

Supplementary Information

“A Diastereoselective Metal Catalyzed [2+2]Cycloaddition of bis-Enones”

JA010800P

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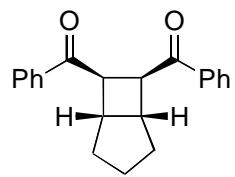
Austin, TX 78712

USA

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I. [2+2] Cycloaddition Products:



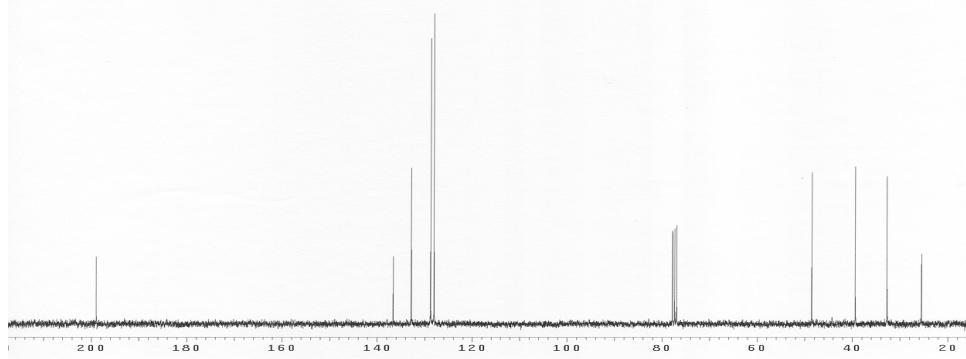
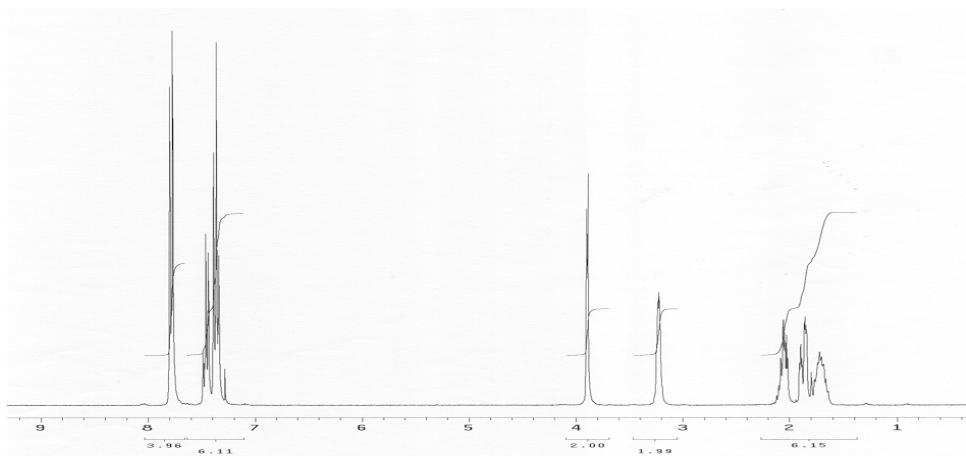
¹H NMR: (300 MHz, CDCl₃) 1.84 (m, 4H), 2.06 (m, 2H), 3.22 (m, 2H), 3.90 (d, *J* 4.2Hz, 2H), 7.42 (m, 6H), 7.78 (m, 4H).

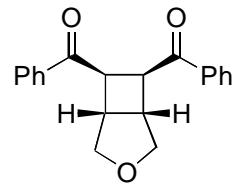
¹³C NMR: (75 MHz, CDCl₃) 25.5, 32.7, 39.3, 48.6, 128.1, 128.7, 136.6, 198.9.

HRMS: Calc'd for C₂₁H₂₁O₂: 305.1541, Found: 305.1538.

FTIR: (KBr) 3054, 2968, 1682, 1447, 1263, 743, 704 cm⁻¹.

m.p.: 155 ~157 °C





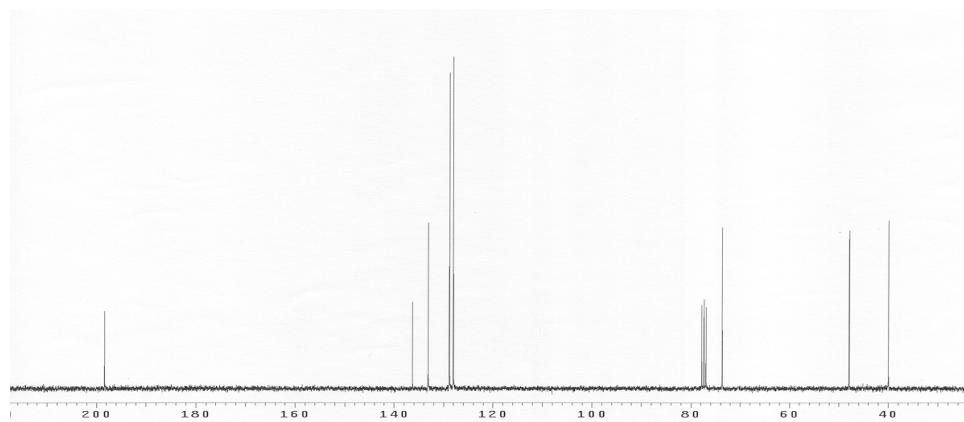
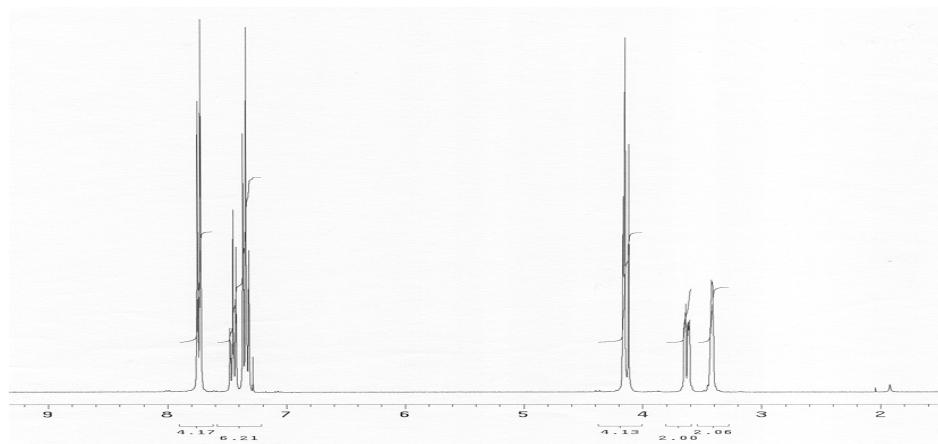
¹H NMR: (300 MHz, CDCl₃) 3.42 (m, 2H), 3.64 (m, 2H), 4.16 (m, 4H), 7.48 (m, 6H), 7.92 (m, 4H).

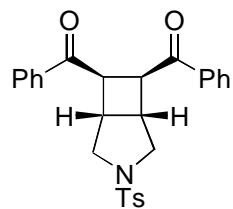
¹³C NMR: (75 MHz, CDCl₃) 39.9, 47.9, 73.7, 128.0, 128.8, 133.1, 136.2, 198.3.

HRMS: Calc'd for C₂₀H₁₉O₃: 307.1334, Found: 307.1336.

FTIR: (KBr) 3055, 2858, 1685, 1448, 1265, 738, 704 cm⁻¹.

m.p.: 163 ~ 165 °C





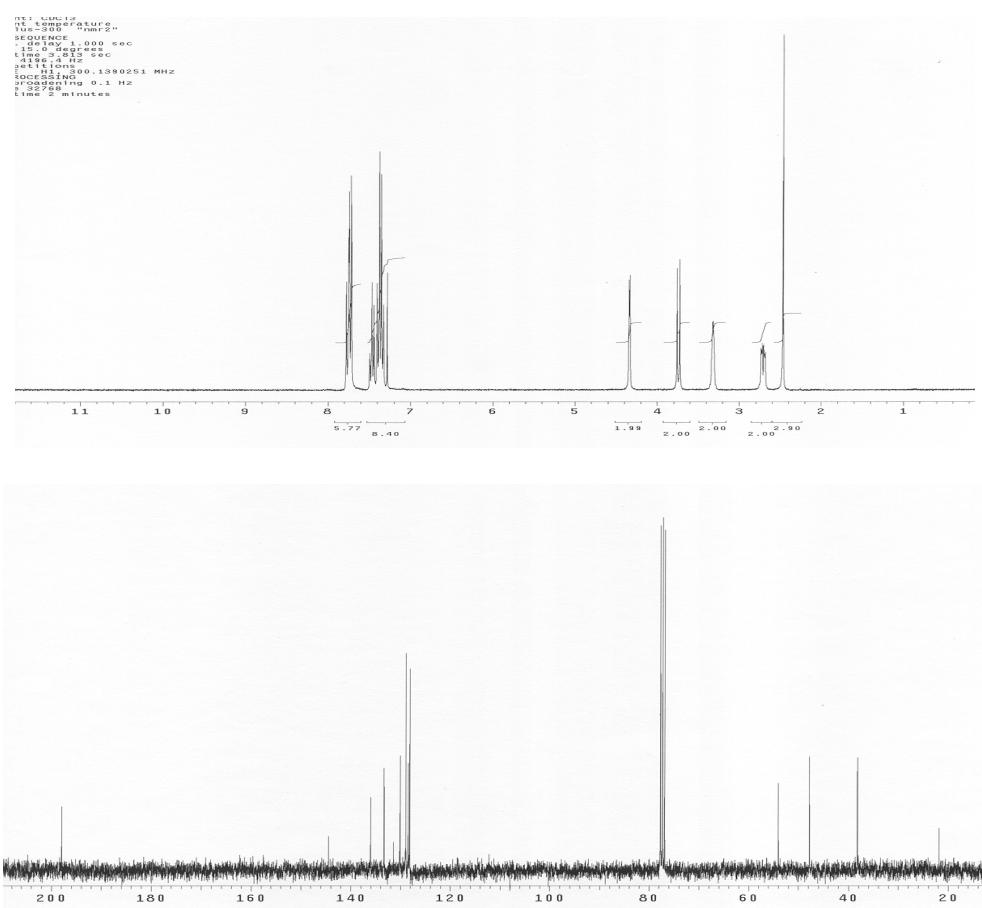
¹H NMR: (300 MHz, CDCl₃) 2.47 (s, 3H), 2.71 (m, 2H), 3.31 (m, 2H), 3.73 (d, *J* 1.8, 2H), 4.33 (d, *J* 4.2, 2H), 7.42 (m, 8H), 7.70 (m, 6H).

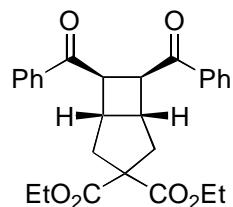
¹³C NMR: (75 MHz, CDCl₃) 21.8, 38.2, 47.7, 54.0, 128.1, 128.4, 128.8, 130.0, 131.3, 133.3, 136.0, 144.4, 197.9.

HRMS: Calc'd for C₂₇H₂₆NO₄S: 460.1582, Found: 460.1587.

FTIR: (KBr) 3056, 2985, 1685, 1346, 1265, 1163, 734, 704, 665 cm⁻¹.

m.p.: 170 ~172 °C





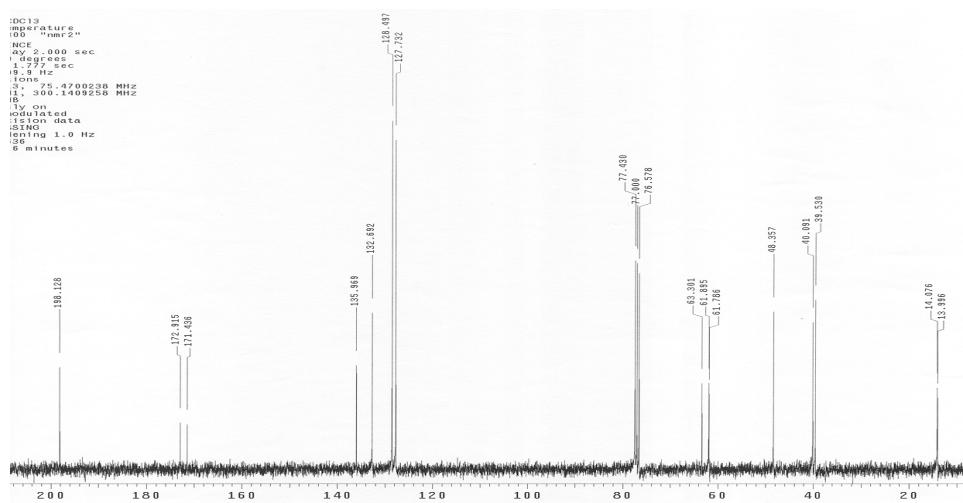
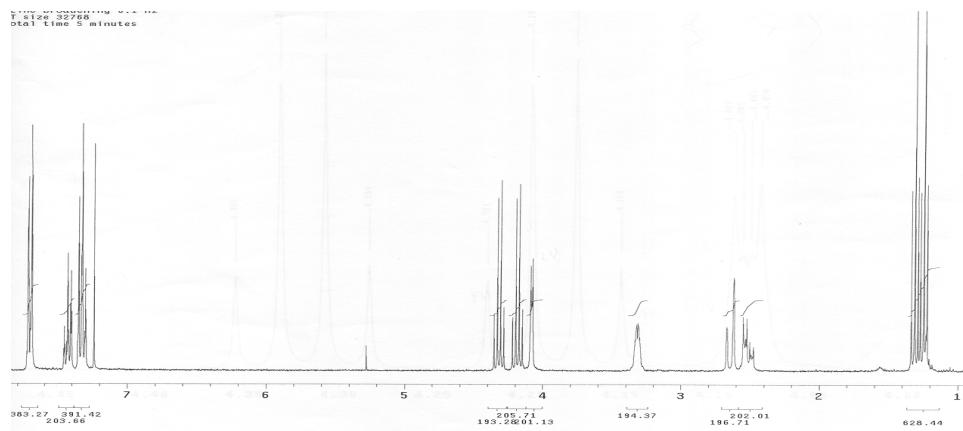
¹H NMR: (300 MHz, CDCl₃) 1.27 (m, 6H), 2.62 (m, 4H), 3.32 (m, 2H), 4.08 (d, *J* 3.9 Hz, 2H), 4.17 (q, *J* 6.9 Hz, 2H), 4.30 (q, *J* 6.3 Hz, 2H), 7.42 (m, 6H), 7.72 (m, 4H).

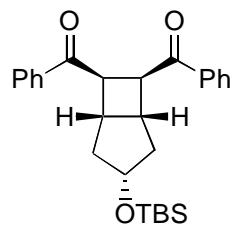
¹³C NMR: (75 MHz, CDCl₃) 13.9, 14.1, 39.5, 40.1, 48.3, 61.8, 61.9, 63.3, 127.7, 128.5, 132.7, 135.9, 171.4, 172.9, 198.1.

HRMS: Calc'd for C₂₇H₂₉O₆: 460.1582, Found: 460.1587.

FTIR: (KBr) 3054, 2985, 2306, 1724, 1686, 1597, 1581, 1448, 1272, 758, 697 cm⁻¹.

m.p.: 96 ~ 98 °C





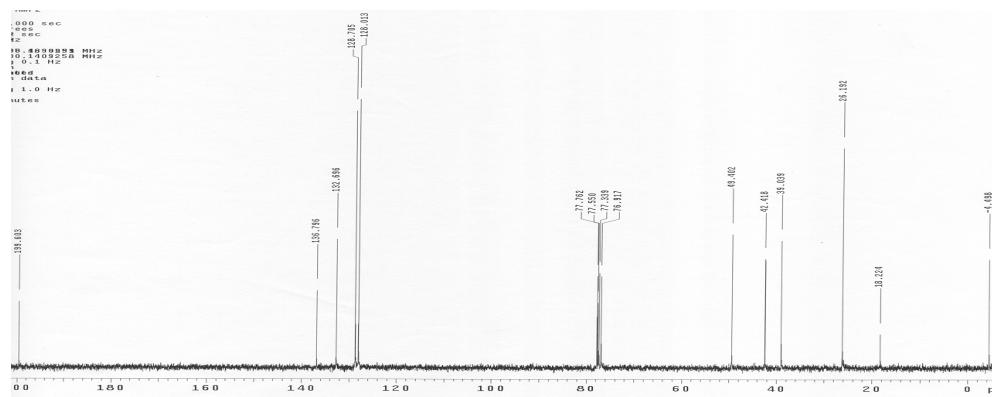
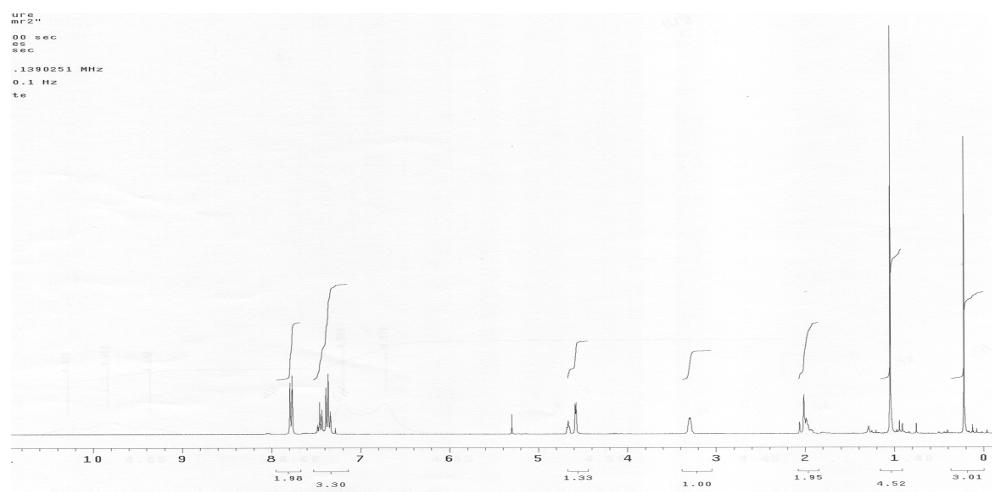
¹H NMR: (300 MHz, CDCl₃) 0.22 (s, 6H), 1.04 (s, 9H), 1.98 (m, 4H), 3.29 (d, *J* 2.7 Hz, 2H), 4.58 (d, *J* 3.9 Hz, 2H), 4.66 (m, 1H), 7.42 (m, 6H), 7.78 (m, 4H).

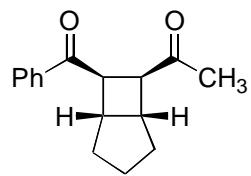
¹³C NMR: (75 MHz, CDCl₃) –4.5, 18.2, 26.2, 39.0, 42.4, 49.4, 128.0, 128.7, 132.7, 136.8, 199.6.

HRMS: Calc'd for C₂₇H₃₅O₃Si: 435.2355, Found: 435.2360.

FTIR: (KBr) 3054, 2954, 2929, 2856, 1684, 1448, 1264, 746, 704 cm⁻¹.

m.p.: 107 ~ 109 °C





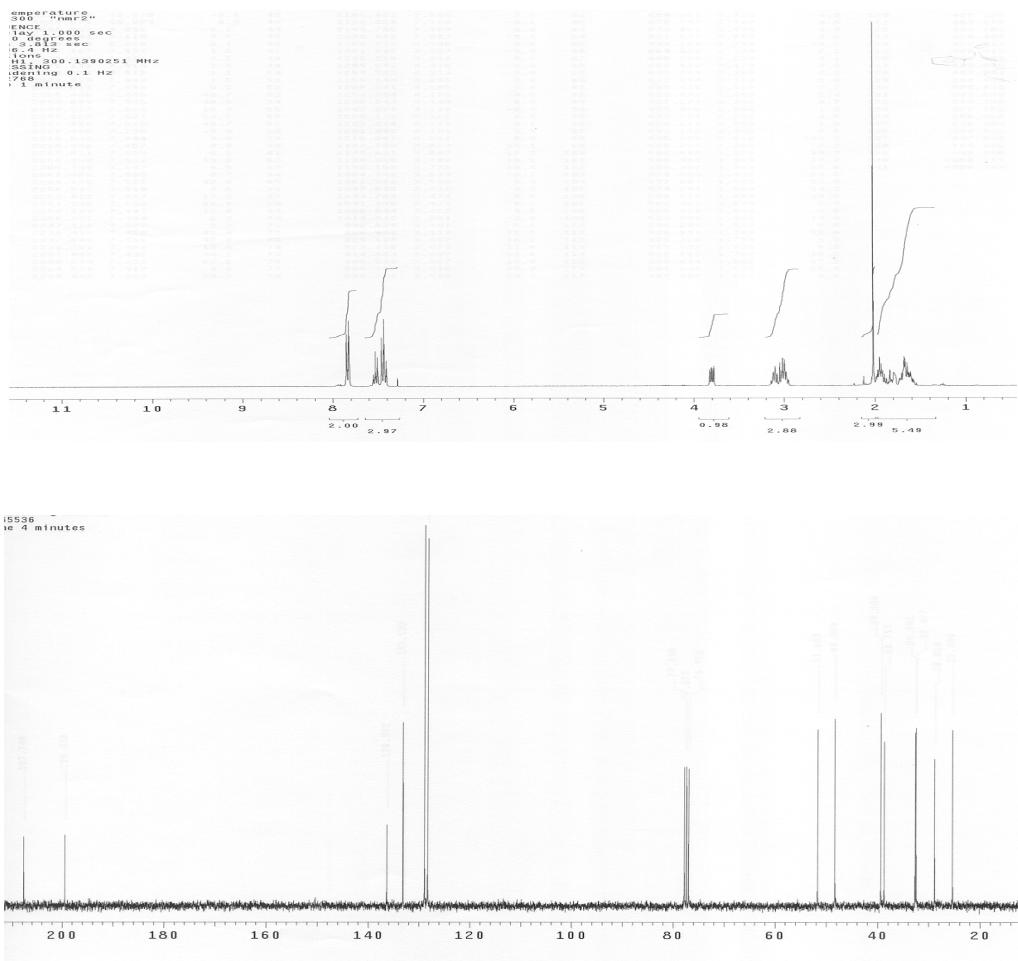
¹H NMR: (300 MHz, CDCl₃) 1.60 ~ 1.98 (m, 6H), 2.02 (s, 3H), 3.02 (m, 3H), 3.80 (dd, *J* 5.1, 9.6 Hz, 1H), 7.46 (m, 3H), 7.81 (m, 2H).

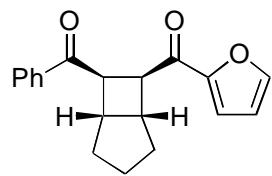
¹³C NMR: (75 MHz, CDCl₃) 25.4, 28.8, 32.5, 32.7, 38.7, 39.4, 48.3, 51.7, 128.2, 128.9, 133.1, 136.4, 199.4, 297.7.

HRMS: Calc'd for C₁₆H₁₉O₂: 243.1385, Found: 243.1387.

FTIR: (KBr) 3055, 2948, 2858, 1706, 1678, 1448, 1356, 1264, 1218, 739 cm⁻¹.

m.p.: 77 ~ 78 °C





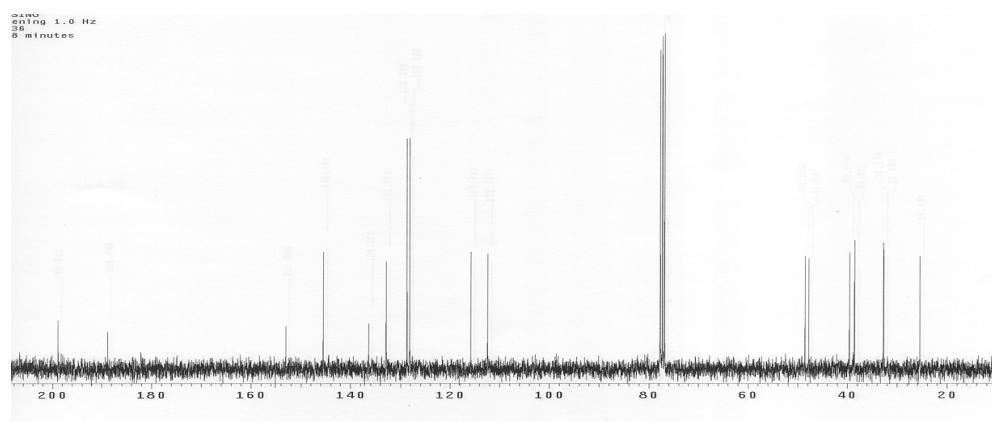
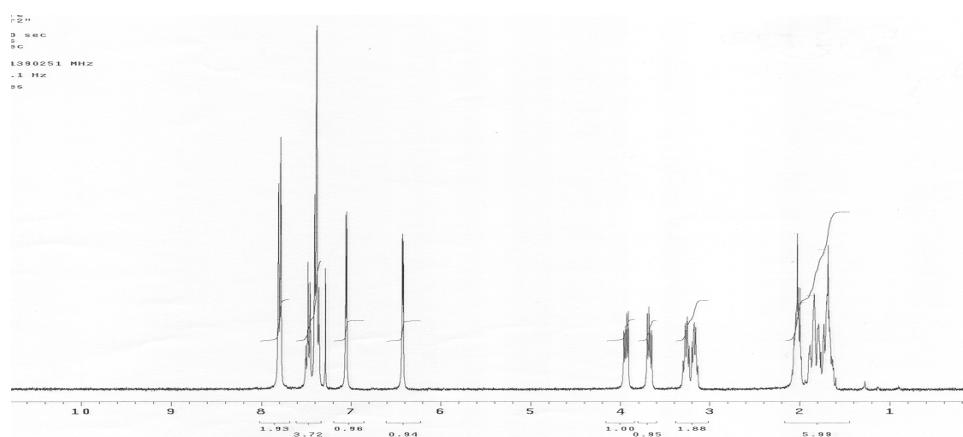
¹H NMR: (300 MHz, CDCl₃) 1.77 (m, 4H), 2.03 (m, 2H), 3.17 (m, 1H), 3.25 (m, 1H), 3.61 (dd, *J* 5.4, 9.9, 1H), 3.93 (dd, *J* 4.8, 9.9, 1H), 6.42 (dd, *J* 1.8, 3.6 Hz, 1H), 7.05 (dd, *J* 0.6, 3.6 Hz, 1H), 7.40 (m, 4H), 7.70 (m, 2H).

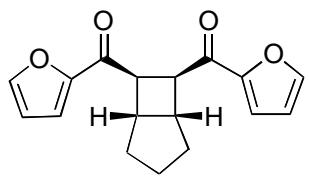
¹³C NMR: (75 MHz, CDCl₃) 25.4, 32.6, 32.7, 38.5, 39.6, 47.8, 48.5, 112.4, 115.7, 128.2, 128.7, 132.9, 136.3, 145.5, 153.0, 188.7, 198.6.

HRMS: Calc'd for C₁₉H₁₉O₃: 295.1334, Found: 295.1335.

FTIR: (KBr) 3054, 2950, 1682, 1467, 1265, 737, 704 cm⁻¹.

m.p.: 130 ~ 132 °C





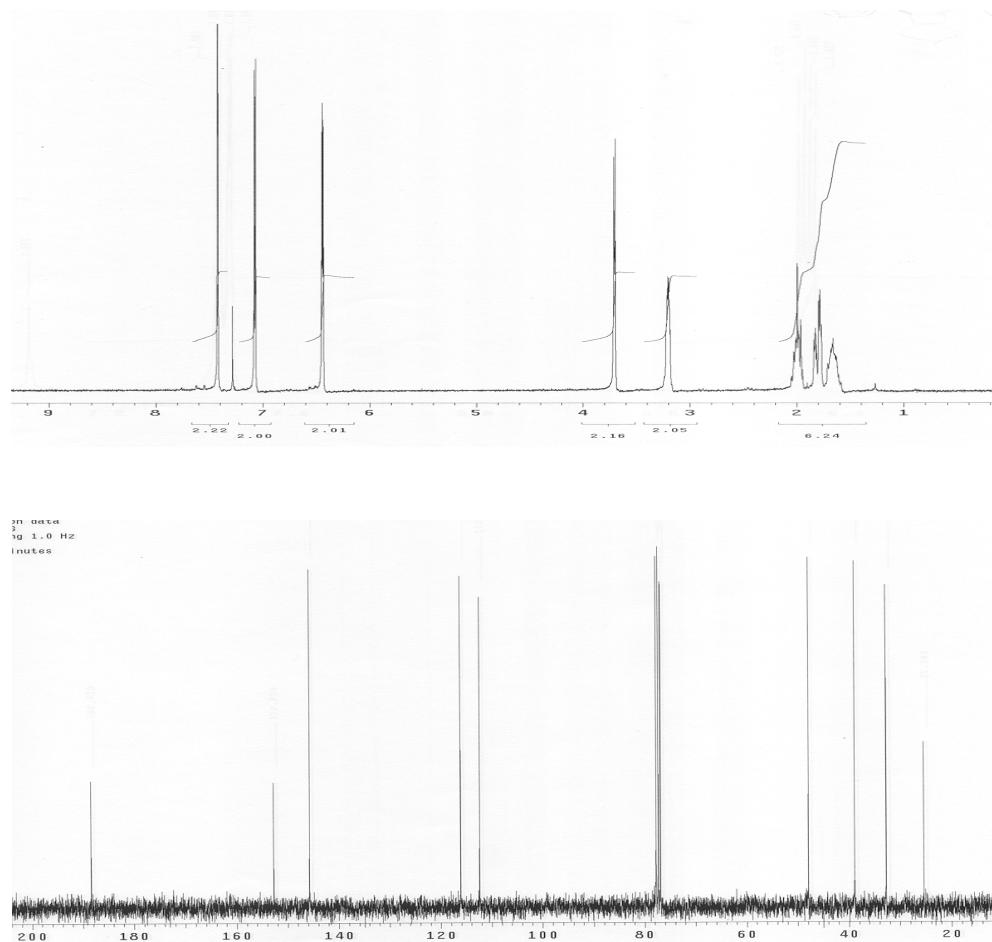
¹H NMR: (300 MHz, CDCl₃) 1.67 ~ 2.04 (m, 6H), 3.20 (m, 2H), 3.70 (d, *J* 4.2 Hz, 2H), 6.44 (dd, *J* 1.8, 3.6 Hz, 2H), 7.07 (dd, *J* 0.6, 3.6 Hz, 2H), 7.42 (dd, *J* 0.9, 1.5, 2H).

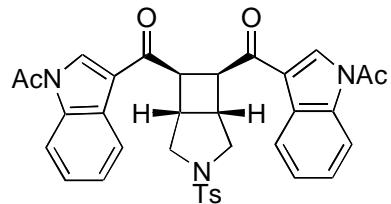
¹³C NMR: (75 MHz, CDCl₃) 25.4, 32.7, 38.9, 47.9, 112.4, 116.1, 145.7, 152.7, 188.7.

HRMS: Calc'd for C₁₇H₁₇O₄: 285.1126, Found: 285.1128.

FTIR: (KBr) 3054, 2953, 1678, 1570, 1468, 1265, 747, 704 cm⁻¹.

m.p.: 156 ~ 157 °C





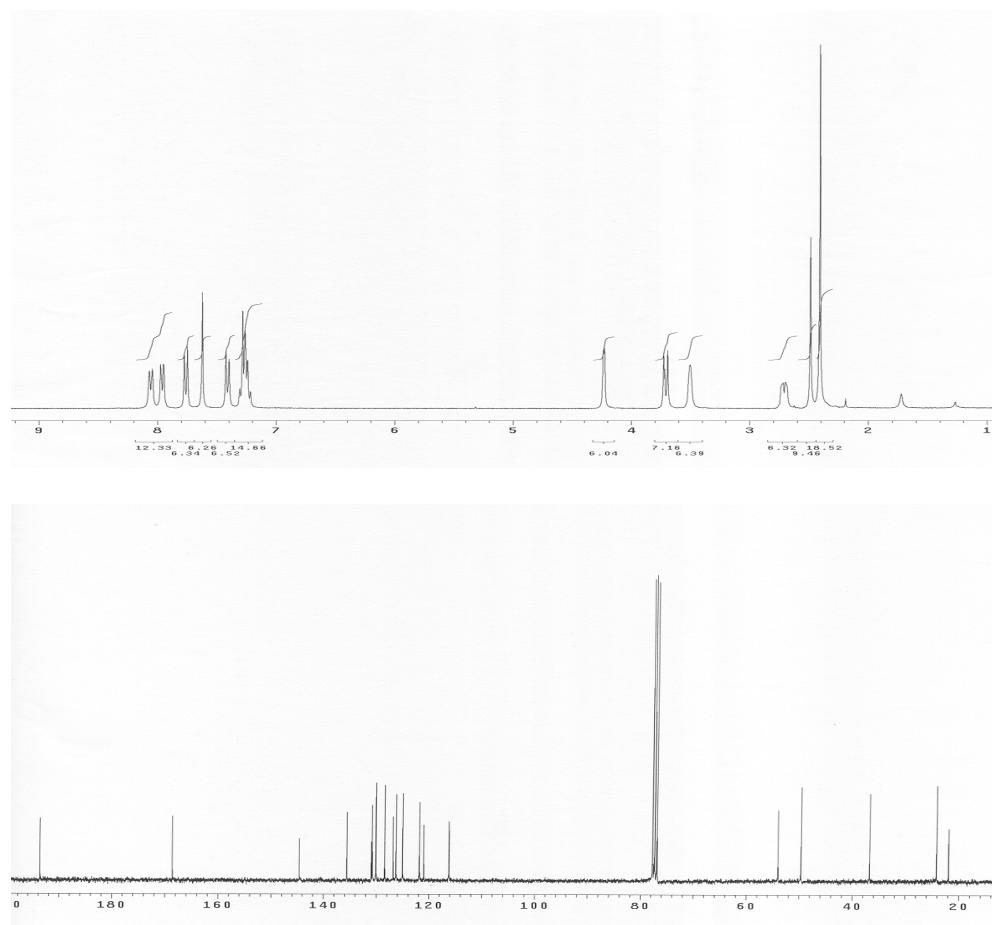
¹H NMR: (300 MHz, CDCl₃) 2.41 (s, 6H), 2.48 (s, 3H), 2.70 (m, 2H), 3.50 (s, 2H), 3.72 (d, *J* 3.0 Hz, 2H), 4.23 (d, *J* 2.8 Hz, 2H), 7.24 (m, 4H), 7.40 (d, *J* 7.9 Hz, 2H), 7.62 (s, 2H), 7.75 (d, *J* 8.4 Hz, 2H), 8.05 (d, *J* 7.9 Hz, 2H), 7.96 (d, *J* 6.9 Hz, 2H), 8.05 (d, *J* 7.9 Hz, 2H).

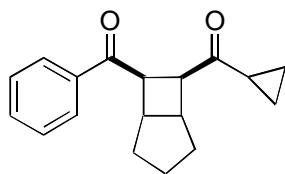
¹³C NMR: (75 MHz, CDCl₃) 21.8, 24.1, 36.7, 49.6, 53.9, 116.2, 121.0, 121.8, 125.0, 126.3, 126.8, 128.4, 130.1, 130.8, 131.0, 135.6, 144.6, 168.5, 193.6.

HRMS: Calc'd for C₃₅H₃₂N₃O₆S: 622.2011, Found: 622.2012.

FTIR: (KBr) 3052, 2984, 1723, 1670, 1545, 1447, 1262, 1213, 737, 703 cm⁻¹.

m.p.: 252 ~ 253 °C





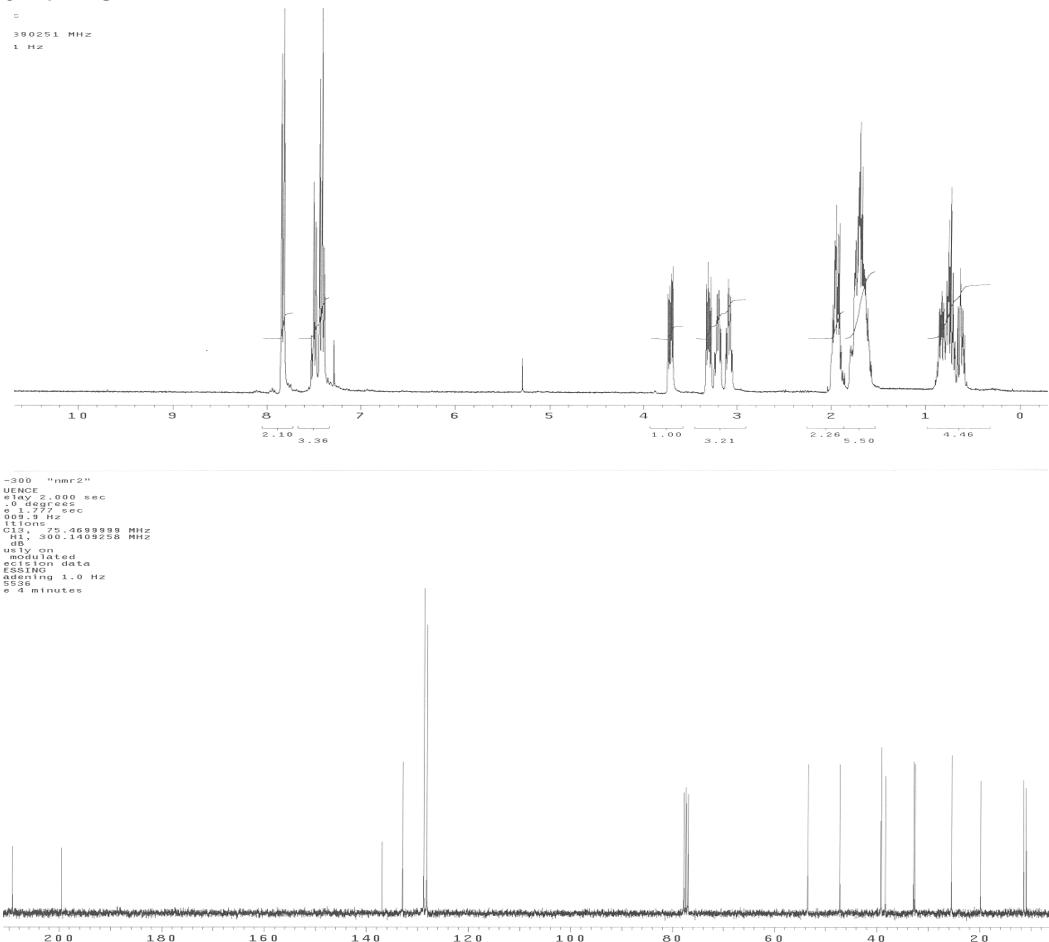
¹H NMR: (300 MHz, CDCl₃) 0.82 (m, 4H), 1.65 (m, 5H), 1.98 (m, 2H), 3.09 (dd, *J* 7.0, 12.7 Hz, 1H), 3.20 (dd, *J* 7.0, 12.7 Hz, 1H), 3.31 (dd, *J* 5.2, 9.7 Hz, 1H), 3.71 (dd, *J* 5.2, 9.7 Hz, 1H), 7.40 (m, 3H), 7.81 (m, 2H)

¹³C NMR: (75 MHz, CDCl₃) 10.9, 11.4, 19.8, 25.5, 32.6, 32.8, 38.3, 39.2, 47.2, 53.5, 128.2, 128.7, 132.8, 136.9, 199.5, 209.4

HRMS: Calc'd for C₁₈H₂₁O₂: 269.1541, Found: 269.1548

FTIR: (KBr) 2944, 1687, 1447, 1385, 1207, 911, 730, 693 cm⁻¹

m.p.: 70 ~ 72 °C



Crystallographic Material for iso **1b**.

X-ray Experimental.

Table 1. Crystallographic Data for 1.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters (\AA^2) for the non-hydrogen atoms of 1.

Table 3. Bond Lengths (\AA) and Angles ($^\circ$) for the non-hydrogen atoms of 1.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of 1.

Table 5. Fractional coordinates and isotropic thermal parameters (\AA^2) for the hydrogen atoms of 1.

Figure 1. View of **1** showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms are drawn to an arbitrary scale.

Figure 2. Unit cell packing diagram for **1**. The view is approximately down the **b** axis.

Table 6. Observed and calculated structure factor amplitudes for 1. Values for F_o , F_c and $\sigma(F_o)$ have been multiplied by 10.

X-ray Experimental for C₂₁H₂₀O₂: Crystals grew as very large, colorless prisms by slow evaporation from ethyl acetate and hexane. The data crystal was cut from a larger crystal and had approximate dimensions; 0.30 x 0.19 x 0.16 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoK α radiation ($\lambda = 0.71073\text{\AA}$). A total of 469 frames of data were collected using ω -scans with a scan range of 1° and a counting time of 29 seconds per frame. The data were collected at -120 °C using a Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.¹ The structure was solved by direct methods using SIR92² and refined by full-matrix least-squares on F² with anisotropic displacement parameters for the non-H atoms using SHELXL-97.³ The hydrogen atoms were observed in a ΔF map and refined with isotropic displacement parameters. The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0415*P)^2 + (0.9360*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.0982, with $R(F)$ equal to 0.0398 and a goodness of fit, S , = 1.072. Definitions used for calculating $R(F), R_w(F^2)$ and the goodness of fit, S , are given below.⁴ The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (6.0(6)\times 10^{-5}) * F_c^2 \lambda^3 / (\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).⁵ All figures were generated using SHELXTL/PC.⁶ Tables of positional and thermal parameters, bond lengths and angles, figures and lists of observed and calculated structure factors are located in tables 1 through 6.

References

- 1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.
- 2) SIR92. (1993). A program for crystal structure solution. Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. J. Appl. Cryst. 26, 343-350.
- 3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.
- 4) $R_w(F^2) = \{\sum w(|F_o|^2 - |F_c|^2)^2 / \sum w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
 $R(F) = \{\sum (|F_o| - |F_c|)^2 / \sum |F_o|\}$ for reflections with $|F_o| > 4(\sigma(F_o))$.
 $S = [\sum w(|F_o|^2 - |F_c|^2)^2 / (n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.
- 5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.
- 6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for 1.

Empirical formula	C21 H20 O2	
Formula weight	304.37	
Temperature	153(2) K	
Wavelength	0.71070 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	$a = 9.1952(2)$ Å	$\alpha = 71.637(1)^\circ$.
	$b = 9.5194(2)$ Å	$\beta = 85.462(1)^\circ$.
	$c = 10.3566(2)$ Å	$\gamma = 67.385(1)^\circ$.
Volume	793.31(3) Å ³	
Z	2	
Density (calculated)	1.274 Mg/m ³	
Absorption coefficient	0.080 mm ⁻¹	
F(000)	324	
Crystal size	0.30 x 0.19 x 0.16 mm	
Theta range for data collection	3.0 to 27.5°.	
Index ranges	-11≤h≤10, -12≤k≤11, -12≤l≤13	
Reflections collected	5529	
Independent reflections	3611 [R(int) = 0.0186]	
Completeness to theta = 27.53°	98.7 %	
Max. and min. transmission	0.9872 and 0.9763	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3611 / 0 / 289	
Goodness-of-fit on F ²	1.072	
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0896	
R indices (all data)	R1 = 0.0606, wR2 = 0.0982	
Extinction coefficient	6.0(6)x10 ⁻⁵	
Largest diff. peak and hole	0.20 and -0.17 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	3762(1)	3250(1)	1728(1)	27(1)
C2	4808(1)	3083(1)	2930(1)	28(1)
C3	6285(1)	2037(2)	2355(1)	31(1)
C4	7062(2)	301(2)	3226(2)	37(1)
C5	5921(2)	-461(2)	3083(1)	36(1)
C6	5351(2)	321(2)	1585(1)	35(1)
C7	5238(1)	2047(2)	1233(1)	30(1)
C8	2354(1)	2780(1)	2063(1)	27(1)
O9	1996(1)	2327(1)	3241(1)	33(1)
C10	1464(1)	2790(1)	910(1)	26(1)
C11	323(1)	2117(2)	1199(1)	33(1)
C12	-449(2)	2012(2)	160(1)	39(1)
C13	-108(2)	2600(2)	-1182(1)	40(1)
C14	992(2)	3302(2)	-1483(1)	39(1)
C15	1785(2)	3393(2)	-442(1)	33(1)
C16	4806(1)	4666(2)	2931(1)	31(1)
O17	5797(1)	5154(1)	2336(1)	53(1)
C18	3520(1)	5696(1)	3598(1)	27(1)
C19	3431(2)	7249(2)	3398(1)	33(1)
C20	2260(2)	8265(2)	3974(1)	37(1)
C21	1164(2)	7749(2)	4755(1)	35(1)
C22	1233(2)	6218(2)	4955(1)	34(1)
C23	2406(1)	5190(2)	4377(1)	29(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for 1.

C1-C8	1.5074(16)	C10-C11	1.3955(17)
C1-C2	1.5641(17)	C11-C12	1.3842(19)
C1-C7	1.5748(16)	C11-H11	0.980(14)
C1-H1	0.969(14)	C12-C13	1.385(2)
C2-C16	1.5071(17)	C12-H12	0.999(16)
C2-C3	1.5477(17)	C13-C14	1.380(2)
C2-H2	1.011(13)	C13-H13	0.985(15)
C3-C4	1.5195(18)	C14-C15	1.3903(19)
C3-C7	1.5617(17)	C14-H14	0.987(16)
C3-H3	0.969(13)	C15-H15	0.969(14)
C4-C5	1.5252(19)	C16-O17	1.2177(15)
C4-H4A	0.992(15)	C16-C18	1.4974(17)
C4-H4B	0.976(15)	C18-C23	1.3910(17)
C5-C6	1.5288(18)	C18-C19	1.3972(17)
C5-H5A	0.990(14)	C19-C20	1.3823(19)
C5-H5B	1.001(14)	C19-H19	0.990(14)
C6-C7	1.5301(18)	C20-C21	1.3825(19)
C6-H6A	1.007(14)	C20-H20	0.987(15)
C6-H6B	1.012(15)	C21-C22	1.3828(18)
C7-H7	0.992(13)	C21-H21	0.972(15)
C8-O9	1.2236(14)	C22-C23	1.3907(18)
C8-C10	1.4960(17)	C22-H22	1.001(14)
C10-C15	1.3905(17)	C23-H23	0.980(13)
C8-C1-C2	118.45(10)	C1-C2-H2	110.5(7)
C8-C1-C7	116.21(10)	C4-C3-C2	116.01(11)
C2-C1-C7	89.64(9)	C4-C3-C7	106.29(10)
C8-C1-H1	108.1(8)	C2-C3-C7	90.72(9)
C2-C1-H1	112.5(8)	C4-C3-H3	114.0(7)
C7-C1-H1	110.9(8)	C2-C3-H3	111.1(7)
C16-C2-C3	115.39(10)	C7-C3-H3	116.6(7)
C16-C2-C1	112.68(10)	C3-C4-C5	104.25(10)
C3-C2-C1	90.03(9)	C3-C4-H4A	108.6(8)
C16-C2-H2	111.8(7)	C5-C4-H4A	109.2(8)
C3-C2-H2	114.7(7)	C3-C4-H4B	112.2(8)

C5-C4-H4B	112.4(8)	C13-C14-H14	122.3(9)
H4A-C4-H4B	109.9(11)	C15-C14-H14	117.4(9)
C4-C5-C6	103.40(11)	C14-C15-C10	120.17(13)
C4-C5-H5A	110.0(8)	C14-C15-H15	119.5(8)
C6-C5-H5A	110.0(7)	C10-C15-H15	120.3(8)
C4-C5-H5B	113.1(8)	O17-C16-C18	119.50(11)
C6-C5-H5B	112.3(8)	O17-C16-C2	120.53(11)
H5A-C5-H5B	108.1(11)	C18-C16-C2	119.87(10)
C5-C6-C7	105.41(10)	C23-C18-C19	119.02(12)
C5-C6-H6A	109.2(8)	C23-C18-C16	123.23(11)
C7-C6-H6A	107.7(8)	C19-C18-C16	117.73(11)
C5-C6-H6B	112.5(8)	C20-C19-C18	120.51(12)
C7-C6-H6B	113.9(8)	C20-C19-H19	122.2(8)
H6A-C6-H6B	108.0(11)	C18-C19-H19	117.3(8)
C6-C7-C3	105.38(10)	C21-C20-C19	120.10(12)
C6-C7-C1	117.21(10)	C21-C20-H20	121.0(8)
C3-C7-C1	89.13(9)	C19-C20-H20	118.9(8)
C6-C7-H7	112.1(7)	C20-C21-C22	120.01(13)
C3-C7-H7	117.5(7)	C20-C21-H21	119.4(8)
C1-C7-H7	113.5(7)	C22-C21-H21	120.5(8)
O9-C8-C10	120.88(11)	C21-C22-C23	120.21(12)
O9-C8-C1	121.37(11)	C21-C22-H22	119.5(8)
C10-C8-C1	117.65(10)	C23-C22-H22	120.3(8)
C15-C10-C11	119.03(11)	C22-C23-C18	120.14(12)
C15-C10-C8	121.87(11)	C22-C23-H23	119.2(8)
C11-C10-C8	119.05(11)	C18-C23-H23	120.6(8)
C12-C11-C10	120.52(12)		
C12-C11-H11	120.2(8)		
C10-C11-H11	119.3(8)		
C13-C12-C11	119.98(14)		
C13-C12-H12	119.7(9)		
C11-C12-H12	120.4(9)		
C14-C13-C12	119.99(13)		
C14-C13-H13	120.8(8)		
C12-C13-H13	119.2(8)		
C13-C14-C15	120.27(13)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	25(1)	26(1)	28(1)	-7(1)	4(1)	-10(1)
C2	25(1)	30(1)	31(1)	-10(1)	4(1)	-13(1)
C3	23(1)	36(1)	38(1)	-14(1)	5(1)	-12(1)
C4	31(1)	39(1)	37(1)	-16(1)	-4(1)	-6(1)
C5	36(1)	30(1)	36(1)	-11(1)	-1(1)	-6(1)
C6	31(1)	35(1)	37(1)	-18(1)	-1(1)	-6(1)
C7	26(1)	36(1)	25(1)	-9(1)	6(1)	-9(1)
C8	25(1)	23(1)	30(1)	-8(1)	5(1)	-8(1)
O9	35(1)	42(1)	29(1)	-12(1)	8(1)	-21(1)
C10	22(1)	26(1)	28(1)	-9(1)	3(1)	-6(1)
C11	29(1)	39(1)	32(1)	-11(1)	3(1)	-14(1)
C12	31(1)	50(1)	42(1)	-19(1)	1(1)	-17(1)
C13	30(1)	48(1)	39(1)	-19(1)	-6(1)	-5(1)
C14	35(1)	42(1)	28(1)	-9(1)	0(1)	-4(1)
C15	28(1)	31(1)	33(1)	-6(1)	3(1)	-8(1)
C16	29(1)	34(1)	35(1)	-10(1)	4(1)	-16(1)
O17	48(1)	49(1)	78(1)	-28(1)	31(1)	-33(1)
C18	27(1)	28(1)	26(1)	-7(1)	-3(1)	-12(1)
C19	36(1)	32(1)	35(1)	-10(1)	0(1)	-19(1)
C20	45(1)	28(1)	40(1)	-11(1)	-4(1)	-16(1)
C21	37(1)	32(1)	34(1)	-14(1)	-1(1)	-9(1)
C22	34(1)	35(1)	31(1)	-10(1)	5(1)	-14(1)
C23	32(1)	26(1)	29(1)	-7(1)	2(1)	-14(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H1	3415(15)	4309(16)	1067(14)	35(3)
H2	4487(14)	2498(14)	3830(13)	28(3)
H3	7013(15)	2573(15)	2045(13)	31(3)
H4A	8074(17)	-199(17)	2830(14)	40(4)
H4B	7248(16)	201(16)	4172(15)	40(4)
H5A	5022(16)	-184(15)	3672(13)	34(3)
H5B	6424(16)	-1656(17)	3333(13)	38(4)
H6A	6178(16)	-217(16)	1011(14)	39(4)
H6B	4332(17)	228(16)	1401(14)	41(4)
H7	5464(14)	2480(15)	269(14)	32(3)
H11	92(15)	1693(16)	2150(14)	37(4)
H12	-1252(19)	1512(18)	371(15)	53(4)
H13	-673(17)	2527(17)	-1913(15)	44(4)
H14	1260(17)	3742(17)	-2426(16)	52(4)
H15	2559(16)	3883(16)	-665(13)	35(4)
H19	4230(17)	7582(17)	2831(14)	42(4)
H20	2205(16)	9366(18)	3796(14)	43(4)
H21	345(17)	8473(17)	5155(14)	42(4)
H22	429(16)	5858(16)	5515(14)	41(4)
H23	2429(15)	4115(16)	4515(13)	31(3)

Figure 1. View of **1** showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms are drawn to an arbitrary scale.

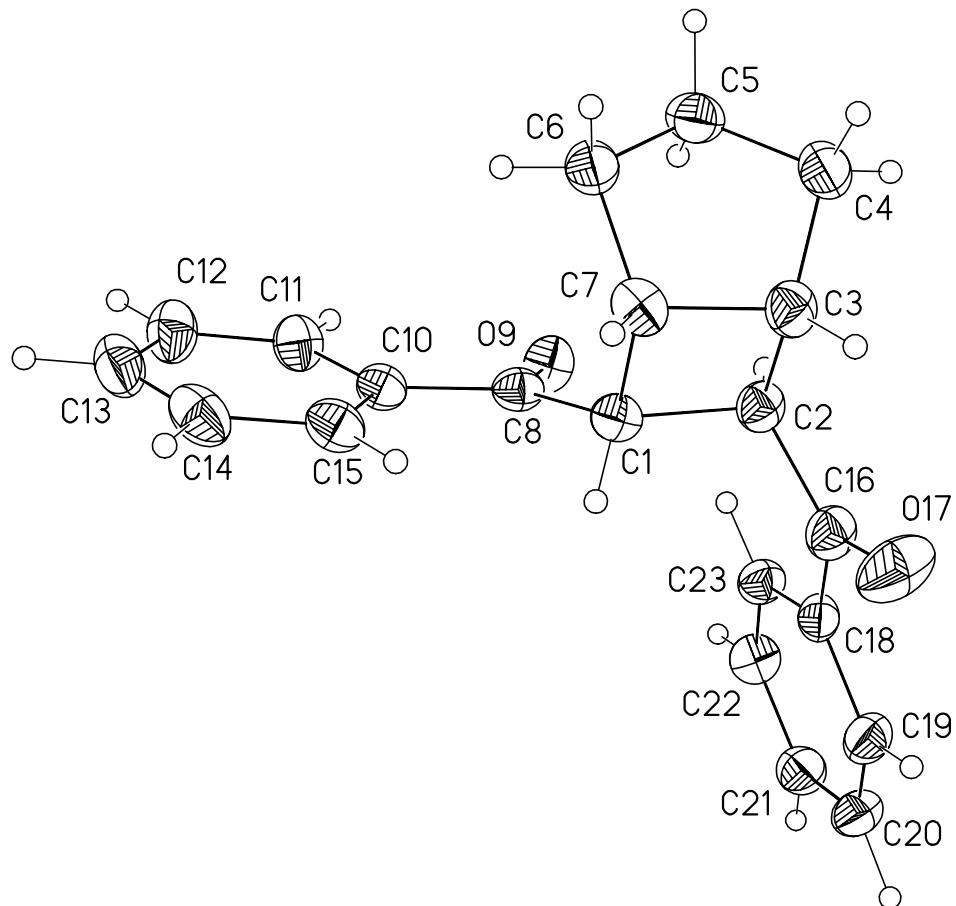


Figure 2. Unit cell packing diagram for **1**. The view is approximately down the **b** axis.

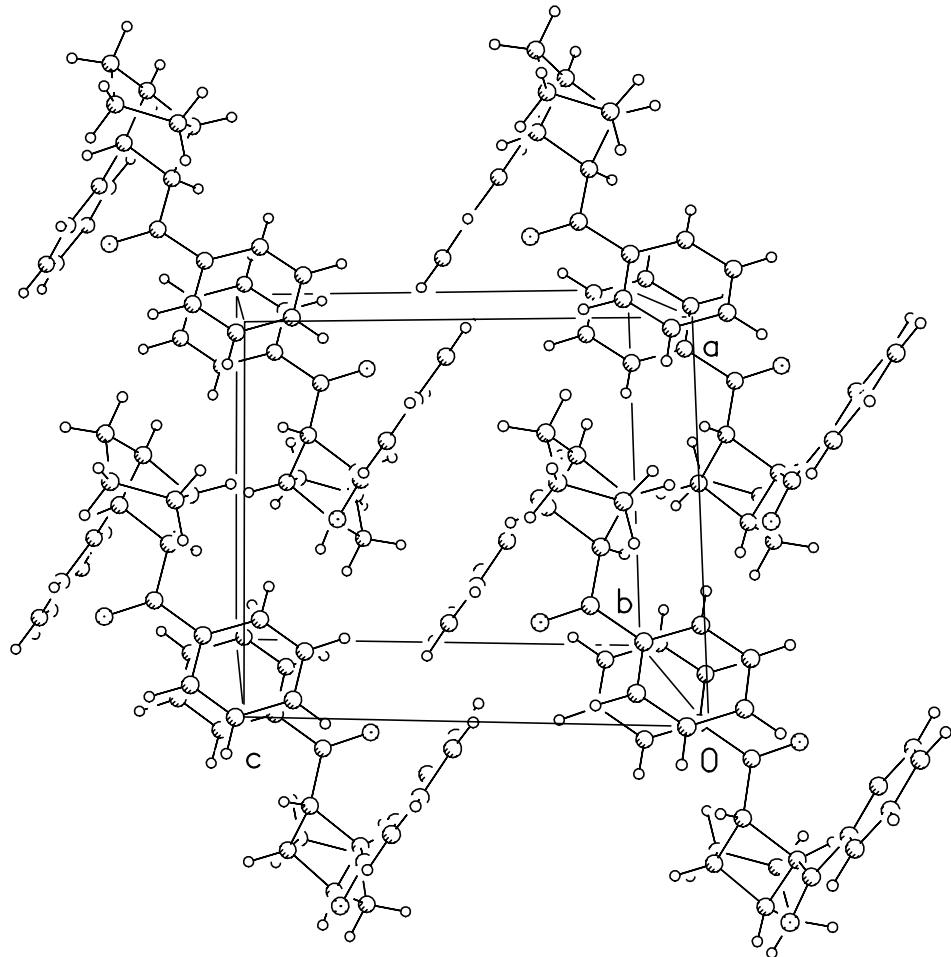


Table 6. Observed and calculated structure factors for 1

Page 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
2	0	0	166	174	1	7	4	0	113	113	1	6	9	0	14	4	7	-10	-6	1	60	58	2
3	0	0	165	171	1	8	4	0	37	43	1	7	9	0	75	76	2	-9	-6	1	63	72	1
4	0	0	33	38	1	9	4	0	52	58	1	8	9	0	0	14	1	-8	-6	1	101	102	2
5	0	0	98	97	1	10	4	0	30	32	2	9	9	0	20	22	4	-7	-6	1	19	26	2
6	0	0	55	55	1	11	4	0	34	31	4	10	9	0	52	47	3	-6	-6	1	95	98	1
7	0	0	77	78	1	-8	5	0	8	1	-1	10	0	6	11	6	-5	-6	1	73	78	1	
8	0	0	108	110	2	-7	5	0	18	27	5	0	10	0	4	8	3	-4	-6	1	159	167	2
9	0	0	20	21	6	-6	5	0	32	30	5	1	10	0	30	27	3	-3	-6	1	42	41	1
10	0	0	5	8	5	-5	5	0	28	27	6	2	10	0	4	5	4	-2	-6	1	65	64	1
11	0	0	0	9	1	-4	5	0	93	90	1	3	10	0	25	29	2	-1	-6	1	71	75	1
-10	1	0	9	1	8	-3	5	0	13	14	2	4	10	0	9	14	8	0	-6	1	95	97	1
-9	1	0	57	61	2	-2	5	0	83	81	1	5	10	0	7	9	7	1	-6	1	42	40	1
-8	1	0	23	23	3	-1	5	0	44	45	1	6	10	0	92	90	2	-2	-6	1	76	75	1
-7	1	0	46	47	1	0	5	0	68	67	1	7	10	0	0	3	1	3	-6	1	77	78	1
-6	1	0	30	34	1	1	5	0	142	138	1	8	10	0	48	50	3	4	-6	1	44	45	1
-5	1	0	11	10	1	2	5	0	38	40	1	9	10	0	0	6	1	5	-6	1	32	34	4
-4	1	0	116	116	1	3	5	0	111	107	1	1	11	0	51	49	3	6	-6	1	6	11	6
-3	1	0	30	33	1	4	5	0	198	196	2	2	11	0	10	18	10	-11	-5	1	0	10	1
-2	1	0	215	217	1	5	5	0	103	107	1	3	11	0	0	0	1	-10	-5	1	38	37	2
-1	1	0	87	87	1	6	5	0	4	9	3	4	11	0	15	22	7	-9	-5	1	171	179	3
2	1	0	170	174	1	7	5	0	9	6	9	5	11	0	24	26	4	-8	-5	1	10	4	5
3	1	0	228	240	1	8	5	0	51	63	1	6	11	0	22	19	6	-7	-5	1	64	63	2
4	1	0	382	378	3	9	5	0	34	33	3	7	11	0	24	21	5	-6	-5	1	94	94	1
5	1	0	12	12	1	10	5	0	61	59	2	8	11	0	0	13	1	-5	-5	1	27	25	1
6	1	0	47	50	1	11	5	0	12	12	7	-7	11	1	6	9	6	-4	-5	1	171	167	2
7	1	0	29	30	1	-7	6	0	25	23	4	-6	11	1	40	33	3	-3	-5	1	66	67	1
8	1	0	103	99	1	-6	6	0	53	52	2	-5	11	1	26	19	11	-2	-5	1	179	169	1
9	1	0	21	21	1	-5	6	0	32	31	2	-4	11	1	9	4	8	-1	-5	1	63	59	1
10	1	0	46	49	2	-4	6	0	43	43	1	-3	11	1	0	8	1	0	-5	1	11	12	2
11	1	0	10	0	10	-3	6	0	108	107	1	-2	11	1	15	5	15	1	-5	1	36	33	1
-10	2	0	64	63	2	-2	6	0	10	11	2	-9	10	1	7	12	6	2	-5	1	79	77	1
-9	2	0	32	32	3	-1	6	0	143	138	1	-8	10	1	30	33	3	-3	-5	1	89	90	1
-8	2	0	19	25	6	0	6	0	70	71	1	-7	10	1	24	26	4	4	-5	1	211	205	2
-7	2	0	51	50	1	1	6	0	17	16	1	-6	10	1	24	26	5	5	-5	1	65	67	2
-6	2	0	84	84	1	2	6	0	66	61	1	-5	10	1	80	74	2	6	-5	1	25	29	2
-5	2	0	129	124	1	3	6	0	40	42	1	-4	10	1	30	22	2	7	-5	1	41	42	2
-4	2	0	94	93	1	4	6	0	28	23	1	-3	10	1	10	1	10	-11	-4	1	35	39	4
-3	2	0	2	0	2	5	6	0	47	54	1	-2	10	1	43	47	2	-10	-4	1	7	8	6
-2	2	0	81	82	1	6	6	0	250	252	3	-1	10	1	9	9	8	-9	-4	1	65	73	3
0	2	0	524	523	19	7	6	0	10	1	0	-10	1	41	40	3	-8	-4	1	36	36	1	
1	2	0	328	333	3	8	6	0	28	33	2	-1	10	1	50	51	4	-7	-4	1	70	72	1
2	2	0	36	38	2	9	6	0	33	32	3	-10	9	1	7	13	7	-6	-4	1	60	55	1
3	2	0	59	55	1	10	6	0	29	31	3	-9	9	1	32	31	3	-5	-4	1	8	8	4
4	2	0	94	90	1	11	6	0	51	57	2	-8	9	1	0	1	1	-4	-4	1	80	75	1
5	2	0	8	7	2	-6	7	0	21	22	5	-7	9	1	0	9	1	-3	-4	1	116	115	1
6	2	0	191	187	1	-5	7	0	56	57	2	-6	9	1	55	47	2	-2	-4	1	231	234	2
7	2	0	123	127	1	-4	7	0	10	12	7	-5	9	1	40	35	2	-1	-4	1	6	0	1
8	2	0	101	100	1	-3	7	0	150	145	2	-4	9	1	0	5	1	0	-4	1	15	9	1
9	2	0	10	9	5	-2	7	0	64	64	1	-3	9	1	47	56	1	1	-4	1	50	50	1
10	2	0	61	61	3	-1	7	0	47	45	1	-2	9	1	102	107	2	2	-4	1	73	73	1
11	2	0	37	31	4	0	7	0	71	72	1	-1	9	1	23	23	2	3	-4	1	87	85	1
-9	3	0	25	28	5	1	7	0	19	18	1	0	-9	1	15	11	6	4	-4	1	33	36	1
-8	3	0	17	8	4	2	7	0	31	33	2	1	-9	1	32	33	2	5	-4	1	38	39	1
-7	3	0	35	35	1	3	7	0	140	137	2	2	-9	1	13	22	13	6	-4	1	18	16	3
-6	3	0	35	32	1	4	7	0	18	21	2	-10	-8	1	0	7	1	7	-4	1	39	41	1
-5	3	0	63	63	1	5	7	0	12	9	4	-9	-8	1	12	4	12	8	-4	1	63	63	2
-4	3	0	74	70	1	6	7	0	125	120	2	-8	8	1	16	15	7	-11	-3	1	20	16	7
-3	3	0	89	89	1	7	7	0	10	4	9	-7	8	1	50	53	2	-10	-3	1	0	9	1
-2	3	0	214	216	2	8	7	0	0	5	1	-6	8	1	54	54	2	-9	-3	1	81	85	2
-1	3	0	139	138	1	-1	8	0	39	36	2	-5	8	1	8	4	8	-8	-3	1	42	44	1
0	3	0	41	39	1	10	7	0	45	37	3	-4	8	1	30	32	1	-7	-3	1	57	59	1
1	3	0	117	119	1	11	7	0	16	17	7	-3	8	1	11	10	5	-6	-3	1	0	9	1
2	3	0	126	124	1	-4	8	0	18	0	9	-2	8	1	13	18	2	-5	-3	1	186	183	1
3	3	0	335	332	3	-3	8	0	21	24	4	-1	8	1	7	5	6	-4	-3	1	47	44	1
4	3	0	249	243	2	-2	8	0	7	8	6	-8	8	1	56	55	1	-3	-3	1	144	149	2
5	3	0	157	150	1	-1	8	0	37	43	1	1	-8	1	6	4	6	-2	-3	1	298	298	3
6	3	0	99	96	1	0	8	0	41	46	1	2	-8	1	75	75	3	-1	-3	1	17	19	1
7	3	0	73	75	1	1	8	0	94	98	1	3	-8	1	32	34	2	0	-3	1	112	109	1
8	3	0	14	13	3	2	8	0	75	83	2												

Table 6. Observed and calculated structure factors for 1

Page 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
5	2	1	3	9	3	-6	7	1	34	36	3	-3	-9	2	30	25	2	2	-4	2	40	41	1
6	2	1	22	20	1	-5	7	1	28	26	4	-2	-9	2	47	48	1	3	-4	2	4	3	4
7	2	1	6	3	6	-4	7	1	71	70	1	-1	-9	2	14	5	13	4	-4	2	94	96	1
8	2	1	40	41	2	-3	7	1	92	93	1	0	-9	2	32	31	2	5	-4	2	40	42	1
9	2	1	19	17	2	-2	7	1	177	176	2	1	-9	2	5	3	4	6	-4	2	53	54	1
10	2	1	82	79	2	-1	7	1	222	220	3	2	-9	2	37	30	5	7	-4	2	85	84	3
11	2	1	0	12	1	0	7	1	41	42	1	-10	-8	2	26	32	5	8	-4	2	34	29	3
-9	3	1	36	38	3	1	7	1	15	14	1	-9	-8	2	55	54	2	-11	-3	2	45	50	5
-8	3	1	24	26	3	2	7	1	72	69	2	-8	-8	2	28	26	3	-10	-3	2	53	53	2
-7	3	1	59	60	1	3	7	1	121	118	1	-7	-8	2	37	34	3	-9	-3	2	51	55	2
-6	3	1	18	23	6	4	7	1	28	33	1	-6	-8	2	49	51	1	-8	-3	2	6	13	6
-5	3	1	126	122	1	5	7	1	101	106	1	-5	-8	2	29	32	2	-7	-3	2	67	68	1
-4	3	1	69	70	1	6	7	1	247	243	4	-4	-8	2	67	70	1	-6	-3	2	38	37	1
-3	3	1	110	110	1	7	7	1	129	132	1	-3	-8	2	106	107	2	-5	-3	2	150	151	1
-2	3	1	468	460	4	8	7	1	19	21	3	-2	-8	2	11	8	2	-4	-3	2	211	203	2
-1	3	1	28	27	1	9	7	1	76	73	1	-1	-8	2	52	57	1	-3	-3	2	35	36	1
0	3	1	449	444	4	10	7	1	34	34	2	0	-8	2	91	90	1	-2	-3	2	178	175	2
1	3	1	35	33	1	11	7	1	11	8	11	1	-8	2	18	24	2	-1	-3	2	78	76	1
2	3	1	59	66	1	-5	8	1	53	43	4	2	-8	2	15	15	3	0	-3	2	76	71	1
3	3	1	408	405	4	-4	8	1	24	1	6	3	-8	2	31	34	3	1	-3	2	170	171	1
4	3	1	17	17	1	-3	8	1	28	36	2	-11	-7	2	16	21	12	2	-3	2	174	173	1
5	3	1	272	270	3	-2	8	1	40	41	1	-10	-7	2	14	7	7	3	-3	2	44	46	1
6	3	1	170	164	1	-1	8	1	50	51	1	-9	-7	2	0	4	1	4	-3	2	0	7	1
7	3	1	99	101	1	0	8	1	16	19	2	-8	-7	2	10	1	9	5	-3	2	133	133	1
8	3	1	47	51	1	1	8	1	72	78	1	-7	-7	2	25	26	2	6	-3	2	26	27	1
9	3	1	20	25	2	2	8	1	11	12	4	-6	-7	2	68	69	1	7	-3	2	63	63	2
10	3	1	21	18	5	3	8	1	117	119	2	-5	-7	2	265	260	4	8	-3	2	46	49	2
11	3	1	0	11	1	4	8	1	9	10	9	-4	-7	2	101	97	1	9	-3	2	7	7	1
-8	4	1	13	1	13	5	8	1	96	97	1	-3	-7	2	40	38	1	-11	-2	2	6	14	6
-7	4	1	65	65	2	6	8	1	71	73	1	-2	-7	2	35	38	1	-10	-2	2	4	0	4
-6	4	1	60	61	1	7	8	1	121	119	2	-1	-7	2	25	32	1	-9	-2	2	116	118	1
-5	4	1	0	4	1	8	8	1	32	32	2	0	-7	2	4	7	3	-8	-2	2	39	42	1
-4	4	1	20	16	1	9	8	1	0	3	1	1	-7	2	84	84	1	7	-2	2	63	62	2
-3	4	1	12	15	2	10	8	1	16	11	6	2	-7	2	10	7	6	-6	-2	2	21	27	1
-2	4	1	453	445	4	11	8	1	34	34	4	3	-7	2	26	26	4	-5	-2	2	22	20	1
-1	4	1	248	248	1	-3	9	1	37	41	4	4	-7	2	39	44	2	-4	-2	2	185	172	1
0	4	1	8	10	3	-2	9	1	0	3	1	5	-7	2	41	41	4	-3	-2	2	241	233	2
1	4	1	53	49	1	-1	9	1	20	18	4	-11	-6	2	18	7	7	-2	-2	2	26	31	1
2	4	1	13	12	1	0	9	1	66	65	1	-10	-6	2	35	40	3	-1	-2	2	143	150	1
3	4	1	154	157	1	1	9	1	14	15	3	-9	-6	2	53	54	2	0	-2	2	65	66	1
4	4	1	20	21	1	2	9	1	66	65	2	-8	-6	2	11	3	7	1	-2	2	16	15	1
5	4	1	111	109	1	3	9	1	10	10	4	-7	-6	2	28	29	2	2	-2	2	109	111	1
6	4	1	6	5	6	4	9	1	12	5	7	-6	-6	2	58	57	1	3	-2	2	15	14	1
7	4	1	51	53	1	5	9	1	42	46	2	-5	-6	2	148	148	1	4	-2	2	156	157	1
8	4	1	40	38	1	6	9	1	36	30	2	-4	-6	2	222	222	3	5	-2	2	50	48	1
9	4	1	31	33	1	7	9	1	5	19	5	-3	-6	2	0	5	1	6	-2	2	39	38	1
10	4	1	26	31	3	8	9	1	18	20	4	-2	-6	2	106	105	1	7	-2	2	126	120	1
11	4	1	17	12	16	9	9	1	0	5	1	-1	-6	2	3	2	2	8	-2	2	28	29	2
-8	5	1	34	27	5	10	9	1	9	3	8	0	-6	2	5	6	5	9	-2	2	130	124	3
-7	5	1	41	41	3	-2	10	1	0	6	1	1	-6	2	22	22	1	-11	-1	2	25	23	10
-6	5	1	15	6	6	-1	10	1	13	0	13	2	-6	2	77	75	1	-10	-1	2	32	33	2
-5	5	1	30	32	1	0	10	1	29	27	2	3	-6	2	82	84	1	9	-1	2	13	6	6
-4	5	1	89	90	1	1	10	1	53	51	2	4	-6	2	28	31	2	-8	-1	2	25	31	2
-3	5	1	152	151	1	2	10	1	17	19	4	5	-6	2	119	114	2	-7	-1	2	103	104	1
-2	5	1	202	200	2	3	10	1	41	43	2	6	-6	2	0	12	1	6	-1	2	15	13	1
-1	5	1	204	202	1	4	10	1	54	52	7	-11	-5	2	65	69	2	-5	-1	2	118	121	1
0	5	1	119	115	1	5	10	1	28	25	3	-10	-5	2	16	24	6	-4	-1	2	41	42	1
1	5	1	61	61	1	6	10	1	15	14	5	-9	-5	2	29	34	3	-3	-1	2	192	189	1
2	5	1	192	195	1	7	10	1	23	22	3	-8	-5	2	60	64	1	-2	-1	2	340	342	3
3	5	1	310	300	3	8	10	1	22	22	5	-7	-5	2	24	24	2	-1	-1	2	9	11	2
4	5	1	80	81	1	9	10	1	0	3	1	-6	-5	2	18	26	3	0	-1	2	250	255	2
5	5	1	118	116	1	0	11	1	54	49	3	-5	-5	2	10	3	3	1	-1	2	647	630	7
6	5	1	25	31	1	1	11	1	0	1	1	-4	-5	2	110	114	2	2	-1	2	43	41	1
7	5	1	31	29	2	2	11	1	34	33	3	-3	-5	2	69	71	1	3	-1	2	14	14	2
8	5	1	64	69	1	3	11	1	0	4	1	-2	-5	2	150	149	1	4	-1	2	97	97	1
9	5	1	45	46	1	4	11	1	35	29	3	-1	-5	2	39	42	1	5	-1	2	116	116	1
10	5	1	170	161	3	5	11	1	16	8	6	0	-5	2	177	167	1	6	-1	2	28	28	1
11	5	1	60	58	4	6	11	1	16	10	7	1	-5	2	24	25	1	7	-1	2	17	19	3
-7	6	1	35	38	3	7																	

Table 6. Observed and calculated structure factors for 1

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<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s
10	4	2	89	87	3	7	9	2	26	30	2	0	-6	3	7	6	6	-11	-1	3	74	76	3
11	4	2	27	23	5	8	9	2	40	42	2	1	-6	3	87	86	1	-10	-1	3	10	1	105
-8	5	2	19	28	18	9	9	2	22	18	3	2	-6	3	58	60	1	-9	-1	3	0	5	1
-7	5	2	10	10	10	10	9	2	19	11	7	3	-6	3	60	58	3	-8	-1	3	34	40	1
-6	5	2	47	47	2	-2	10	2	51	47	4	4	-6	3	95	91	1	-7	-1	3	132	132	1
-5	5	2	10	14	5	-1	10	2	83	79	4	5	-6	3	88	86	2	-6	-1	3	12	13	2
-4	5	2	220	220	3	0	10	2	26	29	4	6	-6	3	19	13	14	-5	-1	3	30	27	2
-3	5	2	20	19	1	1	10	2	28	25	2	-11	-5	3	20	24	8	-4	-1	3	116	115	1
-2	5	2	46	48	1	2	10	2	117	113	2	-10	-5	3	0	1	1	-3	-1	3	36	34	2
-1	5	2	53	54	1	3	10	2	5	1	5	-9	-5	3	17	19	4	-2	-1	3	71	69	1
0	5	2	63	68	1	4	10	2	52	62	2	-8	-5	3	92	96	1	-1	-1	3	125	124	1
1	5	2	157	152	1	5	10	2	42	44	2	-7	-5	3	50	53	1	0	-1	3	78	82	1
2	5	2	169	166	2	6	10	2	42	40	2	-6	-5	3	61	59	2	1	-1	3	171	171	1
3	5	2	55	52	1	7	10	2	23	7	7	-5	-5	3	49	52	6	2	-1	3	70	70	1
4	5	2	132	139	1	8	10	2	25	21	5	-4	-5	3	75	77	1	3	-1	3	39	40	1
5	5	2	42	47	1	9	10	2	19	22	6	-3	-5	3	43	44	1	4	-1	3	255	250	2
6	5	2	18	15	1	10	10	2	35	32	4	-2	-5	3	132	129	1	5	-1	3	30	25	1
7	5	2	0	4	1	0	11	2	18	10	8	-1	-5	3	53	52	1	6	-1	3	173	175	1
8	5	2	24	28	2	1	11	2	26	31	3	0	-5	3	34	34	1	7	-1	3	129	125	1
9	5	2	4	1	4	2	11	2	27	28	3	1	-5	3	17	17	1	8	-1	3	51	50	2
10	5	2	56	52	2	3	11	2	42	35	2	2	-5	3	53	51	1	9	-1	3	44	42	2
11	5	2	42	42	4	4	11	2	44	42	2	3	-5	3	61	64	1	10	-1	3	16	16	2
-7	6	2	0	5	1	5	11	2	37	41	3	4	-5	3	100	100	2	-10	0	3	86	83	3
-6	6	2	27	28	3	6	11	2	11	10	5	-5	-3	3	104	101	2	-9	0	3	40	41	3
-5	6	2	34	37	3	7	11	2	0	4	1	6	-5	3	68	70	2	-8	0	3	43	42	2
-4	6	2	10	14	7	8	11	2	25	11	5	7	-5	3	12	9	12	-7	0	3	156	153	1
-3	6	2	16	15	2	3	12	2	33	34	3	-11	-4	3	17	8	7	-6	0	3	178	180	1
-2	6	2	483	470	4	4	12	2	58	51	3	-10	-4	3	29	27	3	-5	0	3	0	9	1
-1	6	2	116	114	1	5	12	2	31	29	5	-9	-4	3	14	9	9	-4	0	3	78	79	1
0	6	2	59	59	1	6	12	2	0	16	1	-8	-4	3	43	45	2	-3	0	3	101	101	1
1	6	2	129	133	1	-7	10	3	68	61	3	-7	-4	3	140	145	2	-2	0	3	323	329	2
2	6	2	128	130	1	-6	10	3	26	11	9	-6	-4	3	10	1	3	-1	0	3	24	20	1
3	6	2	121	118	1	-5	10	3	35	42	7	-5	-4	3	67	72	1	0	0	3	7	6	7
4	6	2	26	22	1	-4	10	3	127	115	5	-4	-4	3	137	138	1	1	0	3	484	485	4
5	6	2	104	106	1	-3	10	3	28	39	7	-3	-4	3	46	44	1	2	0	3	126	126	1
6	6	2	14	18	9	-2	10	3	0	6	1	-2	-4	3	124	125	1	3	0	3	39	38	1
7	6	2	88	85	4	-1	10	3	15	20	14	-1	-4	3	116	113	1	4	0	3	35	35	1
8	6	2	0	7	1	-9	9	3	0	1	1	0	-4	3	37	40	1	5	0	3	110	110	1
9	6	2	17	15	10	-8	9	3	30	26	3	1	-4	3	165	162	1	6	0	3	32	32	1
10	6	2	34	38	2	-7	9	3	0	6	1	2	-4	3	134	133	1	7	0	3	10	11	9
11	6	2	0	1	1	-6	9	3	18	24	5	3	-4	3	5	2	5	5	0	3	183	173	4
-6	7	2	28	34	3	-5	9	3	27	28	3	4	-4	3	124	121	1	9	0	3	75	79	2
-5	7	2	46	55	2	-4	9	3	57	56	2	5	-4	3	48	47	1	10	0	3	50	55	3
-4	7	2	97	101	2	-3	9	3	58	59	2	6	-4	3	5	11	5	-9	1	3	18	3	6
-3	7	2	44	45	1	-2	9	3	60	57	2	7	-4	3	42	42	2	-8	1	3	20	21	3
-2	7	2	146	144	2	-1	9	3	68	71	3	8	-4	3	0	5	1	-7	1	3	54	56	1
-1	7	2	12	11	2	0	9	3	18	13	6	-11	-3	3	44	42	2	-6	1	3	193	194	2
0	7	2	112	111	1	1	9	3	40	43	4	-10	-3	3	15	0	6	-5	1	3	62	63	1
1	7	2	106	105	1	-10	8	3	0	8	1	-9	-3	3	37	38	2	-4	1	3	216	214	2
2	7	2	167	170	2	-9	8	3	40	33	3	-8	-3	3	46	44	2	-3	1	3	42	41	1
3	7	2	112	115	1	-8	8	3	57	46	3	-7	-3	3	124	129	2	-2	1	3	76	81	1
4	7	2	44	46	1	-7	8	3	0	7	1	-6	-3	3	91	92	1	-1	1	3	63	68	1
5	7	2	4	8	3	-6	8	3	15	17	5	-5	-3	3	45	44	1	0	1	3	352	360	3
6	7	2	69	74	1	-5	8	3	10	6	10	-4	-3	3	79	79	1	1	1	3	191	199	1
7	7	2	88	85	1	-4	8	3	89	88	1	-3	-3	3	19	19	1	2	1	3	622	619	11
8	7	2	56	59	2	-3	8	3	88	90	1	-2	-3	3	26	28	1	3	1	3	157	153	2
9	7	2	6	3	6	-2	8	3	5	6	5	-1	-3	3	227	216	2	4	1	3	181	178	1
10	7	2	38	40	3	-1	8	3	54	53	2	0	-3	3	22	19	1	5	1	3	120	117	1
11	7	2	0	9	1	0	8	3	13	11	12	1	-3	3	64	62	1	6	1	3	34	36	1
-5	8	2	9	13	9	1	-8	3	53	51	1	2	-3	3	78	79	1	7	1	3	76	74	1
-4	8	2	26	27	3	-2	8	3	46	45	2	3	-3	3	81	81	1	8	1	3	243	247	2
-3	8	2	70	77	2	-10	7	3	9	8	4	-4	-3	3	11	12	2	9	1	3	64	63	2
-2	8	2	59	63	1	-9	7	3	10	4	10	5	-3	3	107	105	1	10	1	3	121	116	3
-1	8	2	21	20	1	-8	7	3	36	38	2	6	-3	3	56	56	2	-10	2	3	10	7	10
0	8	2	23	22	1	-7	7	3	48	50	2	7	-3	3	9	9	9	-9	2	3	30	34	3
1	8	2	32	34	1	-6	7	3	11	12	6	8	-3	3	17	20	7	-8	2	3	5	5	4
2	8	2	38	44	1	-5	7	3	150	149	3	-11	-2	3	0	11	1	-7	2	3	14	16	3
3	8	2	43	36	1	-4	7	3	37	37	1	-10	-										

Table 6. Observed and calculated structure factors for 1

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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	7	3	13	13	2	-2	-8	4	27	28	4	4	-3	4	84	83	1	10	1	4	18	19	6
4	7	3	18	21	1	-1	-8	4	12	11	12	5	-3	4	66	65	1	-9	2	4	29	33	2
5	7	3	99	101	1	0	-8	4	23	15	6	6	-3	4	70	67	1	-8	2	4	34	36	2
6	7	3	138	137	2	1	-8	4	42	38	3	7	-3	4	11	12	7	-7	2	4	18	18	2
7	7	3	216	211	2	2	-8	4	21	19	7	8	-3	4	62	58	4	-6	2	4	81	81	1
8	7	3	159	155	3	-10	-7	4	10	6	9	-11	-2	4	11	21	10	-5	2	4	47	49	1
9	7	3	19	19	4	-9	-7	4	46	45	2	-10	-2	4	13	1	-4	2	4	9	15	3	
10	7	3	32	32	2	-8	-7	4	35	33	3	-9	-2	4	47	51	1	-3	2	4	17	12	1
11	7	3	65	51	5	-7	-7	4	23	27	8	-8	-2	4	29	30	2	-2	2	4	353	344	3
-5	8	3	50	48	4	-6	-7	4	8	10	8	-7	-2	4	71	72	1	-1	2	4	181	184	2
-4	8	3	33	40	3	-5	-7	4	152	150	2	-6	-2	4	92	96	1	0	2	4	60	59	1
-3	8	3	129	130	3	-4	-7	4	275	272	6	-5	-2	4	182	184	2	1	2	4	113	113	1
-2	8	3	0	3	1	-3	-7	4	11	11	4	-4	-2	4	65	67	1	2	2	4	185	182	1
-1	8	3	101	101	1	-2	-7	4	7	2	7	-3	-2	4	133	126	1	3	2	4	162	161	1
0	8	3	66	66	1	-1	-7	4	4	10	4	-2	-2	4	168	160	2	4	2	4	129	126	1
1	8	3	72	74	1	0	-7	4	49	47	2	-1	-2	4	19	24	1	5	2	4	63	60	1
2	8	3	7	9	7	1	-7	4	0	0	1	0	-2	4	134	131	1	6	2	4	127	127	1
3	8	3	83	80	1	2	-7	4	20	21	3	1	-2	4	206	203	2	7	2	4	131	131	1
4	8	3	66	72	2	3	-7	4	50	48	3	2	-2	4	16	14	1	8	2	4	80	77	1
5	8	3	44	45	1	4	-7	4	81	77	4	3	-2	4	29	32	1	9	2	4	9	4	8
6	8	3	32	30	2	-10	-6	4	36	40	3	4	-2	4	17	16	1	10	2	4	33	36	5
7	8	3	37	35	2	-9	-6	4	48	53	2	5	-2	4	67	68	2	11	2	4	40	40	3
8	8	3	133	129	2	-8	-6	4	48	47	2	6	-2	4	16	18	1	-9	3	4	41	38	5
9	8	3	7	14	6	-7	-6	4	40	39	2	7	-2	4	29	28	2	-8	3	4	47	45	2
10	8	3	24	22	4	-6	-6	4	26	28	2	8	-2	4	6	7	5	-7	3	4	4	1	3
11	8	3	0	1	1	-5	-6	4	111	111	2	9	-2	4	35	28	4	-6	3	4	27	32	2
-4	9	3	100	94	4	-4	-6	4	39	43	1	-10	-1	4	26	25	3	-5	3	4	57	55	1
-3	9	3	11	19	11	-3	-6	4	221	215	2	-9	-1	4	33	35	4	-4	3	4	93	95	1
-2	9	3	28	27	3	-2	-6	4	50	52	1	-8	-1	4	39	40	2	-3	3	4	119	118	1
-1	9	3	62	60	2	-1	-6	4	18	17	1	-7	-1	4	107	106	2	-2	3	4	53	50	1
0	9	3	0	1	1	0	-6	4	5	7	5	-6	-1	4	116	115	1	-1	3	4	167	168	1
1	9	3	82	75	1	1	-6	4	72	72	1	-5	-1	4	126	128	1	0	3	4	19	22	1
2	9	3	42	42	1	2	-6	4	52	49	1	-4	-1	4	28	34	1	1	3	4	98	105	1
3	9	3	88	96	1	3	-6	4	13	17	13	-3	-1	4	17	12	2	2	3	4	215	214	2
4	9	3	72	75	1	4	-6	4	48	47	2	-2	-1	4	242	234	3	3	3	4	346	339	3
5	9	3	5	4	5	5	-6	4	0	5	1	-1	-1	4	296	294	3	4	3	4	14	16	1
6	9	3	27	26	3	-10	-5	4	6	4	6	0	-1	4	91	94	1	5	3	4	22	18	8
7	9	3	0	2	1	-9	-5	4	65	59	2	1	-1	4	195	193	1	6	3	4	75	78	1
8	9	3	0	9	1	-8	-5	4	25	38	3	2	-1	4	242	237	1	7	3	4	39	37	3
9	9	3	44	44	2	-7	-5	4	0	10	1	3	-1	4	103	104	1	8	3	4	13	10	4
10	9	3	28	20	3	-6	-5	4	160	157	2	4	-1	4	81	80	1	9	3	4	62	63	2
-2	10	3	46	51	4	-5	-5	4	9	2	8	5	-1	4	18	17	1	10	3	4	15	8	14
-1	10	3	41	41	3	-4	-5	4	182	181	2	6	-1	4	32	32	1	11	3	4	5	2	5
0	10	3	40	42	5	-3	-5	4	140	139	1	7	-1	4	38	43	1	-8	4	4	25	22	4
1	10	3	14	13	4	-2	-5	4	23	24	2	8	-1	4	35	36	2	-7	4	4	30	33	3
2	10	3	24	23	2	-1	-5	4	143	136	1	9	-1	4	11	18	10	-6	4	4	47	56	3
3	10	3	21	22	3	0	-5	4	18	17	1	-10	0	4	14	13	13	-5	4	4	68	73	1
4	10	3	0	9	1	1	-5	4	121	120	1	-9	0	4	9	7	9	-4	4	4	57	60	1
5	10	3	39	47	2	2	-5	4	91	90	1	-8	0	4	71	70	1	-3	4	4	20	23	1
6	10	3	0	2	1	3	-5	4	68	69	1	-7	0	4	157	158	1	-2	4	4	41	39	1
7	10	3	26	27	3	4	-5	4	40	39	1	-6	0	4	164	165	1	-1	4	4	93	92	1
8	10	3	10	11	9	5	-5	4	17	14	5	-5	0	4	38	41	2	0	4	4	121	124	1
9	10	3	3	0	3	6	-5	4	39	39	3	-4	0	4	153	154	1	1	4	4	238	242	2
10	10	3	30	21	3	-11	-4	4	0	0	1	-3	0	4	40	39	1	2	4	4	118	117	1
0	11	3	0	11	1	-10	-4	4	31	30	5	-2	0	4	0	5	1	3	4	4	129	126	1
1	11	3	40	39	4	-9	-4	4	28	34	3	-1	0	4	114	115	1	4	4	4	21	19	1
2	11	3	10	4	10	-8	-4	4	59	61	2	0	0	4	123	118	1	5	4	4	189	187	1
3	11	3	0	3	1	-7	-4	4	55	61	1	1	0	4	129	133	1	6	4	4	255	252	2
4	11	3	3	2	3	-6	-4	4	103	97	1	2	0	4	12	14	1	7	4	4	240	238	2
5	11	3	9	12	9	-4	-4	4	165	171	2	3	0	4	217	213	2	8	4	4	45	46	1
6	11	3	35	31	3	-4	-4	4	183	184	2	4	0	4	60	61	1	9	4	4	26	21	5
7	11	3	43	39	2	-3	-4	4	82	82	1	5	0	4	33	33	1	10	4	4	21	22	4
8	11	3	142	125	5	-2	-4	4	18	19	1	6	0	4	27	29	2	11	4	4	62	57	4
9	11	3	57	58	3	-1	-4	4	0	3	1	7	0	4	82	85	1	-8	5	4	16	4	15
2	12	3	7	8	7	0	-4	4	174	169	1	8	0	4	62	64	1	-7	5	4	15	20	6
3	12	3	14	8	13	1	-4	4	48	47	1	9	0	4	72	68	5	-6	5	4	5	12	4
4	12	3	22	17	5	2	-4	4	14	14	1	10	0	4	33	35	4	-5	5	4	11	0	7
5	12	3	4	10	4	3	-4	4	8	3	4	-10	1	4	67	60	4	-4	5	4	117	123	2
6	12	3	14	9	8																		

Table 6. Observed and calculated structure factors for 1

Page 5

<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	
2	12	4	19	5	14	-7	-3	5	122	119	2	3	1	5	372	371	3	11	5	5	15	15	15	
3	12	4	18	26	7	-6	-3	5	18	17	4	4	1	5	100	95	1	-7	6	5	40	37	6	
4	12	4	0	18	1	-5	-3	5	82	78	1	5	1	5	35	33	1	-6	6	5	72	70	2	
5	12	4	3	2	3	-4	-3	5	37	42	1	6	1	5	141	136	1	-5	6	5	22	19	12	
6	12	4	5	9	5	-3	-3	5	39	37	1	7	1	5	8	4	8	-4	6	5	38	41	2	
7	12	4	0	8	1	-2	-3	5	93	89	1	8	1	5	13	13	12	-3	6	5	51	54	1	
-6	-9	5	0	9	1	-1	-3	5	13	11	1	9	1	5	6	7	6	-2	6	5	56	57	1	
-5	-9	5	0	4	1	0	-3	5	82	79	1	10	1	5	14	25	14	-1	6	5	63	70	2	
-4	-9	5	70	68	5	1	-3	5	9	11	4	-9	2	5	93	85	3	0	6	5	222	218	2	
-3	-9	5	30	34	5	2	-3	5	111	112	1	-8	2	5	10	9	9	1	6	5	59	59	1	
-2	-9	5	35	32	5	3	-3	5	103	102	1	-7	2	5	119	112	1	2	6	5	73	78	1	
-1	-9	5	33	30	7	4	-3	5	20	17	1	-6	2	5	90	92	2	3	6	5	25	27	3	
-8	-8	5	0	7	1	5	-3	5	47	48	2	-5	2	5	64	67	2	4	6	5	58	59	1	
-7	-8	5	39	41	3	6	-3	5	30	34	2	-4	2	5	52	54	1	5	6	5	82	82	1	
-6	-8	5	13	11	13	7	-3	5	5	17	5	-3	2	5	198	198	2	6	6	5	280	279	3	
-5	-8	5	34	44	3	-10	-2	5	26	15	6	-2	2	5	77	74	1	7	6	5	28	31	1	
-4	-8	5	19	24	18	-9	-2	5	19	11	4	-1	2	5	101	104	1	8	6	5	120	119	1	
-3	-8	5	3	9	3	-8	-2	5	7	15	7	0	2	5	113	111	1	9	6	5	4	1	4	
-2	-8	5	13	15	7	-7	-2	5	52	54	1	1	2	5	78	79	1	10	6	5	46	38	4	
-1	-8	5	14	17	13	-6	-2	5	236	236	3	2	2	5	239	235	2	11	6	5	20	13	12	
0	-8	5	31	35	3	-5	-2	5	102	102	1	3	2	5	14	18	1	-6	7	5	17	19	17	
1	-8	5	38	42	4	-4	-2	5	32	30	1	4	2	5	11	11	2	-5	7	5	16	9	6	
-9	-7	5	56	51	3	-3	-2	5	144	140	1	5	2	5	121	121	2	-4	7	5	33	34	4	
-8	-7	5	39	32	3	-2	-2	5	15	18	1	6	2	5	107	106	1	-3	7	5	38	36	2	
-7	-7	5	30	29	3	-1	-2	5	281	266	2	7	2	5	87	85	1	-2	7	5	23	23	3	
-6	-7	5	13	11	13	0	-2	5	30	30	1	8	2	5	32	31	4	-1	7	5	64	66	2	
-5	-7	5	37	39	2	1	-2	5	96	98	1	9	2	5	46	50	1	0	7	5	80	82	1	
-4	-7	5	42	48	2	2	-2	5	39	41	1	10	2	5	51	45	3	1	7	5	17	17	9	
-3	-7	5	14	11	4	3	-2	5	27	26	1	-9	3	5	22	22	6	2	7	5	27	28	2	
-2	-7	5	27	30	2	4	-2	5	8	5	4	-8	3	5	60	56	2	3	7	5	23	21	5	
-1	-7	5	57	56	2	5	-2	5	26	28	1	-7	3	5	10	15	10	4	7	5	114	115	1	
0	-7	5	11	10	11	6	-2	5	54	57	1	-6	3	5	4	3	3	5	7	5	52	54	1	
1	-7	5	6	15	6	7	-2	5	22	26	3	-5	3	5	10	5	10	6	7	5	78	73	1	
2	-7	5	18	18	5	8	-2	5	18	17	5	-4	3	5	81	78	1	7	7	5	28	31	1	
3	-7	5	20	26	6	-10	-1	5	66	60	2	-3	3	5	137	134	1	8	7	5	107	108	2	
-9	-6	5	18	25	7	-9	-1	5	12	10	6	-2	3	5	134	131	1	9	7	5	142	135	3	
-8	-6	5	14	18	6	-8	-1	5	112	108	2	-1	3	5	10	8	2	10	7	5	41	40	3	
-7	-6	5	25	21	3	-7	-1	5	66	65	1	0	3	5	105	99	1	11	7	5	17	4	9	
-6	-6	5	48	53	2	-6	-1	5	97	98	1	1	3	5	91	93	1	-5	8	5	43	43	3	
-5	-6	5	174	172	3	-5	-1	5	121	125	1	2	3	5	63	59	1	-4	8	5	100	92	3	
-4	-6	5	0	3	1	-4	-1	5	74	76	1	3	3	5	92	87	1	-3	8	5	70	68	2	
-3	-6	5	5	5	4	-3	-1	5	147	144	1	4	3	5	4	3	3	-2	8	5	46	49	2	
-2	-6	5	83	82	1	-2	-1	5	2	7	2	5	3	5	44	47	1	-1	8	5	59	61	1	
-1	-6	5	66	64	1	-1	-1	5	153	147	1	6	3	5	50	54	1	0	8	5	127	123	2	
0	-6	5	7	8	7	0	-1	5	25	28	1	7	3	5	52	55	1	1	8	5	134	131	2	
1	-6	5	8	12	8	1	-1	5	53	52	1	8	3	5	50	50	1	2	8	5	108	108	2	
2	-6	5	12	10	6	2	-1	5	172	169	1	9	3	5	23	22	2	3	8	5	56	52	2	
3	-6	5	35	39	5	3	-1	5	18	17	1	10	3	5	6	19	6	4	4	8	5	46	44	2
4	-6	5	56	56	3	4	-1	5	42	41	1	11	3	5	0	1	1	5	8	5	132	131	1	
-10	-5	5	83	68	3	5	-1	5	70	71	1	-8	4	5	20	15	4	6	8	5	8	136	133	2
-9	-5	5	78	71	2	6	-1	5	2	10	1	-7	4	5	31	31	2	7	8	5	13	13	3	
-8	-5	5	42	40	2	7	-1	5	136	133	2	-6	4	5	23	19	4	8	8	5	21	18	2	
-7	-5	5	10	16	9	8	-1	5	25	23	4	-5	4	5	40	53	1	9	8	5	116	112	2	
-6	-5	5	69	75	1	9	-1	5	27	30	6	-4	4	5	11	0	5	10	8	5	28	28	4	
-5	-5	5	45	46	1	-10	0	5	55	49	2	-3	4	5	56	56	1	11	8	5	0	2	1	
-4	-5	5	112	109	2	-9	0	5	23	26	3	-2	4	5	23	21	1	-4	9	5	22	18	8	
-3	-5	5	146	142	2	-8	0	5	72	71	1	-1	4	5	13	9	1	-3	9	5	50	44	2	
-2	-5	5	16	15	1	-7	0	5	120	114	1	0	4	5	112	110	1	-2	9	5	17	18	5	
-1	-5	5	32	31	1	-6	0	5	340	335	3	1	4	5	229	228	2	-1	9	5	43	42	2	
0	-5	5	29	29	1	-5	0	5	205	209	2	2	4	5	103	100	1	0	9	5	65	61	1	
1	-5	5	35	36	1	-4	0	5	26	27	1	3	4	5	285	279	3	1	9	5	21	15	4	
2	-5	5	55	53	1	-3	0	5	74	74	1	4	4	5	154	153	1	2	9	5	20	24	3	
3	-5	5	27	27	2	-2	0	5	25	26	1	5	4	5	46	45	1	3	9	5	0	12	1	
4	-5	5	16	16	7	-1	0	5	151	144	1	6	4	5	119	119	2	4	9	5	193	192	3	
5	-5	5	66	65	2	0	0	5	227	219	2	7	4	5	27	31	1	5	9	5	0	7	1	
6	-5	5	86	89	5	1	0	5	92	91	1	8	4	5	16	18	18	2	6	9	5	78	77	1
-10	-4	5	56	48	2	2	0	5	290	285	1	9	4	5	85	84	2	7	9	5	43	41	1	
-9	-4	5	88	83	2	3	0	5	163	161	1	10	4	5										

Table 6. Observed and calculated structure factors for 1

Page 6

<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	
4	-3	6	31	32	1	-2	2	6	63	64	1	11	6	6	10	18	10	-3	-6	7	36	41	3	
5	-3	6	39	36	3	-1	2	6	107	101	1	-6	7	6	104	98	4	-2	-6	7	160	155	3	
6	-3	6	53	55	2	0	2	6	122	122	1	-5	7	6	53	47	3	-1	-6	7	52	49	3	
7	-3	6	22	23	7	1	2	6	99	100	1	-4	7	6	103	94	2	0	-6	7	46	46	2	
-10	-2	6	45	45	5	2	2	6	15	14	1	-3	7	6	26	29	2	1	-6	7	55	57	3	
-9	-2	6	68	64	2	3	2	6	67	69	1	-2	7	6	61	61	2	2	-6	7	26	16	5	
-8	-2	6	80	77	2	4	2	6	73	73	1	-1	7	6	4	3	4	3	-6	7	47	46	5	
-7	-2	6	104	103	2	5	2	6	74	74	1	0	7	6	72	73	2	-8	-5	7	105	101	3	
-6	-2	6	137	136	2	6	2	6	57	57	1	1	7	6	296	292	4	-7	-5	7	21	2	6	
-5	-2	6	54	55	1	7	2	6	27	29	1	2	7	6	25	29	2	-6	-5	7	30	35	3	
-4	-2	6	51	52	1	8	2	6	34	36	2	3	7	6	0	4	1	-5	-5	7	24	28	2	
-3	-2	6	80	77	1	9	2	6	8	2	7	4	7	6	56	60	1	-4	-5	7	21	25	3	
-2	-2	6	84	82	1	10	2	6	24	26	3	5	7	6	31	30	1	-3	-5	7	27	22	2	
-1	-2	6	118	115	1	-8	3	6	104	96	2	6	7	6	35	36	3	-2	-5	7	84	83	1	
0	-2	6	11	13	1	-7	3	6	77	67	1	7	7	6	71	74	3	-1	-5	7	28	28	3	
1	-2	6	56	60	1	-6	3	6	35	45	2	8	7	6	55	52	1	0	-5	7	6	10	6	
2	-2	6	27	30	1	-5	3	6	35	44	1	9	7	6	46	47	2	1	-5	7	28	28	3	
3	-2	6	94	91	1	-4	3	6	47	44	1	10	7	6	55	57	2	2	-5	7	82	80	2	
4	-2	6	93	91	1	-3	3	6	166	165	2	-5	8	6	19	15	11	3	-3	5	7	19	17	5
5	-2	6	0	2	1	-2	3	6	26	23	1	-4	8	6	37	34	6	4	-5	7	89	82	7	
6	-2	6	45	46	2	-1	3	6	104	108	1	-3	8	6	12	14	7	-9	-4	7	14	21	13	
7	-2	6	12	1	11	0	3	6	304	305	3	-2	8	6	30	31	2	-8	-4	7	11	27	11	
8	-2	6	57	56	3	1	3	6	143	143	1	-1	8	6	63	67	3	-7	-4	7	14	14	14	
-10	-1	6	37	32	4	2	3	6	20	15	1	0	8	6	36	40	1	-6	-4	7	74	71	2	
-9	-1	6	57	59	2	3	3	6	10	13	4	1	8	6	177	172	2	-5	-4	7	96	97	5	
-8	-1	6	31	38	2	4	3	6	139	136	2	2	8	6	127	123	2	-4	-4	7	12	6	4	
-7	-1	6	138	140	2	5	3	6	51	51	1	3	8	6	17	16	3	-3	-4	7	20	22	3	
-6	-1	6	280	274	3	6	3	6	54	59	1	4	8	6	75	76	2	-2	-4	7	94	95	1	
-5	-1	6	80	81	2	7	3	6	41	41	1	5	8	6	134	131	2	-1	-4	7	19	15	1	
-4	-1	6	32	29	1	8	3	6	22	25	2	6	8	6	5	7	5	0	-4	7	31	34	2	
-3	-1	6	133	130	1	9	3	6	30	32	2	7	8	6	28	33	2	1	-4	7	88	88	2	
-2	-1	6	26	25	1	10	3	6	50	47	5	8	8	6	34	35	2	2	-4	7	58	60	1	
-1	-1	6	73	67	1	-8	4	6	52	52	2	9	8	6	75	72	2	3	-4	7	51	53	3	
0	-1	6	26	29	1	-7	4	6	38	40	3	10	8	6	14	15	14	4	-4	7	85	74	4	
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2	-1	6	29	28	1	-5	4	6	42	45	3	-2	9	6	24	20	6	-9	-3	7	0	3	1	
3	-1	6	28	30	1	-4	4	6	56	59	1	-1	9	6	30	33	3	-8	-3	7	12	3	11	
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5	-1	6	15	15	3	-2	4	6	86	85	1	1	9	6	90	92	2	-6	-3	7	59	63	2	
6	-1	6	9	12	4	-1	4	6	54	54	1	2	9	6	48	46	2	-5	-3	7	60	63	1	
7	-1	6	18	20	5	0	4	6	86	82	1	3	9	6	37	32	2	-4	-3	7	15	17	3	
8	-1	6	21	23	7	1	4	6	92	94	1	4	9	6	65	64	2	-3	-3	7	18	16	2	
-9	0	6	10	1	9	2	4	6	52	53	1	5	9	6	42	46	3	-2	-3	7	60	55	1	
-8	0	6	68	70	1	3	4	6	107	108	1	6	9	6	46	45	1	-1	-3	7	141	142	2	
-7	0	6	121	115	2	4	4	6	11	1	2	7	9	6	10	10	7	0	-3	7	0	4	1	
-6	0	6	26	26	1	5	4	6	27	27	1	8	9	6	32	33	2	1	-3	7	6	7	6	
-5	0	6	89	86	1	6	4	6	51	54	1	9	9	6	23	24	3	2	-3	7	86	83	1	
-4	0	6	21	26	1	7	4	6	25	25	1	10	9	6	21	13	8	3	-3	7	26	31	5	
-3	0	6	39	40	1	8	4	6	111	111	2	-2	10	6	13	14	13	4	-3	7	124	123	3	
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0	0	6	186	185	1	-7	5	6	67	61	2	1	10	6	42	37	2	-9	-2	7	66	60	2	
1	0	6	2	11	2	-6	5	6	3	3	2	2	10	6	46	44	3	-8	-2	7	14	4	7	
2	0	6	138	134	1	-5	5	6	36	37	2	3	10	6	10	2	10	-7	-2	7	15	22	4	
3	0	6	68	66	1	-4	5	6	106	108	1	4	10	6	109	107	2	-6	-2	7	40	40	1	
4	0	6	90	89	1	-3	5	6	111	110	2	5	10	6	91	85	3	-5	-2	7	33	35	1	
5	0	6	51	50	1	-2	5	6	42	43	1	6	10	6	16	35	7	4	-2	7	63	64	1	
6	0	6	22	20	1	-1	5	6	54	54	1	7	10	6	22	20	5	-3	-2	7	25	29	1	
7	0	6	31	29	2	0	5	6	71	72	1	8	10	6	10	8	10	-2	-2	7	97	98	1	
8	0	6	21	26	4	1	5	6	50	50	1	9	10	6	22	26	5	-1	-2	7	12	6	2	
9	0	6	32	39	6	2	5	6	66	60	1	0	11	6	31	40	5	0	-2	7	50	51	1	
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-7	1	6	0	8	1	5	5	6	161	161	2	3	11	6	79	75	2	3	-2	7	131	126	2	
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-5	1	6	93	97	1	7	5	6	3	3	3	5	11	6	56	59	2	5	-2	7	12	15	1	
-4	1	6	39	39	1	8	5	6	29	29	2	6	11	6	14	13	8	6	-2	7	17	17	5	
-3	1	6	202	195	2	9	5	6	17	12	6	7	11	6	51	54	2	7						

Table 6. Observed and calculated structure factors for 1

Page 7

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	4	7	36	38	1	2	10	7	63	63	2	-5	-1	8	119	114	2	-3	4	8	40	42	1
8	4	7	26	29	2	3	10	7	26	25	4	-4	-1	8	37	37	2	-2	4	8	50	50	2
9	4	7	59	57	2	4	10	7	92	85	3	-3	-1	8	7	0	7	-1	4	8	44	47	1
10	4	7	0	2	1	5	10	7	0	11	1	-2	-1	8	121	122	1	0	4	8	23	22	1
-7	5	7	27	29	6	6	10	7	35	35	4	-1	-1	8	80	85	1	1	4	8	120	120	1
-6	5	7	30	34	3	7	10	7	44	48	3	0	-1	8	24	26	1	2	4	8	149	148	2
-5	5	7	56	62	3	8	10	7	0	4	1	1	-1	8	188	181	2	3	4	8	30	31	1
-4	5	7	35	38	2	9	10	7	0	10	1	2	-1	8	63	63	1	4	4	8	95	95	1
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0	5	7	34	34	1	3	11	7	0	12	1	6	-1	8	12	11	11	8	4	8	13	18	6
1	5	7	31	31	1	4	11	7	17	23	17	7	-1	8	27	24	5	9	4	8	0	3	1
2	5	7	11	12	2	5	11	7	36	39	3	-8	0	8	24	31	5	-6	5	8	11	2	10
3	5	7	48	50	1	6	11	7	37	35	4	-7	0	8	8	6	8	-5	5	8	21	23	3
4	5	7	25	25	1	7	11	7	46	43	4	-6	0	8	20	18	3	-4	5	8	43	44	4
5	5	7	177	180	2	8	11	7	5	5	5	-5	0	8	18	14	4	-3	5	8	58	68	1
6	5	7	53	53	1	4	12	7	89	86	3	-4	0	8	62	62	1	-2	5	8	0	2	1
7	5	7	14	2	3	5	12	7	40	37	3	-3	0	8	39	43	1	-1	5	8	37	36	1
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9	5	7	0	12	1	-3	-7	8	0	17	1	-1	0	8	22	26	1	1	5	8	26	30	1
10	5	7	33	28	3	-2	-7	8	15	6	15	0	0	8	0	2	1	2	5	8	31	30	1
-6	6	7	0	7	1	-6	-6	8	25	31	5	1	0	8	171	168	2	3	5	8	92	89	1
-5	6	7	41	38	3	-5	-6	8	14	20	14	2	0	8	253	247	2	4	5	8	31	30	1
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-3	6	7	27	26	2	-3	-6	8	25	26	3	4	0	8	18	19	1	6	5	8	6	10	5
-2	6	7	22	30	2	-2	-6	8	28	34	3	5	0	8	52	57	1	7	5	8	9	8	0
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1	6	7	42	43	1	1	-6	8	17	4	16	8	0	8	11	15	10	10	5	8	43	42	3
2	6	7	91	92	1	-7	-5	8	72	67	4	-8	1	8	55	47	2	-6	6	8	13	8	11
3	6	7	75	76	3	-6	-5	8	48	52	3	-7	1	8	66	66	1	-5	6	8	17	20	5
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9	6	7	0	2	1	0	-5	8	120	117	3	-1	1	8	0	0	1	1	6	8	122	116	2
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2	8	7	43	47	1	-1	-3	8	36	39	1	6	2	8	53	57	1	9	7	8	116	100	3
3	8	7	94	96	2	0	-3	8	37	40	1	7	2	8	88	91	2	10	7	8	0	15	1
4	8	7	50	55	2	1	-3	8	100	98	2	8	2	8	20	28	6	-4	8	8	12	12	2
5	8	7	65	67	1	2	-3	8	0	3	1	9	2	8	14	4	14	-3	8	8	9	5	9
6	8	7	35	38	2	3	-3	8	87	85	2	-8	3	8	15	2	7	-2	8	8	0	7	1
7	8	7	26	25	2	4	-3	8	36	37	2	-7	3	8	33	31	2	-1	8	8	0	1	5
8	8	7	33	30	2	5	-3	8	21	22	4	-6	3	8	10	11	10	0	8	8	15	12	6
9	8	7	61	57	2	-8	-2	8	48	44	2	-5	3	8	31	32	3	1	8	8	37	36	2</td

Table 6. Observed and calculated structure factors for 1

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<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s
-3	0	9	89	87	1	5	5	9	11	4	4	-5	-2	10	15	8	15	0	4	10	154	149	4
-2	0	9	80	82	1	6	5	9	101	98	2	-4	-2	10	45	45	3	1	4	10	14	11	4
-1	0	9	23	23	2	7	5	9	24	25	4	-3	-2	10	16	12	16	2	4	10	54	56	2
0	0	9	66	67	1	8	5	9	13	4	12	-2	-2	10	0	4	1	3	4	10	45	45	2
1	0	9	77	78	1	9	5	9	35	34	3	-1	-2	10	31	31	5	4	4	10	28	32	2
2	0	9	24	22	1	-5	6	9	38	31	5	0	-2	10	20	19	7	5	4	10	17	13	5
3	0	9	85	85	2	-4	6	9	29	30	2	1	-2	10	0	10	1	6	4	10	0	4	1
4	0	9	13	17	3	-3	6	9	0	11	1	2	-2	10	33	35	4	7	4	10	54	47	2
5	0	9	82	89	3	-2	6	9	16	24	3	3	-2	10	21	16	7	8	4	10	30	33	7
6	0	9	0	12	1	-1	6	9	18	23	4	4	-2	10	21	24	11	-5	5	10	17	0	16
7	0	9	38	27	6	0	6	9	204	198	3	-7	-1	10	23	24	5	-4	5	10	56	58	3
-8	1	9	63	66	3	1	6	9	74	75	4	-6	-1	10	38	37	3	-3	5	10	46	49	3
-7	1	9	33	36	3	2	6	9	102	101	2	-5	-1	10	31	31	3	-2	5	10	51	43	3
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1	1	9	7	7	6	-4	7	9	22	19	6	3	-1	10	16	16	5	6	5	10	56	53	2
2	1	9	117	115	1	-3	7	9	0	5	1	4	-1	10	0	5	1	7	5	10	24	21	3
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5	1	9	96	98	2	0	7	9	43	42	2	-6	0	10	43	49	2	-3	6	10	43	44	4
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7	1	9	59	50	3	2	7	9	62	60	4	-4	0	10	56	57	2	-1	6	10	128	127	4
8	1	9	24	9	7	3	7	9	7	0	7	-3	0	10	145	138	3	0	6	10	173	161	4
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1	3	9	0	4	1	3	9	9	57	57	2	-6	2	10	46	51	3	2	8	10	68	66	3
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3	3	9	32	34	1	5	9	9	12	15	7	-4	2	10	78	80	1	4	8	10	45	47	3
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6	3	9	13	18	5	8	9	9	0	2	1	-1	2	10	24	27	2	7	8	10	23	23	4
7	3	9	0	17	1	0	10	9	39	36	5	0	2	10	132	132	2	8	8	10	42	37	5
8	3	9	25	29	5	1	10	9	44	44	2	1	2	10	9	13	6	-1	9	10	54	48	4
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-3	4	9	14	14	3	5	10	9	7	17	7	5	2	10	10	10	7	-3	3	11	12	14	
-2	4	9	56	58	1	6	10	9	16	14	16	6	2	10	31	37	6	4	9	10	87	85	4
-1	4	9	31	30	1	7	10	9	99	86	6	7	2	10	55	54	4	5	9	10	59	57	4
0	4	9	251	241	5	2	11	9	18	9	14	-6	3	10	51	47	2	7	9	10	43	34	4
1	4	9	172	168	2	3	11	9	39</														

Table 6. Observed and calculated structure factors for 1

Page 9

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	11	29	28	4	2	9	11	40	44	4	-1	2	12	54	54	3	1	5	12	21	26	4	5	8	12	90	89	5
3	6	11	43	38	3	3	9	11	10	0	10	0	2	12	11	14	11	2	5	12	35	41	4	-1	1	13	17	17	11
4	6	11	14	1	8	4	9	11	58	61	4	1	2	12	31	31	4	3	5	12	4	12	4	0	1	13	13	21	12
5	6	11	18	8	4	5	9	11	10	17	10	2	2	12	11	12	11	4	5	12	70	61	4	1	1	13	34	37	6
6	6	11	22	24	5	6	9	11	45	44	5	3	2	12	12	6	12	5	5	12	38	39	3	-2	2	13	12	9	11
7	6	11	20	28	5	-3	-1	12	24	29	7	5	2	12	59	61	6	6	5	12	0	0	1	-1	2	13	89	92	5
-2	7	11	60	59	4	-2	-1	12	0	4	1	-4	3	12	27	24	4	-2	6	12	0	2	1	0	2	13	49	44	4
-1	7	11	18	28	11	-1	-1	12	0	2	1	-3	3	12	18	8	8	-1	6	12	17	17	17	1	2	13	59	61	4
0	7	11	50	50	3	0	-1	12	44	42	4	-2	3	12	22	21	4	0	6	12	0	12	1	2	2	13	36	31	5
1	7	11	65	61	3	1	-1	12	25	25	8	-1	3	12	0	9	1	1	6	12	22	24	5	-2	3	13	33	35	7
2	7	11	10	10	9	-4	0	12	80	68	5	0	3	12	48	51	4	2	6	12	0	12	1	-1	3	13	29	33	6
3	7	11	81	74	3	-3	0	12	50	47	5	1	3	12	22	20	5	3	6	12	68	59	4	0	3	13	0	6	1
4	7	11	34	38	4	-2	0	12	100	99	4	2	3	12	28	34	4	4	6	12	30	31	5	1	3	13	0	10	1
5	7	11	28	24	4	-1	0	12	49	53	4	3	3	12	6	0	6	5	6	12	28	19	6	2	3	13	37	34	9
6	7	11	0	7	1	0	0	12	0	11	1	4	3	12	45	50	3	6	6	12	12	15	9	3	3	13	60	62	4
7	7	11	28	26	4	1	0	12	26	29	7	5	3	12	81	75	5	-1	7	12	0	8	1	-1	4	13	26	20	7
-1	8	11	0	21	1	2	0	12	15	4	10	-3	4	12	3	5	3	0	7	12	0	12	1	0	4	13	0	3	1
0	8	11	10	11	10	-4	1	12	28	28	10	-2	4	12	33	36	4	1	7	12	14	15	14	1	4	13	15	18	10
1	8	11	51	50	4	-3	1	12	20	27	11	-1	4	12	17	4	8	2	7	12	0	6	1	2	4	13	30	34	6
2	8	11	12	2	12	-2	1	12	21	22	11	0	4	12	26	27	3	3	7	12	31	27	3	3	4	13	53	52	4
3	8	11	33	33	3	-1	1	12	100	95	4	1	4	12	14	13	14	4	7	12	36	39	5	-1	5	13	7	5	7
4	8	11	76	79	4	0	1	12	24	8	8	4	4	12	12	4	11	5	7	12	19	2	10	0	6	13	12	17	12
5	8	11	9	6	8	1	1	12	31	29	4	5	4	12	20	17	5	0	8	12	36	41	6	1	6	13	41	40	4
6	8	11	10	12	9	2	1	12	7	2	6	-3	5	12	30	23	6	1	8	12	29	30	6						
7	8	11	18	0	17	-4	2	12	10	4	9	-2	5	12	36	32	5	2	8	12	13	4	12						
0	9	11	31	35	5	-3	2	12	49	42	4	-1	5	12	29	30	6	3	8	12	18	0	17						
1	9	11	0	10	1	-2	2	12	54	58	4	0	5	12	67	62	3	4	8	12	23	15	8						

Crystallographic Material for **1b**

X-ray Experimental.

Table 1. Crystallographic Data for 1.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters (\AA^2) for the non-hydrogen atoms of 1.

Table 3. Bond Lengths (\AA) and Angles ($^\circ$) for the non-hydrogen atoms of 1.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of 1.

Table 5. Fractional coordinates and isotropic thermal parameters (\AA^2) for the hydrogen atoms of 1.

Table 6. Observed and calculated structure factor amplitudes for 1. Values for F_o , F_c and $\sigma(F_o)$ have been multiplied by 10.

Figure 1. View of 1 showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms shown are drawn to an arbitrary scale.

Figure 2. Unit cell packing diagram for 1. The view is approximately down the **c** axis.

Table 6. Observed and calculated structure factor amplitudes 1. Values for F_o , F_c and $\sigma(F_o)$ have been multiplied by 10.

X-ray Experimental for C₂₁H₂₀O₂: Crystals grew as colorless by slow evaporation from ethylacetate and hexane. The data crystal was a long needle that had approximate dimensions; 0.45x0.08x0.08 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoK α radiation ($\lambda = 0.71073\text{\AA}$). A total of 366 frames of data were collected using ω -scans with a scan range of 1° and a counting time of 151 seconds per frame. The data were collected at -120 °C using a Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.¹ The structure was solved by direct methods using SIR92² and refined by full-matrix least-squares on F² with anisotropic displacement parameters for the non-H atoms using SHELXL-97.³ The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached. The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.019*P)^2 + (0.7511*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. R_w(F²) refined to 0.114, with R(F) equal to 0.0553 and a goodness of fit, S, = 1.008. Definitions used for calculating R(F),R_w(F²) and the goodness of fit, S, are given below.⁴ The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (8.4(12)\times 10^{-6}) * F_c^2 \lambda^3 / (\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).⁵ All figures were generated using SHELXTL/PC.⁶ Tables of positional and thermal parameters, bond lengths and angles, figures and lists of observed and calculated structure factors are located in tables 1 through 6.

References

- 1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.
- 2) SIR92. (1993). A program for crystal structure solution. Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. J. Appl. Cryst. 26, 343-350.
- 3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.
- 4) $R_w(F^2) = \{\sum w(|F_o|^2 - |F_c|^2)^2 / \sum w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
 $R(F) = \{\sum (|F_o| - |F_c|)^2 / \sum |F_o|\}$ for reflections with $|F_o| > 4(\sigma(F_o))$.
 $S = [\sum w(|F_o|^2 - |F_c|^2)^2 / (n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.
- 5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.
- 6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for 1.

Empirical formula	C21 H20 O2	
Formula weight	304.37	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 14.4375(5) Å	α= 90°.
	b = 10.6909(4) Å	β= 108.223(2)°.
	c = 10.8075(5) Å	γ= 90°.
Volume	1584.47(11) Å ³	
Z	4	
Density (calculated)	1.276 Mg/m ³	
Absorption coefficient	0.081 mm ⁻¹	
F(000)	648	
Crystal size	0.45 x 0.08 x 0.08 mm	
Theta range for data collection	3.0 to 27.5°.	
Index ranges	-18<=h<=18, -13<=k<=11, -14<=l<=13	
Reflections collected	5650	
Independent reflections	3606 [R(int) = 0.0413]	
Completeness to theta = 27.48°	99.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3606 / 0 / 209	
Goodness-of-fit on F ²	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.0999	
R indices (all data)	R1 = 0.0973, wR2 = 0.1140	
Extinction coefficient	8.4(12)x10 ⁻⁶	
Largest diff. peak and hole	0.25 and -0.24 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	1922(1)	2801(2)	923(2)	24(1)
C2	2975(1)	3018(2)	1870(2)	25(1)
C3	2649(1)	4270(2)	2323(2)	30(1)
C4	3093(2)	5446(2)	1944(2)	43(1)
C5	2602(2)	5554(2)	481(2)	45(1)
C6	1550(2)	5177(2)	285(2)	38(1)
C7	1624(1)	4140(2)	1273(2)	29(1)
C8	1301(1)	1880(2)	1343(2)	26(1)
O9	1569(1)	1420(1)	2432(1)	35(1)
C10	283(1)	1681(2)	453(2)	26(1)
C11	9(1)	1951(2)	-871(2)	31(1)
C12	-946(1)	1749(2)	-1652(2)	35(1)
C13	-1632(1)	1303(2)	-1109(2)	36(1)
C14	-1366(1)	1046(2)	205(2)	36(1)
C15	-410(1)	1215(2)	981(2)	31(1)
C16	3453(1)	2052(2)	2888(2)	26(1)
O17	3646(1)	2277(1)	4051(1)	34(1)
C18	3763(1)	828(2)	2454(2)	23(1)
C19	3726(1)	608(2)	1173(2)	28(1)
C20	4030(1)	-538(2)	826(2)	32(1)
C21	4358(1)	-1465(2)	1746(2)	33(1)
C22	4412(1)	-1250(2)	3032(2)	34(1)
C23	4124(1)	-102(2)	3388(2)	29(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

C1-C8	1.494(2)	C10-C11	1.391(3)
C1-C2	1.562(2)	C11-C12	1.389(3)
C1-C7	1.574(2)	C11-H11	0.96
C1-H1	0.96	C12-C13	1.385(3)
C2-C16	1.509(3)	C12-H12	0.96
C2-C3	1.549(2)	C13-C14	1.378(3)
C2-H2	0.96	C13-H13	0.96
C3-C4	1.524(3)	C14-C15	1.384(3)
C3-C7	1.564(3)	C14-H14	0.96
C3-H3	0.96	C15-H15	0.96
C4-C5	1.522(3)	C16-O17	1.224(2)
C4-H4A	0.96	C16-C18	1.504(2)
C4-H4B	0.96	C18-C19	1.388(3)
C5-C6	1.521(3)	C18-C23	1.396(3)
C5-H5A	0.96	C19-C20	1.392(2)
C5-H5B	0.96	C19-H19	0.96
C6-C7	1.519(3)	C20-C21	1.378(3)
C6-H6A	0.96	C20-H20	0.96
C6-H6B	0.96	C21-C22	1.387(3)
C7-H7	0.96	C21-H21	0.96
C8-O9	1.222(2)	C22-C23	1.389(3)
C8-C10	1.499(3)	C22-H22	0.96
C10-C15	1.390(3)	C23-H23	0.96
C8-C1-C2	116.86(16)	C4-C3-C2	115.67(16)
C8-C1-C7	106.89(14)	C4-C3-C7	105.13(16)
C2-C1-C7	89.49(13)	C2-C3-C7	90.36(14)
C8-C1-H1	113.6	C4-C3-H3	114.6
C2-C1-H1	114.2	C2-C3-H3	113.7
C7-C1-H1	113.1	C7-C3-H3	114.6
C16-C2-C3	118.45(16)	C5-C4-C3	104.05(17)
C16-C2-C1	120.39(15)	C5-C4-H4A	111.4
C3-C2-C1	90.30(13)	C3-C4-H4A	110.8
C16-C2-H2	108.8	C5-C4-H4B	110.2
C3-C2-H2	108.0	C3-C4-H4B	111.3
C1-C2-H2	109.4	H4A-C4-H4B	109.0

C6-C5-C4	104.18(18)	C14-C15-C10	120.5(2)
C6-C5-H5A	110.4	C14-C15-H15	120.1
C4-C5-H5A	110.3	C10-C15-H15	119.4
C6-C5-H5B	111.3	O17-C16-C18	119.78(17)
C4-C5-H5B	111.5	O17-C16-C2	121.32(17)
H5A-C5-H5B	109.0	C18-C16-C2	118.74(16)
C7-C6-C5	104.37(17)	C19-C18-C23	119.32(17)
C7-C6-H6A	110.6	C19-C18-C16	122.37(16)
C5-C6-H6A	111.4	C23-C18-C16	118.29(17)
C7-C6-H6B	111.1	C18-C19-C20	120.02(18)
C5-C6-H6B	110.4	C18-C19-H19	119.2
H6A-C6-H6B	108.9	C20-C19-H19	120.8
C6-C7-C3	106.69(16)	C21-C20-C19	120.34(19)
C6-C7-C1	117.30(17)	C21-C20-H20	120.1
C3-C7-C1	89.27(13)	C19-C20-H20	119.6
C6-C7-H7	113.8	C20-C21-C22	120.16(18)
C3-C7-H7	114.2	C20-C21-H21	119.7
C1-C7-H7	113.0	C22-C21-H21	120.1
O9-C8-C1	121.30(17)	C21-C22-C23	119.76(19)
O9-C8-C10	120.77(16)	C21-C22-H22	119.7
C1-C8-C10	117.37(16)	C23-C22-H22	120.5
C15-C10-C11	119.12(17)	C22-C23-C18	120.36(19)
C15-C10-C8	118.37(17)	C22-C23-H23	120.4
C11-C10-C8	122.51(17)	C18-C23-H23	119.2
C12-C11-C10	120.17(19)		
C12-C11-H11	120.3		
C10-C11-H11	119.6		
C13-C12-C11	120.1(2)		
C13-C12-H12	119.9		
C11-C12-H12	120.0		
C14-C13-C12	119.98(19)		
C14-C13-H13	120.0		
C12-C13-H13	120.0		
C13-C14-C15	120.15(19)		
C13-C14-H14	119.6		
C15-C14-H14	120.3		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	24(1)	23(1)	25(1)	-2(1)	8(1)	0(1)
C2	25(1)	23(1)	27(1)	-2(1)	9(1)	-2(1)
C3	34(1)	24(1)	31(1)	-5(1)	9(1)	-1(1)
C4	33(1)	25(1)	68(2)	-2(1)	11(1)	-1(1)
C5	56(1)	27(1)	62(2)	8(1)	32(1)	7(1)
C6	45(1)	26(1)	40(1)	-1(1)	7(1)	8(1)
C7	27(1)	24(1)	39(1)	-3(1)	13(1)	4(1)
C8	28(1)	21(1)	28(1)	-3(1)	9(1)	0(1)
O9	33(1)	40(1)	30(1)	5(1)	7(1)	-5(1)
C10	26(1)	19(1)	33(1)	-3(1)	10(1)	0(1)
C11	30(1)	28(1)	35(1)	-1(1)	9(1)	-1(1)
C12	33(1)	30(1)	38(1)	0(1)	3(1)	-2(1)
C13	27(1)	25(1)	50(2)	-4(1)	4(1)	-2(1)
C14	28(1)	31(1)	50(1)	-3(1)	14(1)	-5(1)
C15	31(1)	27(1)	38(1)	-2(1)	13(1)	-3(1)
C16	21(1)	27(1)	27(1)	-2(1)	6(1)	-3(1)
O17	37(1)	36(1)	28(1)	-4(1)	6(1)	2(1)
C18	18(1)	25(1)	27(1)	1(1)	6(1)	-3(1)
C19	27(1)	25(1)	30(1)	2(1)	8(1)	-1(1)
C20	31(1)	30(1)	37(1)	-4(1)	13(1)	1(1)
C21	25(1)	25(1)	48(1)	-2(1)	8(1)	4(1)
C22	27(1)	31(1)	40(1)	9(1)	6(1)	5(1)
C23	22(1)	35(1)	28(1)	3(1)	6(1)	2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H1	1887	2720	24	29
H2	3405	3206	1374	30
H3	2639	4257	3207	36
H4A	3787	5362	2154	51
H4B	2952	6171	2379	51
H5A	2899	4990	26	54
H5B	2642	6390	178	54
H6A	1240	4877	-583	46
H6B	1186	5875	448	46
H7	1090	4122	1624	35
H11	483	2275	-1242	38
H12	-1128	1909	-2571	42
H13	-2295	1183	-1645	43
H14	-1847	746	578	43
H15	-220	1005	1890	38
H19	3481	1250	533	33
H20	4018	-676	-56	39
H21	4555	-2257	1494	40
H22	4635	-1902	3666	41
H23	4177	66	4280	35

Figure 1. View of 1 showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms shown are drawn to an arbitrary scale.

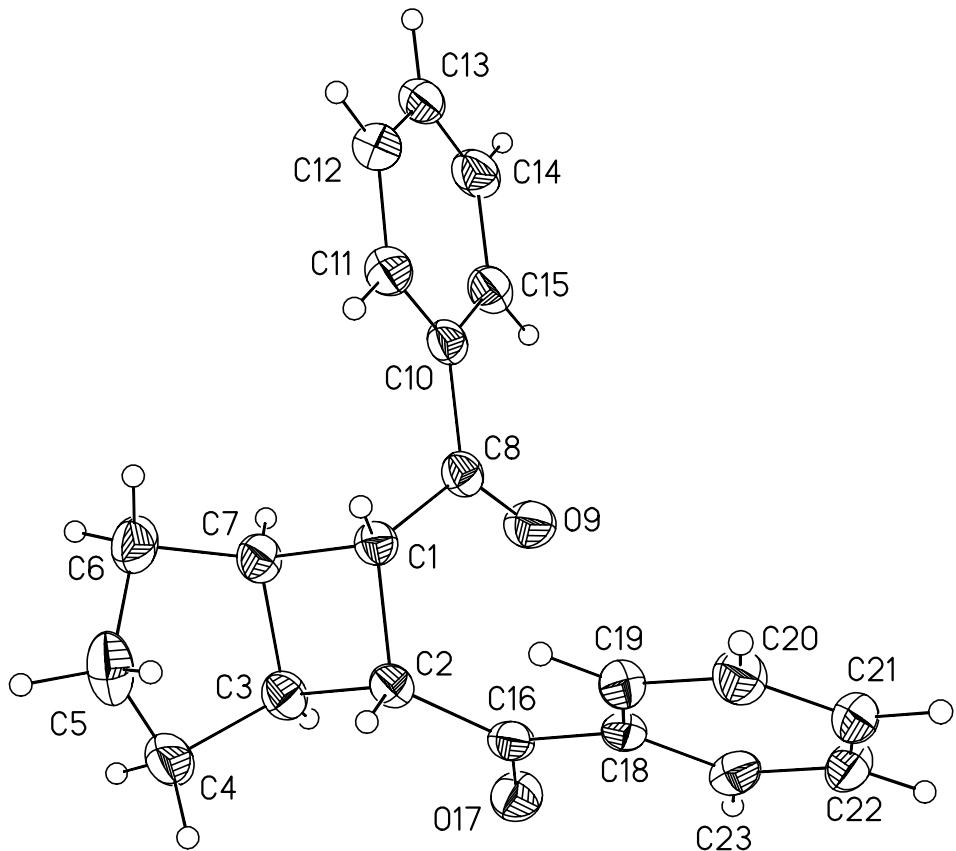


Figure 2. Unit cell packing diagram for 1. The view is approximately down the **c** axis.

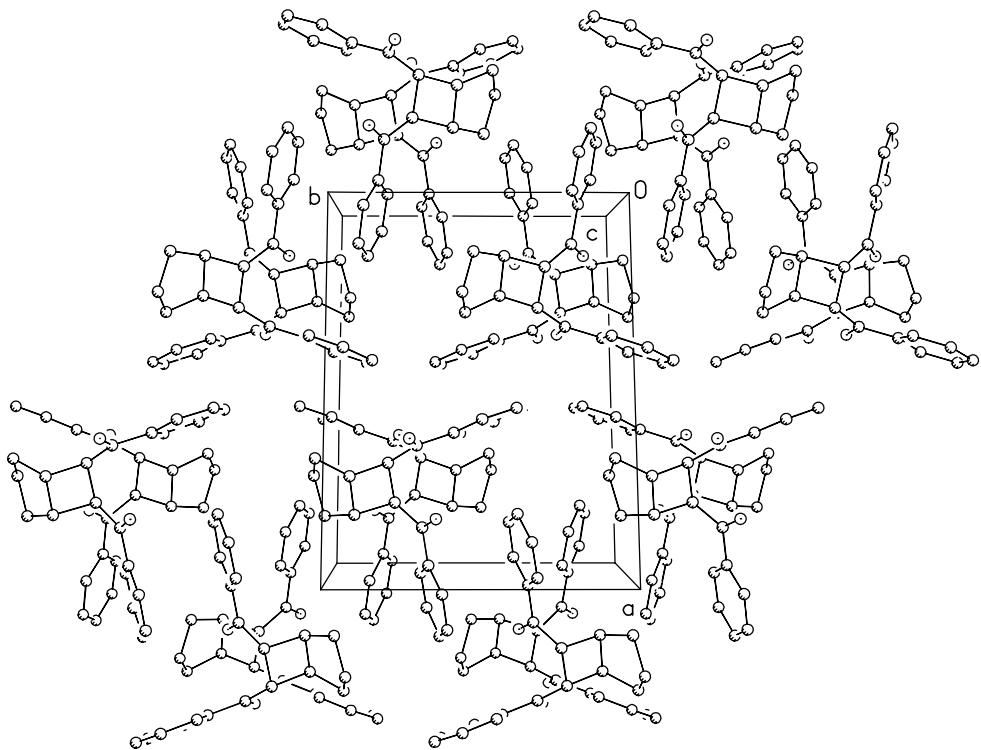


Table 6. Observed and calculated structure factors for 1

Page 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
2	0	0	371	384	5	3	5	0	209	221	2	1	11	0	51	52	3	11	2	1	61	60	3
3	0	0	172	161	1	4	5	0	89	86	1	2	11	0	86	80	3	12	2	1	93	97	2
4	0	0	1132	1112	12	5	5	0	45	42	2	3	11	0	89	83	3	13	2	1	35	30	5
5	0	0	559	550	5	6	5	0	173	174	2	4	11	0	59	57	4	14	2	1	18	8	17
6	0	0	399	396	4	7	5	0	41	38	4	5	11	0	0	9	1	15	2	1	0	10	1
7	0	0	734	704	9	8	5	0	236	231	3	6	11	0	67	64	4	16	2	1	53	40	10
8	0	0	192	183	2	9	5	0	46	42	6	7	11	0	38	29	11	17	2	1	62	53	19
9	0	0	284	273	3	10	5	0	180	179	6	8	11	0	148	145	6	-17	3	1	59	60	14
10	0	0	248	241	3	11	5	0	50	57	4	9	11	0	161	152	6	-16	3	1	0	12	1
11	0	0	134	123	3	12	5	0	238	223	5	10	11	0	10	29	10	-15	3	1	5	14	5
12	0	0	12	0	11	13	5	0	155	157	8	0	12	0	84	89	5	-14	3	1	117	119	5
13	0	0	33	28	7	14	5	0	71	76	5	1	12	0	45	48	4	-13	3	1	8	11	8
14	0	0	68	71	6	15	5	0	76	79	7	2	12	0	56	54	4	-12	3	1	171	174	2
15	0	0	146	152	6	16	5	0	29	39	28	3	12	0	46	38	5	-11	3	1	325	323	3
16	0	0	20	11	19	0	6	0	1	7	1	4	12	0	51	37	7	-10	3	1	72	72	6
17	0	0	62	75	15	1	6	0	266	260	2	5	12	0	35	14	10	-9	3	1	208	200	2
2	1	0	255	258	2	2	6	0	335	326	2	6	12	0	80	82	7	-8	3	1	20	13	4
3	1	0	321	318	2	3	6	0	123	126	2	7	12	0	38	19	17	-7	3	1	516	514	4
4	1	0	288	294	2	4	6	0	51	51	2	8	12	0	113	109	9	-6	3	1	192	191	1
5	1	0	842	841	9	5	6	0	100	87	4	1	13	0	25	33	25	-5	3	1	220	226	3
6	1	0	478	464	4	6	6	0	28	12	12	2	13	0	13	23	13	-4	3	1	98	97	2
7	1	0	144	136	1	7	6	0	255	249	5	3	13	0	21	9	20	-3	3	1	179	172	2
8	1	0	31	33	3	8	6	0	175	173	3	4	13	0	37	15	9	-2	3	1	639	645	6
9	1	0	277	272	5	9	6	0	200	196	4	5	13	0	124	120	7	-1	3	1	1243	1239	12
10	1	0	183	174	2	10	6	0	65	61	6	6	13	0	22	2	21	0	3	1	775	781	8
11	1	0	116	118	2	11	6	0	140	137	4	-18	1	1	34	22	34	1	3	1	210	202	2
12	1	0	62	61	6	12	6	0	124	116	3	-17	1	1	21	20	21	2	3	1	0	25	1
13	1	0	68	71	2	13	6	0	13	23	13	-16	1	1	42	1	41	3	3	1	379	392	4
14	1	0	10	22	10	14	6	0	43	47	11	-15	1	1	49	44	7	4	3	1	192	197	4
15	1	0	41	51	10	15	6	0	57	38	8	-14	1	1	66	65	3	5	3	1	230	232	4
16	1	0	21	14	20	16	6	0	89	101	8	-13	1	1	45	55	3	6	3	1	361	353	7
17	1	0	75	74	8	1	7	0	98	96	1	-12	1	1	98	94	1	7	3	1	242	240	3
0	2	0	16	30	15	2	7	0	169	163	2	-11	1	1	136	128	1	8	3	1	164	156	2
1	2	0	530	547	4	3	7	0	52	44	2	-10	1	1	62	53	2	9	3	1	144	144	2
2	2	0	334	333	3	4	7	0	74	72	3	-9	1	1	63	49	1	10	3	1	109	105	2
3	2	0	176	173	2	5	7	0	69	61	4	-8	1	1	89	88	2	11	3	1	103	98	2
4	2	0	119	115	2	6	7	0	65	58	9	-7	1	1	294	292	3	12	3	1	12	15	11
5	2	0	80	81	1	7	7	0	166	157	8	-6	1	1	261	252	2	13	3	1	31	32	13
6	2	0	457	449	4	8	7	0	74	70	2	-5	1	1	41	39	2	14	3	1	103	110	8
7	2	0	296	299	2	9	7	0	205	197	4	-4	1	1	893	896	7	15	3	1	45	39	9
8	2	0	56	58	4	10	7	0	176	170	4	-3	1	1	1392	1346	30	16	3	1	73	74	20
9	2	0	340	329	7	11	7	0	50	52	7	-2	1	1	212	228	1	-17	4	1	81	73	81
10	2	0	0	1	1	12	7	0	27	28	20	1	1	1	110	123	1	-16	4	1	191	191	8
11	2	0	200	197	2	13	7	0	138	134	4	2	1	1	980	987	19	-15	4	1	94	93	5
12	2	0	101	102	2	14	7	0	40	34	14	3	1	1	743	749	14	-14	4	1	49	59	5
13	2	0	87	95	2	15	7	0	33	0	32	4	1	1	442	463	13	-13	4	1	192	203	6
14	2	0	90	98	3	0	8	0	189	193	2	5	1	1	437	440	5	-12	4	1	223	229	3
15	2	0	19	1	1	1	8	0	0	1	1	6	1	1	159	159	2	-11	4	1	151	147	2
16	2	0	39	27	23	2	8	0	134	137	1	7	1	1	89	81	1	-10	4	1	466	461	5
17	2	0	65	48	12	3	8	0	341	337	7	8	1	1	149	137	2	-9	4	1	131	133	1
1	3	0	674	684	5	4	8	0	81	71	8	9	1	1	13	4	13	-8	4	1	88	81	1
2	3	0	137	137	1	5	8	0	141	132	7	10	1	1	20	20	6	-7	4	1	20	17	20
3	3	0	211	218	2	6	8	0	57	51	10	11	1	1	18	1	18	-6	4	1	82	85	3
4	3	0	0	9	1	7	8	0	48	46	4	12	1	1	130	136	2	-5	4	1	13	11	6
5	3	0	50	47	2	8	8	0	239	237	10	13	1	1	25	38	13	-4	4	1	35	31	3
6	3	0	42	36	5	9	8	0	25	21	25	14	1	1	73	81	4	-3	4	1	515	510	4
7	3	0	235	234	3	10	8	0	202	195	4	15	1	1	25	30	25	-2	4	1	420	430	4
8	3	0	55	54	2	11	8	0	82	96	4	16	1	1	34	23	24	-1	4	1	371	369	3
9	3	0	91	94	1	12	8	0	53	42	8	17	1	1	11	23	11	0	4	1	195	190	2
10	3	0	256	251	3	13	8	0	0	17	1	-17	2	1	75	63	10	1	4	1	168	175	1
11	3	0	30	14	6	14	8	0	0	30	1	-16	2	1	50	45	9	2	4	1	191	190	2
12	3	0	27	23	7	1	9	0	343	334	27	-15	2	1	45	42	8	3	4	1	54	53	1
13	3	0	63	66	2	2	9	0	139	132	3	-14	2	1	27	33	7	4	4	1	178	180	1
14	3	0	114	116	3	3	9	0	67	69	2	-13	2	1	41	45	3	5	4	1	1	55	54
15	3	0	25	9	19	4	9	0	42	41	6	-12	2	1	223	224	2	6	4	1	108	109	2
16	3	0	0	14	1	5	9	0	18	1	-11	2	1	235	228	2	7	4	1	83	86	2	
17	3	0	38	36	37	6	9	0															

Table 6. Observed and calculated structure factors for 1

Page 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
-10	8	1	31	39	16	0	11	1	56	55	3	-6	1	2	82	80	1	11	3	2	102	101	4
-9	8	1	197	199	3	1	11	1	91	96	2	-5	1	2	513	525	4	12	3	2	34	24	6
-8	8	1	164	166	2	2	11	1	34	32	6	-4	1	2	228	233	3	13	3	2	24	0	17
-7	8	1	31	37	5	3	11	1	49	51	4	-3	1	2	635	650	5	14	3	2	70	73	8
-6	8	1	62	65	10	4	11	1	61	66	4	-2	1	2	87	83	3	15	3	2	82	54	14
-5	8	1	67	55	2	5	11	1	62	61	4	-1	1	2	716	747	7	16	3	2	70	59	12
-4	8	1	181	182	3	6	11	1	18	21	17	0	1	2	52	12	13	-17	4	2	41	42	15
-3	8	1	121	121	6	7	11	1	0	24	1	1	1	2	141	132	3	-16	4	2	107	110	6
-2	8	1	252	255	8	8	11	1	130	128	5	2	1	2	263	266	5	-15	4	2	168	181	4
-1	8	1	65	62	9	9	11	1	143	127	7	3	1	2	94	103	2	-14	4	2	38	30	8
0	8	1	29	23	7	10	11	1	27	11	27	4	1	2	47	49	2	-13	4	2	0	17	1
1	8	1	430	434	4	-9	12	1	76	69	8	5	1	2	278	280	4	-12	4	2	0	14	1
2	8	1	91	81	3	-8	12	1	52	47	11	6	1	2	205	203	3	-11	4	2	307	309	5
3	8	1	134	133	8	-7	12	1	15	11	14	7	1	2	171	176	2	-10	4	2	41	39	2
4	8	1	147	139	6	-6	12	1	79	67	4	8	1	2	293	297	4	-9	4	2	111	116	5
5	8	1	195	204	5	-5	12	1	55	46	5	9	1	2	234	233	3	-8	4	2	56	49	4
6	8	1	203	197	13	-4	12	1	136	128	3	10	1	2	94	89	2	-7	4	2	225	226	2
7	8	1	235	241	8	-3	12	1	130	128	2	11	1	2	69	76	4	-6	4	2	17	24	6
8	8	1	41	19	10	-2	12	1	19	3	18	12	1	2	37	51	7	-5	4	2	421	412	3
9	8	1	24	18	23	-1	12	1	28	27	7	13	1	2	42	55	5	-4	4	2	35	21	5
10	8	1	0	19	1	0	12	1	22	20	15	14	1	2	27	17	15	-3	4	2	541	540	4
11	8	1	13	14	13	1	12	1	33	34	7	15	1	2	26	21	25	-2	4	2	58	67	2
12	8	1	20	26	19	2	12	1	8	12	8	16	1	2	42	35	13	-1	4	2	305	310	3
13	8	1	58	54	11	3	12	1	17	19	16	-18	2	2	41	21	20	0	4	2	359	356	3
14	8	1	13	29	13	4	12	1	69	74	4	-17	2	2	16	8	15	1	4	2	96	110	1
-13	9	1	40	29	14	5	12	1	21	24	20	-16	2	2	98	103	7	2	4	2	209	220	3
-12	9	1	40	29	16	6	12	1	13	9	13	-15	2	2	35	8	8	3	4	2	74	78	1
-11	9	1	137	139	4	7	12	1	47	59	11	-14	2	2	147	151	2	4	4	2	224	228	3
-10	9	1	86	82	6	8	12	1	0	5	1	-13	2	2	23	12	7	5	4	2	54	61	2
-9	9	1	22	5	22	-6	13	1	22	17	21	-12	2	2	46	35	2	6	4	2	32	38	4
-8	9	1	27	22	9	-5	13	1	40	48	11	-11	2	2	157	158	4	7	4	2	29	23	8
-7	9	1	74	72	4	-4	13	1	101	108	5	-10	2	2	341	333	4	8	4	2	18	3	18
-6	9	1	68	72	2	-3	13	1	84	84	7	-9	2	2	286	281	3	9	4	2	27	18	9
-5	9	1	172	165	6	-2	13	1	121	114	5	-8	2	2	77	70	1	10	4	2	133	136	4
-4	9	1	169	169	9	-1	13	1	47	61	11	-7	2	2	58	64	2	11	4	2	19	27	19
-3	9	1	142	143	8	0	13	1	104	100	7	-6	2	2	276	283	2	12	4	2	53	56	5
-2	9	1	249	252	10	1	13	1	86	94	5	-5	2	2	583	582	4	13	4	2	119	119	4
-1	9	1	122	119	7	2	13	1	88	93	6	-4	2	2	46	56	2	14	4	2	92	90	5
0	9	1	188	192	3	3	13	1	29	2	13	-3	2	2	348	365	3	15	4	2	12	31	11
1	9	1	59	57	2	4	13	1	25	6	24	-2	2	2	703	717	6	-17	5	2	16	16	15
2	9	1	101	93	9	5	13	1	29	49	28	-1	2	2	225	223	2	-16	5	2	81	82	7
3	9	1	49	53	12	-17	0	2	20	48	19	0	2	2	148	154	5	-15	5	2	62	70	10
4	9	1	133	131	8	-16	0	2	22	2	21	1	2	2	70	81	2	-14	5	2	21	15	20
5	9	1	169	171	7	-15	0	2	84	84	6	2	2	2	351	365	4	-13	5	2	63	69	4
6	9	1	61	56	2	-14	0	2	106	108	3	3	2	2	282	288	5	-12	5	2	248	242	3
7	9	1	52	43	4	-13	0	2	23	22	9	4	2	2	386	395	6	-11	5	2	138	139	5
8	9	1	34	31	9	-12	0	2	70	76	2	5	2	2	47	47	2	-10	5	2	75	75	4
9	9	1	0	9	1	-11	0	2	48	53	3	6	2	2	200	201	4	-9	5	2	54	56	2
10	9	1	77	75	6	-10	0	2	115	110	2	7	2	2	157	165	2	-8	5	2	68	64	1
11	9	1	18	31	17	-9	0	2	219	213	2	8	2	2	28	24	10	-7	5	2	194	195	2
12	9	1	54	9	9	-8	0	2	488	479	5	9	2	2	198	208	3	-6	5	2	17	19	17
13	9	1	68	19	17	-7	0	2	37	36	4	10	2	2	55	59	3	-5	5	2	449	445	3
-12	10	1	147	139	8	-6	0	2	219	231	2	11	2	2	0	16	1	-4	5	2	64	64	2
-11	10	1	92	82	6	-5	0	2	0	19	1	12	2	2	86	82	3	-3	5	2	243	249	2
-10	10	1	0	3	1	-4	0	2	77	73	2	13	2	2	53	34	6	-2	5	2	250	249	3
-9	10	1	69	76	5	-3	0	2	357	380	4	14	2	2	39	40	14	-1	5	2	128	125	1
-8	10	1	34	39	7	-2	0	2	894	918	10	15	2	2	22	9	21	0	5	2	105	107	3
-7	10	1	47	46	9	-1	0	2	2104	1975	37	16	2	2	70	63	13	1	5	2	0	9	1
-6	10	1	161	150	16	0	0	2	335	362	7	-18	3	2	54	39	20	2	5	2	119	127	1
-5	10	1	117	119	6	1	0	2	249	263	7	-17	3	2	46	4	46	3	5	2	359	360	4
-4	10	1	93	93	6	2	0	2	359	372	7	-16	3	2	31	58	16	4	5	2	74	65	2
-3	10	1	84	89	13	3	0	2	23	40	8	-15	3	2	117	123	6	5	5	2	234	240	3
-2	10	1	69	67	2	4	0	2	394	398	8	-14	3	2	24	19	7	6	5	2	29	0	3
-1	10	1	174	171	2	5	0	2	581	578	13	-13	3	2	43	42	3	7	5	2	129	131	4
0	10	1	19	24	10	6	0	2	440	432	8	-12	3	2	49	52	5	8	5	2	65	65	5
1	10	1	24	23	7	7	0	2	84	85	2	-11	3	2	149	140	3	9	5	2	49	44	4
2	10	1	77	75	6	8	0	2	0	3	1												

Table 6. Observed and calculated structure factors for 1

Page 3

<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s						
-4	9	2	58	56	2	2	13	2	41	10	13	-3	3	3	19	25	19	-13	6	3	117	120	4						
-3	9	2	134	141	5	3	13	2	30	29	14	-2	3	3	79	88	2	-12	6	3	49	48	3						
-2	9	2	436	436	15	4	13	2	59	61	9	-1	3	3	176	180	2	-11	6	3	128	122	4						
-1	9	2	91	93	2	-18	1	3	0	11	1	0	3	3	56	62	1	-10	6	3	116	111	2						
0	9	2	170	172	7	-17	1	3	72	85	8	1	3	3	142	144	2	-9	6	3	256	238	4						
1	9	2	134	134	1	-16	1	3	40	24	8	2	3	3	248	244	3	-8	6	3	222	217	5						
2	9	2	101	110	9	-15	1	3	36	55	12	3	3	3	302	297	4	-7	6	3	41	41	3						
3	9	2	164	167	3	-14	1	3	60	57	4	4	3	3	18	5	17	-6	6	3	121	122	1						
4	9	2	209	210	6	-13	1	3	48	44	3	5	3	3	29	23	4	-5	6	3	124	125	1						
5	9	2	112	106	7	-12	1	3	30	5	4	6	3	3	263	260	5	-4	6	3	222	226	2						
6	9	2	105	108	4	-11	1	3	16	1	14	7	3	3	30	9	9	-3	6	3	107	109	1						
7	9	2	150	148	4	-10	1	3	152	151	1	8	3	3	45	48	6	-2	6	3	301	300	3						
8	9	2	21	16	20	-9	1	3	100	100	1	9	3	3	131	129	4	-1	6	3	62	62	2						
9	9	2	55	74	8	-8	1	3	182	190	2	10	3	3	89	94	2	0	6	3	20	15	7						
10	9	2	63	66	7	-7	1	3	73	70	1	11	3	3	15	12	14	1	6	3	76	79	2						
11	9	2	50	53	15	-6	1	3	69	80	1	12	3	3	76	85	9	2	6	3	244	242	7						
12	9	2	105	94	6	-5	1	3	135	131	1	13	3	3	25	17	24	3	6	3	249	241	5						
-12	10	2	51	16	15	-4	1	3	147	153	1	14	3	3	20	24	20	4	6	3	130	129	3						
-11	10	2	0	6	1	-3	1	3	130	156	1	15	3	3	41	22	40	5	6	3	116	119	2						
-10	10	2	75	59	8	-2	1	3	463	482	4	-17	4	3	29	34	28	6	6	3	32	29	2						
-9	10	2	42	40	9	-1	1	3	315	330	3	-16	4	3	0	22	1	7	6	3	44	48	2						
-8	10	2	64	63	4	0	1	3	85	97	2	-15	4	3	153	150	4	8	6	3	89	99	2						
-7	10	2	138	142	2	1	1	3	187	202	3	-14	4	3	153	154	11	9	6	3	123	123	4						
-6	10	2	0	11	1	2	1	3	462	472	7	-13	4	3	100	105	4	10	6	3	159	153	4						
-5	10	2	88	96	17	3	1	3	169	168	10	-12	4	3	191	191	4	11	6	3	0	16	1	11	9	3	93	97	7
-4	10	2	6	8	6	4	1	3	173	173	3	-11	4	3	306	307	9	12	6	3	44	48	10	-13	10	3	107	119	15
-3	10	2	245	248	3	5	1	3	110	97	2	-10	4	3	54	50	2	13	6	3	66	64	9	-12	10	3	47	3	15
-2	10	2	195	196	2	6	1	3	0	11	1	-9	4	3	88	91	3	14	6	3	47	25	17	-11	10	3	6	11	6
-1	10	2	39	42	3	7	1	3	266	257	4	-8	4	3	30	25	6	-16	7	3	41	37	29	-10	10	3	37	1	12
0	10	2	0	2	1	8	1	3	116	109	2	-7	4	3	98	100	1	-15	7	3	50	50	12	-9	10	3	57	55	4
1	10	2	157	155	2	9	1	3	127	126	2	-6	4	3	144	143	1	-14	7	3	41	61	14	-8	10	3	32	44	9
2	10	2	139	142	10	10	1	3	59	52	3	-5	4	3	0	0	1	-13	7	3	40	34	9	-7	10	3	56	63	4
3	10	2	42	48	4	11	1	3	191	194	3	-4	4	3	610	598	6	-12	7	3	34	27	20	-6	10	3	57	59	3
4	10	2	53	49	4	12	1	3	0	13	1	-3	4	3	104	107	1	-11	7	3	0	7	1	-5	10	3	153	156	3
5	10	2	53	57	5	13	1	3	65	75	8	-2	4	3	612	602	6	-10	7	3	50	47	8	-4	10	3	64	65	3
6	10	2	135	129	3	14	1	3	49	46	7	-1	4	3	423	419	4	-9	7	3	47	49	17	-3	10	3	113	113	2
7	10	2	74	74	5	15	1	3	39	21	14	0	4	3	99	99	1	-8	7	3	20	21	12	-2	10	3	128	123	2
8	10	2	0	4	1	16	1	3	0	21	1	1	4	3	29	20	3	-7	7	3	29	21	8	-1	10	3	58	60	3
9	10	2	33	21	19	-18	2	3	41	43	16	2	4	3	171	177	2	-6	7	3	70	67	4	0	10	3	36	30	5
10	10	2	19	2	18	-17	2	3	43	22	28	3	4	3	267	260	3	-5	7	3	69	69	9	1	10	3	85	83	3
11	10	2	32	61	31	-16	2	3	125	134	5	4	4	3	37	35	9	-4	7	3	17	5	14	2	10	3	135	132	6
-11	11	2	79	67	8	-15	2	3	66	66	3	5	4	3	0	1	1	-3	7	3	45	44	3	3	10	3	53	50	3
-10	11	2	121	110	5	-14	2	3	96	100	2	6	4	3	46	33	6	-2	7	3	244	248	2	4	10	3	104	105	3
-9	11	2	20	37	19	-13	2	3	390	382	3	7	4	3	44	40	5	-1	7	3	103	108	1	5	10	3	76	67	5
-8	11	2	82	85	6	-12	2	3	395	381	4	8	4	3	109	109	2	0	7	3	166	163	2	6	10	3	20	19	1
-7	11	2	169	160	3	-11	2	3	37	32	4	9	4	3	166	164	4	1	7	3	21	22	9	7	10	3	46	34	10
-6	11	2	143	132	3	-10	2	3	54	51	2	10	4	3	97	103	3	2	7	3	41	36	3	8	10	3	0	15	1
-5	11	2	131	128	3	-9	2	3	179	176	2	11	4	3	58	54	4	3	7	3	147	143	5	9	10	3	84	71	8
-4	11	2	62	64	3	-8	2	3	30	38	4	12	4	3	61	64	4	4	7	3	76	74	7	7	10	3	25	46	25
-3	11	2	18	14	12	-7	2	3	189	192	2	13	4	3	45	38	8	5	7	3	108	115	3	-11	11	3	28	12	28
-2	11	2	75	78	2	-6	2	3	561	551	4	14	4	3	43	32	13	6	7	3	206	207	10	-10	11	3	15	16	14
-1	11	2	32	30	5	-5	2	3	507	509	4	15	4	3	74	66	13	7	7	3	113	121	6	-9	11	3	95	90	7
0	11	2	48	49	4	-4	2	3	211	219	2	-17	5	3	98	105	13	8	7	3	164	165	4	-8	11	3	0	1	1
1	11	2	55	50	4	-3	2	3	411	421	3	-16	5	3	89	90	7	9	7	3	80	82	5	-7	11	3	112	118	3
2	11	2	53	54	3	-2	2	3	19	44	6	-15	5	3	77	86	6	10	7	3	62	55	7	-6	11	3	60	56	4
3	11	2	99	97	3	-1	2	3	231	236	2	-14	5	3	73	85	4	11	7	3	34	47	12	-5	11	3	239	238	3
4	11	2	37	45	7	0	2	3	51	55	9	-13	5	3	158	158	10	12	7	3	69	74	7	-4	11	3	31	36	8
5	11	2	41	28	8	1	2	3	206	206	2	-12	5	3	56	59	5	13	7										

Table 6. Observed and calculated structure factors for 1

Page 4

<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	
-4	13	3	63	66	7	-7	2	4	276	276	2	14	4	4	54	47	54	8	7	4	92	89	5	
-3	13	3	51	45	9	-6	2	4	21	16	10	-17	5	4	39	17	39	9	7	4	38	20	12	
-2	13	3	59	35	15	-5	2	4	63	54	3	-16	5	4	0	0	1	10	7	4	16	12	15	
-1	13	3	44	45	10	-4	2	4	76	82	2	-15	5	4	0	34	1	11	7	4	54	52	9	
0	13	3	23	21	23	-3	2	4	201	204	1	-14	5	4	183	183	5	12	7	4	0	16	1	
1	13	3	110	111	7	-2	2	4	338	335	3	-13	5	4	109	110	3	-15	8	4	34	34	33	
2	13	3	57	53	8	-1	2	4	326	332	3	-12	5	4	12	15	12	-14	8	4	145	136	9	
3	13	3	34	38	14	0	2	4	351	356	4	-11	5	4	76	78	4	-13	8	4	100	79	8	
-18	0	4	58	76	16	1	2	4	18	30	18	-10	5	4	52	48	3	-12	8	4	43	44	9	
-17	0	4	184	192	8	2	2	4	60	47	9	-9	5	4	170	172	4	-11	8	4	6	2	6	
-16	0	4	65	64	5	3	2	4	230	225	4	-8	5	4	43	45	3	-10	8	4	32	32	7	
-15	0	4	114	119	3	4	2	4	98	83	8	-7	5	4	190	188	2	-9	8	4	92	95	2	
-14	0	4	137	141	3	5	2	4	85	88	4	-6	5	4	379	368	5	-8	8	4	54	60	2	
-13	0	4	228	232	3	6	2	4	109	106	3	-5	5	4	336	330	5	-7	8	4	118	116	5	
-12	0	4	107	105	2	7	2	4	201	204	3	-4	5	4	80	76	1	-6	8	4	84	92	12	
-11	0	4	168	164	2	8	2	4	0	1	1	-3	5	4	8	15	8	-5	8	4	65	58	7	
-10	0	4	126	130	2	9	2	4	15	34	14	-2	5	4	63	67	3	-4	8	4	163	168	7	
-9	0	4	0	3	1	10	2	4	0	36	1	-1	5	4	258	259	2	-3	8	4	159	165	6	
-8	0	4	240	231	3	11	2	4	90	95	2	0	5	4	255	244	2	-2	8	4	48	48	4	
-7	0	4	205	204	3	12	2	4	32	17	12	1	5	4	260	256	3	-1	8	4	115	119	8	
-6	0	4	325	319	4	13	2	4	27	21	26	2	5	4	311	305	3	0	8	4	47	39	4	
-5	0	4	221	219	3	14	2	4	48	18	11	3	5	4	202	200	3	1	8	4	38	32	3	
-4	0	4	253	261	4	15	2	4	32	17	32	4	5	4	85	94	2	2	8	4	0	11	1	
-3	0	4	0	41	1	-18	3	4	0	2	1	5	5	4	94	97	3	3	8	4	96	105	4	
-2	0	4	497	507	6	-17	3	4	46	17	46	6	5	4	76	74	7	4	8	4	114	115	7	
-1	0	4	82	82	3	-16	3	4	69	70	69	7	5	4	154	161	8	5	8	4	33	17	10	
0	0	4	262	257	4	-15	3	4	45	46	13	8	5	4	174	167	10	6	8	4	236	227	4	
1	0	4	55	61	8	-14	3	4	111	112	3	9	5	4	24	21	11	7	8	4	64	54	6	
2	0	4	276	283	5	-13	3	4	113	114	6	10	5	4	104	117	4	8	8	4	51	62	9	
3	0	4	71	67	4	-12	3	4	203	203	4	11	5	4	47	57	8	9	8	4	173	163	4	
4	0	4	483	485	22	-11	3	4	131	129	1	12	5	4	23	38	23	10	8	4	31	36	31	
5	0	4	284	302	15	-10	3	4	121	119	3	13	5	4	51	50	12	11	8	4	31	16	31	
6	0	4	185	196	13	-9	3	4	18	16	11	14	5	4	87	91	8	-14	9	4	13	11	13	
7	0	4	74	78	3	-8	3	4	63	58	2	-16	6	4	104	86	11	-13	9	4	52	29	15	
8	0	4	37	22	6	-7	3	4	9	15	9	-15	6	4	73	65	8	-12	9	4	33	6	32	
9	0	4	59	67	3	-6	3	4	33	30	4	-14	6	4	16	22	15	-11	9	4	46	53	11	
10	0	4	142	155	4	-5	3	4	196	195	1	-13	6	4	74	75	5	-10	9	4	20	24	19	
11	0	4	53	53	4	-4	3	4	41	37	3	-12	6	4	10	5	10	-9	9	4	25	19	5	
12	0	4	41	52	9	-3	3	4	241	245	2	-11	6	4	20	24	7	-9	9	4	137	141	3	
13	0	4	90	87	6	-2	3	4	164	158	4	-10	6	4	59	57	3	-7	9	4	0	11	1	
14	0	4	131	117	8	-1	3	4	90	92	1	-9	6	4	30	37	30	-6	9	4	72	78	4	
15	0	4	27	26	0	3	3	4	72	63	2	-8	6	4	27	1	9	-5	9	4	59	48	3	
16	1	4	16	8	15	1	3	4	195	191	2	-7	6	4	20	11	11	-4	9	4	255	271	3	
17	1	4	16	51	16	2	3	4	28	35	5	-6	6	4	360	355	3	-3	9	4	46	53	4	
18	1	4	34	41	7	3	3	4	272	271	3	-5	6	4	49	44	3	-2	9	4	215	216	6	
19	1	4	60	61	4	4	3	4	0	9	1	-4	6	4	36	39	10	-1	9	4	37	33	16	
20	1	4	162	162	2	5	3	4	55	44	2	-3	6	4	39	38	6	0	9	4	18	25	13	
21	1	4	321	318	5	6	3	4	277	273	5	-2	6	4	52	50	6	1	9	4	72	68	2	
22	1	4	0	2	1	7	3	4	60	52	2	-1	6	4	63	61	3	2	9	4	203	209	5	
23	1	4	41	40	12	8	3	4	93	91	2	0	6	4	0	10	1	3	9	4	167	168	5	
24	1	4	32	18	7	9	3	4	49	42	3	1	6	4	57	52	2	4	9	4	0	17	1	
25	1	4	128	125	1	10	3	4	41	32	4	2	6	4	12	3	11	5	9	4	144	134	4	
26	1	4	321	316	3	11	3	4	0	1	1	3	6	4	74	73	6	6	9	4	64	65	7	
27	1	4	406	396	3	12	3	4	50	60	10	4	6	4	51	55	6	7	9	4	157	153	4	
28	1	4	52	47	6	13	3	4	67	65	5	5	6	4	150	147	7	8	9	4	72	84	6	
29	1	4	212	218	2	14	3	4	0	23	1	6	6	4	77	86	6	9	9	4	41	9	14	
30	4	1	42	40	4	-17	4	4	0	9	1	7	6	4	79	84	2	-1	10	4	118	121	6	
31	3	1	4	135	137	2	-16	4	4	68	58	10	8	6	4	161	159	7	-12	10	4	51	27	17
32	2	1	4	81	81	1	-15	4	4	39	32	10	9	6	4	196	182	5	-11	10	4	53	56	16
33	1	1	4	246	246	4	-14	4	4	186	186	6	10	6	4	102	97	4	-10	10	4	0	18	1
34	0	1	4	23	26	22	-13	4	4	37	48	3	11	6	4	0	8	1	-9	10	4	57	49	5
35	1	1	4	137	137	3	-12	4	4	25	38	6	12	6	4	10	32	10	-8	10	4	65	55	4
36	2	1	4	128	131	6	-11	4	4	98	99	1	13	6	4	26	22	26	-7	10	4	31	34	7
37	3	1	4	73	80	4	-10	4	4	10	9	4	-16	7	4	41	21	18	-6	10	4	38	28	6
38	4	1	4	0	6	1	-9	4	4	59	57	2	-15	7	4	180	182	8	-5	10	4	36	32	6
39	5	1	4	133	135	4	-8	4	4	69	58	3	-14	7	4	38	17	38	-4	10	4</td			

Table 6. Observed and calculated structure factors for 1

Page 5

<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s	<i>h</i>	<i>k</i>	<i>l</i>	10Fo	10Fc	10s
3	2	5	78	84	4	-6	5	5	189	184	4	-5	8	5	56	47	3	1	12	5	82	83	8
4	2	5	327	321	6	-5	5	5	279	275	2	-4	8	5	0	2	1	2	12	5	45	36	13
5	2	5	69	68	5	-4	5	5	240	238	2	-3	8	5	14	12	13	3	12	5	0	24	1
6	2	5	217	216	4	-3	5	5	232	229	5	-2	8	5	26	41	8	4	12	5	40	30	18
7	2	5	253	248	4	-2	5	5	37	33	4	-1	8	5	61	63	3	-18	0	6	106	108	12
8	2	5	86	79	2	-1	5	5	148	148	2	0	8	5	74	84	8	-17	0	6	23	42	23
9	2	5	81	88	2	0	5	5	85	83	3	1	8	5	130	131	3	-16	0	6	51	40	11
10	2	5	119	125	3	1	5	5	28	15	7	2	8	5	27	20	7	-15	0	6	43	50	10
11	2	5	26	20	16	2	5	5	154	157	2	3	8	5	89	88	13	-14	0	6	107	99	4
12	2	5	22	8	22	3	5	5	118	119	2	4	8	5	163	166	8	-13	0	6	87	74	3
13	2	5	104	108	8	4	5	5	116	121	2	5	8	5	0	2	1	-12	0	6	0	18	1
14	2	5	0	47	1	5	5	5	34	29	5	6	8	5	130	129	3	-11	0	6	86	73	4
-18	3	5	103	88	9	6	5	5	117	121	3	7	8	5	73	76	6	-10	0	6	133	82	3
-17	3	5	114	107	14	7	5	5	207	217	6	8	8	5	15	18	14	-9	0	6	281	278	4
-16	3	5	19	18	18	8	5	5	31	39	10	9	8	5	10	15	10	-8	0	6	90	82	3
-15	3	5	83	87	3	9	5	5	81	86	4	10	8	5	47	49	11	-7	0	6	250	238	4
-14	3	5	20	1	20	10	5	5	61	53	7	11	8	5	35	15	34	-6	0	6	280	272	4
-13	3	5	92	94	3	11	5	5	56	64	6	-14	9	5	36	12	17	-5	0	6	85	64	3
-12	3	5	6	9	5	12	5	5	105	99	5	-13	9	5	0	0	1	-4	0	6	419	411	5
-11	3	5	82	74	2	13	5	5	49	35	14	-11	9	5	19	21	18	-3	0	6	477	455	6
-10	3	5	16	9	15	-16	6	5	93	94	11	-10	9	5	16	23	15	-2	0	6	115	71	2
-9	3	5	59	57	2	-15	6	5	0	2	1	-9	9	5	0	34	1	-1	0	6	130	87	4
-8	3	5	257	260	2	-14	6	5	0	14	1	-8	9	5	15	13	14	0	0	6	298	285	6
-7	3	5	67	62	2	-13	6	5	75	85	3	-7	9	5	157	156	2	1	0	6	107	100	3
-6	3	5	43	40	3	-12	6	5	69	68	3	-6	9	5	23	19	13	2	0	6	182	183	3
-5	3	5	24	15	23	-11	6	5	41	30	4	-5	9	5	67	66	11	3	0	6	0	4	1
-4	3	5	199	197	2	-10	6	5	0	14	1	-4	9	5	22	20	10	4	0	6	208	205	4
-3	3	5	205	204	2	-9	6	5	115	117	3	-3	9	5	44	50	5	5	0	6	598	577	14
-2	3	5	164	159	1	-8	6	5	30	9	7	-2	9	5	139	139	5	6	0	6	234	241	11
-1	3	5	26	9	26	-7	6	5	21	22	10	-1	9	5	43	36	10	7	0	6	131	140	7
0	3	5	58	61	3	-6	6	5	151	145	5	0	9	5	68	69	3	8	0	6	308	309	16
1	3	5	287	272	3	-5	6	5	27	15	8	1	9	5	93	91	11	9	0	6	227	214	6
2	3	5	10	22	10	-4	6	5	232	228	4	2	9	5	93	88	5	10	0	6	32	47	12
3	3	5	52	37	6	-3	6	5	160	165	2	3	9	5	78	77	7	11	0	6	230	206	5
4	3	5	154	156	3	-2	6	5	26	19	18	4	9	5	145	140	4	12	0	6	49	43	17
5	3	5	114	107	2	-1	6	5	52	48	3	5	9	5	41	46	9	-18	1	6	88	94	11
6	3	5	200	195	7	0	6	5	138	135	2	6	9	5	54	55	8	-17	1	6	57	34	11
7	3	5	150	151	4	1	6	5	93	89	2	7	9	5	21	27	20	-16	1	6	44	33	8
8	3	5	157	163	3	2	6	5	65	58	4	8	9	5	174	166	5	-15	1	6	88	86	3
9	3	5	128	132	1	3	6	5	82	89	4	9	9	5	51	57	16	-14	1	6	86	84	2
10	3	5	35	35	21	4	6	5	19	7	14	-12	10	5	8	24	8	-13	1	6	39	30	15
11	3	5	28	25	14	5	6	5	103	103	4	-11	10	5	29	43	28	-12	1	6	97	103	2
12	3	5	34	28	16	6	6	5	35	15	26	-10	10	5	23	20	23	-11	1	6	58	46	3
13	3	5	53	45	29	7	6	5	151	157	12	-9	10	5	25	27	25	-10	1	6	73	70	2
14	3	5	54	37	16	8	6	5	34	37	8	-8	10	5	0	13	1	-9	1	6	44	27	5
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Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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7	7																						

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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Table 6. Observed and calculated structure factors for 1

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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	7	9	0	14	1	-10	1	10	51	56	7	5	4	10	0	12	1	-12	1	11	180	187	9		
-7	7	9	30	30	18	-9	1	10	112	119	3	6	4	10	116	98	12	-11	1	11	31	18	11	-6	
-6	7	9	113	117	4	-8	1	10	308	313	4	7	4	10	0	14	1	-10	1	11	78	82	5	-5	
-5	7	9	13	12	13	-7	1	10	136	134	2	-14	5	10	0	43	1	-9	1	11	39	17	11	-3	
-4	7	9	0	16	1	-6	1	10	90	74	4	-13	5	10	52	46	12	-8	1	11	85	91	4	-2	
-3	7	9	40	39	30	-5	1	10	84	92	4	-12	5	10	86	91	6	-7	1	11	46	52	9	-1	
-2	7	9	65	54	5	-4	1	10	131	131	4	-11	5	10	65	71	7	-6	1	11	48	45	13	0	
-1	7	9	35	26	25	-3	1	10	0	39	1	-10	5	10	24	23	23	-5	1	11	64	65	9	1	
0	7	9	59	60	32	-2	1	10	186	193	3	-9	5	10	233	215	5	-4	1	11	104	104	6	2	
1	7	9	0	24	1	-1	1	10	33	17	10	-8	5	10	0	11	1	-3	1	11	94	97	6	3	
2	7	9	72	78	11	0	1	10	125	125	3	-7	5	10	119	127	5	-2	1	11	47	52	47	4	
3	7	9	54	55	18	1	1	10	86	86	3	-6	5	10	80	75	4	-1	1	11	89	63	89	-12	
4	7	9	0	53	1	2	1	10	52	35	7	-5	5	10	64	54	7	0	1	11	47	44	10	-11	
5	7	9	56	37	15	3	1	10	93	83	7	-4	5	10	45	44	9	1	1	11	83	91	8	-10	
6	7	9	30	16	30	4	1	10	17	10	16	-3	5	10	33	33	17	2	1	11	39	26	29	-9	
-12	8	9	0	46	1	5	1	10	25	30	24	-2	5	10	91	99	6	3	1	11	76	60	8	-8	
-11	8	9	56	60	7	6	1	10	33	11	32	-1	5	10	167	168	14	4	1	11	0	8	1	-7	
-10	8	9	117	97	5	7	1	10	20	24	19	0	5	10	21	7	20	5	1	11	0	22	1	-6	
-9	8	9	30	41	30	-16	2	10	57	66	9	1	5	10	38	34	16	-15	2	11	47	46	31	-5	
-8	8	9	70	72	6	-15	2	10	28	5	28	2	5	10	33	3	16	-14	2	11	42	14	41	-4	
-7	8	9	26	19	26	-14	2	10	21	15	21	3	5	10	110	103	11	-13	2	11	104	106	5	-3	
-6	8	9	24	26	23	-13	2	10	62	63	6	4	5	10	64	53	12	-12	2	11	43	20	10	-2	
-5	8	9	79	76	5	-12	2	10	27	23	17	5	5	10	59	6	15	-11	2	11	32	48	31	-1	
-4	8	9	6	0	6	-11	2	10	162	158	4	6	5	10	45	31	39	-10	2	11	74	86	5	0	
-3	8	9	55	48	10	-10	2	10	90	83	4	-14	6	10	97	73	8	-9	2	11	105	113	4	1	
-2	8	9	45	15	45	-9	2	10	40	9	11	-13	6	10	60	46	9	-8	2	11	114	125	4	2	
-1	8	9	60	66	8	-8	2	10	22	4	22	-12	6	10	61	66	10	-7	2	11	18	27	17	3	
0	8	9	38	39	14	-7	2	10	74	75	4	-11	6	10	84	88	8	-6	2	11	27	16	27	-11	
1	8	9	38	75	37	-6	2	10	45	24	24	-10	6	10	93	104	5	-5	2	11	30	40	29	-10	
2	8	9	0	6	1	-5	2	10	84	93	4	-9	6	10	0	3	1	-4	2	11	16	20	15	-9	
3	8	9	29	0	28	-4	2	10	0	0	1	-8	6	10	69	66	7	-3	2	11	183	184	8	-8	
4	8	9	74	47	17	-3	2	10	72	80	5	-7	6	10	31	0	19	-2	2	11	74	64	7	-7	
5	8	9	46	20	28	-2	2	10	43	49	32	-6	6	10	46	39	9	-1	2	11	82	92	7	-6	
-11	9	9	32	47	11	-1	2	10	183	190	3	-5	6	10	80	83	5	0	2	11	21	15	20	-5	
-10	9	9	35	11	19	0	2	10	132	135	4	-4	6	10	25	36	25	1	2	11	63	66	13	-4	
-9	9	9	98	105	6	1	2	10	16	35	15	-3	6	10	50	57	8	2	2	11	26	2	25	-3	
-8	9	9	24	28	23	2	2	10	79	84	9	-2	6	10	40	12	14	3	2	11	47	9	15	-2	
-7	9	9	61	67	7	3	2	10	55	46	10	-1	6	10	77	74	5	4	2	11	46	10	14	-1	
-6	9	9	23	10	23	4	2	10	30	31	18	0	6	10	84	89	5	5	2	11	0	26	1	0	
-5	9	9	87	80	6	5	2	10	56	61	7	1	6	10	0	17	1	6	2	11	62	73	13	1	
-4	9	9	0	4	1	6	2	10	41	26	23	2	6	10	118	97	9	-14	3	11	26	36	25	-8	
-3	9	9	80	73	6	7	2	10	44	15	18	3	6	10	43	12	32	-13	3	11	57	54	8	-7	
-2	9	9	69	66	7	8	2	10	0	16	1	4	6	10	96	85	10	-12	3	11	74	64	8	-6	
-1	9	9	62	47	16	-16	3	10	49	32	13	5	6	10	0	1	1	-11	3	11	29	13	28	-5	
0	9	9	76	35	16	-15	3	10	0	19	1	-12	7	10	32	22	19	-10	3	11	48	50	10	-4	
1	9	9	91	100	11	-14	3	10	45	44	9	-11	7	10	66	65	10	-9	3	11	41	42	14	-3	
2	9	9	84	78	13	-13	3	10	36	37	17	-10	7	10	100	105	6	-8	3	11	16	6	15	-2	
3	9	9	61	20	14	-12	3	10	21	21	20	-9	7	10	66	57	9	-7	3	11	51	36	11	-1	
-8	10	9	136	141	7	-11	3	10	0	37	1	-8	7	10	23	15	23	-6	3	11	40	19	6	-14	
-7	10	9	38	43	15	-10	3	10	72	73	6	-7	7	10	35	1	15	-5	3	11	0	1	-13		
-6	10	9	59	62	9	-9	3	10	76	79	5	-6	7	10	29	27	12	-4	3	11	15	18	14	-12	
-5	10	9	67	78	7	-8	3	10	46	38	10	-5	7	10	0	11	1	-3	3	11	47	63	12	-11	
-4	10	9	46	37	14	-7	3	10	112	108	4	-4	7	10	0	11	1	-2	3	11	35	8	35	-10	
-3	10	9	60	66	8	-6	3	10	84	86	5	-3	7	10	52	18	8	-1	3	11	35	1	27	-9	
-2	10	9	85	72	11	-5	3	10	73	62	5	-2	7	10	87	82	13	0	3	11	87	83	11	-8	
-1	10	9	41	49	28	-4	3	10	76	69	7	-1	7	10	34	16	16	1	3	11	24	31	23	-7	
0	10	9	0	14	1	-3	3	10	79	86	5	0	7	10	51	24	8	2	3	11	131	135	5	-6	
-16	0	10	38	54	37	-2	3	10	154	155	7	1	7	10	58	52	22	3	3	11	18	18	18	-5	
-15	0	10	73	21	17	-1	3	10	126	119	5	2	7	10	71	53	12	4	3	11	54	67	11	-4	
-14	0	10	113	111	6	0	3	10	141	141	4	3	7	10	0	42	1	5	3	11	0	16	1	-3	
-13	0	10	22	6	22	1	3	10	206	214	13	4	7	10	0	0	0	-14	4	11	62	33	9	-2	
-12	0	10	67	88	10	2	3	10	0	21	1	-11	1	8	10	0	11	1	-13	4	11	64	71	9	-1
-11	0	10	30	17	29	3	3	10	52	50	10	-10	8	10	85	82	7	-12	4	11	76	72	7	0	
-10	0	10	0	59	1	4	3																		

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-12	2	12	32	31	31	-3	3	12	63	59	19	-7	5	12	0	5	1	-11	1	13	29	40	29
-11	2	12	123	135	7	-2	3	12	87	72	11	-6	5	12	44	11	18	-10	1	13	27	51	27
-10	2	12	23	23	23	-1	3	12	0	0	1	-5	5	12	54	30	23	-9	1	13	44	31	15
-9	2	12	68	66	7	0	3	12	28	15	27	-4	5	12	86	86	15	-8	1	13	74	11	25
-8	2	12	29	10	28	1	3	12	0	7	1	-3	5	12	0	33	1	-7	1	13	32	14	31
-7	2	12	53	1	14	2	3	12	74	81	12	-2	5	12	0	21	1	-6	1	13	37	45	29
-6	2	12	49	35	14	3	3	12	33	10	33	-1	5	12	44	14	16	-5	1	13	19	31	18
-5	2	12	82	71	8	-12	4	12	0	5	1	0	5	12	0	6	1	-4	1	13	34	67	34
-4	2	12	59	46	16	-11	4	12	0	8	1	1	5	12	0	23	1	-3	1	13	33	12	32
-3	2	12	122	123	5	-10	4	12	89	91	7	-10	6	12	0	20	1	-2	1	13	81	52	13
-2	2	12	20	34	19	-9	4	12	0	13	1	-9	6	12	30	28	30	-1	1	13	49	30	15
-1	2	12	63	66	10	-8	4	12	78	46	8	-8	6	12	22	0	21	0	1	13	0	8	1
0	2	12	43	20	16	-7	4	12	45	53	12	-7	6	12	0	16	1	1	1	13	0	8	1
1	2	12	52	51	12	-6	4	12	40	34	22	-6	6	12	61	42	12	-11	2	13	0	2	1
2	2	12	16	39	15	-5	4	12	81	79	7	-5	6	12	0	2	1	-10	2	13	35	56	34
3	2	12	0	32	1	-4	4	12	0	4	1	-4	6	12	33	6	32	-9	2	13	73	67	15
-13	3	12	0	0	1	-3	4	12	17	21	16	-3	6	12	37	45	23	-8	2	13	58	16	20
-12	3	12	62	60	13	-2	4	12	40	69	40	-2	6	12	38	37	38	-7	2	13	64	58	15
-11	3	12	0	3	1	-1	4	12	42	36	16	-1	6	12	43	57	30	-6	2	13	56	64	16
-10	3	12	78	64	8	0	4	12	0	10	1	0	6	12	39	2	39	-5	2	13	98	94	8
-9	3	12	0	9	1	1	4	12	81	79	11	-7	7	12	89	87	8	-4	2	13	40	23	15
-8	3	12	83	91	7	2	4	12	41	22	40	-6	7	12	33	29	33	-3	2	13	65	6	27
-7	3	12	27	15	27	-11	5	12	37	43	26	-5	7	12	0	13	1	-2	2	13	52	47	21
-6	3	12	49	56	13	-10	5	12	34	11	33	-4	7	12	0	4	1	-1	2	13	22	16	22
-5	3	12	0	15	1	-9	5	12	52	21	11	-3	7	12	137	120	10	0	2	13	50	11	14
-4	3	12	111	96	9	-8	5	12	46	34	12	-12	1	13	32	12	32	-10	3	13	32	28	32

Crystallographic Material for **5b**

X-ray Experimental.

Table 1. Crystallographic Data for **5b**.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters (\AA^2) for the non-hydrogen atoms of **5b**.

Table 3. Bond Lengths (\AA) and Angles ($^\circ$) for the non-hydrogen atoms of **5b**.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of **5b**.

Table 5. Fractional coordinates and isotropic thermal parameters (\AA^2) for the hydrogen atoms of **5b**.

Figure 1. View of 1 showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms shown are drawn to an arbitrary scale.

Figure 2. Unit cell packing diagram for **5b**. The view is approximately down the **c** axis.

Figure 3. Unit cell packing diagram for **5b**. The view is approximately down the **a** axis.

Molecules 2 are shown in wireframe form while molecules **5b** are displayed as ball-and-stick.

Figure 4. View of the fit by least-squares of selected atoms of molecule **5b** (dashed lines) onto the equivalent atoms of molecule 2. The seven atoms of the fused ring system were used in the fit.

Table 6. Observed and calculated structure factor amplitudes 1. Values for F_o , F_c and $\sigma(F_o)$ have been multiplied by 10.

X-ray Experimental for $C_{27}H_{34}SiO_3$: Crystals grew as long colorless lathes and needles by slow evaporation from ethylacetate and hexane. The data crystal was a long lathe that had approximate dimensions; 0.50 x 0.20 x 0.09 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoK α radiation ($\lambda = 0.71073\text{\AA}$). A total of 360 frames of data were collected using ω -scans with a scan range of 1.1° and a counting time of 168 seconds per frame. The data were collected at -120°C using a Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.¹ The structure was solved by direct methods using SIR92² and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.³ The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to $1.2 \times U_{\text{eq}}$ of the attached atom ($1.5 \times U_{\text{eq}}$ for methyl hydrogen atoms). There are two molecules in the asymmetric unit. Atoms of molecule 2 have a ‘ appended to the atom label. The molecules have only slight conformation differences (Figure 4.). The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0244*P)^2 + (1.682*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.117, with $R(F)$ equal to 0.0579 and a goodness of fit, S , = 1.034. Definitions used for calculating $R(F), R_w(F^2)$ and the goodness of fit, S , are given below.⁴ The data were corrected for secondary extinction effects. The correction takes the form: $F_{\text{corr}} = kF_c/[1 + (5.1(5) \times 10^{-6}) * F_c^2 \lambda^3 / (\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).⁵ All figures were generated using SHELXTL/PC.⁶ Tables of positional and thermal parameters, bond lengths and angles, figures and lists of observed and calculated structure factors are located in tables 1 through 6.

References

- 1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.
- 2) SIR92. (1993). A program for crystal structure solution. Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. J. Appl. Cryst. 26, 343-350.
- 3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.
- 4) $R_w(F^2) = \{\sum w(|F_o|^2 - |F_c|^2)^2 / \sum w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
 $R(F) = \{\sum (|F_o| - |F_c|)^2 / \sum |F_o|\}$ for reflections with $|F_o| > 4(\sigma(F_o))$.
 $S = [\sum w(|F_o|^2 - |F_c|^2)^2 / (n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.
- 5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.
- 6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for 5b.

Empirical formula	C27 H34 O3 Si		
Formula weight	434.63		
Temperature	153(2) K		
Wavelength	0.71073 Å		
Crystal system	Triclinic		
Space group	P-1		
Unit cell dimensions	$a = 10.4365(1)$ Å	$\alpha = 92.475(1)^\circ$.	
	$b = 12.1163(2)$ Å	$\beta = 95.407(1)^\circ$.	
	$c = 20.7037(3)$ Å	$\gamma = 107.727(1)^\circ$.	
Volume	$2475.47(6)$ Å ³		
Z	4		
Density (calculated)	1.166 Mg/m ³		
Absorption coefficient	0.119 mm ⁻¹		
F(000)	936		
Crystal size	0.50 x 0.20 x 0.09 mm		
Theta range for data collection	2.94 to 27.50°.		
Index ranges	-13≤h≤13, -15≤k≤12, -26≤l≤26		
Reflections collected	16390		
Independent reflections	11097 [R(int) = 0.0280]		
Completeness to theta = 27.50°	97.4 %		
Absorption correction	None		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	11097 / 0 / 560		
Goodness-of-fit on F ²	1.034		
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1028		
R indices (all data)	R1 = 0.0958, wR2 = 0.1167		
Extinction coefficient	$5.1(5)\times 10^{-6}$		
Largest diff. peak and hole	0.28 and -0.34 e.Å ⁻³		

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	4382(2)	6195(2)	6168(1)	27(1)
C2	4190(2)	7201(2)	6575(1)	30(1)
C3	4965(2)	7217(2)	7241(1)	27(1)
C4	4359(2)	6239(2)	7680(1)	24(1)
C5	5603(2)	5786(2)	7645(1)	23(1)
C6	6098(2)	6665(2)	7119(1)	26(1)
C7	5815(2)	6185(2)	6404(1)	30(1)
O8	3392(1)	5134(1)	6292(1)	28(1)
Si9	2536(1)	4120(1)	5716(1)	25(1)
C10	3655(2)	3340(2)	5403(1)	37(1)
C11	1858(2)	4815(2)	5033(1)	39(1)
C12	1140(2)	3125(2)	6122(1)	34(1)
C13	1707(3)	2865(2)	6786(1)	51(1)
C14	515(3)	1973(2)	5703(1)	55(1)
C15	34(3)	3696(3)	6216(1)	58(1)
C16	3989(2)	6578(2)	8331(1)	26(1)
O17	3882(2)	7539(1)	8448(1)	38(1)
C18	3652(2)	5670(2)	8812(1)	26(1)
C19	3551(2)	6007(2)	9453(1)	38(1)
C20	3246(3)	5182(2)	9907(1)	47(1)
C21	3031(2)	4025(2)	9732(1)	44(1)
C22	3114(2)	3680(2)	9096(1)	36(1)
C23	3428(2)	4498(2)	8639(1)	30(1)
C24	6637(2)	6098(2)	8238(1)	24(1)
O25	6549(1)	6760(1)	8682(1)	31(1)
C26	7816(2)	5640(2)	8259(1)	25(1)
C27	8806(2)	5993(2)	8796(1)	35(1)
C28	9873(2)	5543(2)	8857(1)	46(1)
C29	9969(2)	4743(2)	8387(1)	46(1)
C30	9020(2)	4405(2)	7848(1)	39(1)
C31	7941(2)	4854(2)	7780(1)	30(1)

C1'	5643(2)	1466(2)	8864(1)	30(1)
C2'	5791(2)	2582(2)	8523(1)	29(1)
C3'	4955(2)	2188(2)	7860(1)	26(1)
C4'	5520(2)	1533(2)	7357(1)	22(1)
C5'	4292(2)	417(2)	7377(1)	23(1)
C6'	3842(2)	1029(2)	7957(1)	27(1)
C7'	4193(2)	702(2)	8646(1)	32(1)
O8'	6593(2)	925(1)	8647(1)	33(1)
Si9'	7756(1)	621(1)	9139(1)	32(1)
C10'	8617(3)	1890(2)	9735(1)	55(1)
C11'	6920(3)	-663(2)	9575(1)	47(1)
C12'	8969(2)	337(2)	8586(1)	36(1)
C13'	8211(3)	-586(2)	8041(1)	47(1)
C14'	9694(3)	1448(2)	8273(2)	67(1)
C15'	10024(3)	-98(4)	8972(2)	83(1)
C16'	5849(2)	2070(2)	6722(1)	25(1)
O17'	5873(2)	3069(1)	6649(1)	33(1)
C18'	6255(2)	1376(2)	6208(1)	26(1)
C19'	6367(2)	1776(2)	5588(1)	34(1)
C20'	6707(2)	1139(2)	5098(1)	40(1)
C21'	6949(2)	105(2)	5219(1)	39(1)
C22'	6864(2)	-290(2)	5832(1)	41(1)
C23'	6512(2)	338(2)	6324(1)	32(1)
C24'	3214(2)	143(2)	6809(1)	23(1)
O25'	3296(1)	779(1)	6360(1)	32(1)
C26'	1985(2)	-895(2)	6818(1)	25(1)
C27'	966(2)	-1134(2)	6300(1)	33(1)
C28'	-159(2)	-2106(2)	6281(1)	41(1)
C29'	-282(2)	-2848(2)	6776(1)	40(1)
C30'	710(2)	-2606(2)	7299(1)	38(1)
C31'	1846(2)	-1636(2)	7324(1)	31(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for 1.

C1-O8	1.433(2)	C13-H13B	0.96
C1-C2	1.527(3)	C13-H13C	0.96
C1-C7	1.534(3)	C14-H14A	0.96
C1-H1	0.96	C14-H14B	0.96
C2-C3	1.528(3)	C14-H14C	0.96
C2-H2A	0.96	C15-H15A	0.96
C2-H2B	0.96	C15-H15B	0.96
C3-C4	1.542(3)	C15-H15C	0.96
C3-C6	1.560(3)	C16-O17	1.219(2)
C3-H3	0.96	C16-C18	1.500(3)
C4-C16	1.510(3)	C18-C23	1.392(3)
C4-C5	1.562(3)	C18-C19	1.396(3)
C4-H4	0.96	C19-C20	1.389(3)
C5-C24	1.508(3)	C19-H19	0.96
C5-C6	1.568(3)	C20-C21	1.376(4)
C5-H5	0.96	C20-H20	0.96
C6-C7	1.535(3)	C21-C22	1.382(3)
C6-H6	0.96	C21-H21	0.96
C7-H7A	0.96	C22-C23	1.388(3)
C7-H7B	0.96	C22-H22	0.96
O8-Si9	1.6531(14)	C23-H23	0.96
Si9-C10	1.855(2)	C24-O25	1.223(2)
Si9-C11	1.868(2)	C24-C26	1.493(3)
Si9-C12	1.879(2)	C26-C31	1.389(3)
C10-H10A	0.96	C26-C27	1.398(3)
C10-H10B	0.96	C27-C28	1.379(3)
C10-H10C	0.96	C27-H27	0.96
C11-H11A	0.96	C28-C29	1.375(4)
C11-H11B	0.96	C28-H28	0.96
C11-H11C	0.96	C29-C30	1.378(4)
C12-C13	1.528(3)	C29-H29	0.96
C12-C14	1.536(3)	C30-C31	1.390(3)
C12-C15	1.539(3)	C30-H30	0.96
C13-H13A	0.96	C31-H31	0.96

C1'-O8'	1.439(2)	C13'-H13E	0.96
C1'-C2'	1.525(3)	C13'-H13F	0.96
C1'-C7'	1.527(3)	C14'-H14D	0.96
C1'-H1'	0.96	C14'-H14E	0.96
C2'-C3'	1.529(3)	C14'-H14F	0.96
C2'-H2'A	0.96	C15'-H15D	0.96
C2'-H2'B	0.96	C15'-H15E	0.96
C3'-C4'	1.547(3)	C15'-H15F	0.96
C3'-C6'	1.560(3)	C16'-O17'	1.219(2)
C3'-H3'	0.96	C16'-C18'	1.498(3)
C4'-C16'	1.513(3)	C18'-C23'	1.390(3)
C4'-C5'	1.560(3)	C18'-C19'	1.393(3)
C4'-H4'	0.96	C19'-C20'	1.385(3)
C5'-C24'	1.500(3)	C19'-H19'	0.96
C5'-C6'	1.566(3)	C20'-C21'	1.380(3)
C5'-H5'	0.96	C20'-H20'	0.96
C6'-C7'	1.537(3)	C21'-C22'	1.376(3)
C6'-H6'	0.96	C21'-H21'	0.96
C7'-H7'A	0.96	C22'-C23'	1.388(3)
C7'-H7'B	0.96	C22'-H22'	0.96
O8'-Si9'	1.6478(15)	C23'-H23'	0.96
Si9'-C11'	1.855(3)	C24'-O25'	1.225(2)
Si9'-C10'	1.867(2)	C24'-C26'	1.501(3)
Si9'-C12'	1.880(2)	C26'-C27'	1.391(3)
C10'-H10D	0.96	C26'-C31'	1.398(3)
C10'-H10E	0.96	C27'-C28'	1.382(3)
C10'-H10F	0.96	C27'-H27'	0.96
C11'-H11D	0.96	C28'-C29'	1.382(3)
C11'-H11E	0.96	C28'-H28'	0.96
C11'-H11F	0.96	C29'-C30'	1.381(3)
C12'-C13'	1.528(3)	C29'-H29'	0.96
C12'-C14'	1.534(4)	C30'-C31'	1.387(3)
C12'-C15'	1.533(3)	C30'-H30'	0.96
C13'-H13D	0.96	C31'-H31'	0.96
O8-C1-C2	109.16(16)	C2-C1-C7	104.63(16)
O8-C1-C7	110.84(17)	O8-C1-H1	110.6

C2-C1-H1	110.9	C1-C7-H7B	110.0
C7-C1-H1	110.5	H7A-C7-H7B	108.6
C3-C2-C1	105.27(16)	C1-O8-Si9	123.63(12)
C3-C2-H2A	110.5	O8-Si9-C10	110.26(9)
C1-C2-H2A	110.4	O8-Si9-C11	109.26(9)
C3-C2-H2B	110.5	C10-Si9-C11	109.03(11)
C1-C2-H2B	111.3	O8-Si9-C12	104.90(9)
H2A-C2-H2B	108.8	C10-Si9-C12	111.50(11)
C2-C3-C4	117.76(17)	C11-Si9-C12	111.81(11)
C2-C3-C6	106.09(16)	Si9-C10-H10A	109.6
C4-C3-C6	89.74(15)	Si9-C10-H10B	109.2
C2-C3-H3	114.0	H10A-C10-H10B	109.5
C4-C3-H3	112.8	Si9-C10-H10C	109.6
C6-C3-H3	113.8	H10A-C10-H10C	109.5
C16-C4-C3	117.84(16)	H10B-C10-H10C	109.5
C16-C4-C5	120.21(16)	Si9-C11-H11A	109.4
C3-C4-C5	90.69(14)	Si9-C11-H11B	109.3
C16-C4-H4	108.9	H11A-C11-H11B	109.5
C3-C4-H4	108.8	Si9-C11-H11C	109.7
C5-C4-H4	109.0	H11A-C11-H11C	109.5
C24-C5-C4	115.78(16)	H11B-C11-H11C	109.5
C24-C5-C6	109.03(16)	C13-C12-C14	108.6(2)
C4-C5-C6	88.71(14)	C13-C12-C15	109.1(2)
C24-C5-H5	113.4	C14-C12-C15	109.3(2)
C4-C5-H5	113.9	C13-C12-Si9	109.84(15)
C6-C5-H5	113.6	C14-C12-Si9	109.89(16)
C7-C6-C3	106.26(16)	C15-C12-Si9	110.17(17)
C7-C6-C5	117.44(16)	C12-C13-H13A	109.4
C3-C6-C5	89.79(14)	C12-C13-H13B	109.4
C7-C6-H6	113.5	H13A-C13-H13B	109.5
C3-C6-H6	113.8	C12-C13-H13C	109.6
C5-C6-H6	113.4	H13A-C13-H13C	109.5
C6-C7-C1	106.38(16)	H13B-C13-H13C	109.5
C6-C7-H7A	110.9	C12-C14-H14A	110.2
C1-C7-H7A	111.3	C12-C14-H14B	108.6
C6-C7-H7B	109.7	H14A-C14-H14B	109.5

C12-C14-H14C	109.6	C28-C27-C26	120.6(2)
H14A-C14-H14C	109.5	C28-C27-H27	119.9
H14B-C14-H14C	109.5	C26-C27-H27	119.5
C12-C15-H15A	110.1	C29-C28-C27	119.8(2)
C12-C15-H15B	109.6	C29-C28-H28	120.1
H15A-C15-H15B	109.5	C27-C28-H28	120.0
C12-C15-H15C	108.6	C28-C29-C30	120.4(2)
H15A-C15-H15C	109.5	C28-C29-H29	119.6
H15B-C15-H15C	109.5	C30-C29-H29	119.9
O17-C16-C18	120.65(18)	C29-C30-C31	120.3(2)
O17-C16-C4	121.15(19)	C29-C30-H30	119.6
C18-C16-C4	118.05(17)	C31-C30-H30	120.2
C23-C18-C19	118.7(2)	C26-C31-C30	119.8(2)
C23-C18-C16	122.20(18)	C26-C31-H31	119.9
C19-C18-C16	119.07(19)	C30-C31-H31	120.3
C20-C19-C18	120.0(2)	O8'-C1'-C2'	109.04(16)
C20-C19-H19	120.6	O8'-C1'-C7'	110.40(17)
C18-C19-H19	119.4	C2'-C1'-C7'	104.82(17)
C21-C20-C19	120.8(2)	O8'-C1'-H1'	110.8
C21-C20-H20	119.8	C2'-C1'-H1'	110.6
C19-C20-H20	119.5	C7'-C1'-H1'	111.1
C20-C21-C22	119.6(2)	C3'-C2'-C1'	104.88(16)
C20-C21-H21	120.5	C3'-C2'-H2'A	110.7
C22-C21-H21	119.8	C1'-C2'-H2'A	110.4
C21-C22-C23	120.2(2)	C3'-C2'-H2'B	110.8
C21-C22-H22	120.3	C1'-C2'-H2'B	111.4
C23-C22-H22	119.6	H2'A-C2'-H2'B	108.7
C22-C23-C18	120.6(2)	C2'-C3'-C4'	117.48(17)
C22-C23-H23	120.1	C2'-C3'-C6'	105.85(16)
C18-C23-H23	119.3	C4'-C3'-C6'	89.79(14)
O25-C24-C26	120.20(18)	C2'-C3'-H3'	113.7
O25-C24-C5	120.57(17)	C4'-C3'-H3'	113.1
C26-C24-C5	119.15(17)	C6'-C3'-H3'	114.3
C31-C26-C27	119.09(19)	C16'-C4'-C3'	118.35(16)
C31-C26-C24	122.53(18)	C16'-C4'-C5'	121.10(16)
C27-C26-C24	118.35(18)	C3'-C4'-C5'	90.42(14)

C16'-C4'-H4'	108.5	H11D-C11'-H11E	109.5
C3'-C4'-H4'	108.0	Si9'-C11'-H11F	109.7
C5'-C4'-H4'	108.9	H11D-C11'-H11F	109.5
C24'-C5'-C4'	116.43(16)	H11E-C11'-H11F	109.5
C24'-C5'-C6'	109.78(15)	C13'-C12'-C14'	108.0(2)
C4'-C5'-C6'	89.09(14)	C13'-C12'-C15'	108.6(2)
C24'-C5'-H5'	113.0	C14'-C12'-C15'	109.2(2)
C4'-C5'-H5'	113.5	C13'-C12'-Si9'	110.36(16)
C6'-C5'-H5'	112.8	C14'-C12'-Si9'	110.55(17)
C7'-C6'-C3'	106.34(16)	C15'-C12'-Si9'	110.08(18)
C7'-C6'-C5'	117.27(17)	C12'-C13'-H13D	109.7
C3'-C6'-C5'	89.69(14)	C12'-C13'-H13E	109.3
C7'-C6'-H6'	114.0	H13D-C13'-H13E	109.5
C3'-C6'-H6'	113.8	C12'-C13'-H13F	109.4
C5'-C6'-H6'	113.1	H13D-C13'-H13F	109.5
C1'-C7'-C6'	105.86(17)	H13E-C13'-H13F	109.5
C1'-C7'-H7'A	111.6	C12'-C14'-H14D	109.8
C6'-C7'-H7'A	111.2	C12'-C14'-H14E	108.8
C1'-C7'-H7'B	109.6	H14D-C14'-H14E	109.5
C6'-C7'-H7'B	109.7	C12'-C14'-H14F	109.8
H7'A-C7'-H7'B	108.8	H14D-C14'-H14F	109.5
C1'-O8'-Si9'	123.83(12)	H14E-C14'-H14F	109.5
O8'-Si9'-C11'	108.58(11)	C12'-C15'-H15D	108.5
O8'-Si9'-C10'	109.75(10)	C12'-C15'-H15E	110.3
C11'-Si9'-C10'	109.87(13)	H15D-C15'-H15E	109.5
O8'-Si9'-C12'	104.50(9)	C12'-C15'-H15F	109.7
C11'-Si9'-C12'	112.96(11)	H15D-C15'-H15F	109.5
C10'-Si9'-C12'	111.01(12)	H15E-C15'-H15F	109.5
Si9'-C10'-H10D	110.0	O17'-C16'-C18'	120.82(18)
Si9'-C10'-H10E	109.2	O17'-C16'-C4'	120.82(18)
H10D-C10'-H10E	109.5	C18'-C16'-C4'	118.17(17)
Si9'-C10'-H10F	109.2	C23'-C18'-C19'	118.54(19)
H10D-C10'-H10F	109.5	C23'-C18'-C16'	122.34(18)
H10E-C10'-H10F	109.5	C19'-C18'-C16'	119.12(19)
Si9'-C11'-H11D	109.2	C20'-C19'-C18'	120.5(2)
Si9'-C11'-H11E	109.5	C20'-C19'-H19'	120.0

C18'-C19'-H19'	119.6
C21'-C20'-C19'	120.3(2)
C21'-C20'-H20'	119.8
C19'-C20'-H20'	119.8
C22'-C21'-C20'	119.8(2)
C22'-C21'-H21'	120.4
C20'-C21'-H21'	119.8
C21'-C22'-C23'	120.2(2)
C21'-C22'-H22'	120.0
C23'-C22'-H22'	119.8
C18'-C23'-C22'	120.6(2)
C18'-C23'-H23'	119.3
C22'-C23'-H23'	120.1
O25'-C24'-C5'	121.16(17)
O25'-C24'-C26'	120.26(18)
C5'-C24'-C26'	118.48(17)
C27'-C26'-C31'	119.24(19)
C27'-C26'-C24'	118.68(18)
C31'-C26'-C24'	122.07(18)
C28'-C27'-C26'	120.3(2)
C28'-C27'-H27'	120.2
C26'-C27'-H27'	119.5
C27'-C28'-C29'	120.3(2)
C27'-C28'-H28'	119.9
C29'-C28'-H28'	119.7
C28'-C29'-C30'	119.9(2)
C28'-C29'-H29'	119.8
C30'-C29'-H29'	120.3
C29'-C30'-C31'	120.4(2)
C29'-C30'-H30'	119.8
C31'-C30'-H30'	119.8
C30'-C31'-C26'	119.8(2)
C30'-C31'-H31'	120.8
C26'-C31'-H31'	119.4

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	30(1)	30(1)	20(1)	6(1)	2(1)	6(1)
C2	33(1)	28(1)	28(1)	8(1)	1(1)	9(1)
C3	30(1)	23(1)	25(1)	1(1)	1(1)	7(1)
C4	23(1)	26(1)	21(1)	2(1)	0(1)	8(1)
C5	24(1)	23(1)	23(1)	0(1)	2(1)	9(1)
C6	24(1)	28(1)	23(1)	2(1)	1(1)	4(1)
C7	28(1)	37(1)	24(1)	3(1)	5(1)	7(1)
O8	32(1)	28(1)	21(1)	2(1)	2(1)	3(1)
Si9	26(1)	28(1)	20(1)	1(1)	-1(1)	8(1)
C10	43(1)	44(1)	28(1)	2(1)	6(1)	20(1)
C11	43(1)	40(1)	33(1)	6(1)	-6(1)	13(1)
C12	31(1)	38(1)	28(1)	3(1)	2(1)	3(1)
C13	56(2)	53(2)	32(1)	17(1)	3(1)	-1(1)
C14	53(2)	47(2)	45(2)	1(1)	3(1)	-12(1)
C15	37(1)	80(2)	60(2)	11(2)	18(1)	18(1)
C16	24(1)	33(1)	23(1)	-1(1)	-2(1)	12(1)
O17	48(1)	39(1)	33(1)	-2(1)	3(1)	25(1)
C18	20(1)	37(1)	24(1)	2(1)	2(1)	11(1)
C19	36(1)	46(1)	28(1)	-4(1)	4(1)	7(1)
C20	47(2)	63(2)	23(1)	4(1)	8(1)	6(1)
C21	38(1)	56(2)	35(1)	17(1)	7(1)	8(1)
C22	31(1)	40(1)	39(1)	11(1)	7(1)	13(1)
C23	28(1)	37(1)	27(1)	4(1)	6(1)	14(1)
C24	25(1)	21(1)	23(1)	4(1)	1(1)	5(1)
O25	33(1)	35(1)	25(1)	-5(1)	-2(1)	14(1)
C26	24(1)	24(1)	27(1)	7(1)	4(1)	6(1)
C27	31(1)	40(1)	32(1)	4(1)	2(1)	11(1)
C28	30(1)	58(2)	51(2)	9(1)	-3(1)	17(1)

C29	27(1)	44(1)	73(2)	18(1)	10(1)	16(1)
C30	31(1)	31(1)	59(2)	4(1)	16(1)	12(1)
C31	27(1)	24(1)	38(1)	5(1)	7(1)	5(1)
C1'	34(1)	39(1)	19(1)	-1(1)	1(1)	14(1)
C2'	32(1)	32(1)	25(1)	-4(1)	3(1)	10(1)
C3'	30(1)	27(1)	24(1)	2(1)	3(1)	13(1)
C4'	24(1)	23(1)	20(1)	2(1)	1(1)	6(1)
C5'	27(1)	21(1)	21(1)	5(1)	3(1)	9(1)
C6'	25(1)	33(1)	23(1)	1(1)	3(1)	10(1)
C7'	37(1)	41(1)	19(1)	4(1)	7(1)	12(1)
O8'	38(1)	44(1)	21(1)	2(1)	-3(1)	22(1)
Si9'	39(1)	31(1)	23(1)	1(1)	-8(1)	12(1)
C10'	67(2)	45(2)	45(2)	-12(1)	-23(1)	19(1)
C11'	65(2)	49(2)	28(1)	10(1)	5(1)	17(1)
C12'	31(1)	38(1)	37(1)	6(1)	-4(1)	12(1)
C13'	51(2)	50(2)	39(1)	-3(1)	9(1)	12(1)
C14'	53(2)	50(2)	93(2)	11(2)	26(2)	1(1)
C15'	77(2)	137(3)	60(2)	4(2)	-13(2)	77(2)
C16'	22(1)	26(1)	22(1)	4(1)	-2(1)	1(1)
O17'	42(1)	25(1)	28(1)	5(1)	-1(1)	6(1)
C18'	21(1)	31(1)	21(1)	1(1)	2(1)	2(1)
C19'	29(1)	45(1)	25(1)	8(1)	3(1)	9(1)
C20'	34(1)	62(2)	22(1)	5(1)	6(1)	12(1)
C21'	33(1)	50(2)	30(1)	-8(1)	9(1)	5(1)
C22'	47(1)	35(1)	39(1)	0(1)	15(1)	10(1)
C23'	39(1)	31(1)	25(1)	3(1)	9(1)	7(1)
C24'	26(1)	23(1)	20(1)	1(1)	3(1)	9(1)
O25'	32(1)	33(1)	26(1)	9(1)	-2(1)	3(1)
C26'	25(1)	24(1)	25(1)	1(1)	5(1)	7(1)
C27'	31(1)	35(1)	29(1)	5(1)	2(1)	4(1)
C28'	31(1)	45(1)	36(1)	2(1)	-1(1)	-1(1)
C29'	31(1)	35(1)	46(2)	1(1)	10(1)	-4(1)
C30'	37(1)	33(1)	41(1)	12(1)	12(1)	4(1)
C31'	30(1)	30(1)	31(1)	6(1)	5(1)	7(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H1	4307	6321	5713	33
H2A	3247	7073	6613	36
H2B	4545	7925	6385	36
H3	5294	7970	7473	32
H4	3577	5687	7441	28
H5	5368	4987	7484	28
H6	6999	7185	7234	31
H7A	6470	6649	6150	36
H7B	5856	5404	6374	36
H10A	4352	3867	5196	55
H10B	4061	3033	5760	55
H10C	3133	2714	5095	55
H11A	2598	5314	4837	58
H11B	1303	4223	4713	58
H11C	1326	5265	5195	58
H13A	988	2357	6990	76
H13B	2387	2496	6730	76
H13C	2100	3576	7055	76
H14A	-195	1460	5910	82
H14B	150	2135	5288	82
H14C	1201	1613	5643	82
H15A	-676	3190	6427	87
H15B	419	4417	6477	87
H15C	-331	3842	5797	87
H19	3702	6814	9577	46
H20	3171	5421	10346	56
H21	2832	3459	10048	53
H22	2956	2875	8968	43
H23	3494	4257	8198	36
H27	8722	6532	9130	42

H28	10558	5801	9222	55
H29	10700	4417	8436	55
H30	9111	3861	7519	47
H31	7278	4618	7405	36
H1'	5789	1628	9328	36
H2'A	6723	2961	8472	35
H2'B	5455	3110	8763	35
H3'	4610	2769	7676	31
H4'	6320	1407	7565	27
H5'	4550	-248	7499	27
H6'	2935	1063	7874	32
H7'A	3575	824	8936	38
H7'B	4152	-101	8631	38
H10D	7986	2023	10014	82
H10E	9347	1733	9994	82
H10F	8971	2567	9504	82
H11D	6473	-1309	9264	71
H11E	7587	-856	9860	71
H11F	6266	-491	9825	71
H13D	8839	-724	7762	71
H13E	7763	-1294	8227	71
H13F	7552	-322	7793	71
H14D	10312	1293	7993	101
H14E	9030	1704	8023	101
H14F	10184	2043	8606	101
H15D	10632	-234	8680	125
H15E	10525	472	9315	125
H15F	9579	-810	9155	125
H19'	6203	2496	5502	40
H20'	6779	1421	4672	48
H21'	7171	-337	4874	47
H22'	7036	-1007	5918	49
H23'	6459	64	6752	39

H27'	1050	-619	5956	40
H28'	-856	-2270	5921	49
H29'	-1056	-3531	6754	48
H30'	610	-3111	7649	45
H31'	2540	-1465	7686	37

Figure 1. View of molecule 1 of **5b** showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Most hydrogen atoms have been removed for clarity.

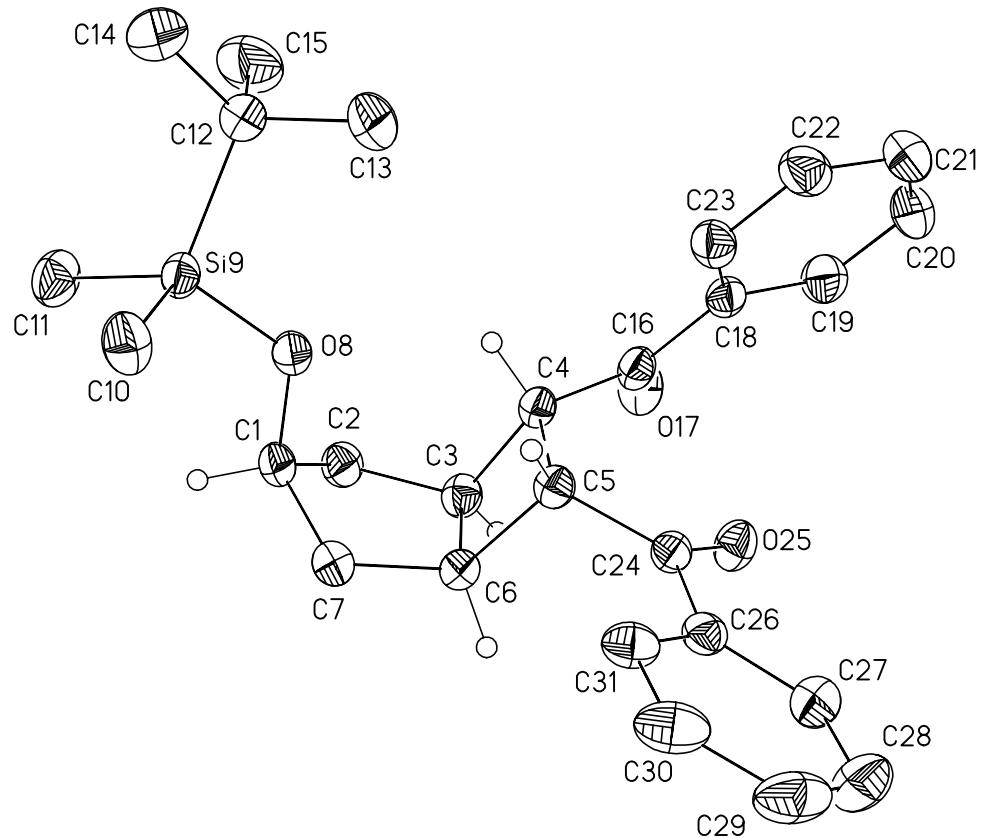


Figure 2. View of molecule 2 of **5b** showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Most hydrogen atoms have been removed for clarity.

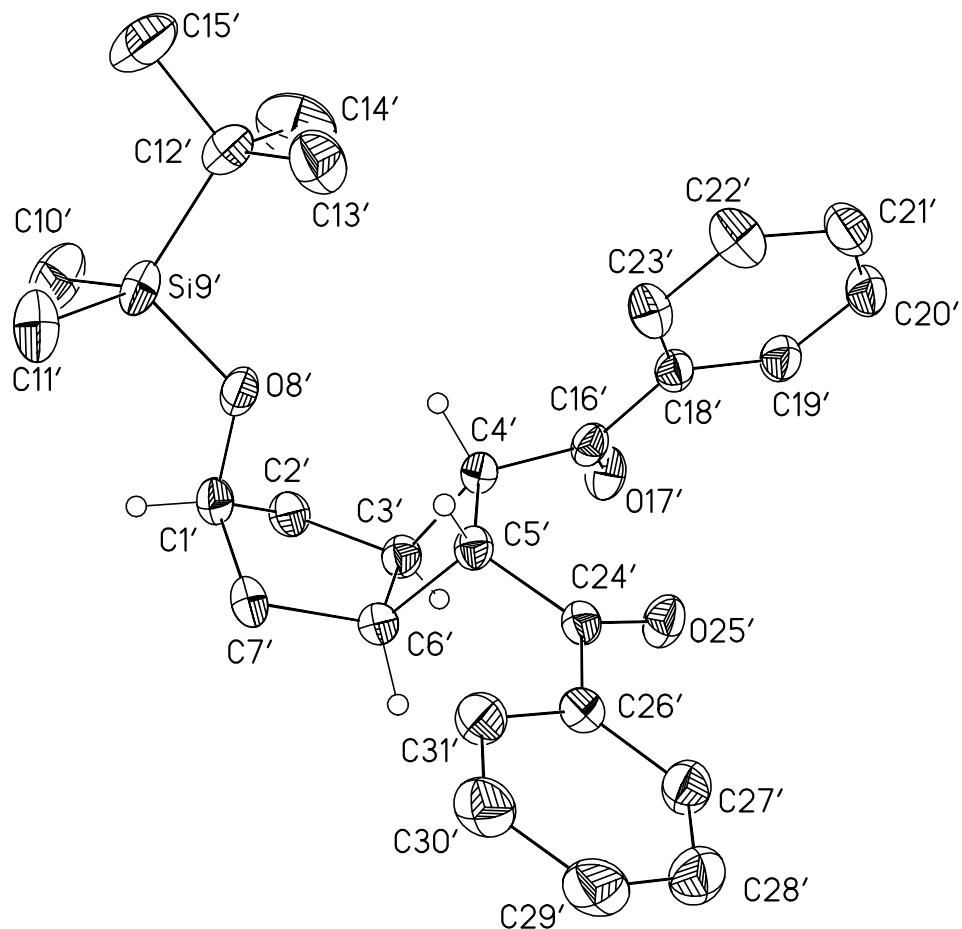


Figure 3. Unit cell packing diagram for **5b**. The view is approximately down the **a** axis. Molecules 2 are shown in wireframe form while molecules **5b** are displayed as ball-and-stick.

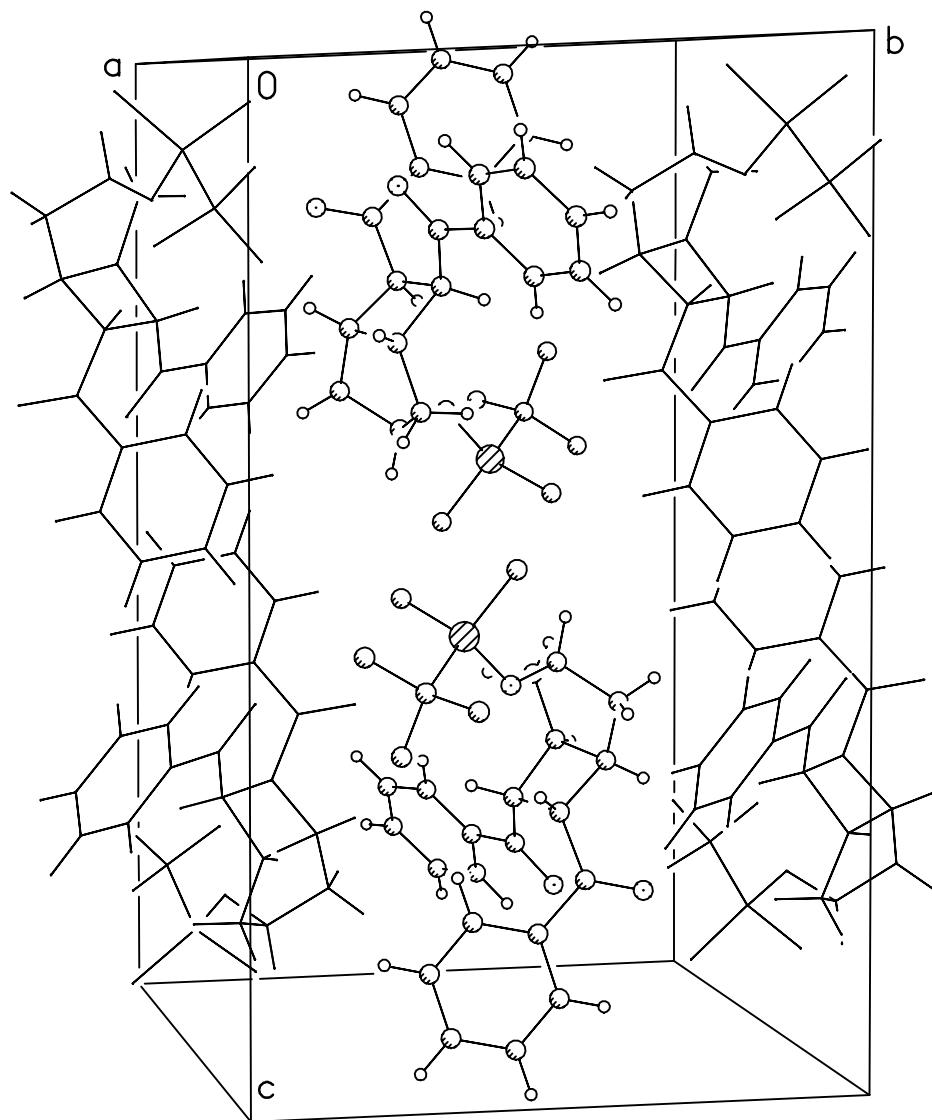


Figure 4. View of the fit by least-squares of selected atoms of molecule **5b** (dashed lines) onto the equivalent atoms of molecule 2. The seven atoms of the fused ring system were used in the fit.

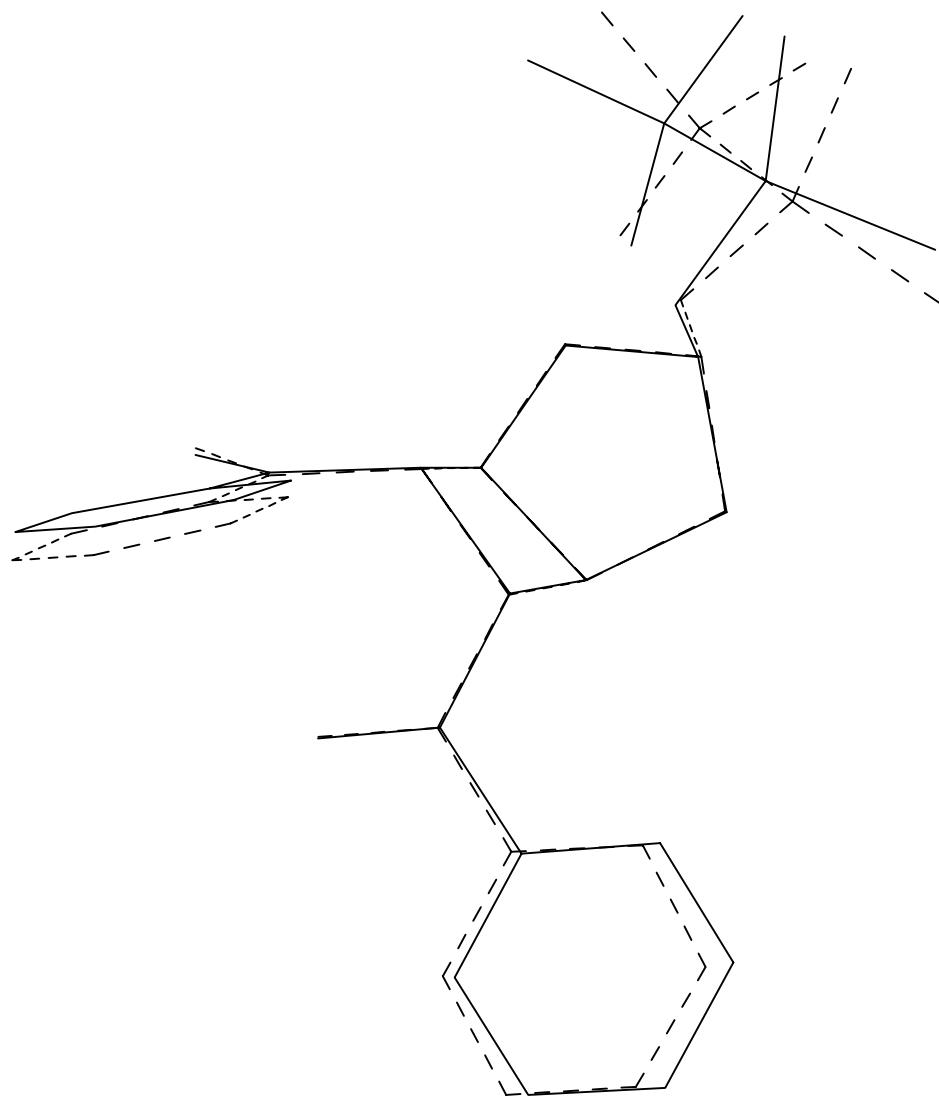


Table 6. Observed and calculated structure factors for 1

Page 1

h	k	l	1	10Fo	10Fc	10s	h	k	l	1	10Fo	10Fc	10s	h	k	l	1	10Fo	10Fc	10s	h	k	l	1	10Fo	10Fc	10s			
2	0	0	64	58	8	-12	4	0	110	122	8	2	7	0	148	159	3	4	11	0	46	15	26	-4	-12	1	33	27	32	
3	0	0	1428	1440	19	-11	4	0	69	63	17	3	7	0	171	175	3	5	11	0	57	38	24	-3	-12	1	37	39	23	
4	0	0	668	665	7	-10	4	0	47	55	3	4	7	0	53	3	9	6	11	0	0	24	1	-2	-12	1	109	97	7	
5	0	0	467	464	7	-9	4	0	111	116	3	5	7	0	49	69	11	-11	12	0	90	80	9	-1	-12	1	161	154	7	
6	0	0	131	130	4	-8	4	0	56	54	7	6	7	0	133	124	5	-10	12	0	26	4	26	0	-12	1	97	117	8	
7	0	0	71	73	3	-7	4	0	132	122	2	7	7	0	37	25	20	-9	12	0	27	35	27	1	-12	1	67	77	11	
8	0	0	55	57	10	-6	4	0	121	122	1	8	7	0	76	64	8	-8	12	0	33	34	18	2	-12	1	279	278	6	
9	0	0	387	401	4	-5	4	0	597	599	5	9	7	0	0	7	1	-7	12	0	48	43	17	3	-12	1	283	273	4	
10	0	0	82	63	5	-4	4	0	392	385	4	-13	8	0	96	108	14	-6	12	0	76	89	5	4	-12	1	103	100	5	
11	0	0	42	33	14	-3	4	0	323	321	3	-12	8	0	23	12	23	-5	12	0	160	167	3	5	-12	1	236	242	11	
12	0	0	146	152	7	-2	4	0	232	227	2	-11	8	0	53	39	13	-4	12	0	142	134	5	6	-12	1	88	85	5	
-13	1	0	115	111	11	-1	4	0	527	526	5	-10	8	0	180	179	5	-3	12	0	52	43	10	7	-12	1	36	32	18	
-12	1	0	76	76	9	0	4	0	182	187	4	-9	8	0	75	75	3	-2	12	0	279	276	5	8	-12	1	47	44	11	
-11	1	0	44	45	34	1	4	0	87	90	8	-8	8	0	101	111	3	-1	12	0	28	27	28	9	-12	1	23	34	23	
-10	1	0	93	94	6	2	4	0	458	447	7	-7	8	0	114	111	6	0	12	0	58	50	12	10	-12	1	81	80	16	
-9	1	0	150	149	6	3	4	0	395	418	5	-6	8	0	52	43	11	1	12	0	43	45	19	11	-12	1	0	4	1	
-8	1	0	150	149	3	4	4	0	52	38	6	-5	8	0	36	20	7	2	12	0	138	124	6	-6	-11	1	53	80	20	
-7	1	0	50	40	5	5	4	0	367	363	4	-4	8	0	27	21	12	3	12	0	50	78	18	-5	-11	1	76	60	11	
-6	1	0	44	46	4	6	4	0	222	223	3	-3	8	0	181	182	2	4	12	0	65	48	21	-4	-11	1	117	120	6	
-5	1	0	239	230	3	7	4	0	169	169	3	-2	8	0	284	288	2	5	12	0	45	60	45	-3	-11	1	71	40	13	
-4	1	0	558	564	7	8	4	0	88	105	5	-1	8	0	27	20	11	-10	13	0	22	19	21	-2	-11	1	132	134	6	
-3	1	0	778	797	9	9	4	0	39	28	10	0	8	0	177	175	2	-9	13	0	119	135	13	-1	-11	1	202	202	5	
-2	1	0	266	270	4	10	4	0	163	171	6	1	8	0	201	202	6	-8	13	0	104	108	5	0	-11	1	0	8	1	
1	1	0	109	105	1	11	4	0	103	95	13	2	8	0	60	48	6	-7	13	0	98	105	6	1	-11	1	193	190	4	
2	1	0	541	553	6	-13	5	0	0	17	1	3	8	0	335	335	4	-6	13	0	44	40	11	2	-11	1	201	199	6	
3	1	0	599	611	6	-12	5	0	172	119	21	4	8	0	56	58	10	-5	13	0	104	113	5	3	-11	1	151	150	9	
4	1	0	568	566	5	-11	5	0	0	49	1	5	8	0	137	157	4	-4	13	0	0	10	1	4	-11	1	24	27	24	
5	1	0	34	17	4	-10	5	0	71	81	2	6	8	0	154	138	6	-3	13	0	47	20	22	5	-11	1	107	120	9	
6	1	0	143	150	2	-9	5	0	21	14	21	7	8	0	75	86	12	-2	13	0	69	28	16	6	-11	1	22	14	21	
7	1	0	195	208	2	-8	5	0	284	290	2	8	8	0	93	100	10	-1	13	0	59	13	20	7	-11	1	57	51	9	
8	1	0	206	202	3	-7	5	0	572	583	5	-12	9	0	98	82	17	0	13	0	36	10	35	8	-11	1	66	42	34	
9	1	0	169	167	2	-6	5	0	373	384	3	-11	9	0	110	92	10	1	13	0	65	76	10	9	-11	1	46	62	12	
10	1	0	55	50	10	-5	5	0	68	66	3	-10	9	0	91	94	10	2	13	0	0	49	1	10	-11	1	102	116	10	
11	1	0	109	123	8	-4	5	0	63	76	3	-9	9	0	188	189	3	3	13	0	0	2	1	11	-11	1	95	18	18	
12	1	0	74	39	25	-3	5	0	0	10	1	-8	9	0	184	189	2	-9	14	0	80	25	17	12	-11	1	51	51	40	
-13	2	0	36	11	30	-2	5	0	160	166	2	-7	9	0	27	13	26	-8	14	0	67	75	13	-7	-10	1	0	52	1	
-12	2	0	16	40	15	-1	5	0	121	122	4	-6	9	0	152	144	13	-7	14	0	57	22	15	-6	-10	1	53	59	13	
-11	2	0	65	64	16	0	5	0	38	49	6	-5	9	0	247	246	2	-6	14	0	53	47	12	-5	-10	1	23	6	23	
-10	2	0	110	117	4	1	5	0	45	59	5	-4	9	0	230	230	6	-5	14	0	55	43	14	-4	-10	1	53	45	21	
-9	2	0	235	236	3	2	5	0	197	180	2	-3	9	0	102	107	3	-4	14	0	253	259	4	-3	-10	1	136	131	6	
-8	2	0	110	109	3	3	5	0	37	43	7	-2	9	0	189	187	3	-3	14	0	102	107	8	-2	-10	1	151	151	5	
-7	2	0	96	85	1	4	5	0	368	366	7	-1	9	0	181	177	3	-2	14	0	0	3	1	-1	-10	1	7	18	7	
-6	2	0	206	215	3	5	5	0	289	282	4	0	9	0	218	223	3	-1	14	0	0	23	1	0	-10	1	322	329	4	
-5	2	0	80	97	2	6	5	0	49	21	12	1	9	0	250	238	3	0	14	0	82	41	15	1	-10	1	136	132	9	
-4	2	0	151	161	1	7	5	0	0	3	1	2	9	0	44	23	18	1	14	0	0	2	1	2	-10	1	144	122	102	
-3	2	0	765	774	7	8	5	0	87	86	5	3	9	0	235	238	3	2	14	0	13	18	12	3	-10	1	52	14	8	
-2	2	0	1439	1411	27	9	5	0	43	3	16	4	9	0	59	45	12	-7	15	0	78	74	12	4	-10	1	179	173	4	
-1	2	0	939	963	10	10	5	0	127	113	6	5	9	0	59	50	10	-6	15	0	86	57	13	5	-10	1	106	110	15	
0	2	0	653	680	7	-13	6	0	101	105	16	6	9	0	0	1	-5	15	0	113	88	10	6	-10	1	254	255	3		
1	2	0	1274	1276	16	-12	6	0	68	81	18	7	9	0	70	62	11	-4	15	0	71	60	18	7	-10	1	43	29	8	
2	2	0	1006	1000	9	-11	6	0	48	36	47	4	8	9	0	101	90	8	-3	15	0	43	24	3	8	-10	1	70	73	5
3	2	0	215	215	3	-10	6	0	88	91	5	-12	10	0	184	166	12	-2	14	1	133	116	7	9	-9	1	23	37	23	
4	2	0	227	232	2	-9	6	0	156	159	2	-11	10	0	96	108	9	-1	15	0										

Table 6. Observed and calculated structure factors for 1

Page 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		
3	-8	1	208	212	2	-5	-4	1	28	14	17	8	-1	1	95	93	2	-4	3	1	481	496	4		
4	-8	1	0	16	1	-4	-4	1	72	82	3	9	-1	1	358	351	4	-3	3	1	748	753	6		
5	-8	1	178	182	2	-3	-4	1	413	399	4	10	-1	1	28	3	27	-2	3	1	38	43	7		
6	-8	1	219	222	2	-2	-4	1	506	480	5	11	-1	1	110	106	6	-1	3	1	271	264	2		
7	-8	1	76	78	9	-1	-4	1	236	231	3	12	-1	1	0	13	1	0	3	1	176	168	2		
8	-8	1	0	2	1	0	-4	1	156	155	5	13	-1	1	35	37	35	1	3	1	130	146	2		
9	-8	1	221	206	8	1	-4	1	297	300	6	-12	0	1	73	25	28	2	3	1	273	279	5		
10	-8	1	74	80	6	2	-4	1	279	292	3	-11	0	1	28	17	28	3	3	1	321	314	3		
11	-8	1	64	78	23	3	-4	1	223	232	2	-10	0	1	213	214	3	4	3	1	275	281	3		
12	-8	1	99	18	42	4	-4	1	435	433	4	-9	0	1	169	164	3	5	3	1	344	340	4		
13	-8	1	91	92	12	5	-4	1	51	36	3	-8	0	1	19	35	19	6	3	1	24	22	24		
-9	-7	1	166	152	6	6	-4	1	291	280	5	-7	0	1	65	75	2	7	3	1	367	368	4		
-8	-7	1	45	14	13	7	-4	1	54	51	3	-6	0	1	163	169	2	8	3	1	94	101	5		
-7	-7	1	70	69	10	8	-4	1	357	367	3	-5	0	1	159	159	2	9	3	1	26	23	11		
-6	-7	1	64	67	14	9	-4	1	91	97	4	-4	0	1	120	124	2	10	3	1	56	11	15		
-5	-7	1	130	130	5	10	-4	1	58	52	4	-3	0	1	65	67	1	11	3	1	78	75	10		
-4	-7	1	23	4	23	11	-4	1	78	62	18	-2	0	1	92	94	4	-13	4	1	72	68	15		
-3	-7	1	396	401	3	12	-4	1	95	82	26	2	0	1	179	185	4	-12	4	1	125	103	10		
-2	-7	1	152	158	3	13	-4	1	39	20	38	3	0	1	77	80	6	-11	4	1	0	35	1		
-1	-7	1	89	58	6	-11	-3	1	75	62	34	4	0	1	74	72	3	-10	4	1	113	127	3		
0	-7	1	419	424	4	-10	-3	1	86	75	8	5	0	1	76	70	17	-9	4	1	130	138	1		
1	-7	1	74	93	4	-9	-3	1	98	101	4	6	0	1	31	31	5	-8	4	1	365	356	3		
2	-7	1	0	41	1	-8	-3	1	235	231	3	7	0	1	72	78	7	-7	4	1	18	16	11		
3	-7	1	132	127	4	-7	-3	1	223	225	3	8	0	1	63	62	14	-6	4	1	251	267	2		
4	-7	1	57	46	7	-6	-3	1	196	198	3	9	0	1	72	72	10	-5	4	1	643	629	5		
5	-7	1	11	11	10	-5	-3	1	7	24	7	10	0	1	86	87	6	-4	4	1	187	177	1		
6	-7	1	539	530	5	-4	-3	1	23	1	23	11	0	1	142	136	8	-3	4	1	300	295	2		
7	-7	1	110	113	2	-3	-3	1	914	902	8	12	0	1	97	98	13	-2	4	1	341	342	3		
8	-7	1	37	55	11	-2	-3	1	218	220	2	-13	1	1	91	61	36	-1	4	1	51	63	3		
9	-7	1	43	43	22	-1	-3	1	84	85	2	-12	1	1	74	68	17	0	4	1	42	50	4		
10	-7	1	117	126	5	0	-3	1	348	329	4	-11	1	1	97	96	7	1	4	1	42	51	8		
11	-7	1	0	39	1	1	-3	1	87	15	4	-10	1	1	177	172	2	2	4	1	235	235	2		
12	-7	1	62	13	47	2	-2	-3	1	82	90	6	-9	1	1	55	59	5	3	4	1	31	38	8	
13	-7	1	82	84	14	3	-3	1	57	55	2	-8	1	1	40	47	19	4	4	1	87	73	3		
-10	-6	1	118	117	6	4	-3	1	277	276	2	-7	1	1	256	255	3	5	4	1	0	1	107	109	6
-9	-6	1	59	50	16	5	-3	1	291	280	3	-6	1	1	546	543	5	6	4	1	102	107	4		
-8	-6	1	10	30	10	6	-3	1	232	223	2	-5	1	1	37	38	11	7	4	1	72	86	4		
-7	-6	1	49	58	13	7	-3	1	173	174	2	-4	1	1	692	697	6	8	4	1	87	84	4		
-6	-6	1	82	84	8	8	-3	1	67	52	10	-3	1	1	976	1002	13	9	4	1	149	156	5		
-5	-6	1	111	120	4	9	-3	1	154	160	8	-2	1	1	485	514	5	10	4	1	57	23	15		
-4	-6	1	75	61	5	10	-3	1	95	92	12	1	1	1	190	192	2	11	4	1	72	40	13		
-3	-6	1	37	2	9	11	-3	1	150	160	10	2	1	1	667	674	9	-13	5	1	83	97	25		
-2	-6	1	87	94	3	12	-3	1	45	31	22	3	1	1	403	414	8	-12	5	1	59	85	15		
-1	-6	1	364	360	3	-12	2	1	73	83	12	4	1	1	86	102	2	-11	5	1	72	21	2		
0	-6	1	291	287	3	-11	-2	1	160	159	6	5	1	1	487	493	9	-10	5	1	113	125	3		
1	-6	1	125	120	5	-10	-2	1	223	225	5	6	1	1	332	339	3	-9	5	1	0	2	1	23	16
2	-6	1	406	381	9	-9	-2	1	163	158	3	7	1	1	47	42	7	-8	5	1	56	44	4		
3	-6	1	350	323	7	-8	-2	1	59	46	6	8	1	1	222	231	3	-7	5	1	96	96	9		
4	-6	1	109	97	2	-7	-2	1	142	146	3	9	1	1	47	48	20	-6	5	1	107	92	1		
5	-6	1	62	68	4	-6	-2	1	61	68	4	10	1	1	48	43	11	-5	5	1	268	287	4		
6	-6	1	402	395	5	-5	-2	1	118	129	2	11	1	1	48	45	33	-4	5	1	592	573	5		
7	-6	1	540	554	6	-4	-2	1	346	358	4	12	1	1	64	69	23	-3	5	1	145	158	4		
8	-6	1	49	10	7	-3	-2	1	522	521	5	-13	2	1	26	12	26	-2	5	1	23	14	23		
9	-6	1	119	126	3	-2	-2	1	856	853	7	-12	2	1	54	44	15	-1	5	1	300	307	3		
10	-6	1	37	35	9	-1	-2	1	1525	1515	27	-11	2	1	18	9	17	0	5	1	110	105	2		
11	-6	1	116	114	11	0	-2	1	560	579	7	-10	2	1	317	318	3	1	5	1	203	212	2		
12	-6	1	101	93	11	1	-2	1	1546	1522	17	-9	2	1	260	254	3	2	5	1	280	270	3		
13	-6	1	65	5	40	2	-2	1	1172	1188	15	-8	2	1	0	16	1	3	5	1	492	495	5		
-10	-5	1	82	49	10	3	-2	1	78	90	3	-7	2	1	396	398	3	4	5	1	339	345	3		
-9	-5	1	80	74	7	4	-2	1	537	535	5	-6	2	1	76	87	1	5	5	1	0	31	1		
-8	-5	1	120	120	4	5	-2	1	79	62	1	-5	2	1	467	465	5	6	5	1	159	154	4		
-7	-5	1	82	102	4	6	-2	1	167	154	2	-4	2	1	529	540	5	7	5	1	59	53	7		
-6	-5	1	180	178	3	7	-2	1	198	190	2	-3	2	1	542	536	5	8	5	1	76	81	5		
-5	-5	1	172	181	3	8	-2	1	300	302	4	-2	2	1	1621	1571	49	9	5	1	154	145	4		
-4	-5	1	106	113	2	9	-2	1	112	118	3	-1	2	1	401	419	3	10	5	1	65	64	13		
-3	-5	1	18	54	18	10	-2	1	62	62	6	0	2	1	1624	1600	16	-13	6	1	109	97	15		
-2	-5	1	308	33																					

Table 6. Observed and calculated structure factors for 1

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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	10	1	53	54	30	9-14	2	73	36	16	9-9	2	48	55	9	3-5	2	197	192	2	-12	-1	2	117	99	12
-12	11	1	37	9	36	-3-13	2	97	66	10	10-9	2	39	21	26	4-5	2	593	573	5	-11	-1	2	79	45	14
-11	11	1	0	0	1	-2-13	2	103	107	9	11-9	2	94	72	11	5-5	2	404	412	3	-10	-1	2	0	27	1
-10	11	1	39	51	38	-1-13	2	97	80	8	12-9	2	102	73	14	6-5	2	146	129	2	-9	-1	2	0	1	1
-9	11	1	35	57	35	0-13	2	78	71	13	-9-8	2	46	23	46	7-5	2	256	264	3	-8	-1	2	40	27	8
-8	11	1	134	126	8	1-13	2	0	23	1	-8-8	2	95	81	7	8-5	2	104	99	3	-7	-1	2	0	23	1
-7	11	1	196	197	3	2-13	2	132	129	5	-7-8	2	61	49	13	9-5	2	293	298	3	-6	-1	2	92	88	3
-6	11	1	25	25	3	3-13	2	88	86	10	-6-8	2	103	110	7	10-5	2	52	42	4	-5	-1	2	233	224	2
-5	11	1	167	163	3	4-13	2	108	105	6	-5-8	2	78	83	10	11-5	2	31	72	31	-4	-1	2	315	307	4
-4	11	1	0	21	1	5-13	2	127	125	5	-4-8	2	111	100	4	12-5	2	53	36	26	-3	-1	2	197	199	2
-3	11	1	53	31	11	6-13	2	79	65	8	-3-8	2	253	251	4	13-5	2	55	82	38	-2	-1	2	118	99	2
-2	11	1	132	135	4	7-13	2	119	113	5	-2-8	2	278	271	9	-11-4	2	70	73	18	-1	-1	2	51	69	4
-1	11	1	0	12	1	8-13	2	70	64	15	-1-8	2	231	228	4	-10-4	2	48	23	18	1	-1	2	13	8	13
0	11	1	42	62	14	9-13	2	0	14	1	0-8	2	143	136	3	-9-4	2	59	64	7	2	-1	2	321	322	5
1	11	1	0	30	1	10-13	2	0	32	1	1-8	2	175	184	3	-8-4	2	80	79	5	3	-1	2	493	491	7
2	11	1	49	43	13	-5-12	2	46	55	38	2-8	2	72	63	4	-7-4	2	108	113	4	4	-1	2	358	354	5
3	11	1	86	62	8	-4-12	2	159	144	8	3-8	2	224	220	2	-6-4	2	329	338	4	5	-1	2	411	408	5
4	11	1	74	66	8	-3-12	2	59	80	11	4-8	2	48	47	8	-5-4	2	57	29	7	6	-1	2	123	130	9
5	11	1	0	40	1	-2-12	2	113	97	8	5-8	2	76	69	4	-4-4	2	467	474	4	7	-1	2	253	256	5
6	11	1	26	0	26	-1-12	2	150	138	6	6-8	2	162	166	2	-3-4	2	44	13	5	8	-1	2	315	323	5
-11	12	1	48	52	23	0-12	2	34	29	34	7-8	2	175	177	3	-2-4	2	249	266	3	9	-1	2	91	82	5
-10	12	1	93	60	19	1-12	2	199	197	6	8-8	2	20	9	20	-1-4	2	64	60	6	10	-1	2	77	70	7
-9	12	1	22	10	21	2-12	2	133	129	5	9-8	2	149	156	6	0-4	2	366	381	3	11	-1	2	56	61	10
-8	12	1	179	174	4	3-12	2	94	87	7	10-8	2	65	53	15	1-4	2	0	9	1	12	-1	2	57	24	57
-7	12	1	63	68	6	4-12	2	184	188	5	11-8	2	170	177	8	2-4	2	16	28	15	-12	0	2	55	48	21
-6	12	1	59	61	6	5-12	2	126	123	5	12-8	2	59	64	30	3-4	2	205	213	2	-11	0	2	132	130	7
-5	12	1	104	109	5	6-12	2	21	9	21	13-8	2	0	21	1	4-4	2	137	148	2	-10	0	2	71	75	4
-4	12	1	428	420	5	7-12	2	77	86	7	-9-7	2	105	113	7	5-4	2	160	147	2	-9	0	2	37	39	9
-3	12	1	80	88	10	8-12	2	81	82	8	-8-7	2	128	119	4	6-4	2	281	275	5	-8	0	2	231	231	2
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-1	12	1	40	38	27	10-12	2	47	83	47	-6-7	2	215	225	4	8-4	2	342	344	4	-6	0	2	37	14	4
0	12	1	83	84	6	11-12	2	50	52	49	-5-7	2	293	295	5	9-4	2	142	147	4	-5	0	2	258	251	3
1	12	1	43	16	19	-6-11	2	0	31	1	-4-7	2	246	241	3	10-4	2	59	52	9	-4	0	2	111	112	1
2	12	1	66	42	10	-5-11	2	46	48	26	-3-7	2	84	83	4	11-4	2	43	46	20	-3	0	2	293	299	2
3	12	1	121	116	6	-4-11	2	34	11	33	-2-7	2	175	165	4	12-4	2	72	48	26	-2	0	2	73	54	11
4	12	1	47	47	32	-3-11	2	43	20	25	-1-7	2	285	275	3	13-4	2	32	48	31	1	0	2	473	487	8
5	12	1	86	95	22	-2-11	2	34	28	34	0-7	2	53	71	6	-11-3	2	21	13	20	3	0	2	1078	1072	11
-10	13	1	81	64	17	-1-11	2	63	75	12	1-7	2	192	203	4	-10-3	2	0	26	1	4	0	2	36	36	3
-9	13	1	45	74	17	0-11	2	131	139	9	2-7	2	16	7	16	-9-3	2	34	29	11	5	0	2	522	538	8
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-7	13	1	47	15	17	2-11	2	143	155	6	4-7	2	20	10	19	-7-3	2	56	49	5	7	0	2	127	109	3
-6	13	1	67	74	7	3-11	2	269	267	10	5-7	2	283	288	3	-6-3	2	276	263	3	8	0	2	480	487	10
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-4	13	1	150	145	4	5-11	2	184	181	9	7-7	2	306	304	3	-4-3	2	359	352	3	10	0	2	308	304	5
-3	13	1	110	104	9	6-11	2	33	43	13	8-7	2	321	321	4	-3-3	2	373	363	3	11	0	2	92	100	12
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1	13	1	18	47	17	10-11	2	64	38	19	12-7	2	92	76	18	1-3	2	213	209	3	-10	1	2	142	143	2
2	13	1	62	48	14	11-11	2	114	102	19	13-7	2	135	134	10	2-3	2	262	268	3	-9	1	2	69	66	9
3	13	1	0	25	1	-7-10	2	72	72	15	-10-6	2	73	52	12	3-3	2	42	36	11	-8	1	2	254	247	3
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-8	14	1	10	2	10	-5-10	2	0	2	1	-8-6	2	97	100	7	5-3	2	77	69	2	-6	1	2	99	89	3
-7	14	1	126	115	4	-4-10	2	52	28	19	-7-6	2	37	12	37	6-3	2	75	57	3	-5	1	2	77	74	2
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-5	14	1	96	81	6	-2-10	2	173	160	5	-5-6	2	234	234	6	8-3	2	386	390	5	-3	1	2	0	7	1
-4	14	1	204	212	5	-1-10	2	0	8	1	-4-6	2	245													

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s				
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6	2	2	282	284	2	-7	6	2	90	77	2	-8	10	2	119	119	3	6-15	3	48	57	15	-4 -9	3	355	350	6
7	2	2	166	159	6	-6	6	2	91	84	2	-7	10	2	67	65	7	7-15	3	18	18	17	-3 -9	3	301	293	5
8	2	2	258	256	2	-5	6	2	250	252	2	-6	10	2	0	20	1	-2-14	3	89	48	24	-2 -9	3	193	198	7
9	2	2	16	2	15	-4	6	2	172	162	2	-5	10	2	460	467	6	-1-14	3	86	90	16	-1 -9	3	82	53	7
10	2	2	0	32	1	-3	6	2	114	101	2	-4	10	2	222	225	3	0-14	3	125	128	8	0 -9	3	45	14	18
11	2	2	114	112	9	-2	6	2	160	152	2	-3	10	2	95	109	3	1-14	3	0	28	1	1 -9	3	263	263	6
12	2	2	59	53	24	-1	6	2	338	347	4	-2	10	2	55	30	14	2-14	3	56	54	21	2 -9	3	89	92	8
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-11	3	2	61	33	27	2	6	2	229	224	4	1	10	2	84	83	7	5-14	3	30	41	30	5 -9	3	250	253	7
-10	3	2	57	54	5	3	6	2	354	363	3	2	10	2	95	97	7	6-14	3	123	130	5	6 -9	3	140	134	3
-9	3	2	270	265	5	4	6	2	253	272	3	3	10	2	0	21	1	7-14	3	34	22	23	7 -9	3	210	209	3
-8	3	2	225	226	3	5	6	2	131	137	3	4	10	2	194	193	6	8-14	3	113	91	8	8 -9	3	52	42	7
-7	3	2	223	228	5	6	6	2	22	24	21	5	10	2	0	19	1	9-14	3	38	13	38	9 -9	3	62	58	9
-6	3	2	378	369	4	7	6	2	125	116	4	6	10	2	41	40	22	-3-13	3	112	91	19	10 -9	3	0	20	1
-5	3	2	109	90	1	8	6	2	85	82	8	7	10	2	93	89	10	-2-13	3	0	22	1	11 -9	3	83	37	50
-4	3	2	40	30	2	9	6	2	44	38	19	-12	11	2	82	74	13	-1-13	3	0	2	1	12 -9	3	53	7	53
-3	3	2	616	635	4	10	6	2	77	75	9	-11	11	2	99	97	10	0-13	3	55	32	16	-9 -8	3	103	97	6
-2	3	2	187	192	1	-13	7	2	133	127	12	-10	11	2	78	64	15	1-13	3	97	96	7	-8 -8	3	32	26	31
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2	3	2	540	523	8	-9	7	2	156	152	4	-6	11	2	190	193	8	5-13	3	29	41	29	-4 -8	3	106	108	5
3	3	2	139	139	2	-8	7	2	432	422	4	-5	11	2	13	24	13	6-13	3	83	80	7	-3 -8	3	249	250	4
4	3	2	91	83	3	-7	7	2	78	67	6	-4	11	2	263	262	3	7-13	3	19	41	19	-2 -8	3	61	59	6
5	3	2	129	131	2	-6	7	2	162	154	2	-3	11	2	132	125	5	8-13	3	0	26	1	-1 -8	3	59	57	10
6	3	2	15	8	14	-5	7	2	119	104	2	-2	11	2	124	124	7	9-13	3	0	9	1	0 -8	3	220	215	6
7	3	2	23	3	12	-4	7	2	28	11	27	-1	11	2	131	140	6	10-13	3	125	103	14	1 -8	3	116	111	3
8	3	2	49	62	4	-3	7	2	210	221	2	0	11	2	0	8	1	-5-12	3	35	42	35	2 -8	3	169	166	3
9	3	2	39	57	17	-2	7	2	119	131	3	1	11	2	45	39	10	-4-12	3	45	59	21	3 -8	3	117	111	8
10	3	2	196	189	6	-1	7	2	105	99	3	2	11	2	114	121	6	-3-12	3	28	47	28	4 -8	3	208	207	2
11	3	2	18	26	17	0	7	2	246	247	2	3	11	2	42	25	18	-2-12	3	40	24	40	5 -8	3	71	58	4
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-6	4	2	368	381	3	8	7	2	7	31	7	-7	12	2	79	83	5	6-12	3	34	29	34	-9 -7	3	140	136	7
-5	4	2	64	46	2	9	7	2	0	36	1	-6	12	2	43	12	9	7-12	3	108	101	7	-8 -7	3	0	11	1
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3	4	2	292	291	5	-6	8	2	231	233	4	2	12	2	81	68	11	-3-11	3	0	54	1	0 -7	3	24	31	23
4	4	2	113	111	2	-5	8	2	53	55	5	3	12	2	68	63	15	-2-11	3	224	218	5	1 -7	3	182	165	3
5	4	2	445	438	5	-4	8	2	28	29	7	4	12	2	141	132	8	-1-11	3	154	152	6	2 -7	3	412	415	4
6	4	2	225	221	3	-3	8	2	85	81	3	-10	13	2	97	96	9	0-11	3	245	236	4	3 -7	3	176	179	3
7	4	2	29	34	11	-2	8	2	63	68	8	-9	13	2	7	8	7	1-11	3	98	110	8	4 -7	3	111	106	3
8	4	2	25	17	25	-1	8	2	216	205	3	-8	13	2	132	136	5	2-11	3	39	45	19	5 -7	3	372	375	3
9	4	2	97	76	5	0	8	2	241	246	3	-7	13</td														

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-10	-5	3	174	150	12	1	-2	3	523	528	5	12	1	3	28	8	28	-1	5	3	153	157	2
-9	-5	3	134	136	4	2	-2	3	463	452	6	-12	2	3	98	95	9	0	5	3	208	177	4
-8	-5	3	18	17	17	3	-2	3	462	480	7	-11	2	3	112	103	5	1	5	3	52	46	3
-7	-5	3	213	224	4	4	-2	3	670	646	7	-10	2	3	141	139	3	2	5	3	222	213	2
-6	-5	3	153	151	4	5	-2	3	710	709	7	-9	2	3	120	117	2	3	5	3	307	308	3
-5	-5	3	37	41	10	6	-2	3	35	32	7	-8	2	3	249	246	2	4	5	3	60	68	5
-4	-5	3	267	269	2	7	-2	3	312	309	5	-7	2	3	232	232	2	5	5	3	355	357	3
-3	-5	3	337	339	3	8	-2	3	258	258	4	-6	2	3	191	203	4	6	5	3	45	32	7
-2	-5	3	303	306	3	9	-2	3	58	59	6	-5	2	3	160	161	2	7	5	3	54	55	9
-1	-5	3	190	189	10	10	-2	3	54	47	6	-4	2	3	42	54	3	8	5	3	24	4	24
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4	-5	3	42	6	7	-11	-1	3	25	15	25	1	2	3	599	608	6	-11	6	3	80	96	6
5	-5	3	346	345	3	-10	-1	3	49	36	5	2	2	3	130	137	2	-10	6	3	131	133	3
6	-5	3	309	306	3	-9	-1	3	135	130	3	3	2	3	511	494	7	-9	6	3	69	67	5
7	-5	3	114	104	3	-8	-1	3	218	211	3	4	2	3	777	773	8	-8	6	3	162	159	4
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9	-5	3	58	65	4	-6	-1	3	241	238	3	6	2	3	296	294	3	-6	6	3	201	196	5
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-11	-4	3	42	65	25	-1	-1	3	1584	1565	18	11	2	3	54	5	23	-1	6	3	188	167	5
-10	-4	3	299	288	6	0	-1	3	574	588	6	-13	3	3	0	4	1	0	6	3	310	300	6
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-8	-4	3	62	51	9	2	-1	3	544	549	15	-11	3	3	165	166	4	2	6	3	96	82	3
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7	-4	3	231	229	3	-8	0	3	174	173	3	4	3	3	224	218	2	-6	7	3	111	114	2
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9	-4	3	34	38	7	-6	0	3	102	100	2	6	3	3	176	174	4	-4	7	3	181	189	2
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12	-4	3	80	78	17	-3	0	3	116	124	1	9	3	3	196	197	4	-1	7	3	225	231	2
13	-4	3	66	60	30	-2	0	3	128	115	5	10	3	3	142	152	7	0	7	3	84	82	7
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-6	-3	3	158	170	2	4	0	3	160	158	3	-9	4	3	222	218	3	6	7	3	33	37	14
-5	-3	3	126	113	2	5	0	3	19	28	18	-8	4	3	35	34	24	8	7	3	93	94	8
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5	-3	3	103	80	17	-10	1	3	31	30	8	2	4	3	25	1	25	-6	8	3	151	149	2
6	-3	3	92	75	6	-9	1																

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s						
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-1	14	3	25	13	25	2-10	4	346	347	5	0	-6	4	141	137	3	13	-3	4	43	43	43	0	1	4	539	549	8	
0	14	3	49	28	38	3-10	4	102	95	4	1	-6	4	91	99	5	-11	-2	4	120	136	7	1	1	4	175	165	3	
1	14	3	0	11	1	4-10	4	56	50	8	2	-6	4	126	119	7	-10	-2	4	29	30	14	2	1	4	327	322	5	
-7	15	3	47	57	47	5-10	4	125	126	3	3	-6	4	791	792	8	-9	-2	4	43	37	9	3	1	4	233	249	6	
-6	15	3	92	69	10	6-10	4	17	18	17	4	-6	4	174	163	2	-8	-2	4	227	217	3	4	1	4	223	231	2	
-5	15	3	43	54	32	7-10	4	56	43	9	5	-6	4	292	303	5	-7	-2	4	281	278	3	5	1	4	0	10	1	
-4	15	3	107	91	15	8-10	4	97	98	5	6	-6	4	65	74	4	-6	-2	4	73	53	3	6	1	4	156	140	4	
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-2	15	3	65	46	17	10-10	4	37	45	37	8	-6	4	100	104	4	-4	-2	4	427	437	4	8	1	4	0	16	1	
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-2-14	4	94	23	15	-2	-9	4	87	84	8	-7	-5	4	0	40	1	5	-2	4	64	47	5	-8	2	4	163	154	2	
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-1-12	4	91	91	10	6	-8	4	178	173	2	-2	-4	4	25	27	20	10	-1	4	182	181	9	-2	3	4	649	656	6	
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5-12	4	43	47</																										

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s				
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-11	5	4	208	198	5	6	8	4	178	183	4	1	13	4	85	95	14	-7-10	5	34	2	33	-7 -6	5	217	219	4
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Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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8	-3	5	435	435	6	-1	1	5	796	813	10	-9	5	5	0	4	1	8	8	5	59	46	21
9	-3	5	215	213	4	0	1	5	218	216	4	-8	5	5	71	58	4	-12	9	5	45	42	34
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Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s		
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3-10	6	43	16	21	4 -6 6	90	110	6	-3 -2 6	381	390	3	-11	2	6	0	7	1	6	5	6	160	168	3	
4-10	6	370	390	4	5 -6 6	194	187	2	-2 -2 6	53	34	4	-10	2	6	100	99	5	7	5	6	71	84	7	
5-10	6	360	361	5	6 -6 6	285	283	3	-1 -2 6	708	694	6	-9	2	6	64	67	6	8	5	6	101	94	6	
6-10	6	56	35	14	7 -6 6	75	84	7	0 -2 6	0	3	1	-8	2	6	102	97	2	9	5	6	34	41	26	
7-10	6	66	69	8	-8 -6 6	46	62	9	1 -2 6	593	585	6	-7	2	6	551	536	6	10	5	6	16	12	16	
8-10	6	252	266	3	9 -6 6	33	25	11	2 -2 6	216	224	3	-6	2	6	294	295	2	-13	6	6	0	24	1	
9-10	6	88	102	10	10 -6 6	37	43	23	3 -2 6	113	117	2	-5	2	6	68	67	3	-12	6	6	97	88	19	
10-10	6	0	14	1	11 -6 6	119	91	20	4 -2 6	75	76	5	-4	2	6	643	638	6	-11	6	6	53	32	12	
11-10	6	92	5	21	12 -6 6	66	49	31	5 -2 6	454	429	5	-3	2	6	197	204	2	-10	6	6	17	7	17	
-8 -9	6	97	110	7	-10 -5 6	122	124	11	6 -2 6	331	347	4	-2	2	6	686	691	7	-9	6	6	0	19	1	
-7 -9	6	56	58	14	-9 -5 6	49	46	11	7 -2 6	286	288	4	-1	2	6	34	24	7	-8	6	6	112	102	4	
-6 -9	6	7	40	7	-8 -5 6	45	42	10	8 -2 6	21	1	21	0	2	6	406	417	5	-7	6	6	0	30	1	
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-3 -9	6	78	74	9	-5 -5 6	58	68	4	11 -2 6	121	115	10	3	2	6	167	170	3	-4	6	6	198	191	2	
-2 -9	6	205	201	5	-4 -5 6	33	25	10	12 -2 6	109	108	11	4	2	6	472	453	5	-3	6	6	60	76	2	
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4 -9	6	230	222	6	2 -5 6	328	313	4	-6 -1 6	276	285	2	10	2	6	51	50	11	3	6	6	41	33	9	
5 -9	6	110	99	4	3 -5 6	510	486	9	-5 -1 6	116	105	3	11	2	6	66	73	12	4	6	6	172	168	3	
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Table 6. Observed and calculated structure factors for 1

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4	9	6	216	206	4	-1-14	7	110	123	10	4-9	7	55	14	8	2-5	7	533	530	10	-3-1	7	0	2	1	
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Table 6. Observed and calculated structure factors for 1

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5	3	7	566	573	5	2	7	7	130	135	3	-4	12	7	95	67	9	10-11	8	265	256	9	5 -6	8	127	124	9
6	3	7	72	73	7	3	7	7	97	91	3	-3	12	7	46	27	24	11-11	8	88	51	38	-4 -6	8	346	345	4
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1	4	7	221	222	3	-1	8	7	239	237	7	1	13	7	51	21	43	9-10	8	57	50	57	-10 -5	8	98	110	14
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Table 6. Observed and calculated structure factors for 1

Page 12

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	
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6	-3	8	126	129	2	-1	1	8	288	276	5	-6	5	8	163	141	2	-4	9	8	31	29	6	
7	-3	8	0	18	1	0	1	8	467	475	7	-5	5	8	652	653	5	-3	9	8	188	183	10	
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9	-1	8	169	171	7	3	3	8	171	163	2	0	7	8	188	184	2	-3	12	8	7	25	7	
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Table 6. Observed and calculated structure factors for 1

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12	-7	9	126	88	12	8	-3	9	251	264	6	1	1	9	135	124	3	-4	5	9	31	25	6	
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-8	-6	9	72	81	7	10	-3	9	0	50	1	3	1	9	144	151	2	-2	5	9	214	204	3	
-7	-6	9	53	47	8	11	-3	9	56	22	29	4	1	9	518	531	6	-1	5	9	72	98	4	
-6	-6	9	50	40	8	12	-3	9	46	6	46	5	1	9	414	415	5	0	5	9	155	141	5	
-5	-6	9	0	0	1	-11	-2	9	39	10	38	6	1	9	172	167	6	1	5	9	55	61	5	
-4	-6	9	223	231	2	-10	-2	9	76	86	6	7	1	9	199	216	6	2	2	5	9	0	13	1
-3	-6	9	135	148	4	-9	-2	9	13	6	12	8	1	9	46	6	18	3	5	9	34	30	11	
-2	-6	9	19	37	19	-8	-2	9	261	259	3	9	1	9	67	75	8	4	5	9	189	190	2	
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0	-6	9	42	47	10	-6	-2	9	155	150	2	11	1	9	100	83	11	6	5	9	110	119	3	
1	-6	9	9	142	142	2	-5	-2	9	142	137	2	-11	2	9	173	172	6	7	5	9	135	132	5
2	-6	9	22	27	21	-4	-2	9	230	239	2	-10	2	9	200	195	3	8	5	9	66	67	11	
3	-6	9	88	87	9	-3	-2	9	169	158	5	-9	2	9	31	43	6	9	5	9	66	83	13	
4	-6	9	54	41	8	-2	-2	9	65	51	3	-8	2	9	40	41	5	-12	6	9	162	162	42	
5	-6	9	62	62	6	-1	-2	9	363	363	3	-7	2	9	58	55	12	-11	6	9	86	65	10	
6	-6	9	66	24	65	0	-2	9	307	303	5	-6	2	9	39	32	5	-10	6	9	75	72	12	
7	-6	9	295	290	4	1	-2	9	666	633	8	-5	2	9	163	162	2	-9	6	9	134	142	4	
8	-6	9	40	46	7	2	-2	9	185	185	5	-4	2	9	45	41	4	-8	6	9	238	235	3	
9	-6	9	83	91	8	3	-2	9	52	61	4	-3	2	9	227	224	2	-7	6	9	76	72	2	
10	-6	9	127	118	19	4	-2	9	127	130	3	-2	2	9	27	10	6	-6	6	9	95	98	3	
11	-6	9	133	145	10	5	-2	9	82	76	3	-1	2	9	409	419	5	-5	6	9	221	223	2	
12	-6	9	78	31	24	6	-2	9	46	52	46	0	2	9	408	388	5	-4	6	9	318	323	3	
-10	-5	9	38	37	38	7	-2	9	51	28	34	1	2											

Table 6. Observed and calculated structure factors for 1

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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	12	9	30	34	30	5-10	10	74	55	13	12 -6 10	61	46	17	8 -2 10	33	46	32	3	2 10	106	105	6
-5	12	9	58	69	10	6-10	10	108	96	6	-10 -5 10	25	19	25	9 -2 10	61	44	30	4	2 10	249	255	3
-4	12	9	79	81	7	7-10	10	61	63	9	-9 -5 10	47	36	16	10 -2 10	62	58	22	5	2 10	236	233	4
-3	12	9	13	15	12	8-10	10	75	26	41	-8 -5 10	61	56	8	11 -2 10	154	143	28	6	2 10	175	169	5
-2	12	9	185	190	5	9-10	10	124	131	12	-7 -5 10	67	54	7	-11 -1 10	111	126	9	7	2 10	59	11	12
-1	12	9	95	99	7	10-10	10	80	52	27	-6 -5 10	17	10	16	-10 -1 10	101	92	10	8	2 10	43	42	17
0	12	9	101	82	10	-7 -9 10	0	1	1	-5 -5 10	51	29	7	-9 -1 10	198	200	3	9	2 10	36	37	16	
1	12	9	24	33	24	-6 -9 10	111	103	6	-4 -5 10	288	280	6	-8 -1 10	13	11	13	10	2 10	167	157	5	
2	12	9	121	130	7	-5 -9 10	51	50	16	-3 -5 10	107	105	3	-7 -1 10	47	37	6	-12	3 10	39	42	39	
3	12	9	28	17	28	-4 -9 10	50	39	16	-2 -5 10	200	191	2	-6 -1 10	61	54	5	-11	3 10	152	146	6	
-8	13	9	71	56	39	-3 -9 10	192	180	5	-1 -5 10	221	233	7	-5 -1 10	233	236	2	-10	3 10	201	199	5	
-7	13	9	76	58	19	-2 -9 10	64	80	14	0 -5 10	121	107	5	-4 -1 10	310	308	2	-9	3 10	239	241	6	
-6	13	9	32	40	31	-1 -9 10	203	209	6	1 -5 10	105	102	8	-3 -1 10	215	215	2	-8	3 10	93	100	5	
-5	13	9	26	24	26	0 -9 10	229	224	6	2 -5 10	147	162	3	-2 -1 10	60	58	5	-7	3 10	105	98	11	
-4	13	9	23	43	23	1 -9 10	57	55	14	3 -5 10	179	180	3	-1 -1 10	152	122	2	-6	3 10	0	14	1	
-3	13	9	0	6	1	2 -9 10	145	133	8	4 -5 10	366	351	5	0 -1 10	299	289	4	-5	3 10	279	279	3	
-2	13	9	25	37	25	3 -9 10	104	105	5	5 -5 10	18	18	17	1 -1 10	335	316	3	-4	3 10	417	400	4	
-1	13	9	0	4	1	4 -9 10	119	124	8	6 -5 10	92	99	4	2 -1 10	179	185	2	-3	3 10	148	154	2	
0	13	9	0	22	1	5 -9 10	46	19	40	7 -5 10	180	183	3	3 -1 10	594	597	8	-2	3 10	164	161	7	
1	13	9	41	48	40	6 -9 10	67	45	17	8 -5 10	76	74	9	4 -1 10	0	7	1	-1	3 10	110	127	2	
-7	14	9	59	73	16	7 -9 10	337	334	6	9 -5 10	143	155	6	5 -1 10	85	86	3	0	3 10	267	255	3	
-6	14	9	99	99	6	8 -9 10	93	84	21	10 -5 10	55	40	35	6 -1 10	226	227	7	1	3 10	531	530	5	
-5	14	9	0	11	1	9 -9 10	110	106	12	11 -5 10	138	139	11	7 -1 10	0	52	1	2	3 10	350	344	3	
-4	14	9	35	41	20	10 -9 10	58	37	58	12 -5 10	116	96	13	8 -1 10	74	67	10	3	3 10	0	21	1	
-3	14	9	0	5	1	11 -9 10	115	103	13	-10 -4 10	34	59	33	9 -1 10	0	68	1	4	3 10	151	146	4	
-2	14	9	75	62	10	-8 -8 10	45	53	14	-9 -4 10	161	165	3	10 -1 10	59	48	13	5	3 10	53	48	6	
-1	14	9	76	79	16	-7 -8 10	62	52	9	-8 -4 10	66	68	5	11 -1 10	166	164	16	6	3 10	78	80	5	
0-14	10	111	97	13	-6 -8 10	149	147	4	-7 -4 10	157	148	3	-11 0 10	0	11	1	7	3 10	32	18	22		
1-14	10	143	109	17	-5 -8 10	159	166	4	-6 -4 10	246	252	6	-10 0 10	144	143	6	8	3 10	57	39	8		
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4-14	10	0	15	1	-2 -8 10	333	327	4	-3 -4 10	138	148	2	-7 0 10	44	49	5	-12	4 10	34	15	34		
5-14	10	54	47	19	-1 -8 10	193	172	18	-2 -4 10	561	577	4	-6 0 10	15	17	14	-11	4 10	13	44	12		
6-14	10	0	12	1	0 -8 10	52	37	11	-1 -4 10	247	258	5	-5 0 10	332	332	3	-10	4 10	0	24	1		
7-14	10	43	72	42	1	-8 -8 10	183	180	3	0 -4 10	477	467	9	-4 0 10	392	398	5	-9 4 10	143	134	5		
-2-13	10	140	126	11	2 -8 10	54	47	10	1 -4 10	84	76	4	-3 0 10	295	292	6	-8 4 10	68	74	6			
-1-13	10	72	50	20	3 -8 10	395	394	5	2 -4 10	462	466	6	-2 0 10	196	218	2	-7 4 10	41	51	9			
0-13	10	65	64	12	4 -8 10	59	49	11	3 -4 10	285	289	3	-1 0 10	420	406	8	-6 4 10	171	155	2			
1-13	10	111	114	9	5 -8 10	223	221	4	4 -4 10	386	387	4	0 0 10	301	286	4	-5 4 10	120	120	2			
2-13	10	87	79	10	6 -8 10	70	63	7	5 -4 10	232	236	3	1 0 10	621	604	11	-4 4 10	100	96	2			
3-13	10	37	20	37	7 -8 10	201	208	5	6 -4 10	67	44	13	2 0 10	323	296	5	-3 4 10	33	34	11			
4-13	10	48	46	22	8 -8 10	75	77	5	7 -4 10	190	188	2	3 0 10	799	794	8	-2 4 10	267	264	3			
5-13	10	56	58	19	9 -8 10	0	2	1	8 -4 10	47	57	16	4 0 10	217	213	3	-1 4 10	91	99	1			
6-13	10	0	36	1	10 -8 10	98	54	27	9 -4 10	86	91	7	5 0 10	182	190	3	0 4 10	537	536	6			
7-13	10	25	21	25	11 -8 10	47	60	26	10 -4 10	123	116	7	6 0 10	296	293	9	1 4 10	139	138	2			
8-13	10	98	68	11	-9 -7 10	59	13	15	11 -4 10	37	18	37	7 0 10	132	119	10	2 4 10	287	292	3			
-4-12	10	0	14	1	-8 -7 10	58	54	12	12 -4 10	89	57	13	8 0 10	42	45	25	3 4 10	236	233	3			
-3-12	10	86	75	13	-7 -7 10	34	33	33	-10 -3 10	147	153	10	9 0 10	80	83	13	4 4 10	28	35	27			
-2-12	10	55	51	15	-6 -7 10	58	53	10	-9 -3 10	35	24	11	10 0 10	69	67	13	5 4 10	141	151	3			
-1-12	10	130	112	8	-5 -7 10	54	43	11	-8 -3 10	50	40	9	11 0 10	37	48	30	6 4 10	65	57	5			
0-12	10	118	103	9	-4 -7 10	46	40	15	-7 -3 10	92	82	3	-11 1 10	131	128	6	7 4 10	158	177	6			
1-12	10	37	11	26	-3 -7 10	409	405	11	-6 -3 10	252	242	3	-10 1 10	73	71	10	8 4 10	106	96	12			
2-12	10	0	6	1	-2 -7 10	179	164	5	-5 -3 10	317	318	3	-9 1 10	165	160	3	9 4 10	108	99	8			
3-12	10	66	69	13	-1 -7 10	239	231	3	-4 -3 10	119	119	3	-8 1 10	197	192	3	-12 5 10	159	100	44			
4-12	10	62	5	16	0 -7 10	81	74	5	-3 -3 10	227	221	2	-7 1 10	234	240	2	-11 5 10	62	51	17			
5-12	10	245	246	5	1 -7 10	173	175	5	-2 -3 10	96	81	2	-6 1 10	261	261	3	-10 5 10	64	76	21			
6-12	10	61	84	18	2 -7 10	128	113	3	-1 -3 10	292	292	3	-5 1 10	126	135	3	-9 5 10	64	68	3			
7-12	10	0	7	1	3 -7 10	215	203	3	0 -3 10	224	201	3	-4 1 10	132	121	3	-8 5 10	200	200	7			
8-12	10	36	3	35	4	-7 -7 10	155	142	12	1 -3 10	31	34	10	-3 1 10	20	2	6	-7 5 10	58	59	6		
9-12	10	83	63	20	5 -7 10	314	314	7	-2 -3 10	487	479	5	-2 1 10	248	237	4	-6 5 10	119	117	2			
-5-11	10	59	59	13	6 -7 10	67	58	8	10 -3 10	40	6	40	6 1 10	59	51	12	2 5 10	31	18	31			
3-11	10	124	112	7	-7 -6 10	122	124	5	-11 2 10														

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s				
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2	6	10	168	162	5	-6	11	10	70	69	7	-4-10	11	36	65	35	3-6	11	229	226	12	1-2	11	14	26	14	
3	6	10	405	404	5	-5	11	10	37	33	12	-3-10	11	60	77	21	4-6	11	56	69	9	2-2	11	45	56	11	
4	6	10	7	26	7	-4	11	10	133	131	6	-2-10	11	64	52	14	5-6	11	109	112	8	3-2	11	0	8	1	
5	6	10	86	93	4	-3	11	10	68	82	7	-1-10	11	34	32	34	6-6	11	255	263	4	4-2	11	175	178	4	
6	6	10	76	74	8	-2	11	10	23	43	23	0-10	11	237	228	4	7-6	11	103	102	9	5-2	11	93	93	3	
7	6	10	169	176	6	-1	11	10	50	59	15	1-10	11	57	62	12	8-6	11	73	58	4	6-2	11	72	65	5	
8	6	10	39	72	38	0	11	10	100	101	7	2-10	11	43	40	13	9-6	11	60	73	25	7-2	11	75	84	40	
-12	7	10	22	0	21	1	11	10	145	143	6	3-10	11	261	265	4	10-6	11	71	78	13	8-2	11	103	101	6	
-11	7	10	118	62	26	2	11	10	50	27	23	4-10	11	172	179	11	11-6	11	36	15	35	9-2	11	165	163	9	
-10	7	10	145	123	9	3	11	10	120	129	9	5-10	11	84	92	13	-10-5	11	39	47	39	10-2	11	39	3	39	
-9	7	10	89	96	9	4	11	10	55	62	47	6-10	11	117	80	21	-9-5	11	119	104	20	11-2	11	101	118	16	
-8	7	10	41	20	8	-10	12	10	90	90	13	7-10	11	75	40	11	-8-5	11	27	4	27	-11-1	11	200	101	50	
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-6	7	10	28	19	8	-8	12	10	0	37	13	21	9-10	11	132	127	11	-6-5	11	79	90	9	-9-1	11	0	4	1
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-4	7	10	385	379	3	-6	12	10	34	31	27	-7-9	11	216	208	5	-4-5	11	253	247	2	-7-1	11	215	213	4	
-3	7	10	69	74	7	-5	12	10	116	122	5	-6-9	11	45	54	17	-3-5	11	136	134	7	-6-1	11	227	230	2	
-2	7	10	523	522	4	-4	12	10	0	6	1	-5-9	11	105	104	7	-2-5	11	58	48	9	-5-1	11	202	202	2	
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0	7	10	201	204	2	-2	12	10	94	88	8	-3-9	11	80	69	11	0-5	11	160	159	6	-3-1	11	191	189	4	
1	7	10	257	259	3	-1	12	10	162	159	7	-2-9	11	45	26	19	1-5	11	130	139	3	-2-1	11	90	77	2	
2	7	10	122	126	5	0	12	10	34	8	33	-1-9	11	239	249	4	2-5	11	93	108	4	-1-1	11	266	272	2	
3	7	10	0	26	1	1	12	10	74	59	11	0-9	11	327	322	7	3-5	11	252	250	4	0	11	98	103	5	
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-8	8	10	192	204	2	-1	13	10	80	64	11	8-9	11	7	53	7	11-5	11	142	114	16	8-1	11	93	110	12	
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-5	8	10	113	117	9	-5	14	10	71	47	10	11-9	11	78	56	23	-8-4	11	66	61	9	11-1	11	100	107	11	
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-1	8	10	70	66	5	0-14	11	0	66	1	-5-8	11	144	138	5	-4-4	11	44	37	7	-8	0	11	181	182		
0	8	10	0	3	1	1-14	11	47	43	47	-4-8	11	93	104	7	-3-4	11	191	186	2	-7	0	11	234	225		
1	8	10	105	104	5	2-14	11	55	24	54	-3-8	11	0	17	1	-2-4	11	84	76	3	-6	0	11	47	52		
2	8	10	308	306	4	3-14	11	31	33	31	-2-8	11	0	3	1	-1-4	11	168	170	2	-5	0	11	154	162		
3	8	10	149	155	3	4-14	11	45	25	45	-1-8	11	114	122	5	0-4	11	256	244	3	-4	0	11	176	172		
4	8	10	77	68	8	5-14	11	28	49	28	-0-8	11	73	83	9	1-4	11	109	109	3	-3	0	11	0	7		
5	8	10	162	150	5	6-14	11	122	97	12	1-8	11	225	226	3	2-4	11	94	97	3	-2	0	11	153	155		
6	8	10	43	9	32	-2-13	11	49	33	49	2-8	11	219	221	3	3-4	11	142	137	3	-1	0	11	220	231		
7	8	10	0	29	1	-1-13	11	34	25	33	3-8	11	44	50	16	4-4	11	92	68	6	0	0	11	38	17		
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-11	9	10	82	50	15	1-13	11	29	64	29	5-8	11	148	147	5	6-4	11	52	49	7	2	0	11	72	68		
-10	9	10	126	120	9	2-13	11	58	28	25	6-8	11	194	186	3	7-4	11	45	51	7	3	0	11	113	120		
-9	9	10	30	10	30	3-13	11	18	32	17	7-8	11	63	34	62	8-4	11	71	88	7	4	0	11	136	145		
-8	9	10	92	92	11	4-13	11	49	15	18	8-8	11	224	183	14	9-4	11	124	111	8	5	0	11	42	57		
-7	9	10	135	134	2	5-13	11	69	57	15	9-8	11	116	100	15	10-4	11	122	113	10	6	0	11	41	28		
-6	9	10	4	4	4	6-13	11	43	8	42	10-8	11	72	49	16	11-4	11	155	121	25	7	0	11	52	49		
-5	9	10	85	89	4	7-13	11	47	13	36	11-8	11	0	5	1	-10-3	11	33	5	32	8	0	11	73	32		
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Table 6. Observed and calculated structure factors for 1

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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	2	11	136	127	2	-7	6	11	294	281	2	4	10	11	79	42	12	3-10	12	86	69	10	-10 -5 12 0 42 1		
-4	2	11	121	117	2	-6	6	11	163	166	2	-10	11	11	136	113	10	4-10	12	90	69	17	-9 -5 12 21 32 20		
-3	2	11	48	65	11	-5	6	11	43	52	13	-9	11	11	187	183	8	5-10	12	114	126	9	-8 -5 12 154 156 4		
-2	2	11	48	28	15	-4	6	11	157	155	2	-8	11	11	62	54	11	6-10	12	68	61	16	-7 -5 12 30 19 16		
-1	2	11	371	356	5	-3	6	11	491	510	5	-7	11	11	34	36	24	7-10	12	43	36	25	-6 -5 12 28 4 13		
0	2	11	117	121	3	-2	6	11	28	42	22	-6	11	11	0	2	1	8-10	12	74	57	25	-5 -5 12 267 260 2		
1	2	11	63	63	4	-1	6	11	237	238	3	-5	11	11	22	15	21	9-10	12	16	49	16	-4 -5 12 43 43 8		
2	2	11	243	233	3	0	6	11	75	64	6	-4	11	11	0	12	1	10-10	12	31	61	31	-3 -5 12 211 202 2		
3	2	11	153	151	2	1	6	11	120	124	4	-3	11	11	23	36	23	-7 -9	12	56	19	17	-2 -5 12 235 226 2		
4	2	11	66	70	3	2	6	11	202	207	3	-2	11	11	29	20	29	-6 -9	12	55	50	17	-1 -5 12 151 156 2		
5	2	11	136	139	6	3	6	11	122	129	6	-1	11	11	39	37	16	-5 -9	12	45	53	14	0 -5 12 287 294 3		
6	2	11	82	91	4	4	6	11	36	31	15	0	11	11	34	2	23	-4 -9	12	82	77	7	1 -5 12 209 202 4		
7	2	11	31	26	25	5	6	11	34	43	16	1	11	11	59	17	15	-3 -9	12	85	84	11	2 -5 12 181 182 5		
8	2	11	86	83	7	6	6	11	118	111	9	2	11	11	83	69	9	-2 -9	12	36	34	25	3 -5 12 135 128 3		
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10	2	11	105	109	7	8	6	11	39	36	24	-9	12	11	60	18	24	0	-9	12	15	2	14	5 -5 12 66 55 5	
-12	3	11	30	21	30	-12	7	11	28	38	28	-8	12	11	0	9	1	1	-9	12	160	166	5	6 -5 12 36 19 13	
-11	3	11	66	79	13	-11	7	11	83	45	18	-7	12	11	80	87	9	2	-9	12	256	255	4	7 -5 12 189 192 3	
-10	3	11	31	46	31	-10	7	11	54	65	12	-6	12	11	42	3	17	3	-9	12	193	189	5	8 -5 12 58 62 16	
-9	3	11	48	53	10	-9	7	11	39	54	16	-5	12	11	58	76	11	4	-9	12	40	18	27	9 -5 12 69 78 19	
-8	3	11	184	184	5	-8	7	11	53	57	9	-4	12	11	23	55	23	5	-9	12	206	196	7	10 -5 12 215 220 7	
-7	3	11	129	108	6	-7	7	11	226	238	3	-3	12	11	100	99	7	6	-9	12	0	35	1	11 -5 12 77 44 25	
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6	4	11	83	81	14	-9	9	11	219	199	7	3	-12	12	117	116	7	3	-7	12	116	118	6	2 -3 12 24	

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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10	-2	12	105	106	9	6	2	12	24	8	9	5	6	12	115	112	7	1	11	12	117	113	7
11	-2	12	77	71	16	7	2	12	83	96	10	6	6	12	258	252	7	2	11	12	88	86	9
-11	-1	12	41	4	33	8	2	12	41	9	18	7	6	12	35	36	22	3	11	12	80	66	23
-10	-1	12	147	146	10	9	2	12	145	117	7	8	6	12	79	75	19	-8	12	12	50	15	49
-9	-1	12	47	38	17	10	2	12	63	58	12	-12	7	12	56	41	25	-7	12	12	22	20	21
-8	-1	12	69	75	3	-12	3	12	119	100	9	-11	7	12	29	3	29	-6	12	12	0	6	1
-7	-1	12	188	184	4	-11	3	12	144	153	8	-10	7	12	51	70	20	-5	12	12	32	31	31
-6	-1	12	212	217	24	-10	3	12	77	73	11	-9	7	12	47	59	13	-4	12	12	42	74	14
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-4	-1	12	242	243	6	-8	3	12	118	130	5	-7	7	12	200	196	4	-2	12	12	71	87	12
-3	-1	12	168	159	2	-7	3	12	56	29	7	-6	7	12	17	27	16	-1	12	12	108	98	9
-2	-1	12	101	97	3	-6	3	12	194	194	3	-5	7	12	203	212	2	0	12	12	58	61	18
-1	-1	12	328	339	3	-5	3	12	143	135	3	-4	7	12	98	98	6	1	12	12	67	71	16
0	-1	12	0	17	1	-4	3	12	189	196	4	-3	7	12	137	131	26	-6	13	12	78	23	20
1	-1	12	110	116	3	-3	3	12	0	5	1	-2	7	12	197	203	3	-5	13	12	189	197	6
2	-1	12	273	272	3	-2	3	12	254	252	4	-1	7	12	243	244	3	-4	13	12	95	102	8
3	-1	12	139	120	10	-1	3	12	110	104	19	0	7	12	18	3	18	-3	13	12	39	6	28
4	-1	12	171	175	3	0	3	12	254	250	2	1	7	12	67	53	6	-2	13	12	69	73	12
5	-1	12	93	91	3	1	3	12	345	341	3	2	7	12	108	108	5	-1	13	12	106	123	10
6	-1	12	28	32	10	2	3	12	86	96	3	3	7	12	0	48	1	2	14	13	0	9	
7	-1	12	19	21	18	3	3	12	249	238	4	4	7	12	90	89	6	3	14	13	85	80	14
8	-1	12	73	77	14	4	3	12	195	183	5	5	7	12	89	83	8	4	14	13	89	17	19
9	-1	12	92	93	11	5	3	12	8	36	8	6	7	12	90	78	10	-1	13	13	39	59	39
10	-1	12	103	82	16	6	3	12	178	180	3	7	7	12	83	50	15	0	13	13	81	83	24
11	-1	12	147	108	10	7	3	12	101	105	7	-12	8	12	103	83	12	1	13	13	63	64	31
-11	0	12	132	128	7	8	3	12	61	2	26	-11	8	12	43	3	43	2	13	13	0	28	1
-10	0	12	21	7	20	9	3	12	44	29	19	-10	8	12	137	133	7	3	13	13	65	65	17
-9	0	12	40	30	29	-12	4	12	65	71	12	-9	8	12	102	126	10	4	13	13	75	87	11
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-7	0	12	161	155	6	-10	4	12	56	52	34	-7	8	12	0	8	1	6	13	13	68	71	26
-6	0	12	216	216	4	-9	4	12	149	156	6	-6	8	12	146	154	2	7	13	13	41	3	41
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-4	0	12	106	101	8	-7	4	12	125	112	2	-4	8	12	90	77	6	-2	12	13	39	57	39
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6	0	12	323	317	8	3	4	12	249	254	3	6	8	12	38	39	38	8	12	13	75	72	58
7	0	12	90	76	15	4	4	12	383	381	4	-11	9	12	79	28	15	-4	11	13	116	106	7
8	0	12	156	147	8	5	4	12	329	334	4	-10	9	12	93	84	14	-3	11	13	105	97	7
9	0	12	53	25	29	6	4	12	156	159	5	-9	9	12	145	152	11	-2	11	13	76	75	13
10	0	12	43	19	42	7	4	12	137	125	7	-8	9	12	101	103	9	-1	11	13	46	13	29
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-10	1	12	226	217	7	9	4	12	39	29	24	-6	9	12	36	12	12	1	11	13	44	37	31
-9	1	12	216	230	5	-12	5	12	72	47	19	-5	9	12	69	52	6	2	11	13	98	96	9
-8	1	12	84	84	3	-11	5	12	59	55	11	-4	9	12	59	69	6	3	11	13	153	163	6
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-2	1	12	207	205	3	-5	5	12	341	333	4	2	9	12	112	113	6	9	11	13	46	30	46
-1	1	12	71	56	12	-4	5	12	97	90	3	3	9	12	45	49	24	-6	10	13	16	22	16
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2	1	12	328	328	4	-1	5	12	60	70	15	-11	10	12	59	39	25	-3	10	13	56	63	17
3	1	12	452	455	6	0	5	12	82	86	6	-10	10	12	57	43	33	-2	10	13	24	7	24
4	1	12	11	11	1	5	12	118	114	3	-9	10	12	152	158	7	-1	10	13	63	50	12	
5	1	12	54	49	8	2	5	12	42	6	10	-8	10	12	62	74	17	0	10				

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	
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-5	-4	13	66	54	7	-7	0	13	61	57	5	-10	4	13	69	62	16	-3	8	13	198	205	6	
-4	-4	13	210	205	3	-6	0	13	68	65	16	-9	4	13	77	87	10	-2	8	13	0	37	1	
-3	-4	13	192	187	2	-5	0	13	331	334	4	-8	4	13	227	219	6	-1	8	13	268	270	3	
-2	-4	13	151	146	2	-4	0	13	48	62	14	-7	4	13	237	244	3	0	8	13	147	150	4	
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6	-4	13	30	24	12	4	0	13	69	70	4	1	4	13	40	23	10	-10	9	13	31	55	31	
7	-4	13	44	47	6	5	0	13	89	91	4	2	4	13	252	238	6	-9	9	13	46	52	38	
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Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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2	-6	14	178	169	3	5	-2	14	322	324	4	5	2	14	82	92	3	7	6	14	113	131	14
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6	-6	14	55	57	13	9	-2	14	0	1	1	9	2	14	40	55	25	-8	7	14	113	124	11
7	-6	14	0	12	1	10	-2	14	57	12	18	-12	3	14	27	28	27	-7	7	14	76	71	4
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9	-6	14	114	97	9	-10	-1	14	72	70	14	-10	3	14	29	22	29	-5	7	14	247	244	3
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Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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2	-7	15	119	119	7	9	-3	15	152	158	7	-11	2	15	46	23	31	-4	6	15	60	71	3
3	-7	15	18	33	17	10	-3	15	0	27	1	-10	2	15	169	148	9	-3	6	15	106	110	4
4	-7	15	280	200	90	-10	-2	15	69	44	16	-9	2	15	109	106	11	-2	6	15	220	209	6
5	-7	15	35	21	35	-9	-2	15	81	37	11	-8	2	15	51	14	12	-1	6	15	35	53	11
6	-7	15	259	259	5	-8	-2	15	94	97	6	-7	2	15	106	108	12	0	6	15	194	188	5
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4	-6	15	259	252	7	9	-2	15	31	8	31	-11	3	15	76	67	18	-1	7	15	167	166	6
5	-6	15	90	89	7	10	-2	15	131	127	12	-10	3	15	44	35	27	0	7	15	23	13	22
6	-6	15	31	1	20	-11	-1	15	59	17	29	-9	3	15	0	12	1	1	7	15	29	39	
7	-6	15	105	97	6	-10	-1	15	169	182	8	-8	3	15	145	141	7	2	7	15	209	210	5
8	-6	15	101	107	10	-9	-1	15	193	191	7	-7	3	15	210	216	3	3	7	15	0	22	1
9	-6	15	72	16	24	-8	-1	15	52	58	22	-6	3	15	73	74	5	4	7	15	159	161	5
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-9	-5	15	0	14	1	-6	-1	15	307	314	7	-4	3	15	266	276	3	6	7	15	120	128	9
-8	-5	15	103	89	7	-5	-1	15	449	458	16	-3	3	15	369	371	5	-11	8	15	59	25	48
-7	-5	15	24	7	24	-4	-1	15	45	39	5	-2	3	15	345	346	4	-10	8	15	73	72	2
-6	-5	15	88	81	6	-3	-1	15	469	458	5	-1	3	15	110	101	4	-9	8	15	116	113	14
-5	-5	15	169	177	3	-2	-1	15	153	151	5	0	3	15	564	566	8	-8	8	15	183	184	8
-4	-5	15	45	52	11	-1	-1	15	55	68	6	1	3	15	33	36	17	-7	8	15	217	215	5
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-2	-5	15	87	95	5	1	-1	15	477	465	5	3	3	15	269	261	4	-5	8	15	101	118	4
-1	-5	15	17	14	16	2	-1	15	42	29	12	4	3	15	82	87	6	-4	8	15	153	153	3
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2	-5	15	149	148	4	5	-1	15	80	76	4	7	3	15	107	102	6	-1	8	15	38	36	21
3	-5	15	213	201	4	6	-1	15	108	112	4	8	3	15	48	44	18	0	8	15	124	135	4
4	-5	15	307	298	6	7	-1	15	81	70	14	-11	4	15	173	152	11	1	8	15	268	263	4
5	-5	15	193	198	5	8	-1	15	0	10	1	-10	4	15	77	62	12	2	8	15	59	72	9
6	-5	15	204	195	4	9	-1	15	51	7	43	-9	4	15	15	1	14	3	8	15	46	22	19
7	-5	15	32	20	15	10	-1	15	143	119	12	-8	4	15	160	152	6	4	8	15	0	9	1
8	-5	15	233	206	8	-11	0	15	29	13	29	-7	4	15	67	71	5	5	8	15	10	19	10
9	-5	15	78	88	12	-10	0	15	77	67	14	-6	4	15	260	260	4	-10	9	15	0	38	1
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-9	-4	15	63	39	25	-8	0	15	214	207	6	-4	4	15	44	40	5	-8	9	15	0	5	1
-8	-4	15	51	51	13	-7	0	15	38	42	14	-3	4	15	160	150	4	-7	9	15	51	30	15
-7	-4	15	133	134	5	-6	0	15	10	41	9	-2	4	15	88	84	3	-6	9	15	42	32	12
-6	-4	15	222	226	14	-5	0	15	110	102	5	-1	4	15	216	205	4	-5	9	15	122	119	10
-5	-4	15	338	333	9	-4	0	15	306	311	3	0	4	15	82	72	3	-4	9	15	89	82	6
-4	-4	15	195	194	4	-3	0	15	214	213	3	1	4	15	344	342	5	-3	9	15	123	127	4
-3	-4	15	41	43	41	-2	0	15	262	257	3	2	4	15	69	67	4	-2	9	15	242	240	3
-2	-4	15	86	82	5	-1	0	15	41	0	15	3	4	15	70	62	4	-1	9	15	93	101	12
-1	-4	15	120	123	6	0	0	15	167	164	3	4	4	15	138	136	3	0	9	15	117	116	4
0	-4	15	269	266	3	1	0	15	259	258	3	5	4	15	109	109	5	1	9	15	130	142	5
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2	-4	15	149	146	4	3	0	15	82	75	7	7	4	15	57	51	20	3	9	15	0	6	1
3	-4	15	71	50	8	4	0	15	130	124	5	8	4	15	60	96	14	4	9	15	161	136	19
4	-4	15	228	229	5	5	0	15	7	26	7	-11	5	15	37	30	36	-9	10	15	164	151	11
5	-																						

Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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-5	-6	16	51	42	11	1	-2	16	370	369	4	5	2	16	56	58	7	-4	7	16	86	97	5
-4	-6	16	152	162	4	2	-2	16	117	127	5	6	2	16	120	122	13	-3	7	16	58	59	9
-3	-6	16	157	167	11	3	-2	16	141	138	5	7	2	16	0	4	1	-2	7	16	86	71	9
-2	-6	16	45	40	13	4	-2	16	342	346	7	8	2	16	141	137	14	-1	7	16	28	22	27
-1	-6	16	136	127	19	5	-2	16	52	53	7	-11	3	16	45	9	20	0	7	16	142	142	4
0	-6	16	112	132	4	6	-2	16	79	87	11	-10	3	16	53	49	16	1	7	16	56	39	26
1	-6	16	132	136	5	7	-2	16	172	149	12	-9	3	16	198	192	7	2	7	16	159	156	5
2	-6	16	72	62	8	8	-2	16	0	3	1	-8	3	16	67	60	16	3	7	16	62	42	13
3	-6	16	209	216	6	9	-2	16	111	133	12	-7	3	16	114	117	11	4	7	16	47	57	15
4	-6	16	0	15	1	-10	-1	16	0	3	1	-6	3	16	81	89	5	5	7	16	52	1	37
5	-6	16	7	29	7	-9	-1	16	79	67	14	-5	3	16	149	162	3	-10	8	16	32	29	31
6	-6	16	109	106	6	-8	-1	16	303	292	7	-4	3	16	162	174	5	-9	8	16	155	157	9
7	-6	16	182	193	8	-7	-1	16	43	3	21	-3	3	16	314	312	3	-8	8	16	110	92	8
8	-6	16	83	85	21	-6	-1	16	69	83	11	-2	3	16	347	347	8	-7	8	16	60	21	28
9	-6	16	138	51	35	-5	-1	16	228	235	6	-1	3	16	40	28	18	-6	8	16	67	51	7
-9	-5	16	26	1	26	-4	-1	16	123	125	2	0	3	16	11	24	10	-5	8	16	27	32	22
-8	-5	16	172	168	6	-3	-1	16	16	18	16	1	3	16	80	77	5	-4	8	16	101	108	5
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-3	-5	16	31	12	30	2	-1	16	50	29	10	6	3	16	55	26	15	1	8	16	60	63	9
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2	-5	16	0	37	1	7	-1	16	108	93	9	-9	4	16	129	130	8	-8	9	16	47	38	29
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7	-5	16	91	106	16	-9	0	16	268	265	9	-4	4	16	147	151	2	-3	9	16	104	100	5
8	-5	16	76	71	12	-8	0	16	10	1	10	-3	4	16	147	150	3	-2	9	16	99	96	5
9	-5	16	216	203	7	-7	0	16	239	240	5	-2	4	16	290	280	6	-1	9	16	80	80	6
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-6	-4	16	243	246	8	-2	0	16	22	36	21	3	4	16	138	132	5	-8	10	16	67	23	18
-5	-4	16	55	59	11	-1	0	16	60	56	17	4	4	16	170	169	2	-7	10	16	73	53	34
-4	-4	16	58	67	8	0	0	16	211	196	3	5	4	16	43	45	13	-6	10	16	34	31	19
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1	-4	16	127	127	4	5	0	16	102	114	5	-9	5	16	155	144	10	-1	10	16	42	42	10
2	-4	16	130	129	4	6	0	16	51	71	16	-8	5	16	100	91	14	0	10	16	137	141	7
3	-4	16	50	56	15	7	0	16	74	92	14	-7	5	16	192	197	5	1	10	16	67	41	20
4	-4	16	41	41	14	8	0	16	0	33	1	-6	5	16	63	53	9	2	10	16	56	62	17
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7	-4	16	30	5	30	-10	1	16	287	264	8	-3	5	16	0	6	1	-3	11	16	92	99	7
8	-4	16	225	219	10	-9	1	16	37	16	37	-2	5	16	57	59	3	-2	11	16	47	17	25
9	-4	16	56	32	56	-8	1	16	95	98	8	-1	5	16	134	130	4	-1	11	16	66	68	13
10	-4	16	63	36	20	-7	1	16	65	67	9	0	5	16	135	131	3	0	11	16	61	56	34
-10	-3	16	79	39	38	-6	1	16	48	37	14	1	5	16	171	173	6	-5	12	16	0	44	1
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-7	-3	16	172	174	15	-3	1	16	71	64	5	4	5	16	237	227	6	0-12	17	68	42	28	-8
-6	-3	16	153	165	4	-2	1	16	394	410	5	5	5	16	31	3	31	-1-12	17	37	45	36	-7
-5	-3	16	99	98	3	-1	1	16	162	151	3	6	5	16	170	161	9	-1-11	17	71	78	11	-6
-4	-3	16	166	169	2	0	1	16	160	150	3	7	5	16	144	143	12	0-11	17	88	90	11	-5
-3	-3	16	80	83	6	1	1	16	343	335	5	-11	6	16	95	92	16	1-11	17	164	168	8	-4
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Table 6. Observed and calculated structure factors for 1

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s					
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2	-4	17	324	321	8	-11	1	17	96	78	28	-2	5	17	27	27	6	3-11	18	89	93	11	3-5	18	45	23	22	
3	-4	17	154	162	8	-10	1	17	36	28	35	-1	5	17	49	52	17	4-11	18	66	71	18	4-5	18	101	112	6	
4	-4	17	199	195	5	-9	1	17	95	84	14	0	5	17	266	267	3	5-11	18	0	37	1	5-5	18	31	20	31	
5	-4	17	125	130	4	-8	1	17	167	172	8	1	5	17	88	91	3	6-11	18	49	41	27	6-5	18	124	112	7	
6	-4	17	115	114	5	-7	1	17	38	50	11	2	5	17	148	151	7	-3-10	18	106	107	9	7-5	18	80	88	13	
7	-4	17	83	51	15	-6	1	17	129	128	12	3	5	17	37	13	16	-2-10	18	49	75	14	8-5	18	58	43	22	
8	-4	17	51	79	38	-5	1	17	237	242	6	4	5	17	31	4	30	-1-10	18	34	35	34	9-5	18	93	64	17	
9	-4	17	191	61	41	-4	1	17	104	109	3	5	5	17	39	21	39	0-10	18	139	138	7	-9-4	18	109	95	12	
-9	-3	17	141	151	16	-3	1	17	27	3	26	6	5	17	0	15	1	1-10	18	189	196	6	-8-4	18	0	2	1	
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-4	-3	17	69	74	7	2	1	17	38	29	37	-6	6	17	165	183	9	6-10	18	98	69	23	-3-4	18	50	52	9	
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-2	-3	17	57	55	9	4	1	17	120	122	5	-4	6	17	55	45	16	-5-9	18	132	125	16	-1-4	18	159	159	5	
-1	-3	17	100	85	9	5	1	17	113	133	4	-3	6	17	0	11	1	-4-9	18	26	46	26	0-4	18	74	85	7	
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1	-3	17	74	82	7	7	1	17	112	113	7	-1	6	17	182	171	8	-2-9	18	53	33	17	2-4	18	34	35	34	
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-4	-2	17	50	49	49	2	2	17	45	21	13	-2	7	17	0	3	1	-1-8	18	40	0	22	-2-3	18	197	200	4	
-3	-2	17	40	43	8	3	2	17	272	274	4	-1	7	17	59	47	11	0-8	18	243	235	5	-1-3	18	35	43	21	
-2	-2	17	201	204	3	4	2	17	203	198	3	0	7	17	0	8	1	1-8	18	100	104	7	0	-3	18	120	124	10
-1	-2	17	291	292	4	5	2	17	34	16	13	1	7	17	101	75	8	2-8	18	151	137	7	1	-3	18	37	52	11
0	-2	17	36	41	17	6	2	17	138	120	137	2	7	17	40	27	40	3-8	18	28	32	28	2-3	18	285	287	7	
1	-2	17	407	409	4	7	2	17	15	20	15	3	7	17	124	90	10	4-8	18	36	2	35	3	-3	18	43	23	42
2	-2	17	51	76	8	8	2	17	0	12	1	4	7	17	43	21	43	5-8	18	77	73	21	4-3	18	10	31	10	
3	-2	17	226	233	6	-11	3	17	0	39	1	5	7	17	135	114	29	6-8	18	86	67	10	5-3	18	61	68	12	
4	-2	17	205	208	5	-10	3	17	0	27	1	-10	8	17	0	35	1	7-8	18	74	61	24	6-3	18	62	27	22	
5	-2	17	77	66	5	-9	3	17	91	111	19	-9	8	17	33	14	32	8-8	18	47	9	46	7-3	18	77	4	25	
6	-2	17	0	14	1	-8	3	17	127	132	11	-8	8	17	97	98	17	-7-7	18	83	73	18	8-3	18	114	74	11	
7	-2	17	124	124	10	-7	3	17	0	49	1	-7	8	17	131	101	15	-6-7	18	23	10	23	9-3	18	0	4	1	
8	-2	17	0	7	1	-6	3	17	86	92	5	-6	8	17	89	86	6	-5-7	18	63	68	13	-9-2	18	0	2	1	
9	-2	17	66	67	17	-5	3	17	30	23	18	-5	8	17	24	17	24	-4-7	18	88	86	7	-8-2	18	72	70	12	
-10	-1	17	60	48	13	-4	3	17	0	9	1	-4	8	17	123	106	6	-3-7	18	89	86	7	-7-2	18	45	0	45	
-9	-1	17	107	93	18	-3	3	17	145	157	3	-3	8	17	5	6	5	-2-7	18	80	92	10	-6-2	18	61	59	6	
-8	-1	17	43	50	28	-2	3	17	48	44	10	-2	8	17	167	173	4	-1-7	18	28	39	28	-5-2	18	75	91	23	
-7	-1	17	192	194	5	-1	3	17	35	5	9	-1	8	17	81	59	6	0-7	18	188	190	5	-4-2	18	97	96	4	
-6	-1	17	98	100	5	0	3	17	255	265	3	0	8	17	208	190	4	1-7	18	60	10	12	-3-2	18	35	29	34	
-5	-1	17	208	225	4	1	3	17	415	425	4	1	8	17	26	25	2	-2-7	18	31	12	31	-2-2	18	139	145	3	
-4	-1	17	238	250	3	2	3	17	237	243	3	2	8	17	54	38	12	3-7										

Table 6. Observed and calculated structure factors for 1

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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	0	18	28	19	28	6	4	18	107	101	10	0-10	19	98	94	9	1	-4	19	0	27	1	-3	1	19	37	40	19		
-6	0	18	59	10	58	-10	5	18	32	45	31	1-10	19	68	81	12	2	-4	19	92	104	8	-2	1	19	105	102	8		
-5	0	18	162	165	4	-9	5	18	45	65	45	2-10	19	23	17	23	3	-4	19	181	189	6	-1	1	19	133	131	6		
-4	0	18	50	45	3	-8	5	18	0	43	1	3-10	19	101	93	8	4	-4	19	107	109	8	0	1	19	69	71	5		
-3	0	18	158	161	3	-7	5	18	131	130	6	4-10	19	79	61	12	5	-4	19	122	114	5	1	1	19	62	70	6		
-2	0	18	328	335	5	-6	5	18	101	89	4	5-10	19	97	93	13	6	-4	19	49	27	48	2	1	19	201	199	6		
-1	0	18	180	179	12	-5	5	18	228	234	5	-4	-9	19	54	6	39	7	-4	19	120	88	12	3	1	19	30	4	30	
0	0	18	29	15	19	-4	5	18	173	193	5	-3	-9	19	61	66	12	8	-4	19	87	96	18	4	1	19	67	69	9	
1	0	18	219	228	10	-3	5	18	54	55	9	-2	-9	19	51	33	15	-9	-3	19	0	24	1	5	1	19	106	100	10	
2	0	18	210	218	5	-2	5	18	15	2	14	-1	-9	19	184	193	7	-8	-3	19	55	35	17	6	1	19	76	59	16	
3	0	18	16	32	15	-1	5	18	90	79	7	0	-9	19	56	49	19	-7	-3	19	65	67	17	7	1	19	134	135	10	
4	0	18	55	24	9	0	5	18	54	55	12	1	-9	19	191	187	6	-6	-3	19	37	52	36	-10	2	19	62	3	27	
5	0	18	81	100	5	1	5	18	217	218	6	2	-9	19	39	68	29	-5	-3	19	70	99	16	-9	2	19	69	75	16	
6	0	18	0	25	1	2	5	18	82	80	6	3	-9	19	0	2	1	-3	-3	19	83	76	6	-8	2	19	215	168	16	
7	0	18	63	71	18	3	5	18	215	212	7	4	-9	19	97	93	9	-2	-3	19	56	45	13	-7	2	19	85	68	16	
8	0	18	69	49	41	4	5	18	38	28	38	5	-9	19	106	96	12	-1	-3	19	118	135	7	-6	2	19	184	188	5	
-10	1	18	48	62	47	5	5	18	128	130	10	6	-9	19	219	233	8	0	-3	19	35	4	35	-5	2	19	290	298	4	
-9	1	18	152	155	12	6	5	18	39	62	38	7	-9	19	92	91	15	1	-3	19	141	139	6	-4	2	19	51	54	10	
-8	1	18	0	50	1	-10	6	18	103	67	12	-5	-8	19	62	77	23	2	-3	19	145	147	5	-3	2	19	334	339	4	
-7	1	18	50	51	22	-9	6	18	7	36	7	-4	-8	19	49	39	17	3	-3	19	28	17	28	-2	2	19	0	5	1	
-6	1	18	32	42	31	-8	6	18	59	64	12	-3	-8	19	154	138	13	4	-3	19	161	171	4	-1	2	19	192	184	4	
-5	1	18	156	153	4	-7	6	18	106	95	8	-2	-8	19	115	113	7	5	-3	19	164	169	5	0	2	19	163	154	4	
-4	1	18	73	79	13	-6	6	18	41	27	41	-1	-8	19	0	8	1	6	-3	19	122	122	12	1	2	19	169	179	4	
-3	1	18	9	34	8	-5	6	18	105	106	8	0	-8	19	82	89	11	7	-3	19	168	184	10	2	2	19	67	68	4	
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-1	1	18	130	128	11	-3	6	18	33	25	20	2	-8	19	75	31	15	-9	-2	19	0	23	1	4	2	19	333	332	5	
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1	1	18	356	360	6	-1	6	18	64	83	12	4	-8	19	164	169	9	-7	-2	19	39	17	38	6	2	19	102	89	9	
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3	1	18	52	61	7	1	6	18	0	15	1	6	-8	19	25	4	25	-5	-2	19	136	149	5	-10	3	19	60	55	21	
4	1	18	42	5	22	2	6	18	82	88	8	7	-8	19	146	136	13	-4	-2	19	142	159	4	-9	3	19	40	52	40	
5	1	18	0	1	1	3	6	18	40	16	22	-6	-7	19	49	10	49	-3	-2	19	100	104	5	-8	3	19	46	9	46	
6	1	18	71	74	11	4	6	18	74	41	23	-5	-7	19	45	30	34	-2	-2	19	52	55	15	-7	3	19	100	46	12	
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8	1	18	0	24	1	-10	7	18	0	32	1	-3	-7	19	37	17	36	0	-2	19	0	25	1	-1	5	3	19	108	110	8
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-9	2	18	77	75	9	-8	7	18	101	78	17	-1	-7	19	137	131	5	2	-2	19	368	379	7	-3	3	19	90	102	5	
-8	2	18	32	3	31	-7	7	18	123	76	17	0	-7	19	51	14	16	3	-2	19	40	42	22	-2	3	19	108	99	7	
-7	2	18	47	46	18	-6	7	18	72	64	17	1	-7	19	38	1	38	4	-2	19	218	218	5	-1	3	19	73	66	11	
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-2	2	18	181	193	3	-1	7	18	58	53	10	6	-7	19	131	132	8	-9	-1	19	46	50	26	4	3	19	8	3	8	
-1	2	18	375	377	5	0	7	18	154	142	6	7	-7	19	92	84	39	-8	-1	19	146	143	11	5	3	19	88	95	12	
0	2	18	102	96	7	1	7	18	90	88	7	8	-7	19	146	143	13	-7	-1	19	211	216	3	-7	4	19	78	86	20	
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2	2	18	44	44	19	3	7	18	89	84	16	-6	-6	19	108	95	10	-5	-1	19	82	82	14	-9	4	19	18	12	17	
3	2	18	0	14	1	4	7	18	93	73	10	-5	-6	19	43	15	17	-4	-1	19	116	111	15	-8	4	19	106	118	11	
4	2	18	136	141	3	-8	8	18	119	47	18	-4	-6	19	36	50	35	-3	-1	19	211	216	3	-7	4	19	78	86	20	
5	2	18	94	81	7	-7	8	18	151	127	11	-3	-6	19	114	96	7	-2	-1	19	155	153	6	-6	4	19	254	246	8	
6	2	18	31	34	31	-6	8	18	172	159	5	-2	-6	19	120	112	7	-1	-1	19	124	118	5	-5	4	19	0	5	1	
7	2	18	127	120	8	-5	8	18	73	48	19	-1	-6	19	23	34</														

Table 6. Observed and calculated structure factors for 1

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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	19	140	135	4	-1	-6	20	172	176	5	4	-1	20	56	44	10	-7	5	20	68	4	15
0	6	19	35	28	21	0	-6	20	7	40	7	5	-1	20	66	72	19	-6	5	20	179	165	12
1	6	19	233	220	5	1	-6	20	87	90	12	6	-1	20	75	71	19	-5	5	20	136	142	8
2	6	19	48	42	11	2	-6	20	159	157	5	7	-1	20	83	51	29	-4	5	20	0	45	1
3	6	19	87	81	10	3	-6	20	82	66	10	-9	0	20	75	75	13	-3	5	20	132	138	4
4	6	19	133	140	7	4	-6	20	110	114	8	-8	0	20	71	84	26	-2	5	20	86	76	13
-8	7	19	92	79	15	5	-6	20	55	31	17	-7	0	20	73	28	20	-1	5	20	165	156	6
-7	7	19	86	87	14	6	-6	20	153	157	8	-6	0	20	225	200	9	0	5	20	237	232	5
-6	7	19	40	29	21	7	-6	20	61	70	25	-5	0	20	233	241	6	1	5	20	80	55	9
-5	7	19	68	42	23	-7	-5	20	122	131	7	-4	0	20	159	157	5	2	5	20	139	130	12
-4	7	19	32	83	31	-6	-5	20	33	6	32	-3	0	20	56	42	29	3	5	20	53	41	19
-3	7	19	40	8	27	-5	-5	20	122	124	7	-2	0	20	249	246	4	4	5	20	153	148	9
-2	7	19	63	53	14	-4	-5	20	59	25	25	-1	0	20	233	238	8	-8	6	20	0	34	1
-1	7	19	0	12	1	-3	-5	20	56	28	17	0	0	20	415	408	11	-7	6	20	64	34	16
0	7	19	107	103	8	-2	-5	20	102	102	6	1	0	20	246	239	5	-6	6	20	30	6	30
1	7	19	0	0	1	-1	-5	20	235	234	8	2	0	20	65	62	8	-5	6	20	25	9	25
2	7	19	72	68	10	0	-5	20	0	33	1	3	0	20	52	51	11	-4	6	20	0	48	1
3	7	19	89	77	15	1	-5	20	210	208	7	4	0	20	27	29	27	-3	6	20	57	55	8
-8	8	19	0	49	1	2	-5	20	187	187	7	5	0	20	129	140	8	-2	6	20	0	19	1
-7	8	19	109	86	9	3	-5	20	77	70	10	6	0	20	168	167	11	-1	6	20	7	19	7
-6	8	19	21	20	21	4	-5	20	0	23	1	7	0	20	45	18	45	0	6	20	0	10	1
-5	8	19	58	70	14	5	-5	20	35	35	24	-9	1	20	0	6	1	1	6	20	0	20	1
-4	8	19	84	71	8	6	-5	20	62	11	41	-8	1	20	106	92	9	2	6	20	37	53	36
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-1	8	19	23	13	22	-7	-4	20	122	135	7	-5	1	20	81	62	10	-8	7	20	0	60	1
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1	8	19	204	201	4	-5	-4	20	143	140	6	-3	1	20	101	97	4	-6	7	20	103	26	54
2	8	19	160	154	8	-4	-4	20	132	118	13	-2	1	20	39	19	11	-5	7	20	54	69	27
-5	9	19	102	88	7	-3	-4	20	149	160	6	-1	1	20	353	348	8	-4	7	20	105	97	11
-4	9	19	64	50	11	-2	-4	20	71	67	18	0	1	20	45	2	20	-3	7	20	41	31	41
-3	9	19	58	47	13	-1	-4	20	59	52	13	1	1	20	156	141	6	-2	7	20	29	25	28
-2	9	19	13	26	12	0	-4	20	63	61	12	2	1	20	106	113	4	-1	7	20	173	168	6
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-5	10	19	74	61	12	4	-4	20	91	82	8	6	1	20	53	15	26	3	7	20	124	117	11
-4	10	19	97	100	19	5	-4	20	279	281	5	7	1	20	40	41	21	-6	8	20	67	53	17
-3	10	19	41	23	19	6	-4	20	307	320	9	-9	2	20	0	30	1	-5	8	20	176	164	6
-2	10	19	43	53	43	7	-4	20	0	17	1	-8	2	20	96	56	18	-4	8	20	147	143	6
-1	10	19	0	23	1	8	-4	20	16	3	16	-7	2	20	39	12	39	-3	8	20	50	4	12
0-10	20	144	138	20	-8	-3	20	56	23	36	-6	2	20	145	135	8	-2	8	20	0	17	1	
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2-10	20	70	40	23	-6	-3	20	110	120	10	-4	2	20	62	55	14	0	8	20	80	86	8	
3-10	20	135	121	16	-5	-3	20	40	48	40	-3	2	20	76	78	7	1	8	20	50	3	26	
4-10	20	95	57	15	-4	-3	20	207	189	9	-2	2	20	168	169	8	-5	9	20	86	89	12	
5-10	20	95	104	11	-3	-3	20	181	188	7	-1	2	20	242	227	5	-4	9	20	131	129	7	
-3-9	20	72	41	20	-2	-3	20	99	102	14	0	2	20	88	88	13	-3	9	20	241	227	6	
-2-9	20	79	87	12	-1	-3	20	89	76	8	-9	3	20	75	66	17	-2	9	20	137	132	9	
-1-9	20	61	80	13	0	-3	20	106	127	5	2	2	20	199	200	4	-1	9	20	53	38	24	
0-9	20	27	42	27	1	-3	-2	20	71	85	12	3	2	20	0	24	1	0	9	20	70	65	12
1-9	20	110	112	7	2	-3	20	176	174	6	4	2	20	27	34	27	-4	10	20	64	52	17	
2-9	20	146	143	6	3	-3	20	109	120	10	5	2	20	0	1	1	-2	10	21	63	9	28	
3-9	20	129	110	14	4	-3	20	77	88	8	6	2	20	46	8	45	3-10	21	112	120	14		
4-9	20	65	24	28	5	-3	20	69	70	8	-9	3	20	75	66	17	-2	9	21	56	6	32	
5-9	20	66	41	65	6	-3	20	115	119	14	-8	3	20	0	29	1	-1	9	21	86	106	13	
6-9	20	49	61	35	7	-3	20	75	85	15	-7	3	20	141	153	6	0	9	21	0	28	1	
-4-8	20	113	96	15	8	-3	20	146	141	14	-6	3	20	51	43	27	1	-1	9	21	102	65	12
-3-8	20	7	47	7	-8	-2	20	25	45	25	-5	3	20	53	54	13	2	-9	21	0	8	1	
-2-8	20	147	153	7	-7	-2	20	97	90	15	-4	3	20	101	95	6	3	-9	21	93	80	14	
-1-8	20	310	285	6	-6	-2	20	74	65	9	-3	3	20	43	54	9	4	-9	21	90	67	20	
0-8	20	27	4	27	-5	-2	20	37	56	37	-2	3	20	182	171	6	5	-9	21	90	71	11	
1-8	20	189	191	6	-4	-2	20	76	51	13	-1	3	20	27	2	27	-4	-8	21	108	18	35	
2-8	20	36	37	35	-3	-2	20	77	12	21	0	3	20	129	132	8	-3	-8	21	0	59	1	
3-8	20	0	23	1	-2	-2	20	87	85	13	1	3	20	72	81	5	-2	-8	21	35	34	35	
4-8	20	191	185	7	-7	-1	20	104	114	10	2	3	20	196	200	6	-1	-8	21	88	58		

Table 6. Observed and calculated structure factors for 1

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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	0	21	59	51	24	-6	6	21	260	222	12	-4	-3	22	75	62	16	1	3	22	105	88	7	
-7	0	21	121	122	9	-5	6	21	172	157	9	-3	-3	22	0	4	1	2	3	22	106	107	7	
-6	0	21	174	179	9	-4	6	21	66	48	24	-2	-3	22	0	45	1	3	3	22	82	73	13	
-5	0	21	40	26	40	-3	6	21	0	14	1	-1	-3	22	64	86	13	4	3	22	47	35	47	
-4	0	21	57	59	20	-2	6	21	28	10	27	0	-3	22	112	120	7	-7	4	22	34	9	33	
-3	0	21	128	125	10	-1	6	21	90	92	6	1	-3	22	255	243	6	-6	4	22	112	79	40	
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-1	0	21	112	119	4	1	6	21	32	19	31	3	-3	22	89	79	19	-4	4	22	52	5	17	
0	0	21	138	133	6	2	6	21	92	105	7	4	-3	22	25	15	25	-3	4	22	95	85	35	
1	0	21	0	34	1	3	6	21	142	141	8	5	-3	22	45	18	45	-2	4	22	31	17	31	
2	0	21	87	82	10	-6	7	21	0	18	1	6	-3	22	68	57	22	-1	4	22	25	22	24	
3	0	21	58	44	10	-5	7	21	102	93	14	-7	-2	22	0	30	1	0	4	22	41	35	17	
4	0	21	47	29	15	-4	7	21	28	1	28	-6	-2	22	98	59	13	1	4	22	62	76	14	
5	0	21	64	45	17	-3	7	21	95	86	12	-5	-2	22	0	53	1	2	4	22	158	139	6	
6	0	21	145	42	58	-2	7	21	50	52	14	-4	-2	22	135	125	11	3	4	22	48	13	47	
-9	1	21	0	48	1	-1	7	21	33	22	25	-3	-2	22	120	124	6	4	4	22	75	62	11	
-8	1	21	38	3	38	0	7	21	42	36	21	-2	-2	22	135	128	9	-7	5	22	177	195	11	
-7	1	21	38	33	38	1	7	21	80	86	11	-1	-2	22	96	103	11	-6	5	22	118	123	10	
-6	1	21	54	45	15	2	7	21	35	18	27	0	-2	22	299	286	6	-5	5	22	59	61	23	
-5	1	21	41	26	40	-5	8	21	71	72	15	1	-2	22	75	59	12	-4	5	22	33	43	32	
-4	1	21	23	47	23	-4	8	21	0	3	1	2	-2	22	111	106	9	-3	5	22	24	31	24	
-3	1	21	6	12	6	-3	8	21	117	86	22	3	-2	22	85	60	10	-2	5	22	117	95	11	
-2	1	21	154	162	6	-2	8	21	86	88	9	4	-2	22	0	19	1	-1	5	22	86	67	8	
-1	1	21	179	175	7	-1	8	21	52	29	24	5	-2	22	172	163	15	0	5	22	216	196	11	
0	1	21	16	26	16	0	8	21	20	12	19	6	-2	22	89	97	12	1	5	22	41	12	32	
1	1	21	117	121	8	-4	9	21	23	23	23	-7	-1	22	59	33	26	2	5	22	148	152	11	
2	1	21	57	55	15	-3	9	21	77	43	13	-6	-1	22	0	2	1	3	5	22	45	45	-2	
3	1	21	69	28	11	-2	9	21	45	14	45	-5	-1	22	62	55	16	-6	6	22	0	12	1	
4	1	21	68	65	19	1	-9	22	0	2	1	-4	-1	22	191	172	8	-5	6	22	110	92	12	
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-5	2	21	102	110	15	0	-8	22	78	65	18	2	-1	22	161	164	9	1	6	22	15	9	15	
-4	2	21	34	17	34	1	-8	22	0	24	1	3	-1	22	88	83	10	2	6	22	55	55	18	
-3	2	21	200	193	4	2	-8	22	0	17	1	4	-1	22	77	75	9	-5	7	22	60	103	59	
-2	2	21	86	80	5	3	-8	22	185	188	8	5	-1	22	127	100	11	-4	7	22	0	23	1	
-1	2	21	92	100	6	4	-8	22	88	91	17	6	-1	22	7	6	7	-3	7	22	88	52	30	
0	2	21	32	30	31	-4	-7	22	0	6	1	-7	0	22	168	167	9	-2	7	22	97	52	20	
1	2	21	132	133	8	-3	-7	22	29	25	29	-6	0	22	184	182	9	-1	7	22	128	121	8	
2	2	21	0	36	1	-2	-7	22	69	62	15	-5	0	22	28	6	28	0	7	22	180	171	9	
3	2	21	153	154	4	-1	-7	22	47	42	23	4	0	22	131	136	8	1	7	22	52	47	51	
4	2	21	55	42	27	0	-7	22	141	122	7	-3	0	22	168	157	7	-4	8	22	0	19	1	
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6	2	21	139	124	13	2	-7	22	107	109	15	-1	0	22	159	157	7	-1	8	22	80	64	8	
-9	3	21	0	16	1	3	-7	22	112	97	10	0	0	22	153	158	6	0	-8	23	19	60	19	
-8	3	21	38	54	30	4	-7	22	87	43	17	1	0	22	95	106	11	1	-8	23	67	17	35	
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-6	3	21	70	66	10	-4	-6	22	0	25	1	3	0	22	92	101	9	3	-8	23	55	4	22	
-5	3	21	157	152	7	-3	-6	22	77	89	13	4	0	22	63	75	20	-3	-7	23	97	91	17	
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-3	3	21	188	184	5	-1	-6	22	53	40	23	6	0	22	157	156	10	0	-7	23	101	101	10	
-2	3	21	0	11	1	0	-6	22	0	2	1	-7	1	22	83	89	14	1	-7	23	50	33	31	
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0	3	21	67	70	6	2	-6	22	129	132	8	-5	1	22	69	42	17	3	-7	23	84	92	15	
1	3	21	39	6	38	3	-6	22	56	53	17	-4	1	22	26	4	26	4	-7	23	41	27	28	
2	3	21	30	42	30	4	-6	22	168	160	9	-3	1	22	149	143	9	-3	-6	23	0	56	1	
3	3	21	72	68	8	5	-6	22	0	7	1	-2	1	22	327	313	5	-2	-6	23	185	170	12	
4	3	21	44	49	43	6	-6	22	114	123	12	-1	1	22	111	113	4	-1	-6	23	0	42	1	
5	3	21	89	83	12	-5	-5	22	49	72	29	0	1	22	140	138	6	0	-6	23	61	73	13	
-8	4	21	86	34	36	-4	-5	22	71	33	12	1	1	22	46	40	14	1	-6	23	96	66	31	
-7	4	21	84	93	16	-3	-5	22	30	53	30	2	1	22	58	52	12	4	-5	23	150	129	6	
-6	4	21	0	41	1	-2	-5	22	130	114	10	3	1	22	65	58	9	3	-6	23	64	25	17	
-5	4	21	248	234	9	-1	-5	22	15	2	14	4	1	22	43	22	42	4	-6	23	93	59	25	
-4	4	21	63	45	20	0	-5	22	106	94	10													

Table 6. Observed and calculated structure factors for 1

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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	23	138	136	12	-2	-3	24	39	4	39	-5	2	24	52	26	51	2	-4	25	47	11	46	2	2	25	181	174	14
2	4	23	52	48	51	-1	-3	24	0	0	1	-4	2	24	37	13	37	3	-4	25	37	18	37	-3	3	25	116	87	22
3	4	23	147	152	12	0	-3	24	101	97	21	-3	2	24	24	33	24	-3	-3	25	76	88	23	-2	3	25	108	111	15
-5	5	23	102	98	12	1	-3	24	91	93	11	-2	2	24	0	7	1	-2	-3	25	118	125	9	-1	3	25	55	74	30
-4	5	23	138	136	15	2	-3	24	31	29	31	-1	2	24	51	49	30	-1	-3	25	127	124	15	0	3	25	73	45	20
-3	5	23	68	66	14	3	-3	24	117	109	10	0	2	24	44	9	17	0	-3	25	63	21	20	1	3	25	44	27	23
-2	5	23	135	129	9	4	-3	24	96	92	15	1	2	24	16	5	16	1	-3	25	101	105	12	-3	4	25	166	148	11
-1	5	23	27	12	26	-5	-2	24	0	57	1	2	24	52	47	16	2	-3	25	37	53	36	-2	4	25	151	140	9	
0	5	23	92	94	7	-4	-2	24	22	58	21	3	2	24	94	90	9	3	-3	25	23	30	23	-1	4	25	41	56	40
1	5	23	63	39	13	-3	-2	24	0	7	1	-5	3	24	44	51	21	-4	-2	25	113	134	13	0	4	25	106	110	9
2	5	23	84	75	27	-2	-2	24	59	3	25	-4	3	24	64	61	41	-3	-2	25	120	91	15	-2	5	25	0	47	1
-4	6	23	99	84	24	-1	-2	24	43	46	28	-3	3	24	105	102	12	-2	-2	25	233	226	11	0	4	26	93	24	15
-3	6	23	118	65	27	0	-2	24	88	82	19	-2	3	24	100	86	11	-1	-2	25	34	22	33	1	-4	26	0	19	1
-2	6	23	140	143	12	1	-2	24	32	16	31	-1	3	24	91	61	21	0	-2	25	128	126	10	-2	3	26	0	2	1
-1	6	23	77	93	20	2	-2	24	157	158	9	0	3	24	121	122	7	1	-2	25	77	42	28	-1	-3	26	72	7	22
0	6	23	67	27	25	3	-2	24	42	25	42	1	3	24	56	26	46	2	-2	25	57	73	26	0	-3	26	50	33	39
1	6	23	64	65	13	4	-2	24	0	9	1	2	3	24	96	89	12	3	-2	25	49	28	48	2	-3	26	150	144	8
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1	-5	24	157	154	6	0	0	24	98	98	16	-1	6	24	57	54	15	-4	1	25	66	50	24	1	0	26	112	103	12
2	-5	24	53	63	23	1	0	24	51	18	22	-0	6	25	97	96	23	-3	1	25	0	23	1	-3	1	26	131	131	12
3	-5	24	71	27	17	2	0	24	94	91	6	1	-6	25	59	70	24	-2	1	25	166	161	10	-2	1	26	0	25	1
-3	-4	24	53	32	36	3	0	24	147	151	6	2	-6	25	41	64	40	-1	1	25	39	26	22	-1	1	26	110	118	9
-2	-4	24	71	40	71	-5	1	24	46	1	46	-1	-5	25	128	90	14	0	1	25	82	78	9	0	1	26	128	129	10
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3	-4	24	78	116	17	0	1	24	70	66	8	-2	-4	25	156	152	9	-2	2	25	194	197	11	-1	3	26	49	63	29
4	-4	24	222	208	9	1	1	24	79	83	9	-1	-4	25	109	113	12	-1	2	25	65	14	26						
-4	-3	24	68	32	33	2	1	24	37	26	36	0	-4	25	63	87	21	0	2	25	152	149	6						
-3	-3	24	0	24	1	4	1	24	90	68	17	1	-4	25	108	84	11	1	2	25	94	71	14						