	27	27	1	3	2	1	167	170	2
5	−13	0	41	42	1	1	4	0	319	318	4	2	−15	1	72	73	1	−4	−7	1	268	270	5	4	2	1	66	71	1
0	−12	0	43	42	1	2	4	0	399	410	4	3	−15	1	48	46	1	−3	−7	1	110	109	1	5	2	1	63	65	1
1	−12	0	76	72	1	3	4	0	250	245	3	−5	−14	1	57	62	1	−2	−7	1	153	142	1	6	2	1	123	120	2
2	−12	0	67	63	1	4	4	0	87	81	1	−4	−14	1	66	72	1	−1	−7	1	391	378	5	7	2	1	130	133	2
3	−12	0	44	40	1	5	4	0	153	154	1	−3	−14	1	7	10	3	0	−7	1	185	171	2	8	2	1	56	50	1
4	−12	0	75	86	1	6	4	0	31	38	1	−2	−14	1	49	45	1	1	−7	1	354	336	4	−8	3	1	22	20	1
5	−12	0	79	74	1	7	4	0	69	74	1	−1	−14	1	63	65	1	2	−7	1	236	227	2	−7	3	1	101	95	1
6	−12	0	66	61	1	8	4	0	12	18	1	0	−14	1	34	35	1	3	−7	1	211	209	3	−6	3	1	74	74	1
1	−11	0	88	88	1	1	5	0	48	55	1	1	−14	1	83	88	1	−3	−6	1	480	451	5	−5	3	1	117	119	1
2	−11	0	105	103	1	2	5	0	241	222	3	2	−14	1	31	30	1	−2	−6	1	598	575	6	−4	3	1	251	235	3
3	−11	0	158	162	1	3	5	0	163	165	2	3	−14	1	10	8	2	−1	−6	1	152	146	1	−3	3	1	143	128	1
4	−11	0	50	52	1	4	5	0	158	167	1	4	−14	1	26	28	1	0	−6	1	303	302	4	−2	3	1	191	189	2
5	−11	0	133	130	2	5	5	0	89	87	1	−5	−13	1	125	128	2	1	−6	1	562	533	6	−1	3	1	406	413	6
6	−11	0	18	22	1	6	5	0	192	193	3	−4	−13	1	41	41	1	2	−6	1	254	234	2	0	3	1	293	280	5
0	−10	0	186	194	1	7	5	0	43	42	1	−3	−13	1	76	76	1	−3	−5	1	126	122	3	1	3	1	364	373	4
1	−10	0	65	57	1	8	5	0	35	37	1	−2	−13	1	57	52	1	−2	−5	1	54	55	1	2	3	1	242	241	2
2	−10	0	167	171	1	0	6	0	382	366	8	−1	−13	1	137	144	1	−1	−5	1	358	351	3	3	3	1	275	287	5
3	−10	0	238	244	1	1	6	0	453	436	8	0	−13	1	91	97	1	0	−5	1	275	275	2	4	3	1	137	135	1
4	−10	0	158	152	2	3	6	0	312	309	4	1	−13	1	193	196	1	1	−5	1	58	66	1	5	3	1	36	39	1
5	−10	0	96	90	1	4	6	0	232	222	1	2	−13	1	199	205	1	2	−5	1	37	36	1	6	3	1	134	135	2
6	−10	0	92	92	1	5	6	0	158	155	1	3	−13	1	82	85	1	−3	−4	1	406	386	10	7	3	1	84	81	1
1	−9	0	185	185	1	6	6	0	170	175	2	4	−13	1	29	27	1	−2	−4	1	198	185	2	8	3	1	45	44	1
2	−9	0	171	177	1	7	6	0	138	133	2	5	−13	1	23	21	1	−1	−4	1	367	368	3	−8	4	1	37	38	1
3	−9	0	86	87	1	8	6	0	57	61	1	−6	−12	1	40	39	1	0	−4	1	229	233	1	−7	4	1	113	118	2
4	−9	0	185	178	3	1	7	0	256	225	4	−5	−12	1	80	74	1	1	−4	1	508	500	5	−6	4	1	116	116	2
5	−9	0	128	130	2	2	7	0	113	122	3	−4	−12	1	88	92	1	2	−4	1	242	228	2	−5	4	1	108	109	1
6	−9	0	53	55	1	3	7	0	87	95	1	−3	−12	1	64	66	1	−3	−3	1	146	127	3	−4	4	1	69	60	1
0	−8	0	262	252	6	4	7	0	119	119	1	−2	−12	1	170	176	1	−2	−3	1	189	189	2	−3	4	1	402	384	6
1	−8	0	168	164	2	5	7	0	180	184	1	−1	−12	1	151	147	1	−1	−3	1	403	412	4	−2	4	1	191	185	2
2	−8	0	44	41	1	6	7	0	25	23	1	0	−12	1	147	146	1	0	−3	1	289	281	2	−1	4	1	365	367	4

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	0	155	149	1	7	7	0	73	73	1	1	−12	1	39	40	1	1	−3	1	377	373	3	0	4	1	227	233	4
4	−8	0	232	231	4	0	8	0	267	253	6	2	−12	1	125	128	1	2	−3	1	240	242	2	1	4	1	504	501	8
5	−8	0	120	115	2	1	8	0	170	164	4	3	−12	1	93	94	1	−2	−2	1	142	145	1	2	4	1	236	228	2
6	−8	0	88	85	1	2	8	0	41	41	1	4	−12	1	30	34	1	−1	−2	1	330	333	3	3	4	1	315	294	4
1	−7	0	254	225	3	3	8	0	154	150	1	5	−12	1	40	35	1	0	−2	1	274	279	2	4	4	1	235	230	2
2	−7	0	120	123	1	4	8	0	231	231	2	−6	−11	1	81	84	1	1	−2	1	375	372	3	5	4	1	243	242	1
3	−7	0	89	96	1	5	8	0	118	115	1	−5	−11	1	66	65	1	2	−2	1	186	196	4	6	4	1	79	80	1
0	−6	0	346	368	9	6	8	0	87	85	1	−4	−11	1	36	33	1	−8	−1	1	23	27	1	7	4	1	48	50	1
1	−6	0	458	436	4	7	8	0	56	57	1	−3	−11	1	10	12	1	−7	−1	1	107	107	1	8	4	1	53	57	1
2	−6	0	246	233	2	1	9	0	180	185	3	−2	−11	1	113	112	1	−2	−1	1	44	48	1	−8	5	1	75	75	1
3	−6	0	318	309	7	2	9	0	171	176	2	−1	−11	1	122	122	1	−1	−1	1	228	240	2	−7	5	1	131	135	2
1	−5	0	47	53	1	3	9	0	87	88	1	0	−11	1	120	110	1	0	−1	1	99	95	1	−6	5	1	218	238	2
2	−5	0	247	222	2	4	9	0	186	178	2	1	−11	1	138	138	1	1	−1	1	339	344	3	−5	5	1	131	120	1
3	−5	0	168	164	4	5	9	0	129	130	1	2	−11	1	268	266	2	2	−1	1	364	386	9	−4	5	1	106	117	1
0	−4	0	922	916	10	6	9	0	50	55	1	3	−11	1	126	119	1	7	−1	1	151	157	2	−3	5	1	129	121	2
1	−4	0	324	317	3	1	10	0	66	57	1	4	−11	1	163	163	2	−8	0	1	6	0	3	−2	5	1	53	56	1
2	−4	0	405	410	4	2	10	0	168	171	2	5	−11	1	35	36	1	−7	0	1	63	70	1	−1	5	1	357	351	4
1	−3	0	141	141	1	3	10	0	237	243	2	6	−11	1	31	32	1	−6	0	1	57	60	1	0	5	1	274	276	4
2	−3	0	269	280	2	4	10	0	154	152	1	−6	−10	1	83	81	1	−3	0	1	226	236	3	1	5	1	57	67	1
0	−2	0	115	113	2	5	10	0	96	90	1	−5	−10	1	166	167	3	−2	0	1	5	9	5	2	5	1	38	37	1
1	−2	0	485	488	5	6	10	0	91	93	1	−4	−10	1	217	215	3	−1	0	1	526	532	5	3	5	1	288	270	4
2	−2	0	217	210	5	1	11	0	90	90	1	−3	−10	1	214	216	1	0	0	1	128	131	1	4	5	1	266	273	2
1	−1	0	460	471	11	2	11	0	105	103	2	−2	−10	1	169	175	1	1	0	1	1440	1454	16	5	5	1	303	307	2
2	−1	0	239	259	6	3	11	0	157	162	2	−1	−10	1	136	145	1	2	0	1	78	75	1	6	5	1	46	52	1
7	−1	0	120	126	2	4	11	0	50	52	1	0	−10	1	287	290	1	3	0	1	393	391	6	7	5	1	92	93	1
1	0	0	86	93	1	5	11	0	133	130	1	1	−10	1	188	180	1	6	0	1	101	102	1	8	5	1	23	28	1
2	0	0	181	158	2	6	11	0	19	22	1	2	−10	1	145	142	1	7	0	1	61	65	1	−8	6	1	61	65	1
3	0	0	173	170	4	3	12	0	44	40	1	3	−10	1	91	93	1	8	0	1	57	56	1	−7	6	1	27	30	1
6	0	0	105	106	1	4	12	0	79	86	1	4	−10	1	119	109	2	−8	1	1	24	27	1	−6	6	1	112	110	1
7	0	0	25	20	1	5	12	0	79	75	1	5	−10	1	67	70	1	−7	1	1	110	107	1	−5	6	1	243	241	3
8	0	0	30	34	1	6	12	0	65	62	1	6	−10	1	42	43	1	−6	1	1	63	58	1	−4	6	1	77	84	1
1	1	0	467	471	5	1	13	0	107	107	2	−6	−9	1	32	35	1	−5	1	1	25	23	1	−3	6	1	484	451	11
2	1	0	253	258	2	2	13	0	77	73	1	−5	−9	1	111	105	2	−4	1	1	311	301	5	−2	6	1	552	575	15
3	1	0	275	267	5	3	13	0	102	95	1	−4	−9	1	22	25	1	−3	1	1	570	528	6	−1	6	1	151	146	2
4	1	0	406	383	7	4	13	0	125	117	1	−3	−9	1	123	121	1	−2	1	1	46	49	1	0	6	1	309	301	5
5	1	0	126	127	2	5	13	0	41	42	1	−2	−9	1	98	101	1	−1	1	1	230	240	2	1	6	1	560	533	9
6	1	0	218	223	3	1	14	0	21	17	2	−1	−9	1	28	17	1	0	1	1	95	94	1	2	6	1	243	234	6
7	1	0	121	126	2	2	14	0	100	96	2	0	−9	1	349	341	2	1	1	1	325	343	6	3	6	1	44	56	1
8	1	0	26	24	1	3	14	0	113	106	1	1	−9	1	96	94	1	2	1	1	372	386	4	4	6	1	178	179	1
0	2	0	115	112	3	4	14	0	25	21	1	2	−9	1	59	51	1	3	1	1	248	249	3	5	6	1	100	100	1
6	6	1	178	184	3	−3	14	1	11	9	2	−7	−9	2	46	48	1	3	0	2	62	71	1	−7	6	2	29	26	1
7	6	1	61	60	1	−2	14	1	49	45	1	−6	−9	2	62	62	1	6	0	2	88	96	1	−6	6	2	107	103	1
−7	7	1	13	13	1	1	14	1	86	88	2	−5	−9	2	30	26	1	7	0	2	77	80	1	−5	6	2	99	101	1
−6	7	1	80	84	1	2	14	1	33	30	1	−4	−9	2	210	206	3	8	0	2	25	23	1	−4	6	2	232	229	1
−5	7	1	233	226	2	3	14	1	10	9	2	−3	−9	2	100	97	1	−8	1	2	15	15	1	−3	6	2	247	241	6
−4	7	1	275	271	2	4	14	1	29	29	1	−2	−9	2	136	142	1	−7	1	2	152	155	2	−2	6	2	380	388	10
−3	7	1	109	109	1	−4	15	1	116	113	2	−1	−9	2	156	157	1	−6	1	2	106	102	1	−1	6	2	213	187	3
−2	7	1	148	142	4	−3	15	1	117	109	1	0	−9	2	97	107	1	−5	1	2	133	137	2	0	6	2	193	179	4
−1	7	1	393	379	6	−2	15	1	104	99	1	1	−9	2	165	164	1	−4	1	2	163	167	2	1	6	2	273	253	5

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	7	1	189	170	3	2	15	1	73	74	1	2	−9	2	273	274	2	−3	1	2	497	473	5	3	6	2	130	136	1
1	7	1	350	336	9	3	15	1	49	46	1	3	−9	2	61	61	1	−2	1	2	212	218	2	4	6	2	263	274	2
2	7	1	234	227	6	−3	16	1	42	39	1	4	−9	2	174	169	3	−1	1	2	664	676	7	5	6	2	107	98	1
3	7	1	212	208	2	−2	16	1	75	77	1	5	−9	2	111	109	2	0	1	2	1028	1060	13	6	6	2	71	75	1
4	7	1	109	108	1	2	16	1	9	6	2	6	−9	2	57	54	1	1	1	2	470	471	5	7	6	2	27	33	1
5	7	1	119	122	1	−3	−16	2	5	2	5	−6	−8	2	55	56	1	2	1	2	101	101	1	−7	7	2	80	80	1
6	7	1	87	89	1	−2	−16	2	101	95	1	−5	−8	2	211	206	3	3	1	2	115	109	1	−6	7	2	102	97	1
7	7	1	23	22	1	−1	−16	2	96	93	1	−4	−8	2	61	65	1	4	1	2	96	103	1	−5	7	2	136	141	1
−7	8	1	30	28	1	0	−16	2	59	57	1	−3	−8	2	122	111	1	5	1	2	64	65	1	−4	7	2	131	128	1
−6	8	1	25	23	1	1	−16	2	39	37	1	−2	−8	2	181	189	1	6	1	2	23	24	1	−3	7	2	133	133	1
−5	8	1	140	141	1	2	−16	2	29	31	1	−1	−8	2	227	225	3	7	1	2	46	44	1	−2	7	2	132	127	4
−4	8	1	25	20	1	−4	−15	2	22	26	1	0	−8	2	47	44	2	8	1	2	16	19	1	−1	7	2	160	135	3
−3	8	1	43	43	1	−3	−15	2	153	147	1	1	−8	2	177	185	1	−8	2	2	26	24	1	0	7	2	266	257	6
−2	8	1	67	64	1	−2	−15	2	75	71	1	2	−8	2	154	153	1	−7	2	2	28	29	1	1	7	2	56	54	2
−1	8	1	103	99	3	−1	−15	2	109	111	1	3	−8	2	140	133	2	−6	2	2	168	167	2	3	7	2	216	211	1
0	8	1	152	161	3	0	−15	2	119	118	1	4	−8	2	127	131	2	−5	2	2	132	134	1	4	7	2	184	197	1
1	8	1	182	190	5	1	−15	2	55	53	1	5	−8	2	249	255	4	−4	2	2	230	224	2	5	7	2	37	32	1
2	8	1	165	151	2	2	−15	2	27	28	1	6	−8	2	56	53	1	−3	2	2	365	363	4	6	7	2	93	91	1
3	8	1	86	79	1	3	−15	2	94	97	1	−6	−7	2	100	97	1	−2	2	2	142	150	1	7	7	2	64	63	1
4	8	1	200	197	1	−5	−14	2	64	62	1	−5	−7	2	135	141	2	−1	2	2	642	650	8	−7	8	2	54	49	1
5	8	1	116	116	1	−4	−14	2	115	114	1	−4	−7	2	131	127	2	0	2	2	581	595	10	−6	8	2	55	56	1
6	8	1	29	28	1	−3	−14	2	50	50	1	−3	−7	2	133	133	1	1	2	2	169	179	1	−5	8	2	209	206	2
7	8	1	42	44	1	−2	−14	2	70	71	1	−2	−7	2	133	127	1	2	2	2	349	336	4	−4	8	2	63	65	1
−6	9	1	32	35	1	−1	−14	2	48	52	1	−1	−7	2	160	135	2	3	2	2	120	113	1	−3	8	2	122	111	1
−5	9	1	111	105	1	0	−14	2	52	50	1	0	−7	2	252	255	3	4	2	2	102	107	1	−2	8	2	181	189	2
−4	9	1	23	24	1	1	−14	2	111	116	1	1	−7	2	58	54	1	5	2	2	195	196	3	−1	8	2	225	224	6
−3	9	1	121	121	1	2	−14	2	45	47	1	2	−7	2	149	153	1	6	2	2	141	139	2	0	8	2	49	44	3
−2	9	1	96	101	1	3	−14	2	23	23	1	3	−7	2	214	211	4	7	2	2	79	80	1	2	8	2	146	154	2
−1	9	1	28	17	1	4	−14	2	46	44	1	4	−7	2	182	198	3	8	2	2	27	24	1	3	8	2	142	133	1
0	9	1	357	341	6	−5	−13	2	25	21	1	−3	−6	2	247	241	3	−8	3	2	43	42	1	4	8	2	128	131	1
1	9	1	99	95	1	−4	−13	2	169	174	3	−2	−6	2	399	389	4	−7	3	2	130	126	2	5	8	2	253	255	3
2	9	1	56	51	1	−3	−13	2	87	89	1	−1	−6	2	207	187	2	−6	3	2	181	168	3	6	8	2	56	53	1
3	9	1	38	37	1	−2	−13	2	234	237	1	0	−6	2	187	178	2	−5	3	2	166	161	1	7	8	2	67	68	1
4	9	1	187	187	2	−1	−13	2	94	92	1	1	−6	2	277	253	3	−4	3	2	425	403	5	−6	9	2	61	63	1
5	9	1	187	181	1	0	−13	2	97	100	1	2	−6	2	303	285	3	−3	3	2	152	139	1	−5	9	2	34	27	1
6	9	1	8	6	1	1	−13	2	83	89	1	−3	−5	2	127	125	1	−2	3	2	176	184	1	−4	9	2	210	206	2
−6	10	1	86	81	1	2	−13	2	129	131	1	−2	−5	2	73	68	1	−1	3	2	512	520	6	−3	9	2	100	97	1
−5	10	1	165	166	2	3	−13	2	111	110	1	−1	−5	2	83	81	1	0	3	2	456	458	7	−2	9	2	137	143	2
−4	10	1	212	214	2	4	−13	2	116	112	2	0	−5	2	512	508	5	1	3	2	676	684	7	−1	9	2	153	157	2
−3	10	1	212	216	2	5	−13	2	76	75	1	1	−5	2	219	202	2	2	3	2	160	155	2	0	9	2	101	108	2
−2	10	1	172	175	2	−6	−12	2	81	76	1	2	−5	2	298	295	3	3	3	2	132	114	1	2	9	2	274	274	4
−1	10	1	134	145	2	−5	−12	2	50	50	1	−3	−4	2	143	136	2	4	3	2	117	125	1	3	9	2	61	61	1
1	10	1	186	180	3	−4	−12	2	93	90	1	−2	−4	2	186	180	2	5	3	2	83	90	1	4	9	2	170	169	1
3	10	1	91	93	1	−3	−12	2	128	127	1	−1	−4	2	314	312	2	6	3	2	175	174	3	5	9	2	106	109	1
4	10	1	111	109	1	−2	−12	2	112	118	1	0	−4	2	99	102	1	7	3	2	77	78	1	6	9	2	56	53	1
5	10	1	68	69	1	−1	−12	2	83	79	1	1	−4	2	795	786	8	8	3	2	22	21	1	−6	10	2	97	97	1
6	10	1	42	43	1	0	−12	2	161	166	1	2	−4	2	299	283	3	−8	4	2	39	36	1	−5	10	2	120	117	2
−6	11	1	81	84	1	1	−12	2	116	112	1	−3	−3	2	146	137	2	−7	4	2	51	62	1	−4	10	2	153	163	2
−5	11	1	67	65	1	2	−12	2	23	28	1	−2	−3	2	176	184	1	−6	4	2	279	284	4	−3	10	2	31	35	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	11	1	33	32	1	3	−12	2	92	101	1	−1	−3	2	514	520	5	−5	4	2	113	114	1	−2	10	2	182	185	2
−3	11	1	12	11	2	4	−12	2	70	68	1	0	−3	2	453	459	4	−4	4	2	99	98	1	−1	10	2	20	14	2
−2	11	1	116	111	2	5	−12	2	53	52	1	1	−3	2	693	684	7	−3	4	2	142	136	2	0	10	2	146	148	4
−1	11	1	118	121	2	−6	−11	2	77	74	1	2	−3	2	159	156	1	−2	4	2	191	181	2	1	10	2	203	208	3
2	11	1	263	266	5	−5	−11	2	52	52	1	−3	−2	2	348	364	4	−1	4	2	315	313	4	2	10	2	53	51	1
3	11	1	128	118	1	−4	−11	2	20	28	1	−2	−2	2	144	150	1	0	4	2	99	103	2	3	10	2	93	91	1
4	11	1	159	163	1	−3	−11	2	143	140	1	−1	−2	2	644	650	6	1	4	2	774	787	19	4	10	2	63	65	1
5	11	1	35	35	1	−2	−11	2	159	158	1	0	−2	2	579	595	5	3	4	2	65	68	1	5	10	2	93	94	1
6	11	1	33	33	1	−1	−11	2	107	107	1	1	−2	2	170	180	1	4	4	2	96	97	1	6	10	2	73	75	1
−6	12	1	38	38	1	0	−11	2	161	161	1	2	−2	2	344	337	3	5	4	2	175	172	1	−6	11	2	75	73	1
−5	12	1	78	74	1	1	−11	2	176	181	1	−8	−1	2	14	15	1	6	4	2	74	80	1	−5	11	2	52	52	1
−4	12	1	92	92	1	2	−11	2	91	94	1	−7	−1	2	149	155	2	7	4	2	54	58	1	−4	11	2	26	29	1
−3	12	1	64	65	1	3	−11	2	101	106	1	−3	−1	2	483	472	5	8	4	2	14	17	1	−3	11	2	140	140	2
−2	12	1	169	176	3	4	−11	2	54	58	1	−2	−1	2	215	218	2	−8	5	2	63	61	1	−2	11	2	161	159	2
−1	12	1	151	147	3	5	−11	2	10	12	2	−1	−1	2	666	677	7	−7	5	2	52	56	1	−1	11	2	105	106	2
1	12	1	37	40	1	6	−11	2	40	46	1	0	−1	2	1043	1061	10	−6	5	2	316	313	3	1	11	2	178	181	2
2	12	1	123	127	2	−6	−10	2	97	96	1	1	−1	2	471	472	4	−5	5	2	248	251	1	2	11	2	90	94	1
3	12	1	92	95	1	−5	−10	2	118	117	2	2	−1	2	99	101	1	−4	5	2	70	71	1	3	11	2	104	106	1
4	12	1	34	35	1	−4	−10	2	157	162	2	7	−1	2	45	44	1	−3	5	2	125	127	2	4	11	2	57	58	1
5	12	1	39	36	1	−3	−10	2	36	36	1	−8	0	2	24	24	1	−2	5	2	73	68	2	5	11	2	10	13	2
−5	13	1	129	128	1	−2	−10	2	181	185	1	−7	0	2	49	50	1	−1	5	2	83	80	1	−6	12	2	81	76	1
−4	13	1	41	41	1	−1	−10	2	22	15	1	−6	0	2	240	262	4	0	5	2	518	509	12	−5	12	2	49	49	1
−3	13	1	75	76	1	0	−10	2	154	148	1	−4	0	2	543	562	10	1	5	2	214	202	2	−4	12	2	93	91	1
1	13	1	191	196	3	1	−10	2	208	209	1	−3	0	2	456	444	5	3	5	2	247	244	3	−3	12	2	128	127	1
2	13	1	201	205	3	2	−10	2	56	51	1	−2	0	2	332	332	3	4	5	2	172	181	1	−2	12	2	115	117	2
3	13	1	82	85	1	3	−10	2	91	91	1	−1	0	2	967	976	10	5	5	2	76	68	1	−1	12	2	85	79	2
4	13	1	26	27	1	4	−10	2	63	64	1	0	0	2	198	202	2	6	5	2	84	101	1	1	12	2	116	113	2
5	13	1	20	20	1	5	−10	2	93	93	1	1	0	2	282	287	3	7	5	2	0	4	1	2	12	2	21	27	1
−4	14	1	71	72	1	6	−10	2	73	75	1	2	0	2	33	49	1	−8	6	2	84	85	1	3	12	2	93	100	1
4	12	2	70	67	1	−5	−10	3	147	150	2	−2	−2	3	513	511	5	−3	4	3	169	164	2	−2	10	3	79	78	1
5	12	2	53	52	1	−4	−10	3	50	55	1	−1	−2	3	621	628	6	−2	4	3	62	70	1	−1	10	3	272	279	4
−5	13	2	25	22	1	−3	−10	3	183	194	1	0	−2	3	994	1008	9	−1	4	3	130	134	1	0	10	3	122	135	2
−4	13	2	175	174	2	−2	−10	3	80	79	1	1	−2	3	465	462	4	0	4	3	176	179	3	1	10	3	138	132	2
−3	13	2	86	89	1	−1	−10	3	271	279	1	2	−2	3	160	168	1	1	4	3	196	194	2	2	10	3	32	29	1
−2	13	2	236	236	4	0	−10	3	126	135	1	7	−2	3	92	97	1	2	4	3	328	305	5	3	10	3	222	221	2
−1	13	2	94	92	2	1	−10	3	138	132	1	−8	−1	3	10	17	1	3	4	3	55	53	1	4	10	3	69	65	1
1	13	2	80	89	2	2	−10	3	29	29	1	−7	−1	3	16	9	1	4	4	3	100	109	1	5	10	3	52	53	1
2	13	2	127	131	1	3	−10	3	222	221	4	−6	−1	3	67	65	1	5	4	3	185	186	1	−6	11	3	69	68	1
3	13	2	114	111	1	4	−10	3	68	64	1	−4	−1	3	327	314	6	6	4	3	59	58	1	−5	11	3	111	114	2
4	13	2	118	111	1	5	−10	3	54	52	1	−3	−1	3	60	62	1	7	4	3	37	33	1	−4	11	3	99	106	1
5	13	2	76	75	1	6	−10	3	27	24	1	−2	−1	3	475	474	5	−8	5	3	22	24	1	−3	11	3	251	251	3
−5	14	2	65	62	1	−7	−9	3	44	45	1	−1	−1	3	219	224	2	−7	5	3	35	28	1	−2	11	3	140	128	2
−4	14	2	117	114	1	−6	−9	3	132	130	2	0	−1	3	807	818	8	−6	5	3	109	104	1	−1	11	3	93	94	2
−3	14	2	51	50	1	−5	−9	3	106	104	2	1	−1	3	206	200	2	−5	5	3	207	205	1	1	11	3	239	244	3
1	14	2	112	116	2	−4	−9	3	95	97	1	2	−1	3	103	104	1	−4	5	3	75	77	1	2	11	3	155	162	2
2	14	2	44	47	1	−3	−9	3	111	103	1	3	−1	3	33	40	1	−3	5	3	200	197	3	3	11	3	81	82	1
3	14	2	24	23	1	−2	−9	3	103	104	1	6	−1	3	118	120	2	−2	5	3	117	111	3	4	11	3	106	104	1
4	14	2	45	44	1	−1	−9	3	153	158	1	7	−1	3	72	74	1	−1	5	3	162	158	3	5	11	3	92	88	1
−4	15	2	26	26	1	0	−9	3	185	193	1	−8	0	3	67	61	1	0	5	3	339	325	5	−6	12	3	52	48	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	15	2	157	147	2	1	-9	3	177	187	1	-7	0	3	17	17	1	1	5	3	703	701	12	-5	12	3	30	27	1
-2	15	2	74	71	1	2	-9	3	125	114	1	-6	0	3	87	91	1	2	5	3	251	257	4	-4	12	3	119	130	1
1	15	2	56	53	1	3	-9	3	75	68	1	-5	0	3	68	76	1	3	5	3	81	86	1	-3	12	3	15	7	2
2	15	2	26	27	1	4	-9	3	182	179	3	-4	0	3	82	68	1	4	5	3	59	59	1	-2	12	3	162	163	3
3	15	2	95	97	1	5	-9	3	123	115	2	-3	0	3	510	487	6	5	5	3	104	106	1	-1	12	3	128	129	2
-3	16	2	3	2	3	6	-9	3	29	28	1	-2	0	3	41	45	1	5	5	3	102	112	1	1	12	3	93	96	2
-2	16	2	100	95	1	-7	-8	3	49	46	1	-1	0	3	962	987	10	7	5	3	40	41	1	2	12	3	172	173	2
2	16	2	27	30	1	-6	-8	3	79	82	1	0	0	3	544	559	7	-8	6	3	34	34	1	3	12	3	71	77	1
-2	-16	3	106	98	2	-5	-8	3	34	32	1	1	0	3	293	301	3	-7	6	3	28	27	1	4	12	3	39	40	1
-1	-16	3	68	65	1	-4	-8	3	151	152	2	2	0	3	386	375	4	-6	6	3	250	250	3	5	12	3	49	49	1
0	-16	3	57	54	1	-3	-8	3	68	72	1	3	0	3	84	85	1	-5	6	3	217	224	1	-5	13	3	101	99	1
1	-16	3	38	35	1	-2	-8	3	172	177	1	5	0	3	179	177	3	-4	6	3	182	188	1	-4	13	3	119	117	2
2	-16	3	43	45	1	-1	-8	3	79	80	1	6	0	3	133	128	2	-3	6	3	37	32	3	-3	13	3	159	157	2
-4	-15	3	124	123	2	0	-8	3	109	99	1	7	0	3	148	158	2	-2	6	3	116	110	3	-2	13	3	146	153	3
-3	-15	3	102	101	1	1	-8	3	181	172	1	-8	1	3	13	18	1	-1	6	3	7	8	6	1	13	3	125	127	2
-2	-15	3	97	95	1	2	-8	3	77	77	1	-7	1	3	14	9	1	0	6	3	311	307	5	2	13	3	134	135	1
-1	-15	3	75	72	1	3	-8	3	18	16	1	-6	1	3	71	66	1	1	6	3	279	255	7	3	13	3	98	96	1
0	-15	3	72	73	1	4	-8	3	130	141	2	-5	1	3	73	76	1	2	6	3	381	377	9	4	13	3	64	61	1
1	-15	3	68	67	1	5	-8	3	138	140	2	-4	1	3	333	314	3	3	6	3	51	47	1	-4	14	3	159	149	2
2	-15	3	47	47	1	6	-8	3	84	82	1	-3	1	3	60	61	1	4	6	3	178	181	1	-3	14	3	51	47	1
3	-15	3	52	53	1	-7	-7	3	85	88	1	-2	1	3	478	474	5	5	6	3	224	219	2	-2	14	3	62	59	1
-5	-14	3	57	57	1	-6	-7	3	110	109	2	-1	1	3	222	224	2	6	6	3	84	83	1	1	14	3	9	12	6
-4	-14	3	154	149	2	-5	-7	3	99	99	2	0	1	3	798	818	10	7	6	3	41	39	1	2	14	3	18	18	1
-3	-14	3	49	47	1	-4	-7	3	76	80	1	1	1	3	201	198	2	-7	7	3	87	88	1	3	14	3	54	54	1
-2	-14	3	61	59	1	-3	-7	3	138	141	1	2	1	3	101	104	1	-6	7	3	115	110	1	4	14	3	70	65	1
-1	-14	3	131	131	1	-2	-7	3	235	237	3	3	1	3	33	41	1	-5	7	3	101	100	1	-4	15	3	124	123	2
0	-14	3	42	36	1	-1	-7	3	57	67	1	4	1	3	143	141	1	-4	7	3	76	80	1	-3	15	3	103	101	1
1	-14	3	9	12	1	0	-7	3	47	42	1	5	1	3	68	65	1	-3	7	3	136	141	1	-2	15	3	96	96	2
2	-14	3	14	18	1	1	-7	3	109	98	1	6	1	3	120	120	2	-2	7	3	236	236	6	1	15	3	67	67	1
3	-14	3	52	53	1	2	-7	3	122	112	1	7	1	3	71	73	1	-1	7	3	57	67	1	2	15	3	45	48	1
4	-14	3	68	65	1	3	-7	3	203	212	3	-8	2	3	17	26	1	0	7	3	48	43	2	3	15	3	53	53	1
-5	-13	3	97	99	2	4	-7	3	102	104	1	-7	2	3	68	64	1	1	7	3	106	98	3	-2	16	3	102	97	1
-4	-13	3	116	117	1	5	-7	3	176	176	3	-6	2	3	31	27	1	2	7	3	122	112	2	2	16	3	47	46	1
-3	-13	3	156	157	1	6	-7	3	81	84	1	-5	2	3	166	176	1	3	7	3	198	211	1	-2	-16	4	48	45	1
-2	-13	3	145	153	1	-7	-6	3	25	27	1	-4	2	3	61	56	1	4	7	3	102	103	1	-1	-16	4	3	3	2
-1	-13	3	241	249	2	-6	-6	3	245	250	4	-3	2	3	261	261	3	5	7	3	174	176	1	0	-16	4	94	97	1
0	-13	3	169	172	1	-5	-6	3	216	224	4	-2	2	3	511	511	5	6	7	3	83	84	1	1	-16	4	28	29	1
1	-13	3	123	127	1	-4	-6	3	181	188	3	-1	2	3	616	629	8	7	7	3	60	61	1	-3	-15	4	29	29	1
2	-13	3	134	136	1	-3	-6	3	37	32	1	0	2	3	988	1007	12	-6	8	3	78	82	1	-2	-15	4	97	95	1
3	-13	3	97	96	1	-2	-6	3	123	111	1	1	2	3	462	462	4	-5	8	3	36	32	1	-1	-15	4	109	107	1
4	-13	3	62	61	1	-1	-6	3	13	7	2	2	2	3	163	168	2	-4	8	3	149	152	1	0	-15	4	51	53	1
5	-13	3	42	38	1	0	-6	3	300	306	4	3	2	3	265	255	3	-3	8	3	68	72	1	1	-15	4	47	45	1
-6	-12	3	54	49	1	1	-6	3	284	255	3	4	2	3	74	81	1	-2	8	3	174	177	2	2	-15	4	74	76	1
-5	-12	3	28	27	1	2	-6	3	385	377	4	5	2	3	162	157	2	-1	8	3	83	79	2	-4	-14	4	59	60	1
-4	-12	3	118	128	2	3	-6	3	49	47	1	6	2	3	75	72	1	0	8	3	109	99	2	-3	-14	4	102	101	1
-3	-12	3	13	6	1	-3	-5	3	202	197	2	7	2	3	95	96	1	1	8	3	182	172	2	-2	-14	4	26	25	1
-2	-12	3	162	163	1	-2	-5	3	124	110	1	-8	3	3	80	77	1	2	8	3	77	77	1	-1	-14	4	35	39	1
-1	-12	3	128	130	1	-1	-5	3	159	158	1	-7	3	3	162	168	2	3	8	3	14	16	1	0	-14	4	99	101	1
0	-12	3	68	67	1	0	-5	3	331	326	3	-6	3	3	170	165	3	4	8	3	131	142	1	1	-14	4	42	40	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	3	93	96	1	1	−5	3	718	700	7	−5	3	3	68	60	1	5	8	3	133	140	1	2	−14	4	67	67	1
2	−12	3	172	174	1	2	−5	3	257	257	2	−4	3	3	76	78	1	6	8	3	83	82	1	3	−14	4	53	54	1
3	−12	3	71	77	1	−3	−4	3	170	164	1	−3	3	3	324	298	4	−6	9	3	131	130	1	4	−14	4	61	62	1
4	−12	3	39	41	1	−2	−4	3	66	69	1	−2	3	3	100	89	1	−5	9	3	102	104	1	−5	−13	4	43	43	1
5	−12	3	50	50	1	−1	−4	3	131	134	1	−1	3	3	400	401	5	−4	9	3	93	96	1	−4	−13	4	92	94	1
−6	−11	3	70	69	1	0	−4	3	173	179	1	0	3	3	654	670	8	−3	9	3	108	103	1	−3	−13	4	123	127	1
−5	−11	3	113	115	2	1	−4	3	198	194	2	1	3	3	379	395	4	−2	9	3	107	105	1	−2	−13	4	118	113	1
−4	−11	3	99	106	2	2	−4	3	327	304	3	2	3	3	277	272	3	−1	9	3	148	158	2	−1	−13	4	92	94	1
−3	−11	3	252	251	2	−7	−3	3	167	168	2	3	3	3	287	285	3	0	9	3	187	194	3	0	−13	4	212	225	1
−2	−11	3	137	128	1	−3	−3	3	321	299	3	4	3	3	61	64	1	1	9	3	176	188	2	1	−13	4	87	92	1
−1	−11	3	93	94	1	−2	−3	3	103	89	1	5	3	3	148	146	2	2	9	3	126	114	1	2	−13	4	125	128	1
0	−11	3	240	240	1	−1	−3	3	397	401	3	6	3	3	118	122	2	3	9	3	74	69	1	3	−13	4	42	43	1
1	−11	3	240	246	1	0	−3	3	668	670	6	7	3	3	52	49	1	4	9	3	181	179	2	4	−13	4	100	96	2
2	−11	3	157	163	1	1	−3	3	388	394	4	−8	4	3	36	39	1	5	9	3	118	115	1	−6	−12	4	61	58	1
3	−11	3	80	83	1	2	−3	3	275	273	2	−7	4	3	60	67	1	−6	10	3	61	61	1	−5	−12	4	36	32	1
4	−11	3	105	105	2	−8	−2	3	17	26	1	−6	4	3	134	131	1	−5	10	3	150	150	2	−4	−12	4	65	69	1
5	−11	3	92	88	1	−7	−2	3	67	65	1	−5	4	3	194	205	1	−4	10	3	48	55	1	−3	−12	4	116	117	1
−6	−10	3	63	61	1	−3	−2	3	261	263	2	−4	4	3	287	288	2	−3	10	3	182	194	2	−2	−12	4	70	72	1
−1	−12	4	61	55	1	6	−6	4	39	36	1	7	0	4	41	41	1	−1	6	4	112	103	2	−2	13	4	119	114	2
0	−12	4	59	62	1	−7	−5	4	39	43	1	−8	1	4	39	38	1	0	6	4	227	220	4	1	13	4	87	92	2
1	−12	4	119	120	1	−6	−5	4	61	60	1	−7	1	4	143	143	2	1	6	4	192	180	5	2	13	4	125	128	1
2	−12	4	52	50	1	−5	−5	4	216	214	3	−6	1	4	54	54	1	2	6	4	37	33	1	3	13	4	45	43	1
3	−12	4	20	20	1	−4	−5	4	57	54	1	−5	1	4	152	146	1	3	6	4	141	136	1	4	13	4	100	95	1
4	−12	4	23	23	1	−3	−5	4	135	141	1	−4	1	4	442	419	5	4	6	4	229	232	1	−4	14	4	61	60	1
5	−12	4	55	51	1	−2	−5	4	419	406	4	−3	1	4	83	83	1	5	6	4	63	61	1	−3	14	4	103	101	1
−6	−11	4	90	86	1	−1	−5	4	294	302	3	−2	1	4	379	377	4	6	6	4	40	35	1	−2	14	4	29	25	2
−5	−11	4	190	190	3	0	−5	4	267	251	3	−1	1	4	376	382	4	7	6	4	96	98	1	1	14	4	42	40	1
−4	−11	4	152	165	3	1	−5	4	693	665	7	0	1	4	260	258	3	−7	7	4	14	13	1	2	14	4	67	67	1
−3	−11	4	117	114	1	2	−5	4	276	267	3	1	1	4	124	115	1	−6	7	4	48	46	1	3	14	4	55	54	1
−2	−11	4	306	307	2	3	−5	4	255	257	4	2	1	4	200	198	2	−5	7	4	182	184	1	4	14	4	67	62	1
−1	−11	4	141	140	1	4	−5	4	261	255	5	3	1	4	83	74	1	−4	7	4	71	70	1	−4	15	4	103	103	2
0	−11	4	78	71	1	5	−5	4	77	84	1	4	1	4	134	130	1	−3	7	4	52	47	1	−3	15	4	28	28	1
1	−11	4	70	73	1	6	−5	4	58	53	1	5	1	4	128	130	2	−2	7	4	231	230	6	1	15	4	47	45	1
2	−11	4	79	85	1	−8	−4	4	97	96	1	6	1	4	135	130	2	−1	7	4	73	77	2	2	15	4	75	76	1
3	−11	4	57	70	1	−7	−4	4	37	33	1	7	1	4	54	55	1	0	7	4	192	186	3	3	15	4	30	30	1
4	−11	4	84	83	1	−6	−4	4	171	172	2	−8	2	4	10	10	2	1	7	4	30	21	3	−2	16	4	52	45	1
5	−11	4	90	89	1	−5	−4	4	154	162	2	−7	2	4	101	100	1	2	7	4	149	151	1	1	16	4	28	29	1
−6	−10	4	92	96	1	−4	−4	4	220	206	2	−6	2	4	130	130	2	3	7	4	121	122	1	−2	−16	5	42	41	1
−5	−10	4	94	99	2	−3	−4	4	107	103	1	−5	2	4	121	129	1	4	7	4	148	143	1	−1	−16	5	26	25	1
−4	−10	4	95	106	2	−2	−4	4	188	191	2	−4	2	4	231	232	2	5	7	4	170	163	1	0	−16	5	24	27	1
−3	−10	4	58	53	1	−1	−4	4	125	128	1	−3	2	4	256	245	3	6	7	4	18	13	1	1	−16	5	102	104	2
−2	−10	4	34	28	1	0	−4	4	384	375	4	−2	2	4	80	78	1	7	7	4	25	32	1	−3	−15	5	26	26	1
−1	−10	4	140	146	1	1	−4	4	199	183	2	−1	2	4	203	205	2	−7	8	4	28	29	1	−2	−15	5	194	186	2
0	−10	4	234	232	1	2	−4	4	198	192	2	0	2	4	563	566	7	−6	8	4	127	131	1	−1	−15	5	59	58	1
1	−10	4	106	103	1	6	−4	4	90	87	1	1	2	4	107	115	1	−5	8	4	150	152	2	0	−15	5	82	82	1
2	−10	4	97	94	1	−8	−3	4	33	27	1	2	2	4	170	169	2	−4	8	4	103	99	1	1	−15	5	99	91	1
3	−10	4	116	123	2	−7	−3	4	60	58	1	3	2	4	144	147	1	−3	8	4	91	89	1	2	−15	5	70	70	1
4	−10	4	123	121	2	−6	−3	4	210	215	3	4	2	4	64	66	1	−2	8	4	62	67	1	−4	−14	5	114	112	1
5	−10	4	29	32	1	−5	−3	4	80	76	1	5	2	4	38	33	1	−1	8	4	68	70	2	−3	−14	5	127	130	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	−10	4	30	31	1	−4	−3	4	107	102	1	6	2	4	195	195	3	0	8	4	155	161	3	−2	−14	5	188	191	1
−7	−9	4	51	48	1	−3	−3	4	145	142	1	7	2	4	30	23	1	1	8	4	130	142	2	−1	−14	5	122	120	1
−6	−9	4	80	77	1	−2	−3	4	209	214	2	−8	3	4	34	27	1	2	8	4	115	113	1	0	−14	5	57	59	1
−5	−9	4	94	96	1	−1	−3	4	189	191	2	−7	3	4	56	57	1	3	8	4	124	118	1	1	−14	5	10	9	1
−4	−9	4	18	19	1	0	−3	4	304	309	2	−6	3	4	215	214	3	4	8	4	212	216	2	2	−14	5	68	67	1
−3	−9	4	137	136	1	1	−3	4	176	180	1	−5	3	4	80	77	1	5	8	4	104	114	1	3	−14	5	59	61	1
−2	−9	4	154	156	1	2	−3	4	281	289	3	−4	3	4	106	102	1	6	8	4	137	138	2	−5	−13	5	23	23	1
−1	−9	4	156	159	1	3	−3	4	107	99	1	−3	3	4	143	142	2	−6	9	4	77	78	1	−4	−13	5	115	116	1
0	−9	4	179	182	1	6	−3	4	61	58	1	−2	3	4	208	214	2	−5	9	4	95	97	1	−3	−13	5	102	99	1
1	−9	4	218	214	1	7	−3	4	68	65	1	−1	3	4	184	191	2	−4	9	4	18	19	1	−2	−13	5	126	125	1
2	−9	4	68	65	1	−8	−2	4	13	10	1	0	3	4	308	311	3	−3	9	4	137	136	1	−1	−13	5	99	107	1
3	−9	4	41	45	1	−7	−2	4	99	99	1	1	3	4	174	180	2	−2	9	4	153	157	2	0	−13	5	114	118	1
4	−9	4	78	78	1	−6	−2	4	126	130	2	2	3	4	285	289	4	−1	9	4	152	158	2	1	−13	5	65	69	1
5	−9	4	125	122	2	−5	−2	4	120	129	1	3	3	4	108	99	1	0	9	4	173	183	3	2	−13	5	37	38	1
6	−9	4	89	92	1	−4	−2	4	231	231	3	4	3	4	73	77	1	1	9	4	218	213	3	3	−13	5	48	55	1
−7	−8	4	29	29	1	−3	−2	4	256	245	2	5	3	4	105	109	1	2	9	4	68	64	1	4	−13	5	32	37	1
−6	−8	4	129	131	2	−2	−2	4	79	78	1	6	3	4	59	58	1	3	9	4	42	45	1	−6	−12	5	52	47	1
−5	−8	4	151	152	2	−1	−2	4	202	204	1	7	3	4	71	65	1	4	9	4	78	77	1	−5	−12	5	91	94	1
−4	−8	4	103	99	2	0	−2	4	559	566	5	−8	4	4	98	96	1	5	9	4	124	122	1	−4	−12	5	47	48	1
−3	−8	4	94	89	1	1	−2	4	109	114	1	−7	4	4	36	33	1	−6	10	4	93	96	1	−3	−12	5	69	70	1
−2	−8	4	64	67	1	2	−2	4	167	169	1	−6	4	4	172	172	2	−5	10	4	100	100	1	−2	−12	5	75	72	1
−1	−8	4	68	70	1	3	−2	4	144	147	2	−5	4	4	154	162	1	−4	10	4	101	106	1	−1	−12	5	226	230	1
0	−8	4	153	160	1	5	−2	4	39	33	1	−4	4	4	215	206	1	−3	10	4	57	53	1	0	−12	5	155	146	1
1	−8	4	130	141	1	6	−2	4	197	195	3	−3	4	4	105	104	2	−2	10	4	36	28	1	1	−12	5	64	61	1
2	−8	4	115	113	1	7	−2	4	30	23	1	−2	4	4	186	191	3	−1	10	4	138	146	2	2	−12	5	163	164	1
3	−8	4	127	119	2	−8	−1	4	40	38	1	−1	4	4	129	127	2	0	10	4	235	232	3	3	−12	5	25	29	1
4	−8	4	211	216	3	−7	−1	4	141	143	2	0	4	4	390	374	6	1	10	4	106	104	2	4	−12	5	46	43	1
5	−8	4	105	113	2	−6	−1	4	54	54	1	1	4	4	196	181	3	2	10	4	96	93	1	−6	−11	5	30	29	1
6	−8	4	140	139	2	−5	−1	4	151	147	2	2	4	4	198	191	3	3	10	4	119	123	1	−5	−11	5	52	57	1
−7	−7	4	13	13	1	−4	−1	4	440	419	5	3	4	4	70	71	1	4	10	4	123	121	1	−4	−11	5	55	54	1
−6	−7	4	49	45	1	−3	−1	4	85	83	1	4	4	4	53	51	1	5	10	4	30	32	1	−3	−11	5	163	156	1
−5	−7	4	185	184	3	−2	−1	4	375	376	4	5	4	4	170	167	1	−6	11	4	87	86	1	−2	−11	5	266	268	2
−4	−7	4	72	69	1	−1	−1	4	374	382	4	6	4	4	84	87	1	−5	11	4	190	190	2	−1	−11	5	304	302	2
−3	−7	4	52	48	1	0	−1	4	261	258	2	7	4	4	43	43	1	−4	11	4	160	164	2	0	−11	5	138	144	1
−2	−7	4	231	230	2	1	−1	4	123	115	1	−8	5	4	30	33	1	−3	11	4	117	114	2	1	−11	5	196	199	1
−1	−7	4	72	76	2	2	−1	4	201	199	2	−7	5	4	40	43	1	−2	11	4	304	307	4	2	−11	5	148	152	1
0	−7	4	189	186	3	3	−1	4	80	75	1	−6	5	4	63	61	1	−1	11	4	140	141	3	3	−11	5	95	99	1
1	−7	4	29	22	1	4	−1	4	132	130	2	−5	5	4	214	213	1	0	11	4	75	71	2	4	−11	5	60	62	1
2	−7	4	153	152	1	5	−1	4	125	130	2	−4	5	4	56	54	1	1	11	4	70	74	1	5	−11	5	93	94	1
3	−7	4	121	122	2	6	−1	4	133	130	2	−3	5	4	135	141	4	2	11	4	78	84	1	−6	−10	5	35	32	1
4	−7	4	149	142	2	7	−1	4	53	55	1	−2	5	4	397	407	10	3	11	4	62	70	1	−5	−10	5	202	209	3
5	−7	4	169	163	3	−8	0	4	28	28	1	−1	5	4	300	302	5	4	11	4	88	83	1	−4	−10	5	185	202	3
6	−7	4	20	12	1	−7	0	4	47	40	1	0	5	4	283	251	4	5	11	4	87	89	1	−3	−10	5	120	123	1
−7	−6	4	53	55	1	−6	0	4	131	132	2	2	5	4	280	266	7	−6	12	4	62	58	1	−2	−10	5	177	171	1
−6	−6	4	187	187	3	−5	0	4	320	331	5	3	5	4	262	257	2	−5	12	4	38	33	1	−1	−10	5	95	96	1
−5	−6	4	140	142	2	−4	0	4	35	22	1	4	5	4	272	254	2	−4	12	4	67	70	1	0	−10	5	97	95	1
−4	−6	4	216	208	3	−3	0	4	103	93	1	5	5	4	80	85	1	−3	12	4	115	117	1	1	−10	5	93	92	1
−3	−6	4	44	41	1	−2	0	4	91	99	1	6	5	4	57	52	1	−2	12	4	69	72	2	2	−10	5	75	77	1
−2	−6	4	110	102	1	−1	0	4	622	630	8	7	5	4	47	44	1	1	12	4	121	120	2	3	−10	5	56	60	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	−6	4	105	102	1	0	0	4	870	877	11	−8	6	4	71	71	1	2	12	4	52	50	1	4	−10	5	17	19	1
0	−6	4	223	219	3	1	0	4	48	52	1	−7	6	4	54	55	1	3	12	4	21	19	1	5	−10	5	61	58	1
1	−6	4	188	180	2	2	0	4	176	173	2	−6	6	4	188	187	3	4	12	4	24	23	1	−7	−9	5	18	21	1
2	−6	4	36	34	1	3	0	4	94	105	1	−5	6	4	136	142	1	5	12	4	55	51	1	−6	−9	5	92	93	1
3	−6	4	142	137	2	4	0	4	53	59	1	−4	6	4	210	208	1	−5	13	4	45	43	1	−5	−9	5	75	75	1
4	−6	4	231	232	4	5	0	4	66	69	1	−3	6	4	43	40	1	−4	13	4	96	95	1	−4	−9	5	141	146	1
5	−6	4	61	61	1	6	0	4	127	124	2	−2	6	4	111	103	3	−3	13	4	124	127	1	−3	−9	5	73	73	1
−2	−9	5	78	77	1	−3	−3	5	177	167	2	4	2	5	108	102	1	−1	8	5	12	11	3	−1	−13	6	122	125	1
−1	−9	5	162	149	1	−2	−3	5	183	175	2	5	2	5	88	85	1	0	8	5	64	69	1	0	−13	6	79	85	1
0	−9	5	120	111	1	−1	−3	5	123	109	1	6	2	5	113	112	2	1	8	5	276	281	4	1	−13	6	127	129	1
1	−9	5	55	55	1	0	−3	5	104	104	1	7	2	5	38	37	1	2	8	5	188	178	2	2	−13	6	43	46	1
2	−9	5	154	149	1	1	−3	5	155	167	1	−8	3	5	39	38	1	3	8	5	212	222	2	3	−13	6	70	75	1
3	−9	5	25	22	1	2	−3	5	69	67	1	−7	3	5	67	79	1	4	8	5	61	64	1	−5	−12	6	65	61	1
4	−9	5	129	131	2	3	−3	5	67	79	1	−6	3	5	124	131	1	5	8	5	74	75	1	−4	−12	6	64	62	1
5	−9	5	51	51	1	4	−3	5	13	10	1	−5	3	5	177	184	1	6	8	5	51	50	1	−3	−12	6	146	146	1
6	−9	5	58	53	1	5	−3	5	88	86	1	−4	3	5	98	92	1	−6	9	5	92	92	1	−2	−12	6	100	95	1
−7	−8	5	94	91	1	6	−3	5	60	61	1	−3	3	5	176	166	2	−5	9	5	79	76	1	−1	−12	6	145	160	1
−6	−8	5	47	44	1	7	−3	5	50	49	1	−2	3	5	178	175	2	−4	9	5	143	146	1	0	−12	6	133	135	1
−5	−8	5	113	112	2	−8	−2	5	83	79	1	−1	3	5	124	110	2	−3	9	5	72	73	1	1	−12	6	102	98	1
−4	−8	5	53	58	1	−7	−2	5	114	119	2	0	3	5	105	104	2	−2	9	5	80	77	1	2	−12	6	56	56	1
−3	−8	5	156	174	1	−6	−2	5	178	177	3	1	3	5	157	168	2	−1	9	5	160	149	2	3	−12	6	54	50	1
−2	−8	5	86	97	1	−5	−2	5	130	131	2	2	3	5	70	67	1	0	9	5	118	111	2	4	−12	6	54	57	1
−1	−8	5	10	11	1	−4	−2	5	180	176	1	3	3	5	67	78	1	1	9	5	57	56	1	−6	−11	6	5	7	5
0	−8	5	64	69	1	−3	−2	5	165	155	1	4	3	5	12	9	1	2	9	5	151	148	2	−5	−11	6	60	58	1
1	−8	5	277	281	2	−2	−2	5	185	181	2	5	3	5	87	87	1	3	9	5	25	22	1	−4	−11	6	62	66	1
2	−8	5	188	177	1	−1	−2	5	246	242	2	6	3	5	59	61	1	4	9	5	129	131	1	−3	−11	6	18	15	1
3	−8	5	217	222	3	0	−2	5	325	312	4	7	3	5	50	48	1	5	9	5	50	51	1	−2	−11	6	71	74	1
4	−8	5	61	64	1	1	−2	5	219	204	2	−8	4	5	52	46	1	−6	10	5	34	32	1	−1	−11	6	204	211	1
5	−8	5	77	76	1	2	−2	5	227	229	2	−7	4	5	62	59	1	−5	10	5	210	209	2	0	−11	6	40	39	1
6	−8	5	51	49	1	3	−2	5	77	83	1	−6	4	5	95	93	1	−4	10	5	195	203	2	1	−11	6	140	138	1
−7	−7	5	57	56	1	4	−2	5	109	103	1	−5	4	5	234	237	1	−3	10	5	120	124	1	2	−11	6	106	117	1
−6	−7	5	107	109	1	5	−2	5	86	84	1	−4	4	5	143	147	1	−2	10	5	178	171	2	3	−11	6	104	108	2
−5	−7	5	43	44	1	6	−2	5	114	112	1	−3	4	5	229	227	6	−1	10	5	92	96	2	4	−11	6	90	87	1
−4	−7	5	163	165	1	7	−2	5	38	36	1	−2	4	5	70	73	1	0	10	5	96	95	1	5	−11	6	113	110	2
−3	−7	5	116	114	1	−8	−1	5	133	120	2	−1	4	5	218	210	3	1	10	5	95	92	1	−6	−10	6	27	23	1
−2	−7	5	66	72	1	−7	−1	5	18	19	1	0	4	5	275	252	4	2	10	5	75	78	1	−5	−10	6	162	171	2
−1	−7	5	97	88	1	−6	−1	5	169	166	3	1	4	5	496	501	9	3	10	5	56	60	1	−4	−10	6	225	234	2
0	−7	5	122	122	1	−5	−1	5	117	119	1	2	4	5	118	122	2	4	10	5	19	19	1	−3	−10	6	124	124	1
1	−7	5	273	279	1	−4	−1	5	315	317	3	3	4	5	55	58	1	5	10	5	60	57	1	−2	−10	6	162	163	1
2	−7	5	199	205	1	−3	−1	5	39	46	1	4	4	5	137	141	1	−6	11	5	30	29	1	−1	−10	6	164	161	1
3	−7	5	48	45	1	−2	−1	5	128	131	1	5	4	5	52	46	1	−5	11	5	52	56	1	0	−10	6	48	43	1
4	−7	5	54	51	1	−1	−1	5	211	223	2	6	4	5	74	76	1	−4	11	5	54	54	1	1	−10	6	96	97	1
5	−7	5	64	61	1	0	−1	5	83	72	1	7	4	5	60	58	1	−3	11	5	161	156	2	2	−10	6	32	33	1
6	−7	5	20	21	1	1	−1	5	190	188	2	−8	5	5	96	95	1	−2	11	5	272	268	5	3	−10	6	48	46	1
−7	−6	5	75	72	1	2	−1	5	253	249	3	−7	5	5	56	63	1	−1	11	5	300	302	6	4	−10	6	46	46	1
−6	−6	5	143	142	1	3	−1	5	90	90	1	−6	5	5	154	158	2	0	11	5	135	144	2	5	−10	6	77	82	1
−5	−6	5	202	199	3	4	−1	5	92	97	1	−5	5	5	227	233	1	1	11	5	196	199	3	−7	−9	6	53	56	1
−4	−6	5	23	21	1	5	−1	5	151	149	2	−4	5	5	190	191	1	2	11	5	149	153	2	−6	−9	6	67	65	1
−3	−6	5	126	127	1	6	−1	5	92	92	1	−3	5	5	232	248	3	3	11	5	90	99	1	−5	−9	6	57	65	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	−6	5	132	130	1	7	−1	5	133	131	2	−2	5	5	114	121	3	4	11	5	63	62	1	−4	−9	6	136	141	1
−1	−6	5	294	309	5	−8	0	5	18	20	1	−1	5	5	332	325	5	5	11	5	90	94	1	−3	−9	6	117	116	1
0	−6	5	208	204	2	−7	0	5	61	71	1	0	5	5	73	67	1	−5	12	5	88	93	1	−2	−9	6	128	124	1
1	−6	5	360	355	4	−6	0	5	46	42	1	1	5	5	128	128	3	−4	12	5	48	48	1	−1	−9	6	137	136	1
2	−6	5	37	25	1	−5	0	5	36	37	1	2	5	5	364	356	5	−3	12	5	68	70	1	0	−9	6	224	219	1
3	−6	5	55	50	1	−4	0	5	500	502	5	3	5	5	77	61	1	−2	12	5	77	71	2	1	−9	6	170	174	1
4	−6	5	32	26	1	−3	0	5	196	207	2	4	5	5	193	198	1	0	12	5	151	147	3	2	−9	6	122	114	1
5	−6	5	137	134	2	−2	0	5	224	231	2	5	5	5	292	291	2	1	12	5	67	62	1	3	−9	6	159	171	3
6	−6	5	30	26	1	−1	0	5	170	178	2	6	5	5	142	139	2	2	12	5	161	164	2	4	−9	6	51	43	1
−8	−5	5	98	96	1	0	0	5	40	40	1	7	5	5	24	22	1	3	12	5	28	29	1	5	−9	6	69	69	1
−7	−5	5	56	63	1	1	0	5	57	50	1	−8	6	5	80	82	1	4	12	5	46	43	1	−7	−8	6	33	35	1
−6	−5	5	155	158	1	2	0	5	129	127	1	−7	6	5	74	73	1	−5	13	5	27	23	1	−6	−8	6	190	191	2
−5	−5	5	230	233	4	3	0	5	68	65	1	−6	6	5	144	143	1	−4	13	5	116	116	1	−5	−8	6	79	79	1
−4	−5	5	190	191	1	4	0	5	37	36	1	−5	6	5	201	199	2	−3	13	5	102	98	1	−4	−8	6	16	14	1
−3	−5	5	233	247	1	5	0	5	43	36	1	−4	6	5	25	22	1	−2	13	5	126	125	2	−3	−8	6	94	104	1
−2	−5	5	113	120	1	6	0	5	198	196	3	−3	6	5	124	127	1	1	13	5	64	69	1	−2	−8	6	24	30	1
−1	−5	5	314	324	4	7	0	5	74	71	1	−2	6	5	125	129	4	2	13	5	37	38	1	−1	−8	6	118	117	1
0	−5	5	70	66	1	−8	1	5	134	120	2	−1	6	5	303	309	5	3	13	5	51	55	1	0	−8	6	250	248	1
1	−5	5	133	128	1	−7	1	5	18	18	1	0	6	5	210	204	3	4	13	5	35	37	1	1	−8	6	65	66	1
2	−5	5	363	357	3	−6	1	5	170	167	3	1	6	5	360	354	9	−4	14	5	117	111	2	2	−8	6	240	233	2
3	−5	5	76	61	1	−5	1	5	115	119	1	2	6	5	37	25	1	−3	14	5	129	130	1	3	−8	6	69	60	1
4	−5	5	193	197	3	−4	1	5	309	317	2	3	6	5	54	50	1	−2	14	5	186	191	3	4	−8	6	171	169	3
5	−5	5	292	291	5	−3	1	5	38	46	1	4	6	5	32	27	1	1	14	5	10	9	4	5	−8	6	119	118	2
6	−5	5	140	139	2	−2	1	5	128	132	1	5	6	5	136	134	1	2	14	5	68	67	1	6	−8	6	54	53	1
−8	−4	5	53	46	1	−1	1	5	212	224	2	6	6	5	28	25	1	3	14	5	61	61	1	−7	−7	6	63	60	1
−7	−4	5	63	60	1	0	1	5	81	71	1	7	6	5	38	41	1	−3	15	5	28	26	1	−6	−7	6	104	103	1
−6	−4	5	94	93	1	1	1	5	192	188	2	−7	7	5	57	57	1	1	15	5	96	91	1	−5	−7	6	7	10	2
−5	−4	5	235	235	2	2	1	5	254	249	3	−6	7	5	104	110	1	2	15	5	69	70	1	−4	−7	6	70	70	1
−4	−4	5	145	147	1	3	1	5	90	90	1	−5	7	5	43	44	1	−3	−15	6	95	90	1	−3	−7	6	54	55	1
−3	−4	5	231	227	2	4	1	5	92	98	1	−4	7	5	163	165	1	−2	−15	6	89	86	1	−2	−7	6	93	90	1
−2	−4	5	70	73	1	5	1	5	152	149	2	−3	7	5	114	114	1	−1	−15	6	165	163	1	−1	−7	6	18	17	1
−1	−4	5	212	210	2	6	1	5	93	92	1	−2	7	5	70	72	1	0	−15	6	73	74	1	0	−7	6	219	210	1
0	−4	5	275	253	3	7	1	5	132	131	1	−1	7	5	100	89	2	1	−15	6	95	89	1	1	−7	6	121	121	1
1	−4	5	513	499	6	−8	2	5	82	79	1	0	7	5	123	122	2	2	−15	6	61	62	1	2	−7	6	92	100	1
2	−4	5	120	122	1	−7	2	5	109	119	2	1	7	5	280	280	4	−4	−14	6	92	95	1	3	−7	6	108	103	2
3	−4	5	54	57	1	−6	2	5	176	177	3	2	7	5	200	206	2	−3	−14	6	153	149	1	4	−7	6	233	238	4
4	−4	5	139	142	2	−5	2	5	131	131	1	3	7	5	46	45	1	−2	−14	6	140	136	1	5	−7	6	87	81	1
5	−4	5	52	46	1	−4	2	5	177	175	1	4	7	5	55	52	1	−1	−14	6	49	51	1	6	−7	6	60	60	1
6	−4	5	77	76	1	−3	2	5	161	156	2	5	7	5	62	61	1	0	−14	6	39	44	1	−7	−6	6	51	52	1
7	−4	5	62	59	1	−2	2	5	184	182	2	6	7	5	18	21	1	1	−14	6	38	38	1	−6	−6	6	63	60	1
−8	−3	5	37	37	1	−1	2	5	244	243	3	−6	8	5	45	44	1	2	−14	6	37	39	1	−5	−6	6	45	47	1
−7	−3	5	75	79	1	0	2	5	318	312	4	−5	8	5	111	112	1	−5	−13	6	53	54	1	−4	−6	6	105	106	1
−6	−3	5	128	131	2	1	2	5	218	203	3	−4	8	5	54	58	1	−4	−13	6	87	87	1	−3	−6	6	93	92	1
−5	−3	5	181	184	2	2	2	5	228	228	3	−3	8	5	159	175	1	−3	−13	6	53	55	1	−2	−6	6	177	173	1
−4	−3	5	101	93	1	3	2	5	77	83	1	−2	8	5	87	98	1	−2	−13	6	99	96	1	−1	−6	6	42	46	1
0	−6	6	101	105	1	−6	0	6	145	155	2	1	5	6	94	95	3	2	12	6	57	56	1	−5	−8	7	186	208	2
1	−6	6	217	220	1	−5	0	6	68	63	1	2	5	6	109	119	1	3	12	6	54	50	1	−4	−8	7	87	90	1
2	−6	6	124	128	1	−4	0	6	79	66	1	3	5	6	143	142	1	4	12	6	55	56	1	−3	−8	7	60	69	1
3	−6	6	149	142	1	−3	0	6	24	10	2	4	5	6	50	53	1	−5	13	6	54	55	1	−2	−8	7	224	237	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	−6	6	48	46	1	−2	0	6	159	167	2	5	5	6	169	162	1	−4	13	6	89	87	1	−1	−8	7	65	53	1
5	−6	6	70	65	1	−1	0	6	435	444	7	6	5	6	80	82	1	−3	13	6	51	55	1	0	−8	7	318	324	2
6	−6	6	76	76	1	0	0	6	265	270	3	−7	6	6	51	51	1	−2	13	6	98	96	2	1	−8	7	397	401	3
−8	−5	6	43	45	1	1	0	6	95	95	1	−6	6	6	62	60	1	0	13	6	79	85	2	2	−8	7	120	114	1
−7	−5	6	55	54	1	2	0	6	82	83	1	−5	6	6	48	47	1	1	13	6	127	130	2	3	−8	7	42	39	1
−6	−5	6	155	153	2	3	0	6	7	9	1	−4	6	6	105	106	1	2	13	6	44	46	1	4	−8	7	18	18	1
−5	−5	6	36	39	1	4	0	6	4	7	4	−3	6	6	94	92	1	3	13	6	71	75	1	5	−8	7	43	43	1
−4	−5	6	24	23	1	5	0	6	54	54	1	−2	6	6	178	174	2	−4	14	6	94	95	1	−7	−7	7	34	34	1
−3	−5	6	113	111	1	6	0	6	59	58	1	−1	6	6	43	46	2	−3	14	6	152	149	2	−6	−7	7	131	130	2
−2	−5	6	107	112	1	7	0	6	43	40	1	0	6	6	103	105	2	−2	14	6	136	136	2	−5	−7	7	58	62	1
−1	−5	6	317	317	5	−8	1	6	45	41	1	1	6	6	219	219	3	1	14	6	38	37	1	−4	−7	7	69	62	1
0	−5	6	332	330	5	−7	1	6	48	43	1	2	6	6	122	128	1	2	14	6	39	40	1	−3	−7	7	56	55	1
1	−5	6	93	96	1	−6	1	6	161	167	2	3	6	6	148	141	1	3	14	6	99	95	2	−2	−7	7	42	43	1
2	−5	6	109	119	1	−5	1	6	150	148	1	4	6	6	47	46	1	−3	15	6	93	90	1	−1	−7	7	67	71	1
3	−5	6	143	142	1	−4	1	6	114	113	1	5	6	6	71	65	1	1	15	6	90	89	1	0	−7	7	118	116	1
4	−5	6	52	53	1	−3	1	6	143	138	2	6	6	6	75	76	1	2	15	6	60	61	1	1	−7	7	65	62	1
5	−5	6	171	162	3	−2	1	6	85	81	1	−7	7	6	57	60	1	−2	−15	7	99	99	1	2	−7	7	147	148	1
6	−5	6	80	83	1	−1	1	6	543	538	9	−6	7	6	102	103	1	−1	−15	7	63	59	1	3	−7	7	71	72	1
−8	−4	6	37	33	1	0	1	6	247	262	3	−5	7	6	7	10	3	0	−15	7	108	110	1	4	−7	7	17	11	1
−7	−4	6	74	78	1	1	1	6	89	82	1	−4	7	6	71	70	1	1	−15	7	77	76	1	5	−7	7	83	81	1
−6	−4	6	50	47	1	2	1	6	182	176	2	−3	7	6	55	54	1	−4	−14	7	62	61	1	6	−7	7	45	41	1
−5	−4	6	46	46	1	3	1	6	48	47	1	−2	7	6	93	91	1	−3	−14	7	39	38	1	−7	−6	7	23	23	1
−4	−4	6	106	107	1	4	1	6	78	85	1	−1	7	6	15	17	2	−2	−14	7	72	74	1	−6	−6	7	16	14	1
−3	−4	6	62	67	1	5	1	6	85	83	1	0	7	6	220	211	3	−1	−14	7	38	34	1	−5	−6	7	196	200	2
−2	−4	6	34	33	1	6	1	6	93	87	1	1	7	6	122	122	2	0	−14	7	59	58	1	−4	−6	7	162	163	1
−1	−4	6	227	221	4	7	1	6	27	29	1	2	7	6	92	100	1	1	−14	7	76	75	1	−3	−6	7	84	83	1
0	−4	6	295	279	4	−8	2	6	52	51	1	3	7	6	105	103	1	2	−14	7	97	96	1	−2	−6	7	114	112	1
1	−4	6	152	148	2	−7	2	6	32	35	1	4	7	6	228	239	2	−4	−13	7	55	53	1	−1	−6	7	44	38	1
2	−4	6	190	194	1	−6	2	6	210	211	2	5	7	6	84	81	1	−3	−13	7	98	97	1	0	−6	7	57	51	1
3	−4	6	51	53	1	−5	2	6	43	37	1	6	7	6	55	60	1	−2	−13	7	93	90	1	1	−6	7	59	57	1
4	−4	6	123	120	2	−4	2	6	146	153	1	−6	8	6	188	191	2	−1	−13	7	75	70	1	2	−6	7	198	199	1
5	−4	6	53	52	1	−3	2	6	139	135	2	−5	8	6	85	80	1	0	−13	7	53	48	1	3	−6	7	122	121	1
6	−4	6	118	112	2	−2	2	6	47	46	1	−4	8	6	21	15	1	1	−13	7	65	65	1	4	−6	7	68	66	1
−8	−3	6	56	47	1	−1	2	6	383	369	6	−3	8	6	96	104	1	2	−13	7	111	113	1	5	−6	7	66	65	1
−7	−3	6	83	82	1	0	2	6	476	464	8	−2	8	6	25	30	1	3	−13	7	90	92	1	6	−6	7	71	67	1
−6	−3	6	38	34	1	1	2	6	403	396	5	−1	8	6	117	116	1	−5	−12	7	23	22	1	−8	−5	7	56	52	1
−5	−3	6	105	106	1	2	2	6	145	145	2	0	8	6	252	248	3	−4	−12	7	132	132	1	−7	−5	7	7	9	6
−4	−3	6	111	116	1	3	2	6	53	53	1	1	8	6	63	65	1	−3	−12	7	29	22	1	−6	−5	7	47	44	1
−3	−3	6	140	140	2	4	2	6	161	158	1	2	8	6	239	232	2	−2	−12	7	98	94	1	−5	−5	7	113	115	1
−2	−3	6	36	35	1	5	2	6	146	151	2	3	8	6	68	60	1	−1	−12	7	87	89	1	−4	−5	7	91	95	1
−1	−3	6	196	199	3	6	2	6	41	42	1	4	8	6	169	169	2	0	−12	7	66	69	1	−3	−5	7	147	145	1
0	−3	6	353	336	4	7	2	6	64	68	1	5	8	6	118	118	2	1	−12	7	114	116	1	−2	−5	7	165	174	1
1	−3	6	147	144	2	−8	3	6	54	47	1	−6	9	6	68	65	1	2	−12	7	94	93	1	−1	−5	7	106	104	1
2	−3	6	99	102	1	−7	3	6	82	81	1	−5	9	6	60	65	1	3	−12	7	10	7	2	0	−5	7	211	208	2
3	−3	6	45	49	1	−6	3	6	36	34	1	−4	9	6	133	140	1	4	−12	7	53	54	1	1	−5	7	107	109	1
4	−3	6	24	25	1	−5	3	6	104	105	1	−3	9	6	119	116	1	−6	−11	7	18	16	1	2	−5	7	125	128	1
5	−3	6	138	143	2	−4	3	6	109	116	1	−2	9	6	127	123	2	−5	−11	7	118	117	1	3	−5	7	105	108	1
6	−3	6	141	135	2	−3	3	6	140	140	4	−1	9	6	134	136	2	−4	−11	7	115	114	1	4	−5	7	66	69	1
7	−3	6	19	14	1	−2	3	6	36	35	2	0	9	6	223	219	3	−3	−11	7	129	135	1	5	−5	7	83	83	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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
−8	−2	6	55	51	1	−1	3	6	208	199	3	1	9	6	167	174	2	−2	−11	7	40	39	1	6	−5	7	15	17	1
−7	−2	6	32	35	1	0	3	6	357	335	6	2	9	6	123	115	1	−1	−11	7	46	46	1	−8	−4	7	18	14	1
−6	−2	6	212	211	3	1	3	6	144	145	4	3	9	6	173	171	2	0	−11	7	51	54	1	−7	−4	7	50	55	1
−5	−2	6	44	38	1	2	3	6	98	101	1	4	9	6	51	44	1	1	−11	7	136	144	1	−6	−4	7	149	151	2
−4	−2	6	147	153	1	3	3	6	46	49	1	5	9	6	70	70	1	2	−11	7	76	84	1	−5	−4	7	39	41	1
−3	−2	6	143	134	2	4	3	6	24	25	1	−6	10	6	25	23	1	3	−11	7	137	135	2	−4	−4	7	199	205	1
−2	−2	6	46	46	1	5	3	6	139	144	2	−5	10	6	165	172	2	4	−11	7	81	80	1	−3	−4	7	111	112	1
−1	−2	6	380	368	6	6	3	6	139	135	2	−4	10	6	231	233	3	−6	−10	7	112	115	2	−2	−4	7	158	160	3
0	−2	6	481	464	6	7	3	6	18	14	1	−3	10	6	125	124	1	−5	−10	7	82	80	1	−1	−4	7	392	399	6
1	−2	6	412	397	5	−8	4	6	37	33	1	−2	10	6	166	163	2	−4	−10	7	212	211	1	0	−4	7	174	173	3
2	−2	6	144	146	1	−7	4	6	70	78	1	−1	10	6	164	162	3	−3	−10	7	165	168	1	1	−4	7	361	375	2
3	−2	6	54	53	1	−6	4	6	50	47	1	0	10	6	46	43	1	−2	−10	7	91	85	1	2	−4	7	67	59	1
4	−2	6	163	157	2	−5	4	6	43	45	1	1	10	6	99	97	2	−1	−10	7	241	238	1	3	−4	7	37	37	1
5	−2	6	153	151	1	−4	4	6	104	107	1	2	10	6	35	34	1	0	−10	7	95	89	1	4	−4	7	101	93	1
6	−2	6	39	41	1	−3	4	6	60	66	1	3	10	6	46	46	1	1	−10	7	54	53	1	5	−4	7	176	173	3
7	−2	6	64	68	1	−2	4	6	33	33	2	4	10	6	47	45	1	2	−10	7	63	56	1	6	−4	7	100	99	1
−8	−1	6	45	41	1	−1	4	6	237	222	4	5	10	6	78	82	1	3	−10	7	39	37	1	−8	−3	7	25	21	1
−7	−1	6	51	44	1	0	4	6	300	278	5	−6	11	6	0	7	1	4	−10	7	43	38	1	−7	−3	7	49	56	1
−6	−1	6	167	166	2	1	4	6	154	148	4	−5	11	6	62	58	1	5	−10	7	76	72	1	−6	−3	7	45	39	1
−5	−1	6	150	149	1	2	4	6	191	195	1	−4	11	6	58	65	1	−7	−9	7	83	84	1	−5	−3	7	171	170	1
−4	−1	6	114	113	1	3	4	6	50	52	1	−3	11	6	20	15	1	−6	−9	7	47	50	1	−4	−3	7	145	143	1
−3	−1	6	145	138	2	4	4	6	122	120	1	−2	11	6	74	74	2	−5	−9	7	114	116	1	−3	−3	7	31	27	1
−2	−1	6	84	80	1	5	4	6	54	53	1	0	11	6	40	38	1	−4	−9	7	57	57	1	−2	−3	7	144	138	2
−1	−1	6	534	537	10	6	4	6	118	113	2	1	11	6	140	139	2	−3	−9	7	136	141	1	−1	−3	7	226	219	4
0	−1	6	249	262	3	7	4	6	46	42	1	2	11	6	106	117	1	−2	−9	7	135	140	1	0	−3	7	115	108	2
1	−1	6	89	81	1	−8	5	6	42	45	1	3	11	6	103	109	1	−1	−9	7	113	109	1	1	−3	7	299	296	4
2	−1	6	177	176	2	−7	5	6	56	55	1	4	11	6	91	87	1	0	−9	7	93	97	1	2	−3	7	19	10	1
3	−1	6	48	48	1	−6	5	6	151	154	1	5	11	6	113	110	2	1	−9	7	254	257	2	3	−3	7	106	109	1
4	−1	6	78	85	1	−5	5	6	39	39	1	−5	12	6	65	61	1	2	−9	7	179	174	1	4	−3	7	169	166	3
5	−1	6	89	84	1	−4	5	6	25	23	1	−4	12	6	66	62	1	3	−9	7	19	18	1	5	−3	7	81	84	1
6	−1	6	95	87	1	−3	5	6	115	111	2	−3	12	6	149	145	2	4	−9	7	44	41	1	6	−3	7	146	142	2
7	−1	6	27	29	1	−2	5	6	111	111	3	−2	12	6	100	95	2	5	−9	7	65	60	1	−8	−2	7	37	33	1
−8	0	6	45	50	1	−1	5	6	319	319	5	0	12	6	134	135	2	−7	−8	7	29	29	1	−7	−2	7	70	67	1
−7	0	6	34	28	1	0	5	6	329	329	5	1	12	6	101	97	2	−6	−8	7	39	45	1	−6	−2	7	162	161	2
−5	−2	7	213	210	1	−8	4	7	13	14	1	2	10	7	62	56	1	1	−9	8	183	188	1	6	−3	8	61	61	1
−4	−2	7	161	155	1	−7	4	7	49	54	1	3	10	7	42	38	1	2	−9	8	81	87	1	−8	−2	8	19	17	1
−3	−2	7	108	111	1	−6	4	7	149	152	1	4	10	7	42	37	1	3	−9	8	40	41	1	−7	−2	8	58	53	1
−2	−2	7	331	340	5	−5	4	7	39	41	1	5	10	7	75	72	1	4	−9	8	58	59	1	−6	−2	8	137	141	2
−1	−2	7	170	169	3	−4	4	7	202	206	1	−6	11	7	18	17	1	5	−9	8	58	63	1	−5	−2	8	242	244	2
0	−2	7	439	422	7	−3	4	7	108	112	1	−5	11	7	121	117	1	−7	−8	8	71	69	1	−4	−2	8	181	178	1
1	−2	7	210	203	2	−2	4	7	158	160	3	−4	11	7	115	114	1	−6	−8	8	18	17	1	−3	−2	8	198	204	1
2	−2	7	94	89	1	−1	4	7	386	399	6	−3	11	7	131	135	1	−5	−8	8	38	38	1	−2	−2	8	410	403	5
3	−2	7	60	58	1	0	4	7	174	173	3	−2	11	7	35	39	2	−4	−8	8	19	20	1	−1	−2	8	201	205	3
4	−2	7	189	191	3	1	4	7	365	375	5	0	11	7	51	54	1	−3	−8	8	11	13	1	0	−2	8	283	288	3
5	−2	7	219	220	3	2	4	7	70	59	1	1	11	7	140	143	2	−2	−8	8	188	191	1	1	−2	8	102	108	1
6	−2	7	152	151	2	3	4	7	38	37	1	2	11	7	77	84	1	−1	−8	8	168	171	1	2	−2	8	22	24	1
−8	−1	7	70	70	1	4	4	7	99	94	1	3	11	7	138	135	1	0	−8	8	160	163	1	3	−2	8	110	109	1
−7	−1	7	106	107	1	5	4	7	175	173	2	4	11	7	83	81	1	1	−8	8	310	308	2	4	−2	8	31	33	1
−6	−1	7	151	151	2	6	4	7	100	99	1	−5	12	7	24	22	1	2	−8	8	184	186	2	5	−2	8	133	139	2

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	38	34	1	−8	5	7	53	52	1	−4	12	7	136	132	1	3	−8	8	125	135	2	6	−2	8	153	148	2
−4	−1	7	189	195	1	−7	5	7	0	8	1	−3	12	7	26	22	1	4	−8	8	130	133	2	−8	−1	8	39	39	1
−3	−1	7	143	137	2	−6	5	7	49	44	1	−2	12	7	97	93	2	5	−8	8	32	31	1	−7	−1	8	84	83	1
−2	−1	7	133	124	2	−5	5	7	114	115	1	0	12	7	64	69	1	−7	−7	8	35	31	1	−6	−1	8	39	40	1
−1	−1	7	128	120	2	−4	5	7	90	95	1	1	12	7	114	115	1	−6	−7	8	147	143	2	−5	−1	8	78	78	1
0	−1	7	44	45	1	−3	5	7	148	145	1	2	12	7	96	92	1	−5	−7	8	21	19	1	−4	−1	8	121	131	1
1	−1	7	27	32	1	−2	5	7	165	174	2	3	12	7	4	7	3	−4	−7	8	69	66	1	−3	−1	8	24	21	1
2	−1	7	79	77	1	−1	5	7	109	104	2	4	12	7	55	54	1	−3	−7	8	27	33	1	−2	−1	8	129	137	2
3	−1	7	64	63	1	0	5	7	216	208	4	−4	13	7	57	53	1	−2	−7	8	68	65	1	−1	−1	8	87	87	2
4	−1	7	36	34	1	1	5	7	109	110	1	−3	13	7	96	96	1	−1	−7	8	45	49	1	0	−1	8	69	72	2
5	−1	7	51	47	1	2	5	7	126	128	1	−2	13	7	90	90	2	0	−7	8	124	127	1	1	−1	8	265	270	2
6	−1	7	153	147	2	3	5	7	105	109	1	0	13	7	49	49	1	1	−7	8	148	146	1	2	−1	8	106	113	1
−8	0	7	169	156	2	4	5	7	65	69	1	1	13	7	64	65	1	2	−7	8	78	74	1	3	−1	8	101	102	1
−7	0	7	116	119	2	5	5	7	82	83	1	2	13	7	116	114	1	3	−7	8	77	82	1	4	−1	8	36	37	1
−6	0	7	28	33	1	6	5	7	17	17	1	3	13	7	92	92	1	4	−7	8	63	71	1	5	−1	8	22	20	1
−5	0	7	52	56	1	−7	6	7	23	23	1	−4	14	7	62	61	1	5	−7	8	101	98	2	6	−1	8	49	47	1
−4	0	7	48	46	1	−6	6	7	16	14	1	−3	14	7	36	38	1	−7	−6	8	63	65	1	−8	0	8	21	11	1
−3	0	7	39	38	1	−5	6	7	200	200	2	−2	14	7	69	74	1	−6	−6	8	154	167	2	−7	0	8	102	93	1
−2	0	7	90	91	2	−4	6	7	162	163	1	1	14	7	75	75	1	−5	−6	8	60	62	1	−6	0	8	216	236	2
−1	0	7	84	99	2	−3	6	7	85	84	1	2	14	7	97	96	1	−4	−6	8	113	112	1	−5	0	8	225	234	1
0	0	7	67	71	1	−2	6	7	115	112	2	1	15	7	74	75	1	−3	−6	8	151	150	1	−4	0	8	87	85	1
1	0	7	229	238	3	−1	6	7	42	38	1	−1	−15	8	26	32	1	−2	−6	8	43	43	1	−3	0	8	14	11	1
2	0	7	281	295	2	0	6	7	58	51	1	−3	−14	8	53	56	1	−1	−6	8	88	85	1	−2	0	8	18	19	3
3	0	7	16	20	1	1	6	7	58	57	1	−2	−14	8	49	49	1	0	−6	8	95	100	1	−1	0	8	215	205	4
4	0	7	38	35	1	2	6	7	198	198	2	−1	−14	8	46	49	1	1	−6	8	75	73	1	0	0	8	49	26	2
5	0	7	53	54	1	3	6	7	120	120	1	0	−14	8	47	47	1	2	−6	8	256	253	2	1	0	8	31	31	1
6	0	7	187	191	3	4	6	7	68	66	1	1	−14	8	83	77	1	3	−6	8	100	98	2	2	0	8	19	19	1
−8	1	7	72	70	1	5	6	7	65	65	1	−4	−13	8	44	44	1	4	−6	8	105	108	2	3	0	8	202	204	1
−7	1	7	103	107	2	6	6	7	70	67	1	−3	−13	8	38	36	1	5	−6	8	9	10	2	4	0	8	47	48	1
−6	1	7	149	151	1	−6	7	7	128	130	1	−2	−13	8	124	120	1	−7	−5	8	14	16	1	5	0	8	39	36	1
−5	1	7	35	33	1	−5	7	7	62	61	1	−1	−13	8	23	23	1	−6	−5	8	32	34	1	6	0	8	27	28	1
−4	1	7	185	194	1	−4	7	7	69	62	1	0	−13	8	37	36	1	−5	−5	8	61	62	1	−8	1	8	39	37	1
−3	1	7	140	136	2	−3	7	7	58	56	1	1	−13	8	30	31	1	−4	−5	8	120	122	1	−7	1	8	85	83	1
−2	1	7	134	125	2	−2	7	7	43	42	1	2	−13	8	9	8	2	−3	−5	8	91	95	1	−6	1	8	39	40	1
−1	1	7	129	120	2	−1	7	7	68	71	1	−5	−12	8	32	29	1	−2	−5	8	103	108	1	−5	1	8	77	78	1
0	1	7	44	45	2	0	7	7	118	116	2	−4	−12	8	39	41	1	−1	−5	8	142	140	1	−4	1	8	122	130	1
1	1	7	27	32	1	1	7	7	66	62	1	−3	−12	8	98	94	1	0	−5	8	107	109	1	−3	1	8	23	21	1
2	1	7	79	78	1	2	7	7	148	149	1	−2	−12	8	63	57	1	1	−5	8	107	114	1	−2	1	8	133	137	2
3	1	7	64	64	1	3	7	7	73	72	1	−1	−12	8	77	81	1	2	−5	8	134	136	1	−1	1	8	86	88	2
4	1	7	35	34	1	4	7	7	15	10	1	0	−12	8	18	19	1	3	−5	8	66	70	1	0	1	8	70	73	2
5	1	7	50	47	1	5	7	7	81	82	1	1	−12	8	98	91	1	4	−5	8	33	35	1	1	1	8	267	271	3
6	1	7	149	147	2	−6	8	7	40	44	1	2	−12	8	44	47	1	5	−5	8	22	19	1	2	1	8	106	112	1
−8	2	7	38	34	1	−5	8	7	205	208	2	3	−12	8	71	74	1	6	−5	8	67	64	1	3	1	8	100	102	1
−7	2	7	67	67	1	−4	8	7	87	90	1	−6	−11	8	26	29	1	−8	−4	8	40	39	1	4	1	8	36	37	1
−6	2	7	161	161	1	−3	8	7	61	69	1	−5	−11	8	101	103	1	−7	−4	8	81	80	1	5	1	8	23	20	1
−5	2	7	212	210	1	−2	8	7	223	237	3	−4	−11	8	33	32	1	−6	−4	8	43	41	1	6	1	8	48	47	1
−4	2	7	160	155	1	−1	8	7	64	53	1	−3	−11	8	92	90	1	−5	−4	8	37	30	1	−8	2	8	16	16	1
−3	2	7	106	111	1	0	8	7	318	324	4	−2	−11	8	173	175	1	−4	−4	8	58	55	1	−7	2	8	58	53	1
−2	2	7	330	340	5	1	8	7	399	401	6	−1	−11	8	89	103	1	−3	−4	8	127	133	1	−6	2	8	146	142	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	2	7	173	169	3	2	8	7	120	115	1	0	−11	8	133	132	1	−2	−4	8	17	20	1	−5	2	8	240	244	2
0	2	7	447	421	7	3	8	7	43	39	1	1	−11	8	55	60	1	−1	−4	8	70	80	1	−4	2	8	181	178	1
1	2	7	210	203	5	4	8	7	19	18	1	2	−11	8	79	79	1	0	−4	8	200	201	1	−3	2	8	198	204	1
2	2	7	93	89	1	5	8	7	42	43	1	3	−11	8	0	7	1	1	−4	8	64	62	1	−2	2	8	400	403	5
3	2	7	59	58	1	−6	9	7	47	50	1	4	−11	8	22	26	1	2	−4	8	150	147	1	−1	2	8	203	204	3
4	2	7	187	191	1	−5	9	7	118	117	1	−6	−10	8	44	45	1	3	−4	8	83	80	1	0	2	8	280	288	5
5	2	7	199	220	2	−4	9	7	57	58	1	−5	−10	8	70	73	1	4	−4	8	104	104	2	1	2	8	102	107	1
6	2	7	151	151	1	−3	9	7	137	141	1	−4	−10	8	66	69	1	5	−4	8	150	147	2	2	2	8	22	25	1
−8	3	7	26	21	1	−2	9	7	133	140	2	−3	−10	8	101	100	1	6	−4	8	116	109	2	3	2	8	109	109	1
−7	3	7	49	56	1	−1	9	7	111	110	2	−2	−10	8	53	58	1	−8	−3	8	29	28	1	4	2	8	33	32	1
−6	3	7	47	39	1	0	9	7	88	97	1	−1	−10	8	175	167	1	−7	−3	8	50	51	1	5	2	8	134	138	2
−5	3	7	172	171	1	1	9	7	253	257	3	0	−10	8	126	131	1	−6	−3	8	140	150	2	6	2	8	149	148	2
−4	3	7	145	143	1	2	9	7	179	174	2	1	−10	8	71	69	1	−5	−3	8	161	165	1	−8	3	8	29	28	1
−3	3	7	30	27	1	3	9	7	21	18	1	2	−10	8	46	50	1	−4	−3	8	145	157	1	−7	3	8	49	51	1
−2	3	7	145	138	2	4	9	7	44	42	1	3	−10	8	116	116	2	−3	−3	8	127	130	1	−6	3	8	152	149	1
−1	3	7	224	219	4	5	9	7	64	61	1	4	−10	8	28	30	1	−2	−3	8	116	115	1	−5	3	8	160	166	1
0	3	7	115	108	2	−6	10	7	113	115	1	−6	−9	8	35	35	1	−1	−3	8	323	314	4	−4	3	8	148	157	1
1	3	7	304	297	7	−5	10	7	80	79	1	−5	−9	8	158	156	2	0	−3	8	147	147	2	−3	3	8	126	130	1
2	3	7	15	11	1	−4	10	7	208	211	2	−4	−9	8	110	113	1	1	−3	8	150	148	1	−2	3	8	115	114	1
3	3	7	105	109	1	−3	10	7	164	168	2	−3	−9	8	71	75	1	2	−3	8	181	182	1	−1	3	8	321	314	5
4	3	7	172	166	1	−2	10	7	91	85	2	−2	−9	8	227	236	1	3	−3	8	76	78	1	0	3	8	148	146	2
5	3	7	75	85	1	0	10	7	94	89	2	−1	−9	8	23	22	1	4	−3	8	226	250	4	1	3	8	152	148	1
6	3	7	146	143	1	1	10	7	54	53	1	0	−9	8	97	98	1	5	−3	8	26	26	1	2	3	8	181	183	1
3	3	8	77	79	1	4	10	8	30	30	1	−7	−7	9	47	47	1	−1	−1	9	152	144	1	0	5	9	51	50	1
4	3	8	246	249	2	−5	11	8	102	103	1	−6	−7	9	47	50	1	0	−1	9	153	158	1	1	5	9	104	111	1
5	3	8	27	27	1	−4	11	8	33	32	1	−5	−7	9	103	104	2	1	−1	9	179	190	1	2	5	9	93	93	1
6	3	8	58	60	1	−3	11	8	94	90	2	−4	−7	9	106	105	1	2	−1	9	111	110	1	3	5	9	60	58	1
−8	4	8	39	38	1	−2	11	8	173	175	3	−3	−7	9	71	69	1	3	−1	9	56	55	1	4	5	9	126	130	1
−7	4	8	80	80	1	0	11	8	131	133	2	−2	−7	9	170	168	1	4	−1	9	78	81	1	5	5	9	53	52	1
−6	4	8	46	40	1	1	11	8	58	61	1	−1	−7	9	111	107	1	5	−1	9	81	80	1	−6	6	9	31	32	1
−5	4	8	36	29	1	2	11	8	79	79	1	0	−7	9	127	130	1	6	−1	9	99	100	1	−5	6	9	155	157	2
−4	4	8	58	55	1	3	11	8	2	7	2	1	−7	9	33	37	1	−8	0	9	129	128	2	−4	6	9	64	67	1
−3	4	8	127	133	1	4	11	8	21	26	1	2	−7	9	145	144	1	−7	0	9	80	86	1	−3	6	9	37	39	1
−2	4	8	17	19	2	−5	12	8	31	29	1	3	−7	9	123	127	2	−6	0	9	124	123	1	−2	6	9	28	33	1
−1	4	8	69	79	2	−4	12	8	37	40	1	4	−7	9	39	39	1	−5	0	9	151	158	1	−1	6	9	110	111	1
0	4	8	207	201	2	−3	12	8	95	93	1	5	−7	9	97	97	1	−4	0	9	132	141	1	0	6	9	219	217	3
1	4	8	64	62	1	−2	12	8	65	57	1	−7	−6	9	65	58	1	−3	0	9	16	18	1	1	6	9	89	93	1
2	4	8	151	147	1	0	12	8	19	19	2	−6	−6	9	37	32	1	−2	0	9	160	183	1	2	6	9	121	119	1
3	4	8	81	79	1	1	12	8	98	91	1	−5	−6	9	152	156	1	−1	0	9	27	25	1	3	6	9	68	66	1
4	4	8	106	104	1	2	12	8	44	46	1	−4	−6	9	65	67	1	0	0	9	321	321	3	4	6	9	61	61	1
5	4	8	148	147	2	3	12	8	72	73	1	−3	−6	9	37	39	1	1	0	9	60	65	1	−6	7	9	48	50	1
6	4	8	110	109	2	−4	13	8	44	43	1	−2	−6	9	30	34	1	2	0	9	171	181	1	−5	7	9	105	104	1
−7	5	8	7	16	7	−3	13	8	39	36	1	−1	−6	9	112	111	1	3	0	9	133	137	1	−4	7	9	104	105	1
−6	5	8	36	34	1	−2	13	8	117	120	2	0	−6	9	222	217	1	4	0	9	59	55	1	−3	7	9	72	70	2
−5	5	8	58	61	1	0	13	8	37	36	1	1	−6	9	89	93	1	5	0	9	219	217	4	−2	7	9	167	169	3
−4	5	8	122	121	1	1	13	8	30	30	1	2	−6	9	125	119	1	6	0	9	104	110	2	−1	7	9	109	107	1
−3	5	8	93	95	1	2	13	8	9	8	2	3	−6	9	65	66	1	−8	1	9	37	32	1	0	7	9	127	129	2
−2	5	8	104	108	1	−3	14	8	52	56	1	4	−6	9	60	62	1	−7	1	9	86	86	1	1	7	9	35	37	1
−1	5	8	139	140	1	1	14	8	80	77	1	5	−6	9	49	48	1	−6	1	9	127	126	1	2	7	9	135	144	2

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	5	8	108	109	1	−2	−14	9	26	27	1	−7	−5	9	44	41	1	−5	1	9	122	122	1	3	7	9	126	127	1
1	5	8	105	114	1	−1	−14	9	7	9	2	−6	−5	9	143	148	2	−4	1	9	47	48	1	4	7	9	38	39	1
2	5	8	137	136	1	0	−14	9	55	51	1	−5	−5	9	91	92	1	−3	1	9	76	77	1	−6	8	9	80	76	1
3	5	8	66	70	1	−4	−13	9	56	56	1	−4	−5	9	232	236	1	−2	1	9	185	186	2	−5	8	9	84	84	1
4	5	8	34	35	1	−3	−13	9	15	14	1	−3	−5	9	40	38	1	−1	1	9	152	144	1	−4	8	9	104	108	2
5	5	8	21	19	1	−2	−13	9	45	46	1	−2	−5	9	9	13	1	0	1	9	153	158	1	−3	8	9	88	88	1
6	5	8	64	64	1	−1	−13	9	26	26	1	−1	−5	9	120	115	1	1	1	9	179	190	1	−2	8	9	107	108	2
−7	6	8	58	66	1	0	−13	9	96	95	1	0	−5	9	50	49	1	2	1	9	111	110	1	−1	8	9	60	61	1
−6	6	8	160	166	1	1	−13	9	55	51	1	1	−5	9	104	112	1	3	1	9	57	55	1	0	8	9	115	121	2
−5	6	8	64	63	1	2	−13	9	36	36	1	2	−5	9	94	93	1	4	1	9	76	81	1	1	8	9	170	169	2
−4	6	8	116	113	1	−4	−12	9	71	71	1	3	−5	9	56	57	1	5	1	9	83	81	1	2	8	9	184	200	2
−3	6	8	151	150	2	−3	−12	9	102	101	1	4	−5	9	122	130	2	6	1	9	97	101	1	3	8	9	45	46	1
−2	6	8	45	43	1	−2	−12	9	68	67	1	5	−5	9	51	52	1	−8	2	9	19	20	1	4	8	9	62	64	1
−1	6	8	86	85	1	−1	−12	9	68	68	1	−7	−4	9	45	45	1	−7	2	9	64	66	1	−6	9	9	31	32	1
0	6	8	95	100	1	0	−12	9	35	33	1	−6	−4	9	35	37	1	−6	2	9	51	46	1	−5	9	9	24	23	1
1	6	8	76	73	1	1	−12	9	35	32	1	−5	−4	9	259	258	3	−5	2	9	70	73	1	−4	9	9	120	122	1
2	6	8	257	252	3	2	−12	9	70	64	1	−4	−4	9	50	53	1	−4	2	9	149	150	1	−3	9	9	166	171	2
3	6	8	100	98	1	−5	−11	9	40	43	1	−3	−4	9	4	8	4	−3	2	9	130	135	1	−2	9	9	122	120	2
4	6	8	107	108	1	−4	−11	9	22	22	1	−2	−4	9	88	85	1	−2	2	9	127	124	1	−1	9	9	313	322	6
5	6	8	2	10	2	−3	−11	9	56	55	1	−1	−4	9	131	130	1	−1	2	9	399	391	4	0	9	9	93	98	2
−6	7	8	147	143	1	−2	−11	9	16	21	1	0	−4	9	209	207	1	0	2	9	151	145	1	1	9	9	144	154	2
−5	7	8	20	20	1	−1	−11	9	84	84	1	1	−4	9	176	182	1	1	2	9	211	208	2	2	9	9	31	30	1
−4	7	8	66	65	1	0	−11	9	83	82	1	2	−4	9	154	156	1	2	2	9	228	231	1	3	9	9	51	49	1
−3	7	8	27	33	1	1	−11	9	99	101	1	3	−4	9	89	87	1	3	2	9	37	40	1	4	9	9	42	39	1
−2	7	8	67	65	1	2	−11	9	138	140	2	4	−4	9	69	77	1	4	2	9	58	55	1	−6	10	9	28	26	1
−1	7	8	44	49	1	3	−11	9	48	49	1	5	−4	9	123	122	2	5	2	9	80	79	1	−5	10	9	41	38	1
0	7	8	126	128	2	−6	−10	9	29	26	1	−8	−3	9	62	58	1	6	2	9	53	53	1	−4	10	9	122	122	1
1	7	8	148	146	1	−5	−10	9	41	38	1	−7	−3	9	66	58	1	−7	3	9	65	59	1	−3	10	9	42	46	1
2	7	8	77	75	1	−4	−10	9	120	122	1	−5	−3	9	227	224	2	−6	3	9	151	151	1	−2	10	9	66	72	2
3	7	8	85	82	1	−3	−10	9	44	45	1	−4	−3	9	154	160	1	−5	3	9	224	223	2	0	10	9	95	96	2
4	7	8	66	71	1	−2	−10	9	68	71	1	−3	−3	9	61	62	1	−4	3	9	156	160	1	1	10	9	100	107	1
−6	8	8	19	17	1	−1	−10	9	89	88	1	−2	−3	9	161	167	1	−3	3	9	62	63	1	2	10	9	91	86	1
−5	8	8	36	37	1	0	−10	9	96	96	1	−1	−3	9	32	37	1	−2	3	9	162	167	1	3	10	9	64	63	1
−4	8	8	18	20	1	1	−10	9	99	107	1	0	−3	9	69	78	1	−1	3	9	32	37	1	4	10	9	46	45	1
−3	8	8	8	13	5	2	−10	9	91	86	1	1	−3	9	175	181	1	0	3	9	68	77	1	−5	11	9	45	43	1
−2	8	8	188	190	3	3	−10	9	63	63	1	2	−3	9	141	148	1	1	3	9	176	181	2	−4	11	9	21	22	1
−1	8	8	166	171	2	4	−10	9	44	45	1	3	−3	9	47	45	1	2	3	9	143	149	1	−3	11	9	55	55	1
0	8	8	161	163	2	−6	−9	9	32	32	1	5	−3	9	165	161	3	3	3	9	49	46	1	−2	11	9	17	20	3
1	8	8	308	308	4	−5	−9	9	25	23	1	6	−3	9	76	74	1	4	3	9	52	45	1	0	11	9	81	83	2
2	8	8	180	186	2	−4	−9	9	123	122	1	−8	−2	9	19	19	1	5	3	9	165	161	3	1	11	9	98	101	1
3	8	8	135	135	1	−3	−9	9	166	171	1	−7	−2	9	64	66	1	6	3	9	75	74	1	2	11	9	143	140	1
4	8	8	128	133	1	−2	−9	9	122	120	1	−6	−2	9	48	46	1	−7	4	9	44	44	1	3	11	9	49	50	1
−6	9	8	36	35	1	−1	−9	9	319	322	2	−5	−2	9	70	73	1	−6	4	9	38	37	1	−4	12	9	71	70	1
−5	9	8	157	156	2	0	−9	9	95	99	1	−4	−2	9	148	150	1	−5	4	9	256	257	5	−3	12	9	103	100	1
−4	9	8	109	113	2	1	−9	9	144	155	1	−3	−2	9	129	135	1	−4	4	9	49	53	1	−2	12	9	65	66	2
−3	9	8	72	75	1	2	−9	9	30	29	1	−2	−2	9	128	124	1	−3	4	9	6	8	6	0	12	9	33	33	1
−2	9	8	232	235	4	3	−9	9	51	50	1	−1	−2	9	407	391	4	−2	4	9	85	85	1	1	12	9	35	32	1
0	9	8	98	99	2	4	−9	9	41	39	1	0	−2	9	152	145	1	−1	4	9	127	129	1	2	12	9	70	64	1
1	9	8	186	188	2	−7	−8	9	19	20	1	1	−2	9	210	207	1	0	4	9	214	208	3	−4	13	9	56	57	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	9	8	81	86	1	-6	-8	9	78	77	1	2	-2	9	228	231	1	1	4	9	178	183	2	-3	13	9	12	13	2
3	9	8	42	41	1	-5	-8	9	87	84	1	3	-2	9	39	40	1	2	4	9	155	155	1	-2	13	9	44	46	1
4	9	8	59	59	1	-4	-8	9	104	108	1	4	-2	9	52	55	1	3	4	9	90	87	1	1	13	9	55	51	1
-6	10	8	44	45	1	-3	-8	9	88	88	1	5	-2	9	80	78	1	4	4	9	76	77	1	2	13	9	37	36	1
-5	10	8	70	73	1	-2	-8	9	109	109	1	6	-2	9	54	53	1	5	4	9	125	123	2	-3	-13	10	27	27	1
-4	10	8	64	69	1	-1	-8	9	63	62	1	-8	-1	9	37	32	1	-7	5	9	42	41	1	-2	-13	10	32	30	1
-3	10	8	102	99	1	0	-8	9	113	120	1	-7	-1	9	86	86	1	-6	5	9	146	148	1	-1	-13	10	13	12	1
-2	10	8	56	58	2	1	-8	9	170	169	1	-6	-1	9	123	127	1	-5	5	9	90	92	2	0	-13	10	45	43	1
0	10	8	124	131	2	2	-8	9	199	199	2	-5	-1	9	123	121	1	-4	5	9	242	237	3	1	-13	10	38	33	1
1	10	8	72	69	1	3	-8	9	43	47	1	-4	-1	9	48	48	1	-3	5	9	40	38	1	-4	-12	10	47	47	1
2	10	8	44	50	1	4	-8	9	60	64	1	-3	-1	9	74	77	1	-2	5	9	6	13	5	-3	-12	10	75	77	1
3	10	8	115	116	1	5	-8	9	50	50	1	-2	-1	9	184	186	1	-1	5	9	118	116	1	-2	-12	10	31	30	1
-1	-12	10	33	33	1	2	-4	10	91	93	1	-2	3	10	123	121	1	-2	11	10	44	46	2	-3	-4	11	140	143	1
0	-12	10	42	44	1	3	-4	10	136	141	2	-1	3	10	19	16	1	0	11	10	100	103	2	-2	-4	11	69	65	1
1	-12	10	2	5	2	4	-4	10	69	68	1	0	3	10	189	186	2	1	11	10	116	120	1	-1	-4	11	52	47	1
-4	-11	10	63	61	1	5	-4	10	44	41	1	1	3	10	208	214	2	2	11	10	61	65	1	0	-4	11	32	25	1
-3	-11	10	73	75	1	-7	-3	10	36	36	1	2	3	10	152	153	1	3	11	10	30	25	1	1	-4	11	98	104	1
-2	-11	10	44	45	1	-6	-3	10	121	121	2	3	3	10	111	113	1	-4	12	10	45	46	1	2	-4	11	201	206	1
-1	-11	10	55	53	1	-5	-3	10	287	283	2	4	3	10	104	102	1	-3	12	10	76	77	1	3	-4	11	43	43	1
0	-11	10	104	103	1	-4	-3	10	221	223	2	5	3	10	79	80	1	-2	12	10	32	30	2	4	-4	11	18	20	1
1	-11	10	116	120	1	-3	-3	10	157	159	1	-6	4	10	27	26	1	0	12	10	42	44	1	-7	-3	11	92	93	1
-5	-10	10	77	79	1	-2	-3	10	122	121	1	-5	4	10	71	70	1	1	12	10	6	5	5	-6	-3	11	103	102	2
-4	-10	10	74	73	1	-1	-3	10	22	16	1	-4	4	10	37	38	1	2	12	10	40	40	1	-5	-3	11	150	148	1
-3	-10	10	55	59	1	0	-3	10	187	186	1	-3	4	10	89	85	1	-3	13	10	28	27	1	-4	-3	11	299	302	3
-2	-10	10	138	140	1	1	-3	10	207	215	1	-2	4	10	75	76	1	0	13	10	42	43	1	-3	-3	11	63	68	1
-1	-10	10	28	31	1	2	-3	10	152	153	1	-1	4	10	182	174	2	1	13	10	38	33	1	-2	-3	11	119	117	1
0	-10	10	153	150	1	3	-3	10	113	114	1	0	4	10	152	152	1	-3	-12	11	66	67	1	-1	-3	11	198	203	1
1	-10	10	136	136	1	4	-3	10	103	102	2	1	4	10	84	82	1	-2	-12	11	21	21	1	0	-3	11	138	130	1
2	-10	10	55	56	1	5	-3	10	78	80	1	2	4	10	90	93	1	-1	-12	11	31	29	1	1	-3	11	188	190	2
3	-10	10	13	16	1	-7	-2	10	61	62	1	3	4	10	138	141	1	0	-12	11	68	70	1	2	-3	11	66	72	1
-6	-9	10	49	48	1	-6	-2	10	76	77	1	4	4	10	69	69	1	1	-12	11	53	49	1	3	-3	11	139	141	1
-5	-9	10	97	99	1	-5	-2	10	158	161	1	5	4	10	42	41	1	-4	-11	11	73	71	1	4	-3	11	32	33	1
-4	-9	10	69	68	1	-4	-2	10	82	89	1	-6	5	10	13	9	1	-3	-11	11	53	54	1	5	-3	11	81	82	1
-3	-9	10	24	19	1	-3	-2	10	48	47	1	-5	5	10	41	38	1	-2	-11	11	65	63	1	-7	-2	11	37	34	1
-2	-9	10	119	124	1	-2	-2	10	40	40	1	-4	5	10	56	56	1	-1	-11	11	19	24	1	-6	-2	11	58	60	1
-1	-9	10	38	38	1	-1	-2	10	231	235	2	-3	5	10	104	107	1	0	-11	11	52	53	1	-5	-2	11	125	127	1
0	-9	10	216	218	2	0	-2	10	70	69	1	-2	5	10	151	151	2	1	-11	11	91	89	1	-4	-2	11	87	90	1
1	-9	10	86	90	1	1	-2	10	176	174	1	-1	5	10	71	72	1	-4	-10	11	28	30	1	-3	-2	11	25	26	1
2	-9	10	75	77	1	2	-2	10	187	187	1	0	5	10	78	83	1	-3	-10	11	128	127	1	-2	-2	11	145	151	1
3	-9	10	78	74	1	3	-2	10	140	137	1	1	5	10	80	80	1	-2	-10	11	74	71	1	-1	-2	11	76	77	1
4	-9	10	28	28	1	4	-2	10	71	73	1	2	5	10	100	105	1	-1	-10	11	68	63	1	0	-2	11	233	234	2
-6	-8	10	83	80	1	5	-2	10	71	73	1	3	5	10	16	19	1	0	-10	11	89	91	1	1	-2	11	116	119	1
-5	-8	10	60	60	1	-7	-1	10	84	83	1	4	5	10	91	92	1	1	-10	11	104	101	1	2	-2	11	56	60	1
-4	-8	10	93	93	1	-6	-1	10	110	112	1	-6	6	10	83	84	1	-4	-9	11	128	129	1	3	-2	11	67	65	1
-3	-8	10	19	17	1	-5	-1	10	19	19	1	-5	6	10	176	178	2	-3	-9	11	104	107	1	4	-2	11	123	125	2
-2	-8	10	50	53	1	-4	-1	10	70	68	1	-4	6	10	110	116	1	-2	-9	11	133	132	1	5	-2	11	71	72	1
-1	-8	10	87	87	1	-3	-1	10	97	97	1	-3	6	10	127	130	1	-1	-9	11	93	91	1	-7	-1	11	20	21	1
0	-8	10	157	157	1	-2	-1	10	66	65	1	-2	6	10	150	153	2	0	-9	11	49	48	1	-6	-1	11	139	136	1
1	-8	10	18	21	1	-1	-1	10	154	153	1	-1	6	10	62	65	1	1	-9	11	117	121	1	-5	-1	11	28	31	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	−8	10	62	63	1	0	−1	10	178	177	1	0	6	10	156	163	2	2	−9	11	82	83	1	−4	−1	11	135	130	1
3	−8	10	107	103	2	1	−1	10	43	43	1	1	6	10	117	123	1	3	−9	11	47	53	1	−3	−1	11	158	158	1
4	−8	10	43	44	1	2	−1	10	25	26	1	2	6	10	89	98	1	−6	−8	11	53	51	1	−2	−1	11	64	66	1
−7	−7	10	44	45	1	3	−1	10	93	91	1	3	6	10	71	70	1	−5	−8	11	49	50	1	−1	−1	11	10	8	2
−6	−7	10	60	58	1	4	−1	10	62	62	1	4	6	10	20	18	1	−4	−8	11	115	117	1	0	−1	11	111	113	1
−5	−7	10	127	130	1	5	−1	10	72	73	1	−6	7	10	60	58	1	−3	−8	11	69	70	1	1	−1	11	129	133	1
−4	−7	10	46	43	1	−7	0	10	84	82	1	−5	7	10	127	130	1	−2	−8	11	51	49	1	2	−1	11	100	104	1
−3	−7	10	8	6	3	−6	0	10	23	25	1	−4	7	10	45	43	1	−1	−8	11	117	121	1	3	−1	11	35	38	1
−2	−7	10	255	252	1	−5	0	10	23	17	1	−3	7	10	13	6	5	0	−8	11	125	126	1	4	−1	11	121	117	2
−1	−7	10	186	190	1	−4	0	10	128	134	1	−2	7	10	251	252	5	1	−8	11	91	93	1	5	−1	11	34	38	1
0	−7	10	128	132	1	−3	0	10	181	183	1	−1	7	10	186	190	2	2	−8	11	61	64	1	−7	0	11	35	34	1
1	−7	10	83	84	1	−2	0	10	44	49	1	0	7	10	132	132	2	3	−8	11	59	60	1	−6	0	11	133	129	1
2	−7	10	98	96	1	−1	0	10	214	206	2	1	7	10	84	84	1	−6	−7	11	69	66	1	−5	0	11	65	69	1
3	−7	10	48	47	1	0	0	10	159	168	1	2	7	10	91	95	1	−5	−7	11	35	35	1	−4	0	11	266	268	3
4	−7	10	49	52	1	1	0	10	101	96	1	3	7	10	50	47	1	−4	−7	11	126	128	1	−3	0	11	138	135	1
−7	−6	10	53	47	1	2	0	10	43	39	1	4	7	10	48	52	1	−3	−7	11	63	66	1	−2	0	11	73	74	1
−6	−6	10	82	84	1	3	0	10	126	131	1	−6	8	10	82	80	1	−2	−7	11	118	120	1	−1	0	11	12	10	2
−5	−6	10	180	178	1	4	0	10	202	199	3	−5	8	10	59	61	1	−1	−7	11	123	125	1	0	0	11	110	110	1
−4	−6	10	111	116	1	5	0	10	39	39	1	−4	8	10	93	93	1	0	−7	11	157	150	1	1	0	11	17	10	1
−3	−6	10	127	130	1	−7	1	10	84	82	1	−3	8	10	19	17	2	1	−7	11	36	41	1	2	0	11	76	78	1
−2	−6	10	155	154	1	−6	1	10	113	112	1	−2	8	10	51	53	2	2	−7	11	69	69	1	3	0	11	16	14	1
−1	−6	10	60	65	1	−5	1	10	24	20	1	−1	8	10	86	87	2	3	−7	11	29	27	1	4	0	11	8	5	3
0	−6	10	157	163	1	−4	1	10	71	67	1	0	8	10	156	157	3	4	−7	11	54	56	1	5	0	11	16	17	1
1	−6	10	117	123	1	−3	1	10	96	97	1	1	8	10	18	21	1	−6	−6	11	53	52	1	−7	1	11	20	21	1
2	−6	10	96	98	1	−2	1	10	66	65	1	2	8	10	57	63	1	−5	−6	11	105	97	1	−6	1	11	137	136	1
3	−6	10	72	71	1	−1	1	10	155	154	1	3	8	10	105	103	1	−4	−6	11	148	154	1	−5	1	11	30	31	1
4	−6	10	22	19	1	0	1	10	177	176	1	4	8	10	44	44	1	−3	−6	11	42	38	1	−4	1	11	130	130	1
5	−6	10	97	99	1	1	1	10	45	43	1	−6	9	10	49	48	1	−2	−6	11	109	111	1	−3	1	11	160	159	1
−7	−5	10	80	80	1	2	1	10	25	27	1	−5	9	10	98	98	1	−1	−6	11	69	69	1	−2	1	11	62	66	1
−6	−5	10	13	8	2	3	1	10	89	91	1	−4	9	10	72	68	1	0	−6	11	134	132	1	−1	1	11	12	9	2
−5	−5	10	38	38	1	4	1	10	63	62	1	−3	9	10	22	19	1	1	−6	11	85	85	1	0	1	11	112	112	1
−4	−5	10	56	56	1	5	1	10	73	73	1	−2	9	10	120	123	2	2	−6	11	83	79	1	1	1	11	130	133	1
−3	−5	10	103	106	1	−7	2	10	62	63	1	−1	9	10	41	38	1	3	−6	11	42	38	1	2	1	11	100	104	1
−2	−5	10	152	151	1	−6	2	10	77	77	1	0	9	10	215	219	4	4	−6	11	83	89	1	3	1	11	34	37	1
−1	−5	10	69	73	1	−5	2	10	158	160	1	1	9	10	89	90	1	−7	−5	11	51	52	1	4	1	11	119	116	2
0	−5	10	78	82	1	−4	2	10	81	88	1	2	9	10	74	76	1	−6	−5	11	96	95	1	5	1	11	36	38	1
1	−5	10	79	80	1	−3	2	10	49	47	1	3	9	10	81	74	1	−5	−5	11	76	77	1	−7	2	11	36	35	1
2	−5	10	101	105	1	−2	2	10	38	40	1	4	9	10	29	28	1	−4	−5	11	75	74	1	−6	2	11	57	60	1
3	−5	10	18	19	1	−1	2	10	231	236	2	−5	10	10	79	79	1	−3	−5	11	58	58	1	−5	2	11	129	127	1
4	−5	10	88	92	1	0	2	10	71	68	1	−4	10	10	74	73	1	−2	−5	11	91	98	1	−4	2	11	86	90	1
5	−5	10	88	86	1	1	2	10	180	174	2	−3	10	10	56	60	1	−1	−5	11	6	6	5	−3	2	11	25	25	1
−7	−4	10	63	59	1	2	2	10	189	186	1	−2	10	10	134	140	3	0	−5	11	142	140	1	−2	2	11	145	151	1
−6	−4	10	30	26	1	3	2	10	139	137	1	−1	10	10	34	30	1	1	−5	11	55	60	1	−1	2	11	77	77	1
−5	−4	10	70	70	1	4	2	10	70	73	1	0	10	10	154	150	3	2	−5	11	98	100	1	0	2	11	236	235	2
−4	−4	10	36	38	1	5	2	10	70	73	1	1	10	10	137	136	1	3	−5	11	90	89	1	1	2	11	117	119	1
−3	−4	10	90	85	1	−7	3	10	34	36	1	2	10	10	59	57	1	4	−5	11	59	59	1	2	2	11	57	59	1
−2	−4	10	76	76	1	−6	3	10	120	121	1	3	10	10	17	16	1	−7	−4	11	81	81	1	3	2	11	66	65	1
−1	−4	10	183	175	1	−5	3	10	286	282	3	−5	11	10	28	30	1	−6	−4	11	123	126	2	4	2	11	121	125	2
0	−4	10	152	153	1	−4	3	10	225	223	3	−4	11	10	66	61	1	−5	−4	11	197	198	2	5	2	11	71	72	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	10	85	82	1	−3	3	10	157	159	1	−3	11	10	73	75	1	−4	−4	11	137	137	1	−6	3	11	104	102	2
−5	3	11	155	149	2	−3	12	11	68	67	1	4	−2	12	94	97	1	−4	7	12	135	142	1	−3	−2	13	109	114	1
−4	3	11	295	302	4	0	12	11	69	70	1	−7	−1	12	37	34	1	−3	7	12	10	17	4	−2	−2	13	76	76	1
−3	3	11	64	67	1	1	12	11	55	49	1	−6	−1	12	80	79	1	−2	7	12	67	67	2	−1	−2	13	65	65	1
−2	3	11	117	117	1	−3	−11	12	73	75	1	−5	−1	12	24	21	1	−1	7	12	119	115	2	0	−2	13	54	54	1
−1	3	11	197	202	2	−2	−11	12	23	23	1	−4	−1	12	141	138	2	0	7	12	99	94	1	1	−2	13	48	50	1
0	3	11	141	130	1	−1	−11	12	113	109	1	−3	−1	12	63	65	1	1	7	12	22	20	1	2	−2	13	20	17	1
1	3	11	188	191	2	0	−11	12	60	59	1	−2	−1	12	117	120	1	2	7	12	61	61	1	−6	−1	13	48	45	1
2	3	11	66	73	1	−4	−10	12	60	57	1	−1	−1	12	64	67	1	3	7	12	101	98	1	−5	−1	13	71	72	1
3	3	11	139	141	1	−3	−10	12	46	47	1	0	−1	12	29	31	1	−5	8	12	95	96	1	−4	−1	13	58	57	1
4	3	11	33	34	1	−2	−10	12	92	87	1	1	−1	12	76	75	1	−4	8	12	50	47	1	−3	−1	13	163	164	1
−6	4	11	126	127	1	−1	−10	12	122	121	1	2	−1	12	25	28	1	−3	8	12	173	177	1	−2	−1	13	26	23	1
−5	4	11	197	198	2	0	−10	12	53	50	1	3	−1	12	37	34	1	−2	8	12	166	161	3	−1	−1	13	109	106	1
−4	4	11	131	136	1	1	−10	12	81	78	1	4	−1	12	36	34	1	−1	8	12	50	53	1	0	−1	13	108	108	1
−3	4	11	140	144	1	−4	−9	12	109	102	1	−6	0	12	74	76	1	0	8	12	72	70	1	1	−1	13	70	68	1
−2	4	11	70	65	1	−3	−9	12	26	25	1	−5	0	12	50	51	1	1	8	12	91	87	1	2	−1	13	40	39	1
−1	4	11	51	47	1	−2	−9	12	62	61	1	−4	0	12	54	49	1	2	8	12	76	73	1	−6	0	13	62	60	1
0	4	11	34	25	1	−1	−9	12	81	84	1	−3	0	12	156	161	1	−5	9	12	10	13	2	−5	0	13	88	85	1
1	4	11	97	104	1	0	−9	12	39	40	1	−2	0	12	110	106	1	−4	9	12	111	102	1	−4	0	13	13	1	2
2	4	11	205	206	2	1	−9	12	60	59	1	−1	0	12	46	52	1	−3	9	12	28	25	1	−3	0	13	48	51	1
3	4	11	43	42	1	−4	−8	12	50	47	1	0	0	12	186	187	2	−2	9	12	60	61	2	−2	0	13	25	24	1
4	4	11	18	20	1	−3	−8	12	175	177	1	1	0	12	25	27	1	−1	9	12	80	84	2	−1	0	13	72	75	1
−6	5	11	97	95	1	−2	−8	12	163	161	1	2	0	12	91	91	1	0	9	12	38	39	1	0	0	13	44	48	1
−5	5	11	76	77	2	−1	−8	12	52	53	1	3	0	12	60	62	1	1	9	12	60	59	1	1	0	13	41	44	1
−4	5	11	71	74	1	0	−8	12	72	69	1	4	0	12	38	41	1	2	9	12	6	4	5	2	0	13	30	30	1
−3	5	11	58	59	1	1	−8	12	89	87	1	−6	1	12	77	78	1	−4	10	12	60	57	1	3	0	13	12	11	1
−2	5	11	92	98	1	−4	−7	12	136	143	1	−5	1	12	25	21	1	−3	10	12	44	46	1	−6	1	13	46	45	1
−1	5	11	6	5	5	−3	−7	12	16	17	1	−4	1	12	140	138	2	−2	10	12	88	87	2	−5	1	13	71	72	1
0	5	11	143	140	1	−2	−7	12	66	68	1	−3	1	12	63	65	1	−1	10	12	118	121	2	−4	1	13	57	57	1
1	5	11	56	60	1	−1	−7	12	118	115	1	−2	1	12	119	120	1	0	10	12	52	50	1	−3	1	13	166	164	1
2	5	11	99	100	1	0	−7	12	98	94	1	−1	1	12	65	67	1	1	10	12	80	77	1	−2	1	13	25	24	1
3	5	11	90	89	1	1	−7	12	24	20	1	0	1	12	31	31	1	−3	11	12	73	75	1	−1	1	13	110	106	1
4	5	11	59	59	1	2	−7	12	63	62	1	1	1	12	74	75	1	0	11	12	60	59	1	0	1	13	113	108	2
−6	6	11	51	52	1	3	−7	12	97	98	2	2	1	12	27	29	1	−3	−10	13	25	23	1	1	1	13	70	68	1
−5	6	11	104	98	1	−6	−6	12	91	94	1	3	1	12	37	33	1	−2	−10	13	21	19	1	2	1	13	39	39	1
−4	6	11	147	153	2	−5	−6	12	88	84	1	4	1	12	36	34	1	−1	−10	13	128	124	1	3	1	13	22	21	1
−3	6	11	41	38	1	−4	−6	12	98	97	1	−6	2	12	82	81	1	0	−10	13	45	43	1	−6	2	13	106	107	2
−2	6	11	110	111	2	−3	−6	12	73	73	1	−5	2	12	69	69	1	−4	−9	13	76	75	1	−5	2	13	31	29	1
−1	6	11	71	69	1	−2	−6	12	84	78	1	−4	2	12	72	74	1	−3	−9	13	151	147	1	−4	2	13	145	147	2
0	6	11	135	132	1	−1	−6	12	74	74	1	−3	2	12	115	109	1	−2	−9	13	68	66	1	−3	2	13	112	113	1
1	6	11	86	85	1	0	−6	12	117	114	1	−2	2	12	57	59	1	−1	−9	13	38	35	1	−2	2	13	79	77	1
2	6	11	83	79	1	1	−6	12	57	57	1	−1	2	12	55	55	1	0	−9	13	75	71	1	−1	2	13	66	66	1
3	6	11	43	38	1	2	−6	12	81	78	1	0	2	12	224	227	2	1	−9	13	34	32	1	0	2	13	56	54	1
4	6	11	86	89	1	3	−6	12	78	76	1	1	2	12	120	128	1	−4	−8	13	115	115	1	1	2	13	47	49	1
−6	7	11	70	66	1	−6	−5	12	135	138	2	2	2	12	102	101	1	−3	−8	13	49	46	1	2	2	13	22	18	1
−5	7	11	31	35	1	−5	−5	12	176	175	3	3	2	12	84	84	1	−2	−8	13	114	109	1	3	2	13	51	51	1
−4	7	11	125	128	1	−4	−5	12	25	23	1	−6	3	12	15	11	2	−1	−8	13	45	48	1	−6	3	13	55	53	1
−3	7	11	61	66	2	−3	−5	12	65	63	1	−5	3	12	97	95	1	0	−8	13	19	20	1	−5	3	13	109	106	1
−2	7	11	122	119	2	−2	−5	12	67	67	1	−4	3	12	59	67	2	1	−8	13	90	84	1	−4	3	13	39	42	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	11	124	126	2	−1	−5	12	25	28	1	−3	3	12	154	161	1	−4	−7	13	99	98	1	−3	3	13	98	95	1
0	7	11	156	150	2	0	−5	12	100	97	1	−2	3	12	79	77	1	−3	−7	13	61	60	1	−2	3	13	42	39	1
1	7	11	34	41	1	1	−5	12	137	141	1	−1	3	12	220	217	3	−2	−7	13	35	36	1	−1	3	13	69	64	1
2	7	11	68	69	1	2	−5	12	92	92	1	0	3	12	179	174	2	−1	−7	13	64	60	1	0	3	13	191	199	3
3	7	11	25	28	1	3	−5	12	53	54	1	1	3	12	80	90	1	0	−7	13	95	95	1	1	3	13	72	74	1
4	7	11	57	57	1	4	−5	12	13	13	1	2	3	12	68	67	1	1	−7	13	42	42	1	2	3	13	69	66	1
−6	8	11	50	51	1	−6	−4	12	120	122	2	3	3	12	129	132	1	−5	−6	13	38	39	1	3	3	13	98	96	1
−5	8	11	51	50	1	−5	−4	12	54	55	1	−6	4	12	117	122	1	−4	−6	13	108	108	1	−6	4	13	28	31	1
−4	8	11	115	117	1	−4	−4	12	122	121	1	−5	4	12	54	54	1	−3	−6	13	94	91	1	−5	4	13	105	105	2
−3	8	11	67	71	1	−3	−4	12	138	140	1	−4	4	12	114	121	1	−2	−6	13	6	8	4	−4	4	13	106	103	1
−2	8	11	51	49	2	−2	−4	12	132	128	1	−3	4	12	140	140	1	−1	−6	13	20	19	1	−3	4	13	87	84	1
−1	8	11	119	121	2	−1	−4	12	79	85	1	−2	4	12	134	129	1	0	−6	13	25	24	1	−2	4	13	106	109	1
0	8	11	123	125	1	0	−4	12	125	119	1	−1	4	12	80	84	1	1	−6	13	91	96	1	−1	4	13	123	111	1
1	8	11	92	93	1	1	−4	12	103	103	1	0	4	12	131	119	1	−5	−5	13	139	137	2	0	4	13	144	146	1
2	8	11	61	64	1	2	−4	12	47	48	1	1	4	12	94	103	1	−4	−5	13	88	87	1	1	4	13	72	73	1
3	8	11	58	61	1	3	−4	12	45	49	1	2	4	12	47	48	1	−3	−5	13	29	25	1	2	4	13	102	102	1
−5	9	11	114	111	1	4	−4	12	20	22	1	3	4	12	47	49	1	−2	−5	13	122	126	1	3	4	13	46	44	1
−4	9	11	129	129	1	−6	−3	12	15	11	2	−6	5	12	136	138	1	−1	−5	13	63	66	1	−6	5	13	55	57	1
−3	9	11	105	108	1	−5	−3	12	97	96	1	−5	5	12	181	175	3	0	−5	13	120	116	1	−5	5	13	140	137	2
−2	9	11	132	132	2	−4	−3	12	67	67	1	−4	5	12	26	23	1	1	−5	13	56	56	1	−4	5	13	89	87	1
−1	9	11	91	91	2	−3	−3	12	150	162	1	−3	5	12	64	63	1	2	−5	13	18	15	1	−3	5	13	28	25	1
0	9	11	50	47	1	−2	−3	12	78	77	1	−2	5	12	66	66	1	−5	−4	13	100	105	2	−2	5	13	120	126	1
1	9	11	117	121	1	−1	−3	12	220	218	2	−1	5	12	25	28	1	−4	−4	13	106	104	1	−1	5	13	64	66	1
2	9	11	83	83	1	0	−3	12	173	174	1	0	5	12	104	98	1	−3	−4	13	85	83	1	0	5	13	120	116	1
3	9	11	50	53	1	1	−3	12	91	90	1	1	5	12	134	142	1	−2	−4	13	107	108	1	1	5	13	57	56	1
−5	10	11	25	23	1	2	−3	12	67	67	1	2	5	12	91	91	1	−1	−4	13	123	112	1	2	5	13	19	16	1
−4	10	11	29	30	1	3	−3	12	126	131	2	3	5	12	53	53	1	0	−4	13	142	146	1	3	5	13	52	53	1
−3	10	11	125	126	2	4	−3	12	49	52	1	−6	6	12	94	95	1	1	−4	13	73	74	1	−5	6	13	40	38	1
−2	10	11	71	71	2	−7	−2	12	92	89	1	−5	6	12	88	84	1	2	−4	13	102	102	1	−4	6	13	113	108	1
−1	10	11	65	63	1	−6	−2	12	81	82	1	−4	6	12	97	97	1	−5	−3	13	107	106	1	−3	6	13	94	90	1
0	10	11	88	91	1	−5	−2	12	67	68	1	−3	6	12	73	74	1	−4	−3	13	41	42	1	−2	6	13	9	8	5
1	10	11	106	101	1	−4	−2	12	74	74	1	−2	6	12	86	78	2	−3	−3	13	90	94	1	−1	6	13	19	19	2
2	10	11	84	88	1	−3	−2	12	112	108	1	−1	6	12	74	74	1	−2	−3	13	40	39	1	0	6	13	25	24	1
−4	11	11	72	71	1	−2	−2	12	56	59	1	0	6	12	118	113	1	−1	−3	13	67	64	1	1	6	13	93	96	1
−3	11	11	51	55	1	−1	−2	12	54	55	1	1	6	12	57	57	1	0	−3	13	187	199	1	2	6	13	37	33	1
−2	11	11	68	63	1	0	−2	12	224	228	2	2	6	12	81	78	1	1	−3	13	74	74	1	3	6	13	16	15	1
0	11	11	52	53	1	1	−2	12	126	128	1	3	6	12	81	76	1	2	−3	13	69	66	1	−5	7	13	115	114	1
1	11	11	91	89	1	2	−2	12	98	101	1	−6	7	12	106	105	2	−5	−2	13	29	30	1	−4	7	13	104	98	1
2	11	11	60	62	1	3	−2	12	85	84	1	−5	7	12	83	80	1	−4	−2	13	147	146	2	−3	7	13	61	60	1
−2	7	13	38	35	2	−3	−3	14	21	20	1	2	3	14	50	49	1	−5	−3	15	70	72	1	0	4	15	88	84	1
−1	7	13	63	60	1	−2	−3	14	87	83	1	−5	4	14	62	64	1	−4	−3	15	39	37	1	1	4	15	16	15	1
0	7	13	95	94	1	−1	−3	14	34	34	1	−4	4	14	97	92	1	−3	−3	15	33	36	1	−4	5	15	70	72	1
1	7	13	43	41	1	0	−3	14	90	90	1	−3	4	14	37	33	1	−2	−3	15	22	20	1	−3	5	15	34	26	1
2	7	13	38	35	1	1	−3	14	112	107	1	−2	4	14	96	97	1	−1	−3	15	37	35	1	−2	5	15	11	5	2
−4	8	13	118	114	1	2	−3	14	51	49	1	−1	4	14	85	81	1	0	−3	15	55	53	1	−1	5	15	77	77	1
−3	8	13	49	46	1	−5	−2	14	40	39	1	0	4	14	118	110	1	1	−3	15	35	30	1	0	5	15	38	36	1
−2	8	13	111	108	2	−4	−2	14	164	161	2	1	4	14	72	75	1	−5	−2	15	51	51	1	1	5	15	109	110	1
−1	8	13	43	47	1	−3	−2	14	207	202	2	2	4	14	73	76	1	−4	−2	15	31	30	1	−3	6	15	54	60	1
0	8	13	19	20	1	−2	−2	14	75	77	1	−5	5	14	37	34	1	−3	−2	15	116	120	1	−2	6	15	25	24	1

TABLE 8-continued

Observed and calculated structure factors for MET-1.

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	8	13	89	84	1	−1	−2	14	66	66	1	−4	5	14	98	95	1	−2	−2	15	72	68	1	−1	6	15	35	36	1
2	8	13	83	81	1	0	−2	14	85	86	1	−3	5	14	21	22	1	−1	−2	15	83	87	1	0	6	15	37	36	1
−4	9	13	73	75	1	1	−2	14	84	83	1	−2	5	14	84	82	1	0	−2	15	155	149	2	−3	7	15	51	47	1
−3	9	13	147	147	2	2	−2	14	34	37	1	−1	5	14	74	69	1	1	−2	15	44	46	1	−2	7	15	77	80	1
−2	9	13	68	67	1	−5	−1	14	81	85	1	0	5	14	57	57	1	−5	−1	15	26	30	1	−1	7	15	14	11	2
−1	9	13	36	35	1	−4	−1	14	117	117	1	1	5	14	70	70	1	−4	−1	15	85	86	1	−3	−4	16	43	42	1
0	9	13	75	71	1	−3	−1	14	47	44	1	2	5	14	49	47	1	−3	−1	15	56	57	1	−2	−4	16	49	51	1
1	9	13	35	32	1	−2	−1	14	26	26	1	−5	6	14	62	62	1	−2	−1	15	31	34	1	−1	−4	16	30	29	1
−3	10	13	24	23	1	−1	−1	14	78	76	1	−4	6	14	125	120	1	−1	−1	15	149	147	1	−3	−3	16	12	10	1
−1	10	13	125	125	1	0	−1	14	149	148	1	−3	6	14	105	102	1	0	−1	15	40	40	1	−2	−3	16	24	25	1
0	10	13	45	43	1	1	−1	14	48	51	1	−2	6	14	28	27	1	1	−1	15	37	36	1	−1	−3	16	49	50	1
−2	−9	14	64	69	1	2	−1	14	17	15	1	−1	6	14	64	62	1	2	−1	15	55	54	1	0	−3	16	45	43	1
−1	−9	14	52	49	1	−5	0	14	38	37	1	0	6	14	28	22	1	−5	0	15	45	45	1	−4	−2	16	40	41	1
−3	−8	14	26	25	1	−4	0	14	17	19	2	1	6	14	55	53	1	−4	0	15	80	82	1	−3	−2	16	34	30	1
−2	−8	14	66	64	1	−3	0	14	43	42	1	2	6	14	126	129	2	−3	0	15	14	9	1	−2	−2	16	54	57	1
−1	−8	14	34	33	1	−2	0	14	95	97	1	−4	7	14	29	30	1	−2	0	15	42	48	1	−1	−2	16	60	57	1
0	−8	14	85	83	1	−1	0	14	132	132	1	−3	7	14	90	83	1	−1	0	15	5	4	5	0	−2	16	117	118	1
−4	−7	14	30	30	1	0	0	14	81	76	1	−2	7	14	129	129	2	0	0	15	10	12	3	−4	−1	16	89	86	1
−3	−7	14	89	83	1	1	0	14	62	60	1	−1	7	14	33	36	1	1	0	15	12	14	1	−3	−1	16	78	78	1
−2	−7	14	130	129	1	2	0	14	4	2	4	0	7	14	66	64	1	2	0	15	54	48	1	−2	−1	16	12	13	1
−1	−7	14	32	36	1	−6	1	14	59	60	1	1	7	14	15	15	1	−5	1	15	26	30	1	−1	−1	16	104	100	1
0	−7	14	67	64	1	−5	1	14	83	85	1	−3	8	14	27	26	1	−4	1	15	86	86	1	0	−1	16	129	129	1
1	−7	14	15	16	1	−4	1	14	117	117	1	−2	8	14	66	64	1	−3	1	15	57	57	1	−4	0	16	106	108	1
−4	−6	14	120	120	1	−3	1	14	47	44	1	−1	8	14	34	32	1	−2	1	15	34	34	1	−3	0	16	4	6	4
−3	−6	14	103	102	1	−2	1	14	25	26	1	0	8	14	85	82	1	−1	1	15	150	147	1	−2	0	16	40	35	1
−2	−6	14	28	27	1	−1	1	14	79	76	1	−1	9	14	53	49	1	0	1	15	41	40	1	−1	0	16	32	33	1
−1	−6	14	66	63	1	0	1	14	150	148	2	−3	−7	15	50	47	1	1	1	15	35	36	1	0	0	16	30	30	1
0	−6	14	27	22	1	1	1	14	47	51	1	−2	−7	15	77	80	1	2	1	15	53	53	1	−4	1	16	86	86	1
1	−6	14	59	53	1	2	1	14	15	16	1	−1	−7	15	10	11	1	−5	2	15	50	51	1	−3	1	16	79	79	1
−5	−5	14	36	34	1	−6	2	14	21	23	1	−3	−6	15	55	60	1	−4	2	15	27	29	1	−2	1	16	13	13	1
−4	−5	14	96	95	1	−5	2	14	42	40	1	−2	−6	15	26	24	1	−3	2	15	118	119	1	−1	1	16	103	100	1
−3	−5	14	25	22	1	−4	2	14	164	160	1	−1	−6	15	35	35	1	−2	2	15	72	68	1	0	1	16	128	129	1
−2	−5	14	86	82	1	−3	2	14	209	202	2	0	−6	15	36	36	1	−1	2	15	83	87	1	−4	2	16	42	41	1
−1	−5	14	76	69	1	−2	2	14	75	76	1	−4	−5	15	75	73	1	0	2	15	156	149	2	−3	2	16	36	30	1
0	−5	14	54	57	1	−1	2	14	66	66	1	−3	−5	15	30	26	1	1	2	15	47	47	1	−2	2	16	54	57	1
1	−5	14	71	71	1	0	2	14	87	87	1	−2	−5	15	9	5	1	−4	3	15	41	37	1	−1	2	16	60	56	1
−5	−4	14	64	65	1	1	2	14	83	83	1	−1	−5	15	77	77	1	−3	3	15	35	36	1	0	2	16	117	118	1
−4	−4	14	94	92	1	2	2	14	33	37	1	0	−5	15	39	35	1	−2	3	15	19	19	1	−3	3	16	13	11	4
−3	−4	14	35	33	1	−5	3	14	27	22	1	1	−5	15	110	110	2	−1	3	15	38	35	1	−2	3	16	25	25	1
−2	−4	14	98	97	1	−4	3	14	34	32	1	−4	−4	15	21	21	1	0	3	15	56	53	1	−1	3	16	49	49	1
−1	−4	14	86	80	1	−3	3	14	20	20	1	−3	−4	15	8	9	3	1	3	15	35	30	1	0	3	16	45	43	1
0	−4	14	118	111	1	−2	3	14	85	83	1	−2	−4	15	35	32	1	−4	4	15	22	21	1	−3	4	16	42	42	1
1	−4	14	72	75	1	−1	3	14	34	34	1	−1	−4	15	38	37	1	−3	4	15	10	9	1	−2	4	16	49	51	1
−5	−3	14	21	22	1	0	3	14	91	90	1	0	−4	15	86	84	1	−2	4	15	34	32	1	−1	4	16	29	29	1
−4	−3	14	32	32	1	1	3	14	113	107	1	1	−4	15	14	15	2	−1	4	15	39	37	1						

TABLE 9

Crystal data and structure refinement for MET-2.		
Empirical formula	C32H56O4	
Formula weight	504.77	
Temperature	298(1) K	
Wavelength	1.54178 Å	
Crystal system, space group	Monoclinic, C2	
Unit cell dimensions	a = 27.3382(16) Å	α = 90°
	b = 6.6860(13) Å	β = 113.57(3)°
	c = 19.221(10) A	γ = 90°
Volume	3320.3(11) $Å^3$	
Z	4	
Calculated density	1.041 Mg/m^3	
Absorption coefficient	0.513 mm^{-1}	
F(000)	1120	
Crystal size	0.36 × 0.17 × 0.03 mm	
Theta range for data collection	2.51 to 58.69°	
Limiting indices	−29 <= h <= 28, −6 <= k <= 6, −21 <= l <= 21	
Reflections collected/unique	10383/3985 [R(int) = 0.0473]	
Data/restraints/parameters	3985/1/325	
Goodness-of-fit on F^2	1.073	
Final R indices [I > 2σ(I)]	R1 = 0.0618, wR2 = 0.1600	
R indices (all data)	R1 = 0.0844, wR2 = 0.1778	
Absolute structure parameter	0.2(4)	
Largest diff. peak and hole	0.140 and −0.190 e/$Å^{-3}$	

TABLE 10

Atomic coordinates ($Å^2 \times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for MET-2 U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(3)	9651(1)	8018(5)	3345(2)	80(1)
C(20)	7634(1)	8343(6)	−2763(2)	67(1)
O(25)	9328(1)	7952(6)	−3391(2)	102(1)
C(13)	7985(1)	7574(6)	−1301(2)	59(1)
C(1)	9449(2)	12075(6)	2708(2)	66(1)
C(17)	8118(1)	8204(6)	−1982(2)	59(1)
O(1)	9565(1)	14167(5)	2735(2)	88(1)
C(10)	8922(2)	11685(7)	2036(2)	73(1)
C(23)	8253(2)	8546(7)	−3469(2)	70(1)
C(2)	9409(2)	11384(7)	3438(2)	67(1)
C(12)	7838(2)	5387(7)	−1291(2)	74(1)
C(14)	8539(1)	7926(6)	−637(2)	64(1)
C(22)	7766(2)	7484(7)	−3431(2)	69(1)
C(18)	7564(2)	8908(7)	−1201(3)	79(1)
C(5)	8739(2)	9568(7)	2011(2)	68(1)
C(3)	9242(2)	9248(7)	3413(2)	68(1)
C(15)	8704(2)	9975(8)	−812(2)	77(1)
C(9)	8370(2)	5285(7)	139(2)	83(1)
C(16)	8471(2)	10076(7)	−1687(2)	76(1)
C(25)	8924(2)	8719(10)	−4091(2)	93(2)
C(8)	8525(2)	7441(7)	118(2)	69(1)
C(30)	7870(2)	5245(7)	−3306(3)	98(2)
C(28)	7279(2)	7779(10)	−4185(2)	103(2)
C(24)	8394(2)	7945(10)	−4124(2)	91(2)
C(11)	7843(2)	4765(8)	−517(2)	83(1)
C(4)	8712(2)	8882(8)	2740(2)	74(1)
C(27)	8974(2)	10999(12)	−4028(4)	134(3)
C(6)	8624(1)	8330(8)	1421(2)	72(1)
C(21)	7379(2)	10414(8)	−2945(3)	98(2)
C(26)	9029(2)	7983(18)	−4745(3)	177(4)
C(7)	8639(2)	8753(7)	686(2)	72(1)
C(29)	9490(2)	12565(9)	4016(2)	97(2)
O(201)	10425(1)	14824(6)	2396(2)	112(1)
C(202)	10381(3)	15282(14)	1660(3)	128(2)
C(201)	10109(4)	17151(16)	1381(5)	185(4)
C(203)	10130(5)	13539(17)	1161(5)	223(5)

TABLE 11

Bond lengths [Å] for MET-2.	
O(3)—C(3)	1.434(5)
C(20)—C(21)	1.527(6)
C(20)—C(17)	1.558(5)
C(20)—C(22)	1.573(5)
O(25)—C(25)	1.451(5)
C(13)—C(12)	1.518(6)
C(13)—C(18)	1.527(6)
C(13)—C(17)	1.549(5)
C(13)—C(14)	1.560(5)
C(1)—O(1)	1.431(5)
C(1)—C(2)	1.521(5)
C(1)—C(10)	1.524(6)
C(17)—C(16)	1.543(6)
C(10)—C(5)	1.495(6)
C(23)—C(24)	1.511(5)
C(23)—C(22)	1.535(6)
C(2)—C(29)	1.308(6)
C(2)—C(3)	1.495(6)
C(12)—C(11)	1.541(5)
C(14)—C(8)	1.501(5)
C(14)—C(15)	1.522(6)
C(22)—C(30)	1.524(7)
C(22)—C(28)	1.541(6)
C(5)—C(6)	1.336(6)
C(5)—C(4)	1.505(5)
C(3)—C(4)	1.527(5)
C(15)—C(16)	1.543(5)
C(9)—C(8)	1.508(7)
C(9)—C(11)	1.527(6)
C(25)—C(26)	1.483(8)
C(25)—C(24)	1.516(7)
C(25)—C(27)	1.532(9)
C(8)—C(7)	1.336(6)
C(6)—C(7)	1.458(5)
O(201)—C(202)	1.405(7)
C(202)—C(201)	1.443(11)
C(202)—C(203)	1.490(11)

TABLE 12

bond angles [°] for MET-2.	
C(21)—C(20)—C(17)	114.1(3)
C(21)—C(20)—C(22)	112.2(4)
C(17)—C(20)—C(22)	112.4(3)
C(12)—C(13)—C(18)	110.1(3)
C(12)—C(13)—C(17)	115.2(3)
C(18)—C(13)—C(17)	113.0(3)
C(12)—C(13)—C(14)	108.1(3)
C(18)—C(13)—C(14)	110.0(3)
C(17)—C(13)—C(14)	99.8(3)
O(1)—C(1)—C(2)	111.1(3)
O(1)—C(1)—C(10)	108.7(4)
C(2)—C(1)—C(10)	109.7(3)
C(16)—C(17)—C(13)	103.5(3)
C(16)—C(17)—C(20)	118.1(3)
C(13)—C(17)—C(20)	115.7(3)
C(5)—C(10)—C(1)	112.3(3)
C(24)—C(23)—C(22)	115.5(4)
C(29)—C(2)—C(3)	123.4(4)
C(29)—C(2)—C(1)	123.4(4)
C(3)—C(2)—C(1)	113.2(3)
C(13)—C(12)—C(11)	111.8(3)
C(8)—C(14)—C(15)	122.2(3)
C(8)—C(14)—C(13)	111.5(3)
C(15)—C(14)—C(13)	103.4(3)
C(30)—C(22)—C(23)	110.6(4)
C(30)—C(22)—C(28)	108.1(4)
C(23)—C(22)—C(28)	109.6(3)
C(30)—C(22)—C(20)	108.7(3)
C(23)—C(22)—C(20)	110.8(3)
C(28)—C(22)—C(20)	109.1(3)
C(6)—C(5)—C(10)	125.2(4)
C(6)—C(5)—C(4)	121.3(4)
C(10)—C(5)—C(4)	113.5(4)

TABLE 12-continued

bond angles [°] for MET-2.	
O(3)—C(3)—C(2)	108.1(3)
O(3)—C(3)—C(4)	109.9(3)
C(2)—C(3)—C(4)	110.8(4)
C(14)—C(15)—C(16)	104.5(3)
C(8)—C(9)—C(11)	112.2(4)
C(17)—C(16)—C(15)	106.9(3)
O(25)—C(25)—C(26)	109.6(5)
O(25)—C(25)—C(24)	106.2(4)
C(26)—C(25)—C(24)	111.0(5)
O(25)—C(25)—C(27)	105.5(5)
C(26)—C(25)—C(27)	110.8(6)
C(24)—C(25)—C(27)	113.4(5)
C(7)—C(8)—C(14)	124.1(4)
C(7)—C(8)—C(9)	125.5(4)
C(14)—C(8)—C(9)	110.4(3)
C(23)—C(24)—C(25)	115.6(4)
C(9)—C(11)—C(12)	112.2(3)
C(5)—C(4)—C(3)	110.9(3)
C(5)—C(6)—C(7)	127.9(4)
C(8)—C(7)—C(6)	125.2(4)
O(201)—C(202)—C(201)	112.8(6)
O(201)—C(202)—C(203)	108.1(7)
C(201)—C(202)—C(203)	113.8(7)

TABLE 13

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(3)	67(2)	71(2)	93(2)	−5(2)	22(1)	−7(2)
C(20)	58(2)	70(3)	67(2)	−4(2)	20(2)	−6(2)
O(25)	79(2)	144(3)	86(2)	43(2)	36(2)	34(2)
C(13)	63(2)	53(3)	67(2)	−10(2)	31(2)	−4(2)
C(1)	73(3)	52(3)	75(3)	−5(2)	31(2)	−8(2)
C(17)	53(2)	65(3)	60(2)	−10(2)	23(2)	−12(2)
O(1)	102(2)	67(2)	87(2)	−11(2)	31(2)	−14(2)
C(10)	76(3)	76(3)	60(2)	−6(2)	18(2)	−3(2)
C(23)	65(2)	79(3)	65(2)	−1(2)	25(2)	−7(2)
C(2)	62(2)	73(3)	63(2)	−7(2)	21(2)	−5(2)
C(12)	88(3)	74(3)	65(2)	−12(2)	37(2)	−23(2)
C(14)	65(2)	65(3)	63(2)	−9(2)	27(2)	−11(2)
C(22)	61(2)	79(3)	64(2)	−9(2)	21(2)	−16(2)
C(18)	68(2)	86(3)	91(3)	−20(2)	38(2)	−8(2)
C(5)	54(2)	82(3)	58(2)	−6(2)	14(2)	−13(2)
C(3)	68(2)	76(3)	59(2)	−4(2)	24(2)	−9(2)
C(15)	78(3)	82(3)	71(2)	−11(2)	30(2)	−23(3)
C(9)	106(3)	76(3)	68(2)	−4(2)	38(2)	−11(3)
C(16)	73(3)	80(3)	73(2)	−7(2)	26(2)	−26(2)
C(25)	68(3)	146(6)	64(3)	17(3)	24(2)	3(3)
C(8)	66(2)	72(3)	65(2)	−4(2)	22(2)	−6(2)
C(30)	152(5)	58(3)	103(3)	−15(3)	70(3)	−17(3)
C(28)	76(3)	148(5)	71(3)	−6(3)	16(2)	−18(3)
C(24)	81(3)	129(5)	65(2)	−4(3)	31(2)	−11(3)
C(11)	108(3)	78(3)	76(3)	−16(2)	49(3)	−37(3)
C(4)	60(2)	97(4)	67(2)	−2(2)	28(2)	−14(2)
C(27)	75(4)	156(7)	150(5)	72(5)	22(3)	−12(4)
C(6)	60(2)	84(3)	67(2)	−7(2)	20(2)	−19(2)
C(21)	88(3)	94(4)	103(3)	10(3)	26(3)	32(3)
C(26)	137(5)	337(12)	83(3)	−5(6)	72(4)	−23(7)
C(7)	65(2)	81(3)	60(2)	−4(2)	15(2)	−17(2)
C(29)	125(4)	92(4)	69(3)	−10(3)	35(3)	−8(3)
O(201)	123(3)	122(3)	96(2)	−17(2)	51(2)	−23(2)
C(202)	113(4)	180(8)	101(4)	−8(5)	54(4)	−21(5)
C(201)	192(8)	180(9)	152(7)	42(6)	36(6)	15(8)
C(203)	305(13)	227(11)	134(6)	−84(7)	85(7)	−25(10)

TABLE 14

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

	x	y	z	U(eq)
H(3A)	9521	6950	3147	120
H(20I)	7360	7457	−2725	80
H(25A)	9621	8007	−3413	153
H(1A)	9733	11326	2636	79
H(17A)	8352	7159	−2035	71
H(1B)	9853	14390	3088	131
H(10A)	8651	12572	2069	88
H(10B)	8963	11988	1569	88
H(23A)	8187	9976	−3499	84
H(23B)	8559	8290	−2999	84
H(12A)	8088	4563	−1405	88
H(12B)	7484	5157	−1683	88
H(14A)	8784	6962	−710	77
H(18A)	7495	8444	−777	119
H(18B)	7241	8859	−1653	119
H(18C)	7693	10260	−1111	119
H(3B)	9203	8917	3885	82
H(15A)	9090	10101	−603	92
H(15B)	8558	11029	−605	92
H(9A)	8338	5027	616	99
H(9B)	8649	4428	116	99
H(16A)	8260	11280	−1864	92
H(16B)	8756	10086	−1867	92
H(30A)	7954	4704	−3709	147
H(30B)	7558	4597	−3304	147
H(30C)	8165	5024	−2829	147
H(28A)	7358	7266	−4595	154
H(28B)	7197	9178	−4264	154
H(28C)	6978	7076	−4166	154
H(24A)	8114	8414	−4591	109
H(24B)	8398	6496	−4147	109
H(11A)	7553	5434	−441	100
H(11B)	7783	3335	−517	100
H(4A)	8627	7467	2706	89
H(4B)	8430	9599	2818	89
H(27A)	9317	11395	−4006	201
H(27B)	8937	11432	−3575	201
H(27C)	8699	11600	−4462	201
H(6A)	8522	7041	1487	87
H(21A)	7302	10877	−2527	148
H(21B)	7054	10341	−3393	148
H(21C)	7620	11328	−3030	148
H(26A)	8994	6554	−4776	265
H(26B)	9385	8347	−4679	265
H(26C)	8778	8571	−5205	265
H(7A)	8736	10038	606	86
H(29A)	9444	12086	4440	116
H(29B)	9594	13885	4003	116
H(20A)	10540	15801	2672	167
H(20B)	10744	15418	1682	154
H(20C)	10300	18216	1714	278
H(20D)	9753	17079	1362	278
H(20E)	10094	17402	881	278
H(20F)	10095	13823	653	334
H(20G)	9784	13292	1161	334
H(20H)	10351	12378	1348	334

TABLE 15

Torsion angles [deg] for MET-2.	
C(12)—C(13)—C(17)—C(16)	−156.5(4)
C(18)—C(13)—C(17)—C(16)	75.8(4)
C(14)—C(13)—C(17)—C(16)	−41.0(4)
C(12)—C(13)—C(17)—C(20)	72.7(5)
C(18)—C(13)—C(17)—C(20)	−55.1(4)
C(14)—C(13)—C(17)—C(20)	−171.9(3)
C(21)—C(20)—C(17)—C(16)	−32.0(5)
C(22)—C(20)—C(17)—C(16)	97.2(4)
C(21)—C(20)—C(17)—C(13)	91.5(5)
C(22)—C(20)—C(17)—C(13)	−139.3(4)
O(1)—C(1)—C(10)—C(5)	−174.1(4)

TABLE 15-continued

Torsion angles [deg] for MET-2.	
C(2)—C(1)—C(10)—C(5)	−52.4(5)
O(1)—C(1)—C(2)—C(29)	−2.0(6)
C(10)—C(1)—C(2)—C(29)	−122.2(5)
O(1)—C(1)—C(2)—C(3)	175.1(4)
C(10)—C(1)—C(2)—C(3)	54.9(5)
C(18)—C(13)—C(12)—C(11)	−64.5(5)
C(17)—C(13)—C(12)—C(11)	166.3(3)
C(14)—C(13)—C(12)—C(11)	55.7(4)
C(12)—C(13)—C(14)—C(8)	−59.9(4)
C(18)—C(13)—C(14)—C(8)	60.3(5)
C(17)—C(13)—C(14)—C(8)	179.4(3)
C(12)—C(13)—C(14)—C(15)	167.1(3)
C(18)—C(13)—C(14)—C(15)	−72.7(4)
C(17)—C(13)—C(14)—C(15)	46.3(4)
C(24)—C(23)—C(22)—C(30)	63.6(5)
C(24)—C(23)—C(22)—C(28)	−55.4(5)
C(24)—C(23)—C(22)—C(20)	−175.9(4)
C(21)—C(20)—C(22)—C(30)	−164.4(4)
C(17)—C(20)—C(22)—C(30)	65.4(4)
C(21)—C(20)—C(22)—C(23)	73.9(4)
C(17)—C(20)—C(22)—C(23)	−56.3(5)
C(21)—C(20)—C(22)—C(28)	−46.8(5)
C(17)—C(20)—C(22)—C(28)	−177.0(4)
C(1)—C(10)—C(5)—C(6)	−124.5(4)
C(1)—C(10)—C(5)—C(4)	53.4(5)
C(29)—C(2)—C(3)—O(3)	−118.5(5)
C(1)—C(2)—C(3)—O(3)	64.5(4)
C(29)—C(2)—C(3)—C(4)	121.0(5)
C(1)—C(2)—C(3)—C(4)	−56.1(4)

TABLE 15-continued

Torsion angles [deg] for MET-2.	
C(8)—C(14)—C(15)—C(16)	−159.9(4)
C(13)—C(14)—C(15)—C(16)	−33.4(4)
C(13)—C(17)—C(16)—C(15)	21.6(4)
C(20)—C(17)—C(16)—C(15)	151.0(3)
C(14)—C(15)—C(16)—C(17)	7.3(5)
C(15)—C(14)—C(8)—C(7)	2.0(6)
C(13)—C(14)—C(8)—C(7)	−120.8(4)
C(15)—C(14)—C(8)—C(9)	−177.6(4)
C(13)—C(14)—C(8)—C(9)	59.6(5)
C(11)—C(9)—C(8)—C(7)	125.6(4)
C(11)—C(9)—C(8)—C(14)	−54.8(5)
C(22)—C(23)—C(24)—C(25)	−170.1(4)
O(25)—C(25)—C(24)—C(23)	59.0(6)
C(26)—C(25)—C(24)—C(23)	178.1(6)
C(27)—C(25)—C(24)—C(23)	−56.4(6)
C(8)—C(9)—C(11)—C(12)	51.6(6)
C(13)—C(12)—C(11)—C(9)	−53.0(5)
C(6)—C(5)—C(4)—C(3)	124.7(4)
C(10)—C(5)—C(4)—C(3)	−53.3(5)
O(3)—C(3)—C(4)—C(5)	−65.7(5)
C(2)—C(3)—C(4)—C(5)	53.8(5)
C(10)—C(5)—C(6)—C(7)	−1.2(7)
C(4)—C(5)—C(6)—C(7)	−179.0(4)
C(14)—C(8)—C(7)—C(6)	179.4(4)
C(9)—C(8)—C(7)—C(6)	−1.1(7)
C(5)—C(6)—C(7)—C(8)	179.2(4)

TABLE 16

Observed and calculated structure factors for MET-2.

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
16	−6	0	23	6	23	8	2	0	224	220	8	−15	−3	1	173	173	6	0	0	1	381	388	6	−12	4	1	124	117	4
9	−5	0	179	178	8	10	2	0	276	310	10	−13	−3	1	172	175	6	2	0	1	833	936	12	−10	4	1	197	179	4
11	−5	0	59	52	13	12	2	0	175	180	7	−11	−3	1	115	118	5	4	0	1	1025	1083	15	−8	4	1	91	99	4
13	−5	0	99	92	9	14	2	0	56	63	14	−9	−3	1	240	217	8	6	0	1	570	567	9	−6	4	1	295	284	5
15	−5	0	0	21	1	18	2	0	194	198	6	−7	−3	1	205	199	8	8	0	1	1171	1214	18	−4	4	1	213	211	4
17	−5	0	60	46	13	20	2	0	86	102	12	−5	−3	1	348	327	10	10	0	1	73	67	4	−2	4	1	387	390	4
19	−5	0	23	27	23	22	2	0	76	77	13	−3	−3	1	592	563	18	12	0	1	331	349	8	0	4	1	224	227	3
4	−4	0	167	167	8	24	2	0	110	145	10	−1	−3	1	463	464	10	14	0	1	13	30	13	2	4	1	452	446	5
6	−4	0	204	189	5	26	2	0	23	38	22	1	−3	1	614	614	12	16	0	1	59	53	7	4	4	1	237	239	4
8	−4	0	112	93	8	1	3	0	862	875	14	3	−3	1	295	286	9	18	0	1	215	210	8	6	4	1	54	49	5
10	−4	0	72	88	8	3	3	0	361	364	7	5	−3	1	244	265	9	20	0	1	0	10	1	8	4	1	68	55	5
12	−4	0	183	165	6	7	3	0	457	449	16	7	−3	1	236	224	9	22	0	1	58	50	20	10	4	1	69	74	5
14	−4	0	196	198	9	9	3	0	222	220	9	9	−3	1	245	235	6	24	0	1	91	86	5	12	4	1	97	91	5
16	−4	0	175	189	8	15	3	0	145	135	11	11	−3	1	122	109	7	−23	1	1	65	87	16	14	4	1	169	156	9
18	−4	0	40	45	24	17	3	0	220	212	8	13	−3	1	157	144	6	−21	1	1	352	352	5	16	4	1	112	138	9
20	−4	0	30	28	30	19	3	0	126	122	9	15	−3	1	72	59	9	−19	1	1	221	213	3	18	4	1	109	114	9
22	−4	0	0	22	1	21	3	0	67	69	15	17	−3	1	171	169	9	−17	1	1	202	194	3	20	4	1	32	31	32
1	−3	0	869	873	18	23	3	0	59	59	16	19	−3	1	52	50	17	−15	1	1	147	143	3	22	4	1	0	11	1
3	−3	0	364	365	11	25	3	0	0	32	1	21	−3	1	72	59	14	−13	1	1	416	412	16	−21	5	1	33	19	33
5	−3	0	400	372	12	0	4	0	429	436	6	23	−3	1	46	46	13	−11	1	1	902	941	20	−19	5	1	0	34	1
7	−3	0	476	447	14	2	4	0	403	390	5	−26	−2	1	61	57	9	−9	1	1	403	389	6	−17	5	1	92	86	10
9	−3	0	232	220	5	4	4	0	170	167	5	−24	−2	1	97	102	16	−7	1	1	587	602	9	−15	5	1	143	128	6
11	−3	0	252	248	6	6	4	0	208	189	4	−22	−2	1	212	217	6	−5	1	1	1112	1157	19	−13	5	1	157	146	5
13	−3	0	126	117	7	8	4	0	111	93	4	−20	−2	1	199	190	5	−3	1	1	965	1044	30	−11	5	1	133	125	5
15	−3	0	138	135	6	10	4	0	77	89	5	−18	−2	1	47	54	10	−1	1	1	1304	1398	16	−9	5	1	41	24	11
17	−3	0	214	212	6	12	4	0	169	165	4	−16	−2	1	214	194	5	1	1	1	1131	1213	15	−7	5	1	110	106	6
19	−3	0	110	122	9	14	4	0	190	198	6	−14	−2	1	274	254	5	3	1	1	395	453	5	−5	5	1	309	295	6
21	−3	0	71	69	13	16	4	0	184	189	8	−12	−2	1	87	85	6	5	1	1	501	544	7	−3	5	1	147	145	3
23	−3	0	41	59	24	18	4	0	52	45	18	−10	−2	1	433	429	14	7	1	1	556	601	7	−1	5	1	28	32	9
25	−3	0	16	32	16	20	4	0	0	28	1	−8	−2	1	134	160	6	9	1	1	322	313	6	1	5	1	90	83	3
0	−2	0	1263	1370	38	22	4	0	41	22	34	−6	−2	1	255	251	6	11	1	1	175	185	13	3	5	1	26	29	13
2	−2	0	379	408	10	1	5	0	130	130	3	−4	−2	1	474	505	10	13	1	1	363	359	8	5	5	1	119	122	5
4	−2	0	107	94	4	3	5	0	66	73	4	−2	−2	1	245	257	5	15	1	1	412	413	5	7	5	1	97	91	6
6	−2	0	224	223	6	5	5	0	35	25	12	0	−2	1	731	763	15	17	1	1	46	47	7	9	5	1	110	108	5
8	−2	0	202	222	13	7	5	0	98	95	6	2	−2	1	266	299	5	19	1	1	162	160	3	11	5	1	130	133	5
10	−2	0	270	310	22	9	5	0	185	178	4	4	−2	1	303	318	5	21	1	1	29	21	14	13	5	1	80	73	7
12	−2	0	175	180	4	11	5	0	11	51	10	6	−2	1	476	490	11	−26	2	1	48	58	21	15	5	1	113	110	8
14	−2	0	64	62	6	13	5	0	111	93	6	8	−2	1	529	557	37	−24	2	1	100	102	10	17	5	1	60	81	10
16	−2	0	136	130	10	15	5	0	27	21	27	10	−2	1	459	504	30	−22	2	1	219	218	9	19	5	1	34	60	21
18	−2	0	192	198	5	17	5	0	28	45	28	12	−2	1	124	130	4	−20	2	1	199	190	7	−16	6	1	10	23	10
20	−2	0	112	102	6	19	5	0	22	27	21	14	−2	1	104	89	6	−18	2	1	63	52	11	−14	6	1	0	20	1
22	−2	0	62	77	17	4	6	0	47	57	11	16	−2	1	290	278	7	−16	2	1	215	194	6	−12	6	1	61	61	10
24	−2	0	119	145	6	6	6	0	57	56	6	18	−2	1	393	384	7	−10	2	1	436	431	14	−10	6	1	28	39	24
26	−2	0	0	38	1	8	6	0	47	52	8	20	−2	1	106	120	21	−8	2	1	134	159	7	−8	6	1	71	79	6
1	−1	0	1074	1170	22	10	6	0	22	12	22	22	−2	1	167	142	11	−6	2	1	252	250	9	−6	6	1	34	39	10
3	−1	0	1769	1951	39	12	6	0	45	37	14	24	−2	1	34	23	20	−2	2	1	249	257	4	−4	6	1	25	26	25
5	−1	0	1600	1755	36	14	6	0	0	24	1	26	−2	1	40	37	23	0	2	1	730	762	10	4	6	1	36	35	9

TABLE 16-continued

Observed and calculated structure factors for MET-2.

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	−1	0	967	1006	20	16	6	0	16	6	16
9	−1	0	38	38	12	−16	−6	1	27	23	26
11	−1	0	201	210	5	−21	−5	1	0	18	1
13	−1	0	262	261	6	−19	−5	1	18	35	18
15	−1	0	273	271	4	−17	−5	1	95	86	9
17	−1	0	232	224	4	−15	−5	1	135	128	8
19	−1	0	311	304	5	−13	−5	1	142	146	8
21	−1	0	44	41	14	−11	−5	1	131	124	8
23	−1	0	87	76	10	−9	−5	1	18	25	17
25	−1	0	46	45	15	9	−5	1	91	108	9
27	−1	0	43	50	13	11	−5	1	111	133	8
2	0	0	312	362	4	13	−5	1	54	73	16
4	0	0	117	119	3	15	−5	1	101	110	9
6	0	0	308	322	5	17	−5	1	83	80	10
8	0	0	345	323	7	19	−5	1	53	60	14
10	0	0	1081	1115	28	−22	−4	1	71	87	11
12	0	0	621	642	13	−20	−4	1	69	76	12
14	0	0	51	44	8	−18	−4	1	42	63	20
16	0	0	42	40	9	−16	−4	1	115	100	9
18	0	0	50	53	11	−14	−4	1	69	57	10
20	0	0	34	31	19	−12	−4	1	137	117	6
22	0	0	92	81	7	−10	−4	1	196	179	6
24	0	0	53	52	8	−8	−4	1	102	99	5
26	0	0	14	7	13	−6	−4	1	289	284	6
1	1	0	1075	1172	16	−4	−4	1	202	211	8
3	1	0	1834	1949	56	4	−4	1	231	239	9
5	1	0	1647	1755	25	6	−4	1	45	49	13
7	1	0	952	1005	15	8	−4	1	70	55	8
9	1	0	36	38	4	10	−4	1	77	74	8
11	1	0	199	210	5	12	−4	1	105	91	7
13	1	0	238	260	9	14	−4	1	174	156	7
15	1	0	271	271	4	16	−4	1	144	138	8
17	1	0	233	224	4	18	−4	1	110	114	9
19	1	0	309	304	4	20	−4	1	28	31	27
21	1	0	41	40	9	22	−4	1	23	11	23
23	1	0	55	76	19	−25	−3	1	0	29	1
0	2	0	1283	1369	22	−23	−3	1	26	19	26
2	2	0	371	406	6	−21	−3	1	43	42	27
4	2	0	102	94	6	−19	−3	1	100	87	10
6	2	0	233	223	8	−17	−3	1	104	102	7
−25	−3	2	0	15	1	−8	0	2	909	967	21
−23	−3	2	48	24	20	−6	0	2	2200	2323	38
−21	−3	2	86	93	11	−4	0	2	598	601	9
−19	−3	2	103	110	10	−2	0	2	670	726	10
−17	−3	2	153	146	7	0	0	2	1279	1357	22
−15	−3	2	90	80	7	2	0	2	585	617	9
−13	−3	2	162	158	5	4	0	2	1340	1409	20
−11	−3	2	334	343	8	6	0	2	1056	1084	16
−9	−3	2	201	191	8	8	0	2	23	31	12

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
−27	−1	1	0	7	1	2	2	1	259	300	3
−25	−1	1	105	98	8	4	2	1	304	317	4
−23	−1	1	97	87	9	6	2	1	485	489	15
−21	−1	1	349	352	6	8	2	1	556	557	17
−19	−1	1	221	214	4	10	2	1	488	503	15
−17	−1	1	204	193	4	12	2	1	134	129	7
−15	−1	1	141	143	4	14	2	1	103	90	10
−13	−1	1	460	413	9	16	2	1	285	278	10
−11	−1	1	909	940	16	20	2	1	108	121	10
−9	−1	1	402	390	10	22	2	1	166	143	9
−7	−1	1	583	602	10	24	2	1	0	23	1
−5	−1	1	1075	1157	19	−25	3	1	54	29	18
−3	−1	1	951	1044	21	−23	3	1	33	20	33
−1	−1	1	1322	1398	27	−21	3	1	61	41	17
1	−1	1	1140	1212	19	−19	3	1	76	86	13
3	−1	1	404	455	7	−17	3	1	91	102	8
5	−1	1	507	544	8	−15	3	1	170	173	11
7	−1	1	560	600	9	−13	3	1	178	175	5
9	−1	1	317	313	9	−11	3	1	114	118	4
11	−1	1	182	183	5	−9	3	1	231	218	6
13	−1	1	376	360	8	−7	3	1	194	198	8
15	−1	1	417	413	6	−5	3	1	337	326	8
17	−1	1	51	47	7	−3	3	1	592	563	9
19	−1	1	164	160	4	−1	3	1	479	464	8
21	−1	1	28	21	27	1	3	1	607	614	11
23	−1	1	147	117	8	3	3	1	288	285	5
25	−1	1	63	65	29	5	3	1	253	265	9
−26	0	1	78	77	5	7	3	1	236	223	9
−24	0	1	0	12	1	9	3	1	235	236	6
−22	0	1	105	94	20	11	3	1	118	108	6
−20	0	1	190	175	5	13	3	1	145	144	8
−18	0	1	383	366	8	17	3	1	179	169	8
−16	0	1	54	57	6	19	3	1	49	50	22
−14	0	1	770	744	17	21	3	1	69	59	15
−12	0	1	19	32	19	23	3	1	74	46	13
−10	0	1	575	593	17	−22	4	1	61	88	16
−8	0	1	543	599	9	−20	4	1	66	75	14
−6	0	1	2059	2218	45	−18	4	1	47	64	21
−4	0	1	1538	1686	33	−16	4	1	112	100	10
−2	0	1	417	443	8	−14	4	1	59	56	8
21	3	2	55	56	18	18	−4	3	74	77	12
23	3	2	34	45	33	20	−4	3	38	25	30
−24	4	2	41	14	31	−25	−3	3	61	63	9
−22	4	2	0	17	1	−23	−3	3	0	35	1
−20	4	2	12	22	12	−21	−3	3	58	53	15
−18	4	2	74	74	13	−19	−3	3	121	114	9
−16	4	2	7	34	6	−17	−3	3	161	151	6
−14	4	2	33	36	17	−15	−3	3	86	82	7
−12	4	2	97	94	5	−13	−3	3	237	228	8

h	k	l	10Fo	10Fc	10s
6	6	1	89	86	4
8	6	1	18	31	18
10	6	1	59	78	8
12	6	1	24	10	23
14	6	1	11	30	10
−16	−6	2	14	13	14
−21	−5	2	75	53	10
−19	−5	2	91	90	9
−17	−5	2	65	78	12
−15	−5	2	52	57	17
−13	−5	2	12	15	12
−11	−5	2	117	119	8
−9	−5	2	172	180	7
9	−5	2	129	118	8
11	−5	2	50	32	17
13	−5	2	0	33	1
15	−5	2	47	32	19
17	−5	2	44	48	19
19	−5	2	56	50	12
−24	−4	2	35	14	35
−22	−4	2	0	17	1
−20	−4	2	32	23	31
−18	−4	2	66	74	12
−16	−4	2	41	34	29
−14	−4	2	46	36	14
−12	−4	2	104	94	7
−10	−4	2	106	95	10
−8	−4	2	108	97	5
−6	−4	2	0	26	1
−4	−4	2	377	362	13
4	−4	2	102	107	8
6	−4	2	131	103	5
8	−4	2	61	56	11
10	−4	2	251	255	6
12	−4	2	140	125	7
14	−4	2	27	33	27
16	−4	2	42	13	25
18	−4	2	114	132	8
20	−4	2	38	58	32
22	−4	2	20	19	19
−14	0	3	214	230	4
−12	0	3	313	309	6
−10	0	3	360	335	5
−8	0	3	1125	1138	19
−6	0	3	1022	1054	15
−4	0	3	227	229	3
−2	0	3	1111	1236	17
0	0	3	744	848	11
2	0	3	1244	1255	19

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	2	764	740	23	10	0	2	71	61	5	−10	4	2	103	95	4	−11	−3	3	372	350	8	4	0	3	222	277	4
−5	−3	2	714	680	21	12	0	2	520	511	17	−8	4	2	103	96	4	−9	−3	3	362	315	12	6	0	3	9	2	9
−3	−3	2	541	545	16	14	0	2	357	365	6	−6	4	2	21	26	21	−7	−3	3	340	301	10	8	0	3	318	290	6
−1	−3	2	523	549	11	16	0	2	302	295	5	−4	4	2	396	362	7	−5	−3	3	219	236	8	10	0	3	872	844	15
1	−3	2	179	169	4	18	0	2	68	57	17	−2	4	2	234	231	2	−3	−3	3	314	326	10	12	0	3	65	71	6
3	−3	2	384	372	12	20	0	2	168	173	6	0	4	2	161	158	2	−1	−3	3	474	491	10	14	0	3	168	161	3
5	−3	2	543	516	16	22	0	2	53	44	11	2	4	2	397	387	4	1	−3	3	248	236	6	16	0	3	48	11	8
7	−3	2	195	188	8	24	0	2	16	38	16	12	4	2	133	125	5	3	−3	3	46	52	15	18	0	3	169	177	6
9	−3	2	108	87	8	−23	1	2	123	155	9	14	4	2	28	33	27	5	−3	3	100	106	8	20	0	3	221	221	6
11	−3	2	224	226	6	−21	1	2	188	174	3	16	4	2	33	13	33	7	−3	3	217	212	8	22	0	3	36	17	31
13	−3	2	226	210	6	−19	1	2	0	19	1	18	4	2	138	132	8	9	−3	3	76	67	7	24	0	3	25	18	24
15	−3	2	175	163	7	−17	1	2	104	86	4	20	4	2	36	58	36	11	−3	3	294	298	7	−23	1	3	63	63	6
17	−3	2	128	115	9	−15	1	2	76	74	6	22	4	2	0	19	1	13	−3	3	120	114	8	−21	1	3	80	78	4
19	−3	2	101	124	10	−13	1	2	352	405	16	−21	5	2	62	53	14	15	−3	3	193	170	7	−19	1	3	50	44	5
21	−3	2	68	56	13	−11	1	2	792	818	18	−19	5	2	68	90	26	17	−3	3	171	195	8	−17	1	3	71	67	3
23	−3	2	0	45	1	−9	1	2	323	318	6	−17	5	2	68	78	10	19	−3	3	76	77	12	−15	1	3	217	211	4
−26	−2	2	35	60	28	−7	1	2	290	295	4	−15	5	2	58	57	10	21	−3	3	115	109	8	−13	1	3	307	277	7
−24	−2	2	90	122	17	−5	1	2	682	732	10	−13	5	2	0	15	1	23	−3	3	20	22	20	−11	1	3	395	389	6
−22	−2	2	111	113	16	−3	1	2	685	708	9	−11	5	2	127	118	11	−28	−2	3	58	55	14	−9	1	3	190	197	3
−20	−2	2	62	31	9	−1	1	2	210	235	3	−9	5	2	183	181	6	−26	−2	3	69	81	8	−7	1	3	514	543	7
−18	−2	2	131	131	6	1	1	2	806	847	11	−7	5	2	184	179	4	−24	−2	3	69	79	15	−5	1	3	649	696	9
−16	−2	2	110	115	5	3	1	2	743	795	10	−5	5	2	148	138	4	−22	−2	3	118	94	8	−3	1	3	1714	1799	23
−14	−2	2	240	231	5	5	1	2	483	506	6	−3	5	2	36	37	8	−20	−2	3	92	70	5	−1	1	3	829	881	14
−12	−2	2	406	382	9	7	1	2	514	546	7	−1	5	2	107	103	3	−18	−2	3	127	115	5	1	1	3	235	237	3
−10	−2	2	337	359	10	9	1	2	149	155	4	1	5	2	113	118	3	−16	−2	3	179	174	5	3	1	3	94	86	2
−8	−2	2	281	276	13	11	1	2	362	383	14	3	5	2	74	75	5	−14	−2	3	138	124	8	5	1	3	248	228	3
−6	−2	2	363	343	8	13	1	2	270	290	5	5	5	2	110	102	4	−12	−2	3	102	96	6	7	1	3	129	129	4
−4	−2	2	155	160	3	15	1	2	173	162	3	7	5	2	26	51	26	−10	−2	3	793	938	23	9	1	3	318	343	8
−2	−2	2	350	360	7	17	1	2	262	253	4	9	5	2	139	118	5	−8	−2	3	395	397	28	11	1	3	117	105	4
0	−2	2	328	334	7	19	1	2	391	384	6	11	5	2	10	32	10	−6	−2	3	152	167	5	13	1	3	224	221	4
2	−2	2	403	425	7	21	1	2	50	46	9	13	5	2	0	32	1	−4	−2	3	181	173	4	15	1	3	287	269	4
4	−2	2	235	216	4	−26	2	2	49	60	21	15	5	2	40	32	16	−2	−2	3	452	478	9	17	1	3	62	56	6
6	−2	2	329	334	6	−24	2	2	102	122	10	17	5	2	44	48	25	0	−2	3	283	274	6	19	1	3	94	97	5
8	−2	2	252	273	18	−22	2	2	114	114	10	19	5	2	36	50	35	2	−2	3	410	412	15	21	1	3	104	107	4
10	−2	2	258	257	7	−20	2	2	50	32	17	−16	6	2	2	13	1	4	−2	3	179	185	4	−26	2	3	81	81	12
12	−2	2	344	339	6	−18	2	2	125	131	6	−14	6	2	38	36	19	6	−2	3	41	45	6	−24	2	3	61	79	17
14	−2	2	180	174	6	−16	2	2	110	115	6	−12	6	2	33	28	32	8	−2	3	394	395	24	−22	2	3	112	95	10
16	−2	2	112	102	7	−14	2	2	236	231	6	−10	6	2	0	21	1	10	−2	3	170	167	4	−20	2	3	87	71	16
18	−2	2	146	142	13	−12	2	2	396	381	9	−8	6	2	0	35	1	12	−2	3	223	212	6	−18	2	3	126	115	7
20	−2	2	131	147	14	−10	2	2	311	361	19	−6	6	2	17	41	17	14	−2	3	50	42	13	−16	2	3	182	174	5
22	−2	2	48	43	12	−8	2	2	281	274	16	−4	6	2	15	19	15	16	−2	3	126	142	7	−14	2	3	137	124	12
24	−2	2	40	38	17	−6	2	2	369	342	8	4	6	2	43	48	6	18	−2	3	140	136	10	−12	2	3	99	96	9
−27	−1	2	57	64	23	−4	2	2	167	160	4	6	6	2	50	51	7	20	−2	3	140	155	12	−10	2	3	767	938	24
−25	−1	2	83	70	10	−2	2	2	347	358	4	8	6	2	38	29	11	22	−2	3	32	51	32	−8	2	3	402	398	22
−23	−1	2	120	155	5	0	2	2	321	335	4	10	6	2	20	20	20	24	−2	3	50	47	11	−6	2	3	153	167	6
−21	−1	2	192	174	5	2	2	2	413	426	5	12	6	2	0	18	1	−27	−1	3	130	110	6	−4	2	3	183	171	3
−19	−1	2	0	18	1	4	2	2	233	215	3	14	6	2	48	38	12	−25	−1	3	27	15	26	−2	2	3	441	477	5
−17	−1	2	97	87	4	6	2	2	327	334	5	−16	−6	3	45	20	15	−23	−1	3	38	63	16	0	2	3	273	276	3
−15	−1	2	65	74	5	8	2	2	271	272	7	−21	−5	3	52	18	13	−21	−1	3	73	78	6	2	2	3	406	413	5

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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
−13	−1	2	370	405	6	10	2	2	259	257	5	−19	−5	3	45	44	18	−19	−1	3	36	44	11	4	2	3	172	185	3
−11	−1	2	813	818	14	12	2	2	346	340	4	−17	−5	3	0	30	1	−17	−1	3	72	66	4	6	2	3	40	45	5
−9	−1	2	325	320	6	14	2	2	178	174	3	−15	−5	3	33	58	32	−15	−1	3	217	211	6	8	2	3	394	394	9
−7	−1	2	288	296	5	16	2	2	93	102	11	−13	−5	3	122	154	8	−13	−1	3	323	277	6	10	2	3	172	166	4
−5	−1	2	685	732	12	20	2	2	126	147	9	−11	−5	3	102	105	8	−11	−1	3	412	390	8	12	2	3	223	211	3
−3	−1	2	654	708	12	22	2	2	15	42	14	−9	−5	3	20	16	20	−9	−1	3	186	196	4	14	2	3	51	42	4
−1	−1	2	205	233	4	24	2	2	6	38	6	9	−5	3	157	156	8	−7	−1	3	530	541	9	16	2	3	127	142	9
1	−1	2	815	849	15	−25	3	2	22	15	22	11	−5	3	66	56	13	−5	−1	3	661	696	11	20	2	3	127	155	9
3	−1	2	759	794	13	−23	3	2	27	24	26	13	−5	3	148	141	8	−3	−1	3	1674	1797	32	22	2	3	47	51	20
5	−1	2	492	505	8	−21	3	2	90	93	12	15	−5	3	50	53	16	−1	−1	3	809	881	14	24	2	3	33	47	33
7	−1	2	522	546	14	−19	3	2	96	109	11	17	−5	3	44	50	19	1	−1	3	231	236	4	−25	3	3	38	63	38
9	−1	2	162	156	4	−17	3	2	143	147	12	−24	−4	3	33	12	33	3	−1	3	93	86	4	−23	3	3	32	35	32
11	−1	2	381	386	6	−15	3	2	84	80	13	−22	−4	3	54	32	16	5	−1	3	244	228	5	−21	3	3	45	53	29
13	−1	2	274	291	6	−13	3	2	159	158	6	−20	−4	3	0	28	1	7	−1	3	130	129	5	−19	3	3	103	113	11
15	−1	2	172	162	4	−11	3	2	326	343	6	−18	−4	3	60	46	13	9	−1	3	338	343	6	−17	3	3	161	152	6
17	−1	2	270	253	4	−9	3	2	197	189	6	−16	−4	3	64	78	13	11	−1	3	125	105	4	−15	3	3	76	82	7
19	−1	2	388	384	6	−7	3	2	768	740	17	−14	−4	3	0	21	1	13	−1	3	219	221	4	−13	3	3	224	227	5
21	−1	2	23	45	22	−5	3	2	706	681	15	−12	−4	3	104	106	6	15	−1	3	284	270	5	−11	3	3	360	350	7
23	−1	2	87	76	10	−3	3	2	545	546	9	−10	−4	3	175	167	5	17	−1	3	55	57	8	−9	3	3	366	316	8
25	−1	2	17	14	16	−1	3	2	519	550	17	−8	−4	3	148	135	5	19	−1	3	95	97	9	−7	3	3	330	302	8
−26	0	2	43	34	9	1	3	2	166	172	4	−6	−4	3	121	119	5	21	−1	3	106	107	11	−5	3	3	220	237	6
−24	0	2	135	129	6	3	3	2	384	371	7	−4	−4	3	164	143	7	23	−1	3	69	65	12	−3	3	3	324	326	6
−22	0	2	41	49	41	5	3	2	521	517	18	4	−4	3	272	273	6	25	−1	3	57	43	10	−1	3	3	481	492	14
−20	0	2	76	62	5	7	3	2	185	188	9	6	−4	3	61	56	20	−26	0	3	35	27	35	1	3	3	234	237	5
−18	0	2	115	91	6	9	3	2	106	87	7	8	−4	3	156	171	6	−24	0	3	47	44	12	3	3	3	46	53	4
−16	0	2	174	176	3	11	3	2	224	226	6	10	−4	3	35	31	25	−22	0	3	0	6	1	5	3	3	102	106	4
−14	0	2	213	236	4	13	3	2	228	210	8	12	−4	3	158	156	13	−20	0	3	15	9	14	7	3	3	218	211	8
−12	0	2	266	266	5	17	3	2	122	115	10	14	−4	3	202	205	8	−18	0	3	87	83	4	9	3	3	77	68	6
−10	0	2	881	931	13	19	3	2	96	124	10	16	−4	3	189	196	8	−16	0	3	138	114	3	11	3	3	307	298	9
13	3	3	114	114	10	14	−4	4	93	77	11	−16	0	4	117	118	5	9	3	4	99	99	7	−27	−3	5	86	76	6
15	3	3	201	169	9	16	−4	4	15	35	14	−14	0	4	261	256	5	11	3	4	102	107	10	−25	−3	5	88	76	7
19	3	3	81	77	12	18	−4	4	54	51	16	−12	0	4	547	540	9	13	3	4	108	96	10	−23	−3	5	0	23	1
21	3	3	80	109	12	20	−4	4	18	35	18	−10	0	4	24	15	13	15	3	4	227	228	9	−21	−3	5	30	18	30
23	3	3	35	22	35	−27	−3	4	48	39	11	−8	0	4	834	878	15	19	3	4	26	4	25	−19	−3	5	70	65	20
−24	4	3	0	12	1	−25	−3	4	20	23	19	−6	0	4	80	82	3	21	3	4	50	55	19	−17	−3	5	92	80	13
−22	4	3	31	32	31	−23	−3	4	17	31	17	−4	0	4	1279	1392	23	−24	4	4	0	32	1	−15	−3	5	69	72	8
−20	4	3	35	28	35	−21	−3	4	178	154	8	−2	0	4	315	357	5	−22	4	4	61	35	17	−13	−3	5	255	231	6
−18	4	3	56	46	18	−19	−3	4	12	2	11	0	0	4	1116	1209	17	−20	4	4	45	35	24	−11	−3	5	349	338	7
−16	4	3	57	78	17	−17	−3	4	70	77	14	2	0	4	444	445	7	−18	4	4	87	85	11	−9	−3	5	360	349	7
−14	4	3	0	21	1	−15	−3	4	139	130	5	4	0	4	135	130	3	−16	4	4	168	153	9	−7	−3	5	244	225	8
−12	4	3	101	105	5	−13	−3	4	99	104	6	6	0	4	185	185	3	−14	4	4	191	198	5	−5	−3	5	160	143	7
−10	4	3	173	168	4	−11	−3	4	284	269	6	8	0	4	770	754	13	−12	4	4	81	86	5	−3	−3	5	262	276	6
−8	4	3	140	135	4	−9	−3	4	146	162	8	10	0	4	564	516	10	−10	4	4	0	22	1	−1	−3	5	21	26	20
−6	4	3	130	119	4	−7	−3	4	237	264	9	12	0	4	199	188	3	−8	4	4	175	179	3	1	−3	5	268	280	8
−4	4	3	162	144	5	−5	−3	4	118	125	7	14	0	4	179	164	3	−6	4	4	18	22	18	3	−3	5	163	170	8
−2	4	3	164	155	2	−3	−3	4	114	105	5	16	0	4	0	9	1	−4	4	4	154	151	3	5	−3	5	105	108	6
0	4	3	80	77	2	−1	−3	4	95	83	9	18	0	4	162	146	6	−2	4	4	289	281	4	7	−3	5	89	90	14
2	4	3	208	195	3	1	−3	4	77	76	5	20	0	4	0	12	1	0	4	4	274	263	3	9	−3	5	268	270	7
4	4	3	282	272	6	3	−3	4	330	311	10	22	0	4	92	84	14	2	4	4	125	129	2	11	−3	5	258	248	7

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	4	3	73	56	6	5	−3	4	97	101	9	24	0	4	22	34	21	4	4	4	162	153	4	13	−3	5	187	182	15
8	4	3	158	172	4	7	−3	4	229	227	6	−23	1	4	0	27	1	6	4	4	80	70	6	15	−3	5	94	111	10
10	4	3	51	31	11	9	−3	4	107	98	6	−21	1	4	197	192	3	8	4	4	133	137	8	17	−3	5	23	34	22
14	4	3	199	206	8	11	−3	4	111	107	7	−19	1	4	114	104	3	10	4	4	276	267	5	19	−3	5	127	103	8
16	4	3	189	196	8	13	−3	4	112	96	7	−17	1	4	131	119	3	16	4	4	21	35	20	21	−3	5	53	43	15
18	4	3	70	76	13	15	−3	4	241	228	8	−15	1	4	67	65	4	18	4	4	72	51	12	−28	−2	5	0	17	1
20	4	3	25	26	24	17	−3	4	135	128	9	−13	1	4	189	198	5	20	4	4	60	35	14	−26	−2	5	0	10	1
−21	5	3	4	18	4	19	−3	4	0	3	1	−11	1	4	327	317	5	−21	5	4	33	25	32	−24	−2	5	77	111	7
−19	5	3	51	44	12	21	−3	4	57	55	14	−9	1	4	977	1049	13	−19	5	4	33	44	32	−22	−2	5	64	55	9
−17	5	3	36	30	36	−28	−2	4	85	98	9	−7	1	4	166	184	3	−17	5	4	93	122	18	−20	−2	5	107	100	7
−15	5	3	57	58	10	−26	−2	4	55	65	10	−5	1	4	477	502	6	−15	5	4	65	75	9	−18	−2	5	147	125	7
−13	5	3	144	154	18	−24	−2	4	77	91	7	−3	1	4	266	278	4	−13	5	4	31	42	30	−16	−2	5	89	89	6
−11	5	3	118	105	10	−22	−2	4	130	133	12	−1	1	4	991	1024	23	−11	5	4	160	169	5	−14	−2	5	325	326	6
−9	5	3	34	16	20	−20	−2	4	108	93	7	1	1	4	413	429	6	−9	5	4	117	103	6	−12	−2	5	75	82	6
−7	5	3	135	135	5	−18	−2	4	162	147	4	3	1	4	28	30	6	−7	5	4	342	333	8	−10	−2	5	328	327	12
−5	5	3	19	14	19	−16	−2	4	130	116	13	5	1	4	372	385	5	−5	5	4	198	205	5	−8	−2	5	554	568	18
−3	5	3	385	387	6	−14	−2	4	326	327	6	7	1	4	191	195	4	−3	5	4	187	183	3	−6	−2	5	424	432	7
−1	5	3	156	149	2	−12	−2	4	549	586	17	9	1	4	139	157	5	−1	5	4	28	44	5	−4	−2	5	201	208	4
1	5	3	106	105	3	−10	−2	4	84	114	16	11	1	4	342	332	4	1	5	4	36	37	8	−2	−2	5	373	376	8
3	5	3	62	54	6	−8	−2	4	215	240	21	13	1	4	229	203	4	3	5	4	144	129	4	0	−2	5	443	432	9
5	5	3	44	38	10	−6	−2	4	237	241	4	15	1	4	261	249	4	5	5	4	95	99	6	2	−2	5	369	382	8
7	5	3	140	131	5	−4	−2	4	153	148	3	17	1	4	70	53	5	7	5	4	255	244	8	4	−2	5	253	257	6
9	5	3	157	156	5	−2	−2	4	189	193	5	19	1	4	88	83	6	9	5	4	58	62	9	6	−2	5	213	203	12
11	5	3	51	55	11	0	−2	4	484	496	10	21	1	4	29	27	13	11	5	4	103	94	6	8	−2	5	270	272	9
13	5	3	145	141	5	2	−2	4	513	527	9	−26	2	4	64	65	16	13	5	4	53	46	10	10	−2	5	86	76	7
15	5	3	54	53	12	4	−2	4	413	435	7	−24	2	4	85	91	12	15	5	4	26	23	25	12	−2	5	29	27	29
17	5	3	49	50	14	6	−2	4	267	255	6	−22	2	4	126	133	10	17	5	4	0	19	1	14	−2	5	79	83	9
−16	6	3	0	20	1	8	−2	4	172	159	9	−20	2	4	103	93	8	−16	6	4	20	8	20	16	−2	5	25	15	24
−14	6	3	31	25	31	10	−2	4	178	182	5	−18	2	4	161	148	6	−14	6	4	0	15	1	18	−2	5	163	142	8
−12	6	3	0	11	1	12	−2	4	309	321	7	−16	2	4	128	116	5	−12	6	4	73	60	15	20	−2	5	56	50	29
−10	6	3	32	31	17	14	−2	4	106	113	13	−14	2	4	315	327	7	−10	6	4	132	133	5	22	−2	5	0	9	1
−8	6	3	41	44	9	16	−2	4	68	70	20	−12	2	4	567	585	36	−8	6	4	76	71	5	−29	−1	5	50	50	8
−6	6	3	128	137	5	18	−2	4	2	25	2	−10	2	4	84	116	15	−6	6	4	130	130	7	−27	−1	5	74	83	8
4	6	3	113	116	3	20	−2	4	56	59	11	−8	2	4	226	241	8	4	6	4	71	75	4	−25	−1	5	87	70	10
6	6	3	64	57	5	22	−2	4	46	64	21	−6	2	4	240	241	3	6	6	4	86	85	4	−23	−1	5	45	63	44
8	6	3	48	53	10	−29	−1	4	71	74	5	−4	2	4	150	149	2	8	6	4	0	28	1	−21	−1	5	69	77	6
10	6	3	29	38	23	−27	−1	4	34	38	34	−2	2	4	187	194	3	10	6	4	17	30	17	−19	−1	5	163	159	4
12	6	3	0	5	1	−25	−1	4	25	28	24	0	2	4	479	497	6	12	6	4	33	61	22	−17	−1	5	180	172	3
14	6	3	33	46	20	−23	−1	4	29	27	28	2	2	4	522	527	8	−21	−5	5	38	51	23	−15	−1	5	35	26	14
−16	−6	4	0	8	1	−21	−1	4	195	193	4	4	2	4	420	436	6	−19	−5	5	56	72	13	−13	−1	5	311	262	6
−21	−5	4	5	25	4	−19	−1	4	126	104	4	6	2	4	265	255	7	−17	−5	5	78	76	11	−11	−1	5	411	422	7
−19	−5	4	24	44	23	−17	−1	4	130	119	3	8	2	4	164	158	4	−15	−5	5	144	127	8	−9	−1	5	300	317	5
−17	−5	4	122	122	8	−15	−1	4	59	65	8	10	2	4	176	183	3	−13	−5	5	81	78	10	−7	−1	5	442	458	8
−15	−5	4	68	75	11	−13	−1	4	194	198	4	12	2	4	316	321	4	−11	−5	5	199	193	8	−5	−1	5	539	543	9
−13	−5	4	50	42	17	−11	−1	4	328	315	6	14	2	4	119	112	3	7	−5	5	83	99	10	−3	−1	5	393	406	6
−11	−5	4	171	169	7	−9	−1	4	1002	1049	17	16	2	4	67	71	6	9	−5	5	50	46	17	−1	−1	5	451	460	7
9	−5	4	74	62	11	−7	−1	4	174	185	5	18	2	4	0	25	1	11	−5	5	0	35	1	1	−1	5	188	199	3
11	−5	4	98	93	9	−5	−1	4	484	501	8	20	2	4	47	59	23	13	−5	5	0	14	1	3	−1	5	280	296	8
13	−5	4	0	46	1	−3	−1	4	268	279	5	22	2	4	48	64	19	15	−5	5	31	55	31	5	−1	5	218	233	10

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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
15	−5	4	23	23	23	−1	−1	4	958	1024	15	−27	3	4	44	39	22	−24	−4	5	48	61	17	7	−1	5	264	257	11
17	−5	4	11	19	11	1	−1	4	393	426	7	−25	3	4	42	23	39	−22	−4	5	103	87	9	9	−1	5	637	624	10
−24	−4	4	46	32	18	3	−1	4	20	27	19	−23	3	4	37	31	36	−20	−4	5	91	113	9	11	−1	5	206	201	4
−22	−4	4	45	35	20	5	−1	4	395	387	8	−21	3	4	161	155	9	−18	−4	5	25	30	24	13	−1	5	156	142	4
−20	−4	4	0	36	1	7	−1	4	188	195	4	−19	3	4	0	3	1	−16	−4	5	69	41	12	15	−1	5	115	110	5
−18	−4	4	70	86	11	9	−1	4	141	156	4	−17	3	4	72	77	16	−14	−4	5	80	63	8	17	−1	5	52	55	10
−16	−4	4	156	153	8	11	−1	4	335	333	5	−15	3	4	141	130	6	−12	−4	5	224	209	6	19	−1	5	163	161	8
−14	−4	4	205	198	6	13	−1	4	221	205	4	−13	3	4	92	103	5	−10	−4	5	282	270	6	21	−1	5	0	9	1
−12	−4	4	94	86	7	15	−1	4	258	249	5	−11	3	4	274	269	5	−8	−4	5	205	205	5	23	−1	5	0	18	1
−10	−4	4	23	22	23	17	−1	4	50	52	10	−9	3	4	166	162	5	−6	−4	5	61	57	18	−26	0	5	67	70	8
−8	−4	4	167	179	5	19	−1	4	92	83	7	−7	3	4	246	263	6	4	−4	5	69	74	8	−24	0	5	117	132	6
−6	−4	4	44	22	10	21	−1	4	0	27	1	−5	3	4	119	125	3	6	−4	5	265	270	6	−22	0	5	17	41	17
−4	−4	4	143	151	7	23	−1	4	79	61	10	−3	3	4	110	105	3	8	−4	5	327	322	10	−20	0	5	43	46	11
4	−4	4	157	154	5	−26	0	4	0	13	1	−1	3	4	82	84	6	10	−4	5	294	307	7	−18	0	5	103	112	4
6	−4	4	76	70	7	−24	0	4	118	108	11	1	3	4	77	77	3	12	−4	5	82	68	12	−16	0	5	158	157	3
8	−4	4	138	138	6	−22	0	4	49	47	10	3	3	4	327	311	6	14	−4	5	17	35	17	−14	0	5	248	236	5
10	−4	4	261	266	7	−20	0	4	170	168	4	5	3	4	99	102	2	16	−4	5	65	39	14	−12	0	5	325	311	6
12	−4	4	398	404	12	−18	0	4	248	225	4	7	3	4	232	227	5	18	−4	5	61	69	13	−10	0	5	153	155	4
−8	0	5	322	330	5	21	3	5	45	43	21	−13	−3	6	208	190	5	10	0	6	90	96	4	−4	4	6	81	81	3
−6	0	5	128	120	3	−24	4	5	57	61	17	−11	−3	6	259	234	6	12	0	6	215	207	3	−2	4	6	286	261	3
−4	0	5	496	544	7	−22	4	5	114	87	10	−9	−3	6	170	156	4	14	0	6	127	136	4	0	4	6	225	211	3
−2	0	5	229	251	4	−20	4	5	89	113	11	−7	−3	6	43	40	15	16	0	6	0	3	1	2	4	6	68	66	3
0	0	5	293	313	4	−18	4	5	52	30	20	−5	−3	6	104	106	7	18	0	6	14	28	13	4	4	6	202	188	3
2	0	5	228	235	4	−16	4	5	52	41	21	−3	−3	6	151	150	5	20	0	6	0	9	1	6	4	6	218	225	5
4	0	5	1383	1397	21	−14	4	5	78	64	10	−1	−3	6	260	272	6	22	0	6	28	45	22	8	4	6	214	211	6
6	0	5	710	692	13	−12	4	5	215	209	4	1	−3	6	72	76	6	−23	1	6	108	115	6	10	4	6	32	44	32
8	0	5	186	186	4	−10	4	5	279	271	5	3	−3	6	111	115	5	−21	1	6	55	63	7	12	4	6	170	155	6
10	0	5	245	213	5	−8	4	5	210	205	4	5	−3	6	136	132	7	−19	1	6	71	69	4	16	4	6	38	25	38
12	0	5	38	8	8	−6	4	5	56	57	6	7	−3	6	224	224	6	−17	1	6	31	22	9	18	4	6	57	78	13
14	0	5	160	160	3	−4	4	5	116	96	4	9	−3	6	98	87	7	−15	1	6	176	177	3	−21	5	6	17	40	16
16	0	5	153	140	7	−2	4	5	102	103	2	11	−3	6	111	98	7	−13	1	6	61	71	4	−19	5	6	57	81	10
18	0	5	187	174	8	0	4	5	136	130	2	13	−3	6	0	49	1	−11	1	6	260	281	5	−17	5	6	29	26	29
20	0	5	90	95	8	2	4	5	127	117	2	15	−3	6	31	45	31	−9	1	6	831	852	20	−15	5	6	56	68	10
22	0	5	36	49	15	4	4	5	77	74	5	17	−3	6	75	52	13	−7	1	6	476	515	7	−13	5	6	160	146	5
−23	1	5	67	63	5	6	4	5	262	270	5	19	−3	6	17	34	17	−5	1	6	482	526	7	−11	5	6	254	246	6
−21	1	5	80	77	4	8	4	5	330	323	7	−28	−2	6	122	102	8	−3	1	6	802	822	12	−9	5	6	127	123	8
−19	1	5	165	158	3	10	4	5	306	307	6	−26	−2	6	108	85	6	−1	1	6	676	668	10	−7	5	6	234	237	6
−17	1	5	180	172	3	12	4	5	87	68	8	−24	−2	6	43	65	13	1	1	6	800	784	12	−5	5	6	86	72	5
−15	1	5	33	26	9	16	4	5	23	39	22	−22	−2	6	52	41	11	3	1	6	319	330	6	−3	5	6	76	85	4
−13	1	5	302	262	7	18	4	5	31	70	30	−20	−2	6	56	41	9	5	1	6	844	811	15	−1	5	6	88	84	2
−11	1	5	401	423	6	−21	5	5	44	51	22	−18	−2	6	186	172	4	7	1	6	586	575	10	1	5	6	239	243	4
−9	1	5	300	319	7	−19	5	5	66	72	9	−16	−2	6	92	97	5	9	1	6	188	187	3	9	5	6	48	38	11
−7	1	5	442	457	6	−17	5	5	95	76	7	−14	−2	6	230	217	5	11	1	6	129	121	3	11	5	6	49	53	11
−5	1	5	523	543	7	−15	5	5	140	127	6	−12	−2	6	457	423	10	13	1	6	11	8	11	13	5	6	0	18	1
−3	1	5	406	407	7	−13	5	5	84	78	7	−10	−2	6	151	160	16	15	1	6	87	68	5	15	5	6	0	5	1
−1	1	5	458	460	9	−11	5	5	211	193	5	−8	−2	6	177	173	4	17	1	6	41	36	13	−16	6	6	98	96	8
1	1	5	190	199	4	−9	5	5	178	176	6	−6	−2	6	286	277	6	19	1	6	76	65	5	−14	6	6	71	58	10
3	1	5	287	296	4	−7	5	5	213	197	5	−4	−2	6	219	222	5	−26	2	6	78	85	13	−12	6	6	23	43	22
5	1	5	222	233	4	−5	5	5	170	157	4	−2	−2	6	573	568	12	−24	2	6	68	65	15	−10	6	6	36	49	14

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	1	5	262	258	8	−3	5	5	196	204	3	0	−2	6	251	235	6	−22	2	6	47	41	28	−8	6	6	51	52	7
9	1	5	658	623	8	−1	5	5	68	70	3	2	−2	6	271	276	6	−20	2	6	63	41	12	−6	6	6	74	81	4
11	1	5	213	201	3	1	5	5	194	195	5	4	−2	6	164	161	6	−18	2	6	186	172	6	4	6	6	69	68	4
13	1	5	150	142	3	3	5	5	168	171	4	6	−2	6	99	103	4	−16	2	6	94	97	6	6	6	6	48	47	7
15	1	5	134	110	8	5	5	5	180	172	7	8	−2	6	258	259	11	−14	2	6	232	218	6	8	6	6	42	45	10
17	1	5	51	55	9	7	5	5	89	99	8	10	−2	6	186	173	8	−12	2	6	463	422	7	10	6	6	0	18	1
19	1	5	156	161	4	9	5	5	45	46	12	12	−2	6	74	75	11	−10	2	6	162	158	4	−21	−5	7	45	59	16
21	1	5	0	9	1	11	5	5	43	35	13	14	−2	6	34	59	34	−8	2	6	182	174	3	−19	−5	7	0	18	1
−26	2	5	17	10	16	13	5	5	10	14	10	16	−2	6	0	14	1	−6	2	6	292	278	4	−17	−5	7	70	79	11
−24	2	5	84	111	12	15	5	5	27	55	26	18	−2	6	85	91	16	−4	2	6	222	222	4	−15	−5	7	30	42	30
−22	2	5	58	55	19	−16	6	5	28	37	27	20	−2	6	64	62	9	−2	2	6	572	568	9	−13	−5	7	46	38	17
−20	2	5	112	100	7	−14	6	5	65	55	11	22	−2	6	57	63	9	0	2	6	254	232	4	−11	−5	7	124	153	8
−18	2	5	147	125	13	−12	6	5	92	97	6	−29	−1	6	33	39	15	2	2	6	278	276	5	7	−5	7	101	120	9
−16	2	5	89	89	7	−10	6	5	126	138	5	−27	−1	6	48	58	19	4	2	6	175	162	3	9	−5	7	94	77	9
−14	2	5	327	326	7	−8	6	5	85	88	4	−25	−1	6	65	91	12	6	2	6	106	104	3	11	−5	7	76	56	11
−12	2	5	69	81	7	−6	6	5	84	79	4	−23	−1	6	112	115	6	8	2	6	264	259	4	13	−5	7	0	33	1
−10	2	5	342	327	6	4	6	5	29	31	11	−21	−1	6	52	62	7	10	2	6	184	173	3	−24	−4	7	51	35	15
−8	2	5	564	567	13	6	6	5	84	88	4	−19	−1	6	65	69	5	12	2	6	76	75	4	−22	−4	7	0	26	1
−6	2	5	431	432	6	8	6	5	31	25	30	−17	−1	6	41	23	8	14	2	6	59	58	5	−20	−4	7	140	138	8
−4	2	5	200	207	3	10	6	5	58	64	10	−15	−1	6	178	177	4	16	2	6	14	14	13	−18	−4	7	144	128	8
−2	2	5	379	376	6	12	6	5	34	48	18	−13	−1	6	64	72	5	18	2	6	78	91	14	−16	−4	7	53	54	16
0	2	5	450	433	9	−21	−5	6	28	40	28	−11	−1	6	266	283	5	20	2	6	60	62	14	−14	−4	7	74	87	8
2	2	5	380	381	8	−19	−5	6	58	81	13	−9	−1	6	807	851	59	22	2	6	46	63	17	−12	−4	7	41	46	15
4	2	5	261	258	5	−17	−5	6	52	25	15	−7	−1	6	497	517	19	−27	3	6	54	15	17	−10	−4	7	14	20	13
6	2	5	210	203	4	−15	−5	6	63	69	13	−5	−1	6	508	526	8	−25	3	6	52	43	22	−8	−4	7	307	323	7
8	2	5	280	272	3	−13	−5	6	148	146	8	−3	−1	6	794	821	12	−23	3	6	95	104	12	−6	−4	7	240	240	6
10	2	5	91	76	3	7	−5	6	68	67	12	−1	−1	6	662	670	10	−21	3	6	106	126	10	2	−4	7	199	192	8
12	2	5	25	27	15	9	−5	6	60	38	13	1	−1	6	768	785	13	−19	3	6	41	61	41	4	−4	7	98	107	8
14	2	5	86	83	3	11	−5	6	58	53	14	3	−1	6	317	329	14	−17	3	6	136	113	20	6	−4	7	51	59	14
16	2	5	0	15	1	13	−5	6	0	18	1	5	−1	6	834	812	18	−15	3	6	73	69	8	8	−4	7	134	157	9
18	2	5	149	143	10	15	−5	6	29	5	28	7	−1	6	585	575	10	−13	3	6	206	190	5	10	−4	7	127	127	9
20	2	5	24	50	24	−24	−4	6	52	7	15	9	−1	6	186	187	4	−11	3	6	256	234	5	12	−4	7	101	97	10
22	2	5	0	9	1	−22	−4	6	39	49	27	11	−1	6	117	122	4	−9	3	6	151	156	4	14	−4	7	66	45	14
−27	3	5	76	76	12	−20	−4	6	49	57	16	13	−1	6	19	8	18	−7	3	6	51	40	3	16	−4	7	39	48	29
−25	3	5	106	76	11	−18	−4	6	108	103	9	15	−1	6	80	68	6	−5	3	6	102	106	4	−27	−3	7	101	92	6
−23	3	5	0	23	1	−16	−4	6	204	196	8	17	−1	6	37	37	23	−3	3	6	152	150	3	−25	−3	7	124	115	8
−21	3	5	18	19	17	−14	−4	6	164	165	12	19	−1	6	61	65	24	−1	3	6	271	271	4	−23	−3	7	103	78	9
−19	3	5	72	65	19	−12	−4	6	168	157	6	21	−1	6	31	26	30	1	3	6	74	76	3	−21	−3	7	16	69	15
−17	3	5	91	80	8	−10	−4	6	141	137	5	−26	0	6	19	35	19	3	3	6	119	115	2	−19	−3	7	64	60	13
−15	3	5	61	72	9	−8	−4	6	166	176	5	−24	0	6	67	59	8	5	3	6	136	131	2	−17	−3	7	251	222	6
−13	3	5	241	230	5	−6	−4	6	149	155	5	−22	0	6	134	127	8	7	3	6	230	224	2	−15	−3	7	121	119	5
−11	3	5	338	339	6	4	−4	6	191	188	6	−20	0	6	215	205	5	9	3	6	95	87	2	−13	−3	7	85	87	6
−9	3	5	351	349	6	6	−4	6	213	225	6	−18	0	6	107	109	4	11	3	6	111	98	11	−11	−3	7	114	109	5
−7	3	5	236	224	7	8	−4	6	218	211	6	−16	0	6	221	203	4	13	3	6	48	49	26	−9	−3	7	87	92	5
−5	3	5	171	144	3	10	−4	6	53	44	19	−14	0	6	123	110	4	15	3	6	37	45	37	−7	−3	7	88	90	5
−3	3	5	257	276	4	12	−4	6	175	155	8	−12	0	6	157	171	4	19	3	6	0	34	1	−5	−3	7	173	170	8
−1	3	5	36	25	6	14	−4	6	62	67	15	−10	0	6	85	66	4	−24	4	6	32	7	32	−3	−3	7	194	205	5
1	3	5	267	280	4	16	−4	6	0	25	1	−8	0	6	341	313	7	−22	4	6	57	49	18	−1	−3	7	119	114	10
3	3	5	169	169	3	18	−4	6	57	78	14	−6	0	6	349	364	5	−20	4	6	22	57	22	1	−3	7	78	82	5

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	3	5	104	108	3	−27	−3	6	9	15	8	−4	0	6	51	72	4	−18	4	6	104	103	10	3	−3	7	64	70	11
7	3	5	97	91	2	−25	−3	6	41	43	22	−2	0	6	15	38	14	−16	4	6	208	196	8	5	−3	7	50	44	12
9	3	5	272	270	12	−23	−3	6	93	104	9	0	0	6	248	265	4	−14	4	6	154	165	9	7	−3	7	260	243	7
11	3	5	259	248	9	−21	−3	6	121	125	9	2	0	6	63	56	4	−12	4	6	168	156	5	9	−3	7	188	183	6
13	3	5	204	182	8	−19	−3	6	65	60	17	4	0	6	110	110	6	−10	4	6	142	137	4	11	−3	7	145	145	23
15	3	5	81	111	13	−17	−3	6	121	113	10	6	0	6	0	18	1	−8	4	6	168	177	4	13	−3	7	118	135	9
19	3	5	88	103	11	−15	−3	6	76	69	9	8	0	6	664	610	12	−6	4	6	170	156	4	15	−3	7	50	46	19
17	−3	7	123	94	9	−7	1	7	447	467	9	−11	5	7	161	153	5	6	−2	8	53	56	10	−14	2	8	208	200	3
19	−3	7	57	59	13	−5	1	7	433	473	9	−9	5	7	79	85	10	8	−2	8	140	123	6	−12	2	8	172	160	3
−28	−2	7	55	68	18	−3	1	7	151	169	3	−7	5	7	48	61	12	10	−2	8	88	79	8	−10	2	8	279	284	4
−26	−2	7	65	59	8	−1	1	7	652	668	10	−5	5	7	156	162	5	12	−2	8	188	159	9	−8	2	8	400	403	8
−24	−2	7	137	146	5	1	1	7	340	341	7	−3	5	7	191	183	3	14	−2	8	165	153	8	−6	2	8	238	220	4
−22	−2	7	37	29	16	3	1	7	322	323	8	−1	5	7	156	148	2	16	−2	8	81	73	8	−4	2	8	162	166	4
−20	−2	7	117	109	7	5	1	7	251	250	5	1	5	7	43	29	42	18	−2	8	0	14	1	−2	2	8	347	323	5
−18	−2	7	143	142	6	7	1	7	449	431	6	9	5	7	75	77	7	20	−2	8	36	36	15	0	2	8	118	111	4
−16	−2	7	4	37	4	9	1	7	363	359	5	11	5	7	54	56	12	−29	−1	8	55	48	9	2	2	8	220	212	3
−14	−2	7	218	201	5	11	1	7	161	155	4	13	5	7	0	33	1	−27	−1	8	39	40	17	4	2	8	159	144	3
−12	−2	7	313	294	6	13	1	7	15	28	15	−16	6	7	40	25	19	−25	−1	8	74	75	10	6	2	8	52	57	6
−10	−2	7	207	228	8	15	1	7	100	88	10	−14	6	7	45	60	15	−23	−1	8	111	127	9	8	2	8	135	123	4
−8	−2	7	181	170	5	17	1	7	78	75	5	−12	6	7	64	70	12	−21	−1	8	121	109	5	10	2	8	91	79	4
−6	−2	7	207	214	5	19	1	7	45	46	7	−10	6	7	64	75	7	−19	−1	8	85	94	4	12	2	8	175	159	5
−4	−2	7	159	173	5	−28	2	7	49	68	21	−8	6	7	25	28	24	−17	−1	8	245	242	5	14	2	8	159	153	4
−2	−2	7	217	213	5	−26	2	7	74	59	14	−6	6	7	33	33	9	−15	−1	8	97	92	4	16	2	8	56	73	21
0	−2	7	94	94	5	−24	2	7	150	146	9	4	6	7	72	75	4	−13	−1	8	282	287	5	18	2	8	0	15	1
2	−2	7	161	149	8	−22	2	7	58	29	18	6	6	7	32	39	11	−11	−1	8	127	137	7	20	2	8	17	36	17
4	−2	7	171	178	4	−20	2	7	119	110	7	8	6	7	40	45	14	−9	−1	8	758	744	16	−27	3	8	85	69	12
6	−2	7	133	130	4	−18	2	7	150	142	6	−21	−5	8	0	33	1	−7	−1	8	423	407	9	−25	3	8	99	82	11
8	−2	7	267	252	7	−16	2	7	25	37	24	−19	−5	8	46	38	17	−5	−1	8	566	606	10	−23	3	8	23	21	22
10	−2	7	76	71	11	−14	2	7	220	201	3	−17	−5	8	40	29	22	−3	−1	8	446	460	15	−21	3	8	97	95	10
12	−2	7	57	62	18	−12	2	7	311	294	4	−15	−5	8	83	89	9	−1	−1	8	382	391	7	−19	3	8	33	12	33
14	−2	7	166	122	9	−10	2	7	216	228	5	−13	−5	8	54	62	14	1	−1	8	583	575	12	−17	3	8	94	100	8
16	−2	7	115	87	7	−8	2	7	190	170	4	−11	−5	8	24	35	23	3	−1	8	143	139	4	−15	3	8	37	23	18
18	−2	7	86	116	7	−6	2	7	205	214	5	7	−5	8	94	100	9	5	−1	8	255	249	4	−13	3	8	53	50	11
20	−2	7	16	19	15	−4	2	7	156	173	3	9	−5	8	0	17	1	7	−1	8	242	234	4	−11	3	8	57	51	6
−29	−1	7	40	43	15	−2	2	7	215	213	4	11	−5	8	21	39	20	9	−1	8	45	43	8	−9	3	8	89	83	2
−27	−1	7	133	126	7	0	2	7	99	94	4	13	−5	8	0	36	1	11	−1	8	111	104	5	−7	3	8	110	114	2
−25	−1	7	57	47	14	2	2	7	161	150	3	−24	−4	8	0	31	1	13	−1	8	24	34	24	−5	3	8	59	64	4
−23	−1	7	24	15	23	4	2	7	183	178	3	−22	−4	8	105	87	9	15	−1	8	65	47	11	−3	3	8	114	115	3
−21	−1	7	50	48	7	6	2	7	132	130	3	−20	−4	8	74	90	10	17	−1	8	109	104	6	−1	3	8	124	108	2
−19	−1	7	243	229	4	8	2	7	280	253	4	−18	−4	8	58	61	14	19	−1	8	40	52	16	1	3	8	41	38	6
−17	−1	7	83	83	4	10	2	7	82	71	4	−16	−4	8	152	125	8	−28	0	8	0	12	1	3	3	8	109	105	3
−15	−1	7	96	98	4	12	2	7	62	61	6	−14	−4	8	71	68	11	−26	0	8	67	64	7	5	3	8	171	172	2
−13	−1	7	123	135	4	14	2	7	147	122	4	−12	−4	8	97	92	7	−24	0	8	110	124	6	7	3	8	116	112	3
−11	−1	7	154	161	4	16	2	7	85	88	14	−10	−4	8	225	219	6	−22	0	8	15	14	15	9	3	8	46	46	6
−9	−1	7	207	214	9	18	2	7	93	116	12	−8	−4	8	220	223	6	−20	0	8	261	264	6	11	3	8	133	140	10
−7	−1	7	474	467	9	20	2	7	0	19	1	−6	−4	8	76	71	9	−18	0	8	129	135	7	13	3	8	55	63	18
−5	−1	7	438	473	11	−27	3	7	100	92	10	2	−4	8	136	132	8	−16	0	8	30	25	9	15	3	8	67	89	16
−3	−1	7	162	170	3	−25	3	7	132	115	9	4	−4	8	141	129	6	−14	0	8	117	95	4	−24	4	8	0	31	1
−1	−1	7	648	666	10	−23	3	7	84	78	12	6	−4	8	114	116	7	−12	0	8	444	426	8	−22	4	8	98	87	11

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	7	338	339	8	−21	3	7	62	69	16	8	−4	8	205	199	8	−10	0	8	42	55	8	−20	4	8	79	90	12
3	−1	7	325	324	10	−19	3	7	46	59	46	10	−4	8	53	46	19	−8	0	8	321	317	6	−18	4	8	33	60	32
5	−1	7	253	250	5	−17	3	7	251	223	7	12	−4	8	123	105	9	−6	0	8	330	316	5	−16	4	8	153	125	9
7	−1	7	446	432	7	−15	3	7	113	119	6	14	−4	8	24	25	24	−4	0	8	545	598	12	−14	4	8	67	68	8
9	−1	7	357	359	5	−13	3	7	80	88	7	16	−4	8	73	50	10	−2	0	8	7	6	6	−12	4	8	101	91	5
11	−1	7	167	153	6	−11	3	7	108	110	4	−27	−3	8	79	68	6	0	0	8	145	144	8	−10	4	8	220	219	4
13	−1	7	33	27	17	−9	3	7	89	91	2	−25	−3	8	98	82	6	2	0	8	426	432	11	−8	4	8	231	223	4
15	−1	7	78	88	8	−7	3	7	94	89	2	−23	−3	8	7	21	7	4	0	8	193	194	4	−6	4	8	70	70	3
17	−1	7	64	75	10	−5	3	7	182	170	3	−21	−3	8	73	95	11	6	0	8	224	200	3	−4	4	8	136	130	3
19	−1	7	39	46	17	−3	3	7	204	205	3	−19	−3	8	27	13	26	8	0	8	48	58	6	−2	4	8	126	114	4
21	−1	7	0	25	1	−1	3	7	130	115	2	−17	−3	8	111	100	6	10	0	8	23	7	22	0	4	8	83	83	3
−28	0	7	0	12	1	1	3	7	88	82	3	−15	−3	8	0	24	1	12	0	8	125	125	5	2	4	8	139	133	3
−26	0	7	21	36	21	3	3	7	74	70	3	−13	−3	8	36	49	16	14	0	8	80	75	6	4	4	8	141	129	3
−24	0	7	137	155	6	5	3	7	41	44	5	−11	−3	8	59	51	8	16	0	8	0	19	1	6	4	8	108	117	8
−22	0	7	36	49	15	7	3	7	264	242	3	−9	−3	8	90	83	6	18	0	8	64	77	13	8	4	8	196	199	10
−20	0	7	249	257	6	9	3	7	180	184	3	−7	−3	8	101	114	5	20	0	8	0	0	1	10	4	8	21	46	20
−18	0	7	65	51	5	11	3	7	147	144	9	−5	−3	8	56	64	7	−23	1	8	125	127	3	12	4	8	102	105	11
−16	0	7	119	96	3	13	3	7	110	135	10	−3	−3	8	111	114	12	−21	1	8	117	108	3	16	4	8	47	50	16
−14	0	7	183	188	5	15	3	7	29	46	28	−1	−3	8	106	108	4	−19	1	8	90	94	4	−21	5	8	17	33	17
−12	0	7	87	107	4	19	3	7	43	59	22	1	−3	8	46	38	11	−17	1	8	250	242	3	−19	5	8	43	39	16
−10	0	7	669	637	12	−24	4	7	39	35	39	3	−3	8	111	106	6	−15	1	8	101	92	3	−17	5	8	0	30	1
−8	0	7	247	229	4	−22	4	7	32	26	31	5	−3	8	167	173	12	−13	1	8	273	287	4	−15	5	8	81	89	9
−6	0	7	546	524	8	−20	4	7	125	137	9	7	−3	8	126	112	7	−11	1	8	128	135	5	−13	5	8	70	63	9
−4	0	7	481	488	7	−18	4	7	123	128	9	9	−3	8	6	45	5	−9	1	8	736	743	17	−11	5	8	38	34	19
−2	0	7	280	291	4	−16	4	7	22	54	21	11	−3	8	140	139	9	−7	1	8	408	404	11	−9	5	8	91	104	9
0	0	7	230	268	5	−14	4	7	88	86	6	13	−3	8	58	63	15	−5	1	8	585	605	10	−7	5	8	113	95	6
2	0	7	204	214	8	−12	4	7	52	46	8	15	−3	8	73	89	13	−3	1	8	450	459	7	−5	5	8	125	121	5
4	0	7	547	532	10	−10	4	7	0	20	1	17	−3	8	48	56	19	−1	1	8	384	391	6	−3	5	8	96	88	3
6	0	7	149	148	5	−8	4	7	310	323	5	−28	−2	8	68	90	7	1	1	8	573	575	19	−1	5	8	49	49	5
8	0	7	208	209	3	−6	4	7	246	240	5	−26	−2	8	44	47	12	3	1	8	141	138	4	11	5	8	34	39	17
10	0	7	42	42	7	−4	4	7	59	64	4	−24	−2	8	60	61	9	5	1	8	263	248	4	13	5	8	34	36	14
12	0	7	165	166	3	−2	4	7	84	69	3	−22	−2	8	69	78	9	7	1	8	243	234	3	−16	6	8	47	55	14
14	0	7	0	9	1	0	4	7	62	57	4	−20	−2	8	47	44	10	9	1	8	31	42	11	−14	6	8	12	32	11
16	0	7	149	127	10	2	4	7	215	193	3	−18	−2	8	107	99	9	11	1	8	111	104	5	−12	6	8	21	26	20
18	0	7	0	9	1	4	4	7	121	107	4	−16	−2	8	115	101	6	13	1	8	17	34	16	−10	6	8	55	54	8
20	0	7	112	104	6	6	4	7	51	58	10	−14	−2	8	207	200	5	15	1	8	49	46	11	−8	6	8	47	38	13
22	0	7	0	13	1	8	4	7	150	158	7	−12	−2	8	173	160	5	17	1	8	99	104	4	−6	6	8	54	43	4
−23	1	7	4	14	4	10	4	7	123	127	6	−10	−2	8	286	284	6	19	1	8	53	52	7	4	6	8	0	32	1
−21	1	7	47	49	6	12	4	7	75	96	9	−8	−2	8	403	403	12	−28	2	8	34	90	34	6	6	8	57	64	5
−19	1	7	240	229	3	16	4	7	40	48	23	−6	−2	8	241	221	6	−26	2	8	34	47	34	−21	−5	9	0	19	1
−17	1	7	95	82	5	−21	5	7	55	59	17	−4	−2	8	158	166	5	−24	2	8	34	61	34	−19	−5	9	0	35	1
−15	1	7	95	98	3	−19	5	7	22	18	22	−2	−2	8	349	323	9	−22	2	8	67	78	15	−17	−5	9	27	20	26
−13	1	7	113	134	4	−17	5	7	56	79	11	0	−2	8	124	110	5	−20	2	8	62	43	11	−15	−5	9	31	37	31
−11	1	7	146	161	7	−15	5	7	55	43	11	2	−2	8	221	214	5	−18	2	8	113	100	7	−13	−5	9	13	31	13
−9	1	7	212	215	5	−13	5	7	18	39	18	4	−2	8	156	145	9	−16	2	8	117	100	3	−11	−5	9	46	53	16
7	−5	9	33	40	32	11	−1	9	55	41	10	−3	3	9	71	64	3	1	−3	10	225	218	6	−9	1	10	412	408	6
9	−5	9	68	85	11	13	−1	9	107	91	9	−1	3	9	79	75	3	3	−3	10	72	84	9	−7	1	10	232	229	4
11	−5	9	104	106	7	15	−1	9	13	24	13	1	3	9	203	204	3	5	−3	10	100	96	7	−5	1	10	224	223	4
−24	−4	9	9	30	8	17	−1	9	54	49	18	3	3	9	49	45	6	7	−3	10	30	24	29	−3	1	10	289	284	5

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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
−22	−4	9	37	27	27	19	−1	9	0	30	1	5	3	9	90	77	3	9	−3	10	109	90	10	−1	1	10	132	139	3
−20	−4	9	32	26	32	−28	0	9	24	35	23	7	3	9	44	35	7	11	−3	10	133	130	8	1	1	10	328	341	4
−18	−4	9	81	93	10	−26	0	9	49	56	13	9	3	9	166	176	6	13	−3	10	67	68	14	3	1	10	115	104	3
−16	−4	9	88	80	9	−24	0	9	29	39	29	11	3	9	88	107	12	15	−3	10	76	61	11	5	1	10	122	118	3
−14	−4	9	50	33	12	−22	0	9	207	206	5	13	3	9	16	48	16	−28	−2	10	115	97	5	7	1	10	154	136	3
−12	−4	9	246	243	8	−20	0	9	181	170	5	15	3	9	33	19	32	−26	−2	10	119	113	5	9	1	10	181	177	3
−10	−4	9	115	117	6	−18	0	9	44	50	6	−24	4	9	33	30	33	−24	−2	10	58	40	9	11	1	10	33	33	32
−8	−4	9	240	235	6	−16	0	9	98	90	3	−22	4	9	0	27	1	−22	−2	10	42	41	13	13	1	10	136	150	5
−6	−4	9	243	265	9	−14	0	9	100	101	4	−20	4	9	37	26	37	−20	−2	10	234	220	5	15	1	10	14	14	14
2	−4	9	193	182	8	−12	0	9	260	261	5	−18	4	9	95	92	11	−18	−2	10	125	126	6	17	1	10	0	17	1
4	−4	9	67	66	11	−10	0	9	641	625	11	−16	4	9	47	80	24	−16	−2	10	17	41	17	−28	2	10	100	97	11
6	−4	9	154	132	8	−8	0	9	1007	926	17	−14	4	9	24	32	24	−14	−2	10	211	200	7	−26	2	10	116	113	10
8	−4	9	132	141	9	−6	0	9	559	566	10	−12	4	9	242	243	5	−12	−2	10	28	41	25	−24	2	10	43	40	37
10	−4	9	0	9	1	−4	0	9	410	437	13	−10	4	9	130	118	4	−10	−2	10	224	228	5	−22	2	10	46	40	29
12	−4	9	71	50	13	−2	0	9	114	107	7	−8	4	9	240	235	4	−8	−2	10	207	195	4	−20	2	10	234	220	7
14	−4	9	45	51	20	0	0	9	0	13	1	−6	4	9	267	265	5	−6	−2	10	144	132	5	−18	2	10	129	127	5
−27	−3	9	27	5	26	2	0	9	142	138	5	−4	4	9	139	137	3	−4	−2	10	212	201	3	−16	2	10	33	41	11
−25	−3	9	30	51	30	4	0	9	148	158	3	−2	4	9	31	38	11	−2	−2	10	179	174	4	−14	2	10	207	200	3
−23	−3	9	77	83	11	6	0	9	371	334	5	0	4	9	84	79	3	0	−2	10	90	84	4	−12	2	10	37	42	8
−21	−3	9	90	110	9	8	0	9	10	21	9	2	4	9	184	182	3	2	−2	10	116	118	4	−10	2	10	212	228	3
−19	−3	9	47	64	18	10	0	9	40	44	9	4	4	9	77	66	3	4	−2	10	47	59	9	−8	2	10	205	194	3
−17	−3	9	92	83	12	12	0	9	41	59	10	6	4	9	141	132	6	6	−2	10	90	93	8	−6	2	10	144	133	3
−15	−3	9	109	107	11	14	0	9	0	7	1	8	4	9	134	142	9	8	−2	10	150	152	16	−4	2	10	206	200	3
−13	−3	9	74	62	12	16	0	9	57	57	17	10	4	9	26	9	25	10	−2	10	135	119	9	−2	2	10	175	174	2
−11	−3	9	129	133	12	18	0	9	14	19	14	12	4	9	43	50	32	12	−2	10	31	35	30	0	2	10	83	84	3
−9	−3	9	315	304	7	20	0	9	49	57	7	−21	5	9	29	19	28	14	−2	10	42	46	28	2	2	10	130	117	3
−7	−3	9	187	188	5	−25	1	9	103	111	11	−19	5	9	33	35	32	16	−2	10	57	68	17	4	2	10	72	60	5
−5	−3	9	155	156	5	−23	1	9	35	36	11	−17	5	9	12	20	12	−29	−1	10	107	106	5	6	2	10	101	94	5
−3	−3	9	58	65	6	−21	1	9	64	58	5	−15	5	9	47	37	14	−27	−1	10	51	44	16	8	2	10	155	151	5
−1	−3	9	73	74	6	−19	1	9	115	115	5	−13	5	9	37	31	21	−25	−1	10	82	89	9	10	2	10	117	119	8
1	−3	9	200	205	9	−17	1	9	160	150	3	−11	5	9	45	52	14	−23	−1	10	145	135	5	12	2	10	34	35	13
3	−3	9	52	46	11	−15	1	9	128	133	4	−9	5	9	8	12	7	−21	−1	10	74	83	5	14	2	10	37	46	10
5	−3	9	85	77	10	−13	1	9	91	75	4	−7	5	9	145	161	8	−19	−1	10	255	258	5	16	2	10	44	68	29
7	−3	9	52	35	15	−11	1	9	64	67	6	−5	5	9	43	41	10	−17	−1	10	148	137	4	−27	3	10	70	81	14
9	−3	9	157	175	9	−9	1	9	568	580	10	−3	5	9	105	93	3	−15	−1	10	159	160	4	−25	3	10	111	111	10
11	−3	9	100	107	10	−7	1	9	679	679	12	−1	5	9	186	186	3	−13	−1	10	218	209	4	−23	3	10	155	135	9
13	−3	9	37	48	37	−5	1	9	632	620	11	3	5	9	34	25	28	−11	−1	10	268	273	4	−21	3	10	17	43	16
15	−3	9	0	19	1	−3	1	9	291	281	5	11	5	9	84	106	6	−9	−1	10	426	409	6	−19	3	10	85	86	12
17	−3	9	16	16	16	−1	1	9	169	188	4	−16	6	9	51	50	12	−7	−1	10	234	229	5	−17	3	10	112	116	7
−28	−2	9	0	20	1	1	1	9	390	410	6	−14	6	9	44	47	11	−5	−1	10	225	224	6	−15	3	10	126	113	15
−26	−2	9	103	87	6	3	1	9	371	364	4	−12	6	9	41	33	11	−3	−1	10	291	284	7	−13	3	10	191	178	6
−24	−2	9	88	66	13	5	1	9	175	177	3	−10	6	9	35	44	10	−1	−1	10	136	139	5	−11	3	10	329	330	4
−22	−2	9	75	82	7	7	1	9	337	331	4	−8	6	9	33	46	9	1	−1	10	329	341	5	−9	3	10	198	193	3
−20	−2	9	38	33	25	9	1	9	96	107	4	4	6	9	38	49	6	3	−1	10	114	105	6	−7	3	10	221	223	3
−18	−2	9	10	21	9	11	1	9	39	41	13	6	6	9	33	41	7	5	−1	10	119	118	4	−5	3	10	125	118	3
−16	−2	9	86	88	12	13	1	9	94	91	6	−21	−5	10	0	12	1	7	−1	10	158	137	4	−3	3	10	65	50	4
−14	−2	9	134	127	5	15	1	9	38	24	15	−19	−5	10	40	28	21	9	−1	10	171	176	10	−1	3	10	141	146	3
−12	−2	9	167	164	7	17	1	9	48	49	8	−17	−5	10	0	30	1	11	−1	10	25	33	24	1	3	10	221	219	3
−10	−2	9	59	56	7	−28	2	9	16	20	16	−15	−5	10	43	30	19	13	−1	10	158	150	8	3	3	10	82	84	7

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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
−8	−2	9	249	271	4	−26	2	9	110	87	11	−13	−5	10	42	39	20	15	−1	10	19	14	18	5	3	10	102	96	3
−6	−2	9	135	107	14	−24	2	9	56	66	20	−11	−5	10	55	57	13	17	−1	10	0	17	1	7	3	10	0	24	1
−4	−2	9	252	244	6	−22	2	9	86	82	12	7	−5	10	102	101	9	−28	0	10	128	124	6	9	3	10	92	90	4
−2	−2	9	75	75	15	−20	2	9	46	33	17	9	−5	10	59	60	12	−26	0	10	128	123	7	11	3	10	119	130	10
0	−2	9	183	180	4	−18	2	9	23	21	15	−24	−4	10	52	9	14	−24	0	10	29	34	29	13	3	10	40	68	39
2	−2	9	112	110	4	−16	2	9	95	88	3	−22	−4	10	61	55	13	−22	0	10	115	102	10	15	3	10	53	61	20
4	−2	9	123	111	5	−14	2	9	128	127	3	−20	−4	10	117	128	8	−20	0	10	251	255	8	−24	4	10	0	9	1
6	−2	9	65	80	9	−12	2	9	166	164	3	−18	−4	10	39	56	23	−18	0	10	93	80	3	−22	4	10	0	55	1
8	−2	9	188	175	6	−10	2	9	63	56	4	−16	−4	10	109	118	8	−16	0	10	73	74	4	−20	4	10	103	128	10
10	−2	9	44	42	17	−8	2	9	246	271	3	−14	−4	10	6	5	5	−14	0	10	653	620	8	−18	4	10	63	56	16
12	−2	9	143	151	9	−6	2	9	130	107	4	−12	−4	10	154	144	13	−12	0	10	173	181	5	−16	4	10	112	118	10
14	−2	9	58	49	18	−4	2	9	251	243	4	−10	−4	10	204	188	6	−10	0	10	354	302	6	−14	4	10	20	5	19
16	−2	9	40	38	19	−2	2	9	81	76	4	−8	−4	10	351	334	8	−8	0	10	264	271	5	−12	4	10	160	144	5
18	−2	9	12	28	12	0	2	9	182	180	3	−6	−4	10	268	280	9	−6	0	10	444	458	8	−10	4	10	199	187	5
−29	−1	9	41	38	40	2	2	9	114	111	2	2	−4	10	86	95	11	−4	0	10	324	302	6	−8	4	10	357	334	4
−27	−1	9	45	31	15	4	2	9	116	111	3	4	−4	10	106	102	9	−2	0	10	179	183	4	−6	4	10	281	281	3
−25	−1	9	100	111	8	6	2	9	84	80	5	6	−4	10	98	68	10	0	0	10	218	211	3	−4	4	10	108	119	5
−23	−1	9	38	36	14	8	2	9	188	175	3	8	−4	10	70	87	14	2	0	10	117	117	3	−2	4	10	114	111	3
−21	−1	9	60	57	6	10	2	9	23	42	23	10	−4	10	61	58	15	4	0	10	255	243	3	0	4	10	28	37	13
−19	−1	9	114	115	5	12	2	9	154	151	7	12	−4	10	0	22	1	6	0	10	150	160	3	2	4	10	94	94	4
−17	−1	9	162	150	3	14	2	9	65	50	6	−27	−3	10	55	81	9	8	0	10	291	283	4	4	4	10	102	102	3
−15	−1	9	133	133	3	16	2	9	19	38	18	−25	−3	10	110	111	7	10	0	10	72	90	5	6	4	10	85	68	14
−13	−1	9	86	75	4	−27	3	9	0	5	1	−23	−3	10	151	135	8	12	0	10	0	4	1	8	4	10	55	87	12
−11	−1	9	70	66	5	−25	3	9	37	51	36	−21	−3	10	0	43	1	14	0	10	57	42	8	10	4	10	23	59	23
−9	−1	9	590	580	20	−23	3	9	81	84	13	−19	−3	10	77	85	10	16	0	10	21	32	21	12	4	10	0	23	1
−7	−1	9	685	680	15	−21	3	9	78	110	12	−17	−3	10	120	116	9	18	0	10	0	16	1	−21	5	10	16	12	16
−5	−1	9	625	619	25	−19	3	9	79	64	12	−15	−3	10	129	113	11	−25	1	10	84	89	14	−19	5	10	0	28	1
−3	−1	9	286	280	7	−17	3	9	87	83	20	−13	−3	10	189	178	6	−23	1	10	148	135	9	−17	5	10	35	29	34
−1	−1	9	172	190	5	−15	3	9	103	107	8	−11	−3	10	315	330	7	−21	1	10	78	83	6	−15	5	10	48	30	14
1	−1	9	380	410	9	−13	3	9	72	62	10	−9	−3	10	195	192	5	−19	1	10	250	258	4	−13	5	10	49	39	13
3	−1	9	364	363	5	−11	3	9	122	133	2	−7	−3	10	220	223	5	−17	1	10	144	137	3	−11	5	10	73	58	8
5	−1	9	175	177	5	−9	3	9	313	303	3	−5	−3	10	113	119	5	−15	1	10	162	160	4	−9	5	10	76	81	10
7	−1	9	334	331	7	−7	3	9	195	188	3	−3	−3	10	56	50	6	−13	1	10	217	209	3	−7	5	10	93	111	15
9	−1	9	101	106	5	−5	3	9	159	156	3	−1	−3	10	133	146	5	−11	1	10	264	274	4	−5	5	10	81	92	5
−3	5	10	207	207	3	−1	−1	11	191	208	4	−9	3	11	32	36	9	−24	−2	12	0	19	1	−28	2	12	0	23	1
−1	5	10	80	78	5	1	−11	1	104	100	4	−7	3	11	70	67	4	−22	−2	12	126	119	17	−26	2	12	12	2	11
1	5	10	47	68	12	3	−1	11	135	138	4	−5	3	11	34	35	9	−20	−2	12	118	135	5	−24	2	12	50	19	24
3	5	10	59	75	12	5	−1	11	122	118	4	−3	3	11	163	159	4	−18	−2	12	231	223	8	−22	2	12	118	119	10
−14	6	10	19	13	19	7	−1	11	74	74	8	−1	3	11	62	61	5	−16	−2	12	166	161	6	−20	2	12	130	135	10
−12	6	10	38	40	11	9	−1	11	73	82	9	1	3	11	92	96	4	−14	−2	12	29	30	29	−18	2	12	225	223	4
−10	6	10	37	35	9	11	−1	11	97	104	7	3	3	11	71	71	5	−12	−2	12	19	28	19	−16	2	12	164	161	4
−8	6	10	28	34	10	13	−1	11	25	16	24	5	3	11	51	50	8	−10	−2	12	55	68	13	−14	2	12	10	30	9
−19	−5	11	0	41	1	15	−1	11	28	49	27	7	3	11	92	92	4	−8	−2	12	0	10	1	−12	2	12	27	28	25
−17	−5	11	32	28	32	17	−1	11	23	4	23	9	3	11	70	64	7	−6	−2	12	71	67	5	−10	2	12	62	67	7
−15	−5	11	45	52	17	−28	0	11	135	125	10	11	3	11	91	103	12	−4	−2	12	199	197	4	−8	2	12	17	9	16
−13	−5	11	0	22	1	−26	0	11	30	26	30	13	3	11	53	60	18	−2	−2	12	119	109	4	−6	2	12	67	68	4
−11	−5	11	41	36	20	−24	0	11	32	6	25	−24	4	11	41	57	31	0	−2	12	59	58	7	−4	2	12	196	197	3
−24	−4	11	63	57	11	−22	0	11	192	174	7	−22	4	11	25	64	25	2	−2	12	109	121	5	−2	2	12	117	110	3
−22	−4	11	53	64	15	−20	0	11	211	206	5	−20	4	11	89	73	12	4	−2	12	83	76	7	0	2	12	64	59	4

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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
−20	−4	11	71	73	11	−18	0	11	0	5	1	−18	4	11	38	36	37	6	−2	12	162	159	8	2	2	12	122	122	5
−18	−4	11	59	37	13	−16	0	11	355	335	4	−16	4	11	12	12	12	8	−2	12	50	60	17	4	2	12	78	75	5
−16	−4	11	0	12	1	−14	0	11	128	119	3	−14	4	11	158	130	6	10	−2	12	73	78	12	6	2	12	147	160	6
−14	−4	11	130	131	8	−12	0	11	328	331	4	−12	4	11	379	361	8	12	−2	12	0	37	1	8	2	12	54	60	9
−12	−4	11	370	362	11	−10	0	11	408	371	5	−10	4	11	247	228	4	14	−2	12	22	39	21	10	2	12	71	78	6
−10	−4	11	241	227	8	−8	0	11	246	232	4	−8	4	11	39	33	7	−29	−1	12	31	37	25	12	2	12	46	38	8
−8	−4	11	45	34	29	−6	0	11	214	203	3	−6	4	11	31	17	11	−27	−1	12	84	63	9	14	2	12	26	39	26
−6	−4	11	0	17	1	−4	0	11	103	98	3	−4	4	11	151	150	4	−25	−1	12	41	42	12	−25	3	12	22	14	22
2	−4	11	197	185	8	−2	0	11	139	153	4	−2	4	11	155	159	4	−23	−1	12	91	75	6	−23	3	12	53	60	20
4	−4	11	127	121	9	0	0	11	120	99	5	0	4	11	127	116	6	−21	−1	12	224	212	5	−21	3	12	112	149	9
6	−4	11	26	27	25	2	0	11	261	259	4	2	4	11	189	186	3	−19	−1	12	145	145	6	−19	3	12	91	130	11
8	−4	11	72	68	13	4	0	11	207	203	3	4	4	11	110	120	3	−17	−1	12	102	106	9	−17	3	12	153	174	9
10	−4	11	44	54	24	6	0	11	61	64	6	6	4	11	36	26	33	−15	−1	12	272	254	5	−15	3	12	106	82	10
12	−4	11	0	65	1	8	0	11	89	95	4	8	4	11	61	68	10	−13	−1	12	141	137	3	−13	3	12	83	82	4
−27	−3	11	73	75	6	10	0	11	71	83	7	10	4	11	21	54	20	−11	−1	12	111	98	5	−11	3	12	100	96	4
−25	−3	11	46	34	11	12	0	11	0	28	1	−19	5	11	56	41	10	−9	−1	12	146	143	4	−9	3	12	175	183	3
−23	−3	11	48	28	17	14	0	11	15	10	15	−17	5	11	42	27	13	−7	−1	12	246	238	4	−7	3	12	41	51	8
−21	−3	11	53	42	13	16	0	11	42	29	26	−15	5	11	23	52	23	−5	−1	12	114	96	8	−5	3	12	67	58	5
−19	−3	11	121	123	8	−25	1	11	0	35	1	−13	5	11	0	23	1	−3	−1	12	204	217	4	−3	3	12	65	58	4
−17	−3	11	235	248	8	−23	1	11	62	69	7	−11	5	11	52	36	10	−1	−1	12	306	303	5	−1	3	12	101	101	4
−15	−3	11	246	234	6	−21	1	11	86	74	5	−9	5	11	140	118	7	1	−1	12	78	68	8	1	3	12	94	86	5
−13	−3	11	127	134	7	−19	1	11	376	361	6	−7	5	11	105	120	8	3	−1	12	108	99	6	3	3	12	211	209	6
−11	−3	11	170	161	5	−17	1	11	142	126	5	−5	5	11	67	71	8	5	−1	12	195	204	4	5	3	12	42	52	10
−9	−3	11	49	35	10	−15	1	11	192	183	3	−3	5	11	65	55	4	7	−1	12	143	140	5	7	3	12	121	116	4
−7	−3	11	70	67	8	−13	1	11	233	221	3	−1	5	11	60	57	4	9	−1	12	67	58	9	9	3	12	138	131	9
−5	−3	11	0	35	1	−11	1	11	367	356	4	1	5	11	111	120	7	11	−1	12	32	27	32	11	3	12	32	62	32
−3	−3	11	153	159	4	−9	1	11	223	236	4	3	5	11	25	52	24	13	−1	12	28	47	27	13	3	12	25	42	25
−1	−3	11	57	61	9	−7	1	11	87	91	5	−14	6	11	43	46	9	15	−1	12	10	10	10	−24	4	12	50	45	18
1	−3	11	94	96	7	−5	1	11	539	532	6	−12	6	11	45	48	8	−28	0	12	0	23	1	−22	4	12	0	29	1
3	−3	11	73	70	9	−3	1	11	165	172	3	−10	6	11	39	33	7	−26	0	12	11	36	10	−20	4	12	82	63	12
5	−3	11	70	49	13	−1	1	11	188	208	3	−8	6	11	31	22	7	−24	0	12	24	33	23	−18	4	12	114	112	10
7	−3	11	100	91	11	1	1	11	95	100	4	−19	−5	12	0	27	1	−22	0	12	0	4	1	−16	4	12	159	135	8
9	−3	11	60	64	16	3	1	11	147	138	3	−17	−5	12	42	48	19	−20	0	12	199	187	4	−14	4	12	168	153	6
11	−3	11	118	103	9	5	1	11	127	118	5	−15	−5	12	0	20	1	−18	0	12	391	374	5	−12	4	12	69	72	9
13	−3	11	53	60	17	7	1	11	73	75	5	−13	−5	12	67	78	11	−16	0	12	181	180	3	−10	4	12	125	139	9
−28	−2	11	0	23	1	9	1	11	59	82	9	−24	−4	12	53	45	13	−14	0	12	140	130	3	−8	4	12	0	23	1
−26	−2	11	46	50	12	11	1	11	103	104	18	−22	−4	12	7	29	7	−12	0	12	0	13	1	−6	4	12	92	91	4
−24	−2	11	64	66	8	13	1	11	0	16	1	−20	−4	12	70	62	11	−10	0	12	534	518	6	−4	4	12	115	128	5
−22	−2	11	73	81	18	15	1	11	39	49	27	−18	−4	12	133	112	8	−8	0	12	290	275	4	−2	4	12	111	122	6
−20	−2	11	202	218	11	17	1	11	0	4	1	−16	−4	12	154	135	8	−6	0	12	80	77	4	0	4	12	107	112	7
−18	−2	11	0	32	1	−28	2	11	40	22	39	−14	−4	12	152	153	8	−4	0	12	366	356	5	2	4	12	66	65	6
−16	−2	11	136	132	10	−26	2	11	30	50	29	−12	−4	12	54	71	15	−2	0	12	26	28	22	4	4	12	126	131	6
−14	−2	11	60	61	9	−24	2	11	84	66	13	−10	−4	12	119	139	8	0	0	12	289	286	5	6	4	12	38	17	19
−12	−2	11	146	142	6	−22	2	11	83	81	13	−8	−4	12	0	23	1	2	0	12	433	429	7	8	4	12	64	93	9
−10	−2	11	324	320	7	−20	2	11	213	218	9	−6	−4	12	109	91	8	4	0	12	41	44	10	10	4	12	36	43	35
−8	−2	11	56	66	7	−18	2	11	9	32	8	2	−4	12	52	65	19	6	0	12	0	9	1	−19	5	12	47	27	10
−6	−2	11	127	125	3	−16	2	11	138	131	4	4	−4	12	131	131	8	8	0	12	77	67	7	−17	5	12	24	48	23
−4	−2	11	87	84	4	−14	2	11	62	61	6	6	−4	12	0	17	1	10	0	12	140	128	6	−15	5	12	26	20	26
−2	−2	11	0	13	1	−12	2	11	146	142	4	8	−4	12	92	93	10	12	0	12	15	21	14	−13	5	12	88	78	6

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	11	101	99	4	−10	2	11	309	321	4	10	−4	12	51	43	16	14	0	12	25	11	25	−11	5	12	36	30	27
2	−2	11	154	162	7	−8	2	11	51	65	10	−25	−3	12	0	14	1	16	0	12	37	60	18	−9	5	12	70	82	9
4	−2	11	160	154	5	−6	2	11	129	125	2	−23	−3	12	60	60	13	−25	1	12	38	42	38	−7	5	12	40	27	12
6	−2	11	160	151	8	−4	2	11	86	84	3	−21	−3	12	116	149	7	−23	1	12	80	75	6	−5	5	12	90	74	13
8	−2	11	119	108	9	−2	2	11	12	14	11	−19	−3	12	93	130	8	−21	1	12	219	212	8	−3	5	12	28	24	12
10	−2	11	26	45	25	0	2	11	97	100	3	−17	−3	12	157	174	7	−19	1	12	163	145	5	−1	5	12	108	110	9
12	−2	11	29	38	29	2	2	11	159	162	5	−15	−3	12	81	82	10	−17	1	12	111	106	4	−10	6	12	58	61	4
14	−2	11	68	57	13	4	2	11	162	154	3	−13	−3	12	68	82	33	−15	1	12	270	254	5	−17	−5	13	28	26	27
16	−2	11	35	24	18	6	2	11	155	151	6	−11	−3	12	93	97	18	−13	1	12	137	137	3	−15	−5	13	84	113	8
−29	−1	11	34	31	20	8	2	11	101	107	6	−9	−3	12	182	183	5	−11	1	12	114	98	4	−13	−5	13	43	50	16
−27	−1	11	44	46	19	10	2	11	40	45	13	−7	−3	12	42	51	14	−9	1	12	147	144	3	−22	−4	13	32	21	32
−25	−1	11	33	35	18	12	2	11	44	38	9	−5	−3	12	78	58	10	−7	1	12	235	237	3	−20	−4	13	43	46	19
−23	−1	11	55	69	9	14	2	11	57	57	18	−3	−3	12	52	57	13	−5	1	12	108	95	4	−18	−4	13	4	34	3
−21	−1	11	95	73	5	16	2	11	0	24	1	−1	−3	12	96	101	6	−3	1	12	209	216	3	−16	−4	13	71	62	11
−19	−1	11	382	362	8	−27	3	11	88	75	10	1	−3	12	115	86	10	−1	1	12	311	303	4	−14	−4	13	69	79	11
−17	−1	11	133	126	5	−25	3	11	66	34	16	3	−3	12	230	209	8	1	1	12	81	68	4	−12	−4	13	63	66	13
−15	−1	11	195	183	4	−23	3	11	0	28	1	5	−3	12	46	51	28	3	1	12	102	100	5	−10	−4	13	154	151	8
−13	−1	11	223	221	4	−21	3	11	29	42	28	7	−3	12	142	116	8	5	1	12	203	204	4	−8	−4	13	54	33	14
−11	−1	11	364	358	5	−19	3	11	123	123	9	9	−3	12	149	131	8	7	1	12	150	141	5	−6	−4	13	70	69	11
−9	−1	11	227	235	3	−17	3	11	244	248	9	11	−3	12	66	62	13	9	1	12	56	58	12	2	−4	13	140	135	8
−7	−1	11	86	90	4	−15	3	11	245	235	7	13	−3	12	11	42	11	11	1	12	30	27	30	4	−4	13	72	61	12
−5	−1	11	538	532	8	−13	3	11	139	133	4	−28	−2	12	3	23	3	13	1	12	27	47	27	6	−4	13	30	10	29
−3	−1	11	169	171	3	−11	3	11	164	161	3	−26	−2	12	24	2	24	15	1	12	0	10	1	8	−4	13	0	17	1
−25	−3	13	0	29	1	−19	1	13	302	281	5	−18	−4	14	72	68	10	−25	1	14	51	55	24	2	−4	15	71	76	11
−23	−3	13	46	52	17	−17	1	13	231	218	4	−16	−4	14	110	89	8	−23	1	14	91	88	7	4	−4	15	60	22	13
−21	−3	13	26	27	26	−15	1	13	175	166	4	−14	−4	14	40	52	23	−21	1	14	99	111	7	−23	−3	15	76	77	9
−19	−3	13	0	26	1	−13	1	13	61	54	5	−12	−4	14	128	120	8	−19	1	14	101	98	6	−21	−3	15	0	24	1
−17	−3	13	90	125	8	−11	1	13	144	149	6	−10	−4	14	40	38	25	−17	1	14	101	98	5	−19	−3	15	104	81	8
−15	−3	13	67	65	11	−9	1	13	116	115	3	−8	−4	14	101	96	9	−15	1	14	345	321	6	−17	−3	15	64	57	11
−13	−3	13	145	129	8	−7	1	13	73	63	5	−6	−4	14	21	48	21	−13	1	14	311	293	4	−15	−3	15	47	33	16
−11	−3	13	75	80	8	−5	1	13	253	244	3	2	−4	14	64	63	13	−11	1	14	96	89	5	−13	−3	15	158	138	7
−9	−3	13	0	19	1	−3	1	13	186	186	4	4	−4	14	38	31	32	−9	1	14	74	61	5	−11	−3	15	78	69	11
−7	−3	13	66	80	9	−1	1	13	28	31	16	6	−4	14	21	25	20	−7	1	14	89	92	4	−9	−3	15	65	53	14
−5	−3	13	51	43	10	1	1	13	230	220	3	−25	−3	14	29	24	29	−5	1	14	165	143	3	−7	−3	15	64	83	14
−3	−3	13	153	159	5	3	1	13	83	69	5	−23	−3	14	59	50	12	−3	1	14	160	164	8	−5	−3	15	94	100	7
−1	−3	13	101	109	6	5	1	13	220	212	7	−21	−3	14	38	45	24	−1	1	14	306	301	4	−3	−3	15	156	155	8
1	−3	13	54	31	17	7	1	13	152	152	5	−19	−3	14	57	65	12	1	1	14	367	351	5	−1	−3	15	58	65	16
3	−3	13	83	57	11	9	1	13	31	24	21	−17	−3	14	72	91	9	3	1	14	137	130	5	1	−3	15	139	141	8
5	−3	13	129	134	9	11	1	13	51	63	13	−15	−3	14	74	87	10	5	1	14	72	77	7	3	−3	15	76	60	13
7	−3	13	108	114	10	13	1	13	59	55	9	−13	−3	14	149	132	8	7	1	14	140	124	5	5	−3	15	19	15	18
9	−3	13	45	67	22	−28	2	13	0	27	1	−11	−3	14	29	27	29	9	1	14	14	31	14	7	−3	15	46	34	19
11	−3	13	44	42	20	−26	2	13	92	72	11	−9	−3	14	0	27	1	11	1	14	93	94	5	−26	−2	15	50	55	9
−28	−2	13	28	27	28	−24	2	13	57	82	18	−7	−3	14	122	116	8	−26	2	14	0	24	1	−24	−2	15	57	82	9
−26	−2	13	84	72	6	−22	2	13	50	68	22	−5	−3	14	131	128	5	−24	2	14	28	36	28	−22	−2	15	75	84	8
−24	−2	13	55	82	9	−20	2	13	169	184	5	−3	−3	14	50	38	12	−22	2	14	90	80	11	−20	−2	15	190	185	8
−22	−2	13	49	68	11	−18	2	13	62	55	7	−1	−3	14	188	163	8	−20	2	14	160	160	4	−18	−2	15	118	134	8
−20	−2	13	179	184	7	−15	2	13	38	45	12	1	−3	14	220	205	8	−18	2	14	101	94	5	−16	−2	15	80	87	9
−18	−2	13	64	54	12	−14	2	13	185	189	4	3	−3	14	195	186	7	−16	2	14	192	186	5	−14	−2	15	80	61	10
−16	−2	13	51	45	12	−12	2	13	137	126	4	5	−3	14	78	81	12	−14	2	14	112	109	4	−12	−2	15	13	51	12

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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
−14	−2	13	194	189	18	−10	2	13	50	50	9	7	−3	14	36	38	35	−12	2	14	101	89	5	−10	−2	15	282	245	6
−12	−2	13	144	126	6	−8	2	13	103	103	5	9	−3	14	53	39	16	−10	2	14	29	39	28	−8	−2	15	128	121	11
−10	−2	13	51	50	11	−6	2	13	120	119	4	−26	−2	14	0	24	1	−8	2	14	154	147	3	−6	−2	15	163	153	5
−8	−2	13	109	102	5	−4	2	13	141	135	3	−24	−2	14	43	36	12	−6	2	14	134	135	5	−4	−2	15	113	99	7
−6	−2	13	114	118	6	−2	2	13	137	146	4	−22	−2	14	96	80	12	−4	2	14	68	77	4	−2	−2	15	80	75	8
−4	−2	13	136	134	4	0	2	13	223	219	4	−20	−2	14	173	160	7	−2	2	14	235	228	3	0	−2	15	237	237	6
−2	−2	13	130	146	7	2	2	13	117	108	5	−18	−2	14	107	94	8	0	2	14	110	113	6	2	−2	15	21	34	21
0	−2	13	215	219	4	4	2	13	86	93	6	−14	−2	14	118	109	18	2	2	14	85	87	6	4	−2	15	0	43	1
2	−2	13	120	108	5	6	2	13	64	80	9	−12	−2	14	104	90	7	4	2	14	100	95	5	6	−2	15	55	35	15
4	−2	13	88	93	7	8	2	13	116	124	9	−10	−2	14	44	39	16	6	2	14	90	84	20	8	−2	15	33	30	32
6	−2	13	70	80	12	10	2	13	69	73	6	−8	−2	14	150	147	4	8	2	14	64	66	8	−27	−1	15	41	40	22
8	−2	13	99	125	10	12	2	13	28	24	13	−6	−2	14	131	136	5	10	2	14	69	77	5	−25	−1	15	38	40	14
10	−2	13	50	73	20	−25	3	13	35	29	34	−4	−2	14	78	77	6	−25	3	14	44	24	20	−23	−1	15	27	26	27
12	−2	13	19	24	18	−23	3	13	42	52	29	−2	−2	14	236	228	4	−23	3	14	48	50	19	−21	−1	15	47	40	11
−29	−1	13	70	55	9	−21	3	13	0	27	1	0	−2	14	125	113	6	−21	3	14	46	45	20	−19	−1	15	81	95	7
−27	−1	13	8	35	8	−19	3	13	29	25	28	2	−2	14	97	87	7	−19	3	14	67	66	12	−17	−1	15	272	248	6
−25	−1	13	24	36	23	−17	3	13	103	125	9	4	−2	14	83	95	7	−17	3	14	85	91	10	−15	−1	15	55	47	9
−23	−1	13	65	64	7	−15	3	13	66	65	15	6	−2	14	56	84	14	−15	3	14	81	87	7	−13	−1	15	150	151	9
−21	−1	13	72	70	7	−13	3	13	136	130	6	8	−2	14	59	66	15	−13	3	14	148	132	10	−11	−1	15	6	40	6
−19	−1	13	312	281	6	−11	3	13	87	80	4	10	−2	14	92	77	9	−11	3	14	33	27	15	−9	−1	15	30	21	19
−17	−1	13	234	218	4	−9	3	13	24	20	23	−27	−1	14	26	25	26	−9	3	14	0	28	1	−7	−1	15	98	105	11
−15	−1	13	173	166	4	−7	3	13	70	81	5	−25	−1	14	63	55	8	−7	3	14	117	116	4	−5	−1	15	267	248	5
−13	−1	13	67	54	6	−5	3	13	47	43	7	−23	−1	14	96	88	6	−5	3	14	118	128	4	−3	−1	15	193	194	6
−11	−1	13	144	149	4	−3	3	13	157	158	3	−21	−1	14	77	111	10	−3	3	14	30	38	16	−1	−1	15	307	295	7
−9	−1	13	116	116	4	−1	3	13	108	110	9	−19	−1	14	91	98	6	−1	3	14	176	163	5	1	−1	15	69	60	9
−7	−1	13	66	63	6	1	3	13	41	32	16	−17	−1	14	107	99	5	1	3	14	211	205	6	3	−1	15	147	150	6
−5	−1	13	255	244	4	3	3	13	64	58	6	−15	−1	14	351	321	5	3	3	14	177	186	4	5	−1	15	74	84	9
−3	−1	13	185	186	4	5	3	13	125	134	12	−13	−1	14	311	294	6	5	3	14	68	81	6	7	−1	15	40	28	17
−1	−1	13	0	31	1	7	3	13	120	115	7	−11	−1	14	92	90	8	7	3	14	23	37	23	9	−1	15	25	54	25
1	−1	13	230	220	4	9	3	13	51	67	20	−9	−1	14	69	60	6	9	3	14	27	39	27	−28	0	15	0	3	1
3	−1	13	92	69	6	11	3	13	42	41	24	−7	−1	14	84	92	5	−22	4	14	34	11	34	−26	0	15	82	64	7
5	−1	13	216	211	7	−22	4	13	38	21	25	−5	−1	14	152	142	7	−20	4	14	37	56	28	−24	0	15	52	41	13
7	−1	13	148	152	6	−20	4	13	18	46	17	−3	−1	14	155	165	9	−18	4	14	69	68	12	−22	0	15	34	1	33
9	−1	13	36	24	21	−18	4	13	0	33	1	−1	−1	14	311	302	6	−16	4	14	83	90	12	−20	0	15	38	25	14
11	−1	13	65	64	9	−16	4	13	67	61	18	1	−1	14	358	351	6	−14	4	14	62	53	9	−18	0	15	93	72	5
13	−1	13	56	55	9	−14	4	13	86	79	7	3	−1	14	128	130	11	−12	4	14	132	119	8	−16	0	15	35	3	13
−28	0	13	25	12	24	−12	4	13	39	66	35	5	−1	14	61	77	10	−10	4	14	47	37	6	−14	0	15	191	183	9
−26	0	13	0	0	1	−10	4	13	168	151	8	7	−1	14	146	124	7	−8	4	14	112	96	3	−12	0	15	0	7	1
−24	0	13	32	42	31	−8	4	13	36	34	14	9	−1	14	12	31	12	−6	4	14	38	48	12	−10	0	15	98	104	4
−22	0	13	53	42	16	−6	4	13	68	70	6	11	−1	14	106	94	11	−4	4	14	71	79	6	−8	0	15	86	89	6
−20	0	13	138	145	8	−4	4	13	30	43	21	−28	0	14	4	3	3	−2	4	14	210	217	6	−6	0	15	181	177	4
−18	0	13	184	169	3	−2	4	13	52	53	7	−26	0	14	65	42	9	0	4	14	37	38	10	−4	0	15	159	160	7
−16	0	13	301	255	4	0	4	13	69	67	9	−24	0	14	38	2	18	2	4	14	58	63	5	−2	0	15	105	110	8
−14	0	13	0	22	1	2	4	13	139	135	8	−22	0	14	42	43	23	4	4	14	33	31	27	2	0	15	76	73	9
−12	0	13	94	85	4	4	4	13	59	61	10	−20	0	14	198	198	4	6	4	14	23	24	23	4	0	15	108	96	6
−10	0	13	53	37	6	6	4	13	20	9	19	−18	0	14	22	2	22	−17	5	14	43	69	10	6	0	15	10	13	9
−8	0	13	231	213	4	8	4	13	0	17	1	−16	0	14	86	79	4	−15	5	14	28	54	28	8	0	15	45	29	10
−6	0	13	97	98	4	−17	5	13	28	26	27	−14	0	14	190	166	3	−13	5	14	74	62	5	10	0	15	36	11	13
−4	0	13	38	38	10	−15	5	13	88	114	6	−12	0	14	72	75	5	−11	5	14	25	16	24	−25	1	15	25	40	25

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	0	13	221	221	4	−13	5	13	41	50	13	−10	0	14	0	18	1	−9	5	14	70	66	6	−23	1	15	23	27	23
0	0	13	407	423	7	−11	5	13	72	71	9	−8	0	14	469	448	10	−7	5	14	77	71	5	−21	1	15	36	40	16
2	0	13	46	55	11	−9	5	13	76	71	6	−6	0	14	45	36	9	−5	5	14	16	23	15	−19	1	15	97	95	9
4	0	13	248	258	4	−7	5	13	26	27	26	−4	0	14	292	275	5	−1	5	14	52	35	13	−17	1	15	275	248	6
6	0	13	337	340	6	−5	5	13	79	78	5	−2	0	14	191	196	4	1	5	14	50	46	16	−15	1	15	40	47	12
8	0	13	114	109	8	−3	5	13	53	50	6	0	0	14	248	239	4	−20	−4	15	30	16	30	−13	1	15	155	152	4
10	0	13	37	59	14	−1	5	13	30	48	30	2	0	14	98	106	5	−18	−4	15	77	74	9	−11	1	15	41	39	12
12	0	13	21	12	21	−17	−5	14	54	69	11	4	0	14	420	408	7	−16	−4	15	73	66	10	−9	1	15	0	21	1
14	0	13	73	60	11	−15	−5	14	43	54	16	6	0	14	99	75	6	−14	−4	15	0	34	1	−7	1	15	106	104	7
−25	1	13	23	35	22	−13	−5	14	75	63	9	8	0	14	0	12	1	−12	−4	15	60	49	14	−5	1	15	269	247	4
−23	1	13	63	65	9	−22	−4	14	0	11	1	10	0	14	95	96	11	−10	−4	15	59	51	14	−3	1	15	193	194	4
−21	1	13	89	70	10	−20	−4	14	35	57	28	12	0	14	16	13	15	−8	−4	15	27	65	26	−1	1	15	296	295	7
1	1	15	54	60	9	−6	−2	16	165	158	6	−1	3	16	84	67	16	−7	1	17	0	17	1	−6	0	18	61	44	9
3	1	15	150	150	29	−4	−2	16	107	104	6	1	3	16	28	15	19	−5	1	17	121	105	10	−4	0	18	47	64	13
5	1	15	90	84	7	−2	−2	16	37	43	21	3	3	16	38	52	10	−3	1	17	126	111	12	−2	0	18	118	107	6
7	1	15	16	29	15	0	−2	16	73	78	10	5	3	16	24	16	13	−1	1	17	15	23	14	0	0	18	41	30	17
9	1	15	50	54	12	2	−2	16	49	40	12	−18	4	16	28	53	27	1	1	17	56	64	8	2	0	18	0	5	1
−26	2	15	49	55	19	4	−2	16	0	22	1	−16	4	16	30	29	25	3	1	17	20	12	20	4	0	18	84	79	8
−24	2	15	78	82	11	6	−2	16	35	22	34	−14	4	16	18	31	18	5	1	17	8	15	8	−23	1	18	79	67	11
−22	2	15	85	84	11	−27	−1	16	39	14	27	−12	4	16	50	42	10	−24	2	17	46	47	19	−21	1	18	43	40	12
−20	2	15	188	185	5	−25	−1	16	38	31	38	−10	4	16	73	94	7	−22	2	17	54	65	15	−19	1	18	52	37	10
−18	2	15	119	134	5	−23	−1	16	26	27	26	−8	4	16	131	121	7	−20	2	17	0	4	1	−17	1	18	0	14	1
−16	2	15	77	87	7	−21	−1	16	190	161	5	−6	4	16	61	62	6	−18	2	17	74	81	7	−15	1	18	34	35	34
−14	2	15	70	60	7	−19	−1	16	70	95	8	−4	4	16	34	38	13	−16	2	17	38	39	13	−13	1	18	144	153	6
−12	2	15	49	51	13	−17	−1	16	90	84	17	−2	4	16	56	57	6	−14	2	17	40	39	13	−11	1	18	101	93	7
−10	2	15	277	245	5	−15	−1	16	59	48	10	0	4	16	24	40	14	−12	2	17	122	145	6	−9	1	18	33	28	17
−8	2	15	132	121	8	−13	−1	16	69	86	9	−16	−4	17	26	49	25	−10	2	17	30	30	30	−7	1	18	68	60	7
−6	2	15	162	154	4	−11	−1	16	60	52	10	−14	−4	17	5	33	4	−8	2	17	121	113	6	−5	1	18	108	94	11
−4	2	15	101	98	5	−9	−1	16	175	177	6	−12	−4	17	75	67	10	−6	2	17	51	58	8	−3	1	18	28	9	27
−2	2	15	70	75	6	−7	−1	16	207	207	8	−10	−4	17	40	17	22	−4	2	17	61	67	7	−1	1	18	43	36	11
0	2	15	240	237	9	−5	−1	16	167	168	6	−21	−3	17	0	7	1	−2	2	17	0	7	1	1	1	18	66	71	7
2	2	15	33	33	17	−3	−1	16	25	47	25	−19	−3	17	21	29	20	0	2	17	14	29	13	3	1	18	32	38	15
4	2	15	30	43	29	−1	−1	16	127	123	16	−17	−3	17	19	34	19	2	2	17	31	28	19	−22	2	18	25	17	24
6	2	15	47	35	11	1	−1	16	25	31	25	−15	−3	17	13	36	13	4	2	17	28	39	28	−20	2	18	0	25	1
8	2	15	17	30	17	3	−1	16	0	38	1	−13	−3	17	51	49	18	−21	3	17	0	7	1	−18	2	18	0	14	1
−23	3	15	66	77	12	5	−1	16	72	65	9	−11	−3	17	47	31	22	−19	3	17	0	30	1	−16	2	18	89	97	6
−21	3	15	43	24	20	7	−1	16	31	18	31	−9	−3	17	0	28	1	−17	3	17	44	34	18	−14	2	18	32	48	26
−19	3	15	89	81	10	−26	0	16	25	20	25	−7	−3	17	65	82	13	−15	3	17	48	36	9	−12	2	18	61	45	15
−17	3	15	39	57	24	−24	0	16	17	5	17	−5	−3	17	37	47	36	−13	3	17	47	49	10	−10	2	18	115	108	5
−15	3	15	38	33	10	−22	0	16	52	14	18	−3	−3	17	0	43	1	−11	3	17	39	31	11	−8	2	18	59	77	8
−13	3	15	142	137	10	−20	0	16	80	75	6	−1	−3	17	0	17	1	−9	3	17	0	28	1	−6	2	18	37	38	12
−11	3	15	61	69	10	−18	0	16	23	3	22	1	−3	17	39	27	34	−7	3	17	69	82	8	−4	2	18	45	51	9
−9	3	15	64	54	7	−16	0	16	52	62	19	−24	−2	17	30	47	30	−5	3	17	48	48	8	−2	2	18	48	64	8
−7	3	15	73	83	8	−14	0	16	70	90	7	−22	−2	17	40	64	13	−3	3	17	34	43	12	0	2	18	36	28	13
−5	3	15	93	101	4	−12	0	16	0	8	1	−20	−2	17	26	4	25	−1	3	17	31	17	18	2	2	18	26	10	25
−3	3	15	147	155	8	−10	0	16	25	22	25	−18	−2	17	60	81	13	1	3	17	25	27	24	−19	3	18	39	35	20
−1	3	15	75	65	6	−8	0	16	151	137	6	−16	−2	17	18	39	18	−16	4	17	42	49	11	−17	3	18	0	1	1
1	3	15	144	141	4	−6	0	16	234	249	6	−14	−2	17	43	39	20	−14	4	17	49	33	13	−15	3	18	23	6	22
3	3	15	64	60	6	−4	0	16	77	81	8	−12	−2	17	151	145	8	−12	4	17	76	66	20	−13	3	18	19	26	19

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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	3	15	12	15	12	−2	0	16	328	334	7	−10	−2	17	31	30	31	−10	4	17	28	17	27	−11	3	18	93	99	4
7	3	15	28	34	28	0	0	16	174	168	6	−8	−2	17	132	113	8	−8	4	17	28	29	15	−9	3	18	0	16	1
−20	4	15	17	16	16	2	0	16	87	87	10	−6	−2	17	62	58	10	−6	4	17	0	11	1	−7	3	18	55	54	7
−18	4	15	85	74	10	4	0	16	54	66	9	−4	−2	17	59	67	36	−4	4	17	79	78	4	−5	3	18	16	30	16
−16	4	15	65	65	13	6	0	16	15	8	15	−2	−2	17	0	7	1	−19	−3	18	56	35	13	−3	3	18	63	49	6
−14	4	15	31	34	28	8	0	16	162	143	9	0	−2	17	19	29	19	−17	−3	18	23	1	23	−1	3	18	22	27	22
−12	4	15	51	49	28	−25	1	16	34	31	33	2	−2	17	24	29	24	−15	−3	18	32	7	32	−15	−3	19	30	25	30
−10	4	15	62	51	9	−23	1	16	34	27	17	4	−2	17	43	39	23	−13	−3	18	38	27	38	−13	−3	19	53	42	16
−8	4	15	65	65	5	−21	1	16	170	162	12	−25	−1	17	0	17	1	−11	−3	18	70	99	12	−11	−3	19	0	17	1
−6	4	15	85	89	5	−19	1	16	96	95	11	−23	−1	17	124	129	8	−9	−3	18	20	16	20	−9	−3	19	32	48	32
−4	4	15	120	146	5	−17	1	16	89	83	7	−21	−1	17	21	3	21	−7	−3	18	65	54	13	−7	−3	19	12	40	12
−2	4	15	37	35	12	−15	1	16	46	49	12	−19	−1	17	49	67	26	−5	−3	18	26	30	25	−20	−2	19	32	14	32
0	4	15	20	20	20	−13	1	16	83	85	6	−17	−1	17	25	20	25	−3	−3	18	59	48	13	−18	−2	19	35	47	35
2	4	15	72	77	7	−11	1	16	39	52	16	−15	−1	17	27	55	27	−1	−3	18	23	26	22	−16	−2	19	38	21	34
4	4	15	29	22	29	−9	1	16	165	178	7	−13	−1	17	102	114	7	−22	−2	18	0	17	1	−14	−2	19	86	64	11
−13	5	15	55	60	10	−7	1	16	200	207	6	−11	−1	17	189	173	8	−20	−2	18	17	25	17	−12	−2	19	97	93	10
−11	5	15	52	46	11	−5	1	16	157	167	8	−9	−1	17	105	114	6	−18	−2	18	0	13	1	−10	−2	19	0	16	1
−9	5	15	68	68	6	−3	1	16	46	47	16	−7	−1	17	47	17	13	−16	−2	18	67	97	13	−8	−2	19	41	33	17
−7	5	15	58	53	9	−1	1	16	106	123	17	−5	−1	17	128	105	9	−14	−2	18	31	48	30	−6	−2	19	33	34	25
−5	5	15	28	35	11	1	1	16	18	31	17	−3	−1	17	126	111	18	−12	−2	18	61	45	15	−4	−2	19	32	27	31
−18	−4	16	59	53	12	3	1	16	20	38	19	−1	−1	17	0	23	1	−10	−2	18	110	108	6	−2	−2	19	59	57	14
−16	−4	16	17	29	17	5	1	16	83	65	9	1	−1	17	54	64	12	−8	−2	18	41	77	30	−21	−1	19	75	73	8
−14	−4	16	2	31	2	7	1	16	0	18	1	3	−1	17	0	12	1	−6	−2	18	39	38	21	−19	−1	19	0	26	1
−12	−4	16	50	41	16	−24	2	16	67	70	12	5	−1	17	22	15	22	−4	−2	18	45	51	14	−17	−1	19	0	28	1
−10	−4	16	72	94	10	−22	2	16	54	65	15	−26	0	17	71	56	7	−2	−2	18	57	64	17	−15	−1	19	60	40	10
−8	−4	16	126	121	8	−20	2	16	86	114	10	−24	0	17	17	15	17	0	−2	18	14	27	14	−13	−1	19	69	55	9
−23	−3	16	40	34	17	−18	2	16	108	122	8	−22	0	17	38	25	37	2	−2	18	0	10	1	−11	−1	19	73	74	9
−21	−3	16	29	41	29	−16	2	16	20	28	19	−20	0	17	42	28	13	−23	−1	18	68	67	8	−9	−1	19	66	70	10
−19	−3	16	0	11	1	−14	2	16	43	61	12	−18	0	17	14	35	13	−21	−1	18	30	40	30	−7	−1	19	22	34	21
−17	−3	16	58	48	13	−12	2	16	21	29	20	−16	0	17	127	120	5	−19	−1	18	35	37	35	−5	−1	19	0	6	1
−15	−3	16	47	71	18	−10	2	16	136	129	5	−14	0	17	179	158	5	−17	−1	18	7	14	6	−3	−1	19	0	10	1
−13	−3	16	59	52	14	−8	2	16	50	48	11	−12	0	17	202	206	8	−15	−1	18	24	35	23	−1	−1	19	56	49	11
−11	−3	16	59	48	15	−6	2	16	156	159	5	−10	0	17	110	89	13	−13	−1	18	153	153	18	1	−1	19	19	27	19
−9	−3	16	63	74	14	−4	2	16	102	104	8	−8	0	17	0	21	1	−11	−1	18	99	93	10	−22	0	19	0	46	1
−7	−3	16	34	21	34	−2	2	16	28	44	23	−6	0	17	80	85	7	−9	−1	18	0	27	1	−20	0	19	34	47	17
−5	−3	16	43	52	14	0	2	16	89	78	5	−4	0	17	113	161	6	−7	−1	18	66	59	10	−18	0	19	28	22	28
−3	−3	16	110	106	9	2	2	16	46	40	10	−2	0	17	64	62	9	−5	−1	18	106	94	7	−16	0	19	45	40	12
−1	−3	16	49	66	19	4	2	16	12	21	12	0	0	17	91	104	7	−3	−1	18	0	9	1	−14	0	19	36	33	17
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3	−3	16	42	52	30	−23	3	16	30	34	30	4	0	17	53	51	9	1	−1	18	81	71	11	−10	0	19	125	108	6
5	−3	16	14	15	13	−21	3	16	43	41	19	6	0	17	73	70	6	3	−1	18	46	38	19	−8	0	19	0	8	1
−24	−2	16	52	70	9	−19	3	16	22	11	22	−25	1	17	37	17	37	−24	0	18	0	23	1	−6	0	19	45	28	15
−22	−2	16	47	64	11	−17	3	16	68	47	12	−23	1	17	132	129	9	−22	0	18	28	38	28	−4	0	19	36	23	22
−20	−2	16	88	114	9	−15	3	16	70	71	10	−21	1	17	0	3	1	−20	0	18	28	6	27	−2	0	19	33	44	32
−18	−2	16	92	122	9	−13	3	16	46	52	10	−19	1	17	65	67	9	−18	0	18	0	3	1	0	0	19	81	64	15
−16	−2	16	22	28	22	−11	3	16	54	48	9	−17	1	17	42	20	17	−16	0	18	45	71	12	−21	1	19	67	73	6
−14	−2	16	66	62	12	−9	3	16	62	73	8	−15	1	17	40	55	14	−14	0	18	0	48	1	−19	1	19	0	26	1
−12	−2	16	51	29	16	−7	3	16	27	21	27	−13	1	17	91	114	10	−12	0	18	17	24	16	−17	1	19	28	28	27
−10	−2	16	131	129	6	−5	3	16	56	51	8	−11	1	17	176	173	11	−10	0	18	42	56	17	−15	1	19	55	40	12

TABLE 16-continued

Observed and calculated structure factors for MET-2.

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
−8	−2	16	41	48	16	−3	3	16	110	106	4	−9	1	17	107	113	5	−8	0	18	74	95	8	−13	1	19	61	55	8
−11	1	19	69	74	7	−6	2	19	24	34	24	−19	−1	20	40	58	16	−10	0	20	0	0	1	−14	2	20	40	47	39
−9	1	19	64	71	8	−4	2	19	38	27	10	−17	−1	20	0	39	1	−8	0	20	0	23	1	−12	2	20	23	14	22
−7	1	19	27	34	27	−2	2	19	60	57	6	−15	−1	20	0	34	1	−6	0	20	13	32	12	−10	2	20	33	48	16
−5	1	19	4	6	3	−15	3	19	47	25	15	−13	−1	20	69	62	21	−4	0	20	19	12	19	−8	2	20	63	66	10
−3	1	19	0	10	1	−13	3	19	48	42	6	−11	−1	20	0	15	1	−19	1	20	47	58	9	−6	2	20	29	23	15
−1	1	19	55	49	8	−11	3	19	0	17	1	−9	−1	20	33	21	32	−17	1	20	31	39	30	−13	−1	21	26	20	25
1	1	19	36	27	12	−9	3	19	46	48	8	−7	−1	20	49	13	13	−15	1	20	45	34	10	−11	−1	21	29	22	29
−20	2	19	27	14	26	−7	3	19	34	40	12	−5	−1	20	41	29	17	−13	1	20	53	62	9	−16	0	21	0	27	1
−18	2	19	56	47	15	−16	−2	20	25	14	25	−3	−1	20	27	24	26	−11	1	20	19	15	18	−14	0	21	24	5	24
−16	2	19	29	21	28	−14	−2	20	42	47	25	−20	0	20	59	58	8	−9	1	20	18	21	17	−12	0	21	11	6	11
−14	2	19	81	63	14	−12	−2	20	0	14	1	−18	0	20	51	20	9	−7	1	20	0	13	1	−10	0	21	25	36	25
−12	2	19	101	93	11	−10	−2	20	52	48	11	−16	0	20	58	54	8	−5	1	20	21	29	21	−8	0	21	0	10	1
−10	2	19	20	16	20	−8	−2	20	76	66	7	−14	0	20	14	21	14	−3	1	20	31	24	16	−13	1	21	0	20	1
−8	2	19	28	34	28	−6	−2	20	30	23	29	−12	0	20	29	37	29	−16	2	20	0	14	1	−11	1	21	41	21	15

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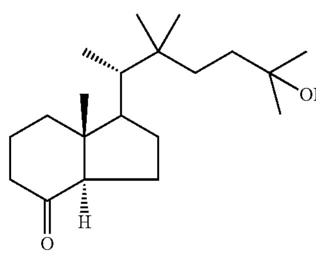
Example 3

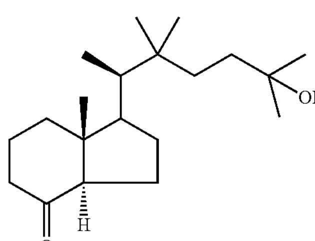
Synthesis of MET-1 and MET-2

The preparation of MET-1 and MET-2 having the basic structures I and II can be accomplished by a common general method otherwise referred to as the condensation of a bicyclic Windaus-Grundmann type ketone IIIa or IIIb with the allylic phosphine oxide IV to the corresponding 2-methylene-19-nor-vitamin D analog Va or Vb followed by deprotection at C-1 and C-3 in the latter compound Va or Vb to obtain compound I (MET-1) or compound II (MET-2).

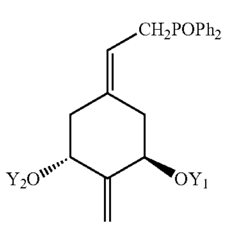
IIIa



IIIb

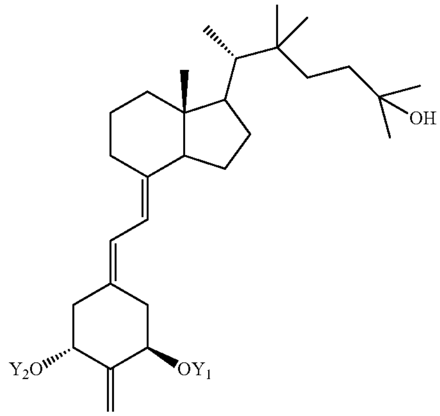


IV

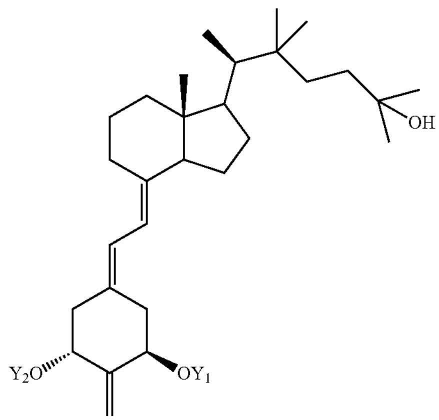


-continued

Va



Vb



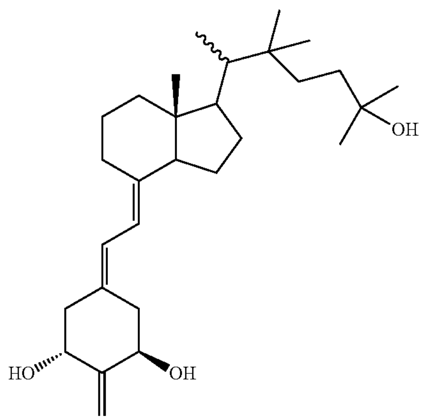
In phosphine oxide IV, Y_1 and Y_2 are preferably hydroxy-protecting groups such as silyl protecting groups. The t-butyldimethylsilyl (TMDMS) group is an example of a particularly useful hydroxy-protecting group. The process described above represents an application of the convergent synthesis concept, 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 IV 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.

An overall process for the synthesis of compounds I and II 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. patent application Ser. No. 13/053,844 filed Mar. 22, 2011, entitled "(20S)-2-Methylene-19-Nor-22-Dimethyl-1α,25-Dihydroxyvitamin D_3 and (20R)-2-Methylene-19-Nor-22-Dimethyl-1α,25-Hydroxyvitamin D_3" published as U.S. Publication No. US 2011/0237556A1 the specification of which is specifically incorporated herein by reference.

We claim:

1. A compound having the formula



in crystalline form, wherein the methyl group attached to carbon 20 may be in its R or S orientation.

2. (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 in crystalline form.

3. A crystalline form of (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 having molecular packing arrangement defined by space group P2(1) and unit cell dimensions a=7.57 Å b=14.79 Å c=14.48 Å α=90°, β=102.2° and γ=90°.

4. A three dimensional structure for (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 as defined by the molecular packing arrangement set forth in claim **3**.

5. A method of purifying (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3, comprising the steps of:

(a) preparing a solvent comprising diethyl ether;

(b) dissolving a product containing (20S)-2-methylene-19-nor-22-dimethyl-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 (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 crystals; and

(d) separating the (20S)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 crystals from the solvent.

6. The method of claim **5** including the further step of allowing said solvent and dissolved product to cool to ambient temperature prior to cooling below ambient temperature.

7. The method of claim **5** wherein said solvent comprises 100% diethyl ether, by volume.

8. The method of claim **5** wherein the step of separating comprises filtering the solvent and precipitate to obtain the crystals.

9. The method of claim **5** 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. (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 in crystalline form.

11. A crystalline form of (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 having molecular packing arrangement defined by space group C2 and unit cell dimensions a=27.33 Å b=6.68 Å c=19.22 Å α=90°, β=113.57° and γ=90°.

12. A three dimensional structure for (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 as defined by the molecular packing arrangement set forth in claim **11**.

13. A method of purifying (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3, comprising the steps of:

(a) preparing a solvent comprising hexane;

(b) adding a product containing (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 to be purified to said hexane to form a suspension of the product in the hexane;

(c) adding 2-propanol dropwise to the suspension to form a mixture of the product in the hexane and 2-propanol;

(d) heating the mixture to dissolve the product containing (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 to be purified in said mixture;

(e) cooling said mixture and dissolved product below ambient temperature for a sufficient amount of time to form a precipitate of (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 crystals; and

(f) separating the (20R)-2-methylene-19-nor-22-dimethyl-1α,25-dihydroxyvitamin D_3 crystals from the mixture.

14. The method of claim **13** including the further step of allowing said mixture and dissolved product to cool to ambient temperature prior to cooling below ambient temperature.

15. The method of claim **13** wherein the step of separating comprises filtering the mixture and precipitate to obtain the crystals.

16. The method of claim **13** including a further step (g) comprising repeating steps (a) through (f) using the recovered crystals from step (f) as the product of step (b).

17. The method of claim **13** wherein said mixture comprises about 15% 2-propanol and about 85% hexane, by volume.

* * * * *