CHEMISTRY OF MATERIALS
Chem. Mater., 1996, 8(6), 1229-1235, DOI:10.1021/cm950524b

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I-1235-1

Table 1. Crystal data and structure refinement for 1.

Identification code	4clbzmal
Empirical formula	$C_{18}H_{24}Cl_2N_2O_6$
Formula weight	435.29
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 4.8350(10) Å α = 96.13° b = 5.7450(10) Å β = 92.62° c = 17.676(3) Å γ = 95.43°
Volume	485.2(2) Å^3
Z	1
Density (calculated)	1.490 Mg/m^3
Absorption coefficient	0.373 mm^{-1}
F(000)	228
Crystal size	0.76 x 0.35 x 0.11 mm
θ range for data collection	2.32 to 24.96°
Index ranges	$-1 \le h \le 5$, $-6 \le k \le 6$, $-20 \le \ell \le 20$
Reflections collected	2353
Independent reflections	2353 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2353 / 3 / 253
Goodness-of-fit on F^2	1.073
Final R indices [I>2σ(I)]	R1 = 0.0357, wR2 = 0.0908
R indices (all data)	R1 = 0.0418, wR2 = 0.0954
Absolute structure parameter	−0.04(8)
Largest diff. peak and hole	0.260 and −0.262 eÅ^{-3}

I-1235-2

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 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)
O(12)	-5222(7)	-5984(5)	-10769(2)	36(1)
O(11)	-2391(7)	-2956(5)	-11055(2)	37(1)
C(1)	-3023(9)	-4617(7)	-10651(2)	28(1)
C(2)	-1014(9)	-4912(7)	-9989(2)	28(1)
C(3)	-1908(8)	-3691(6)	-9237(2)	23(1)
O(3)	-1854(6)	-1219(4)	-9254(1)	34(1)
C(4)	-17(9)	-4295(6)	-8589(2)	22(1)
O(41)	2184(7)	-3035(5)	-8398(2)	35(1)
O(42)	-740(7)	-6182(5)	-8309(2)	33(1)
C(7A)	-3585(9)	-9009(7)	-6739(2)	27(1)
C(8A)	-2478(10)	-8055(7)	-6016(2)	34(1)
C(9A)	-607(11)	-9207(8)	-5609(2)	37(1)
C(10A)	177(11)	-11340(7)	-5926(2)	36(1)
Cl(1A)	2466(2)	-12814(2)	-5408(1)	50(1)
C(11A)	-838(10)	-12289(7)	-6649(2)	34(1)
C(12A)	-2704(9)	-11144(7)	-7047(2)	31(1)
C(6A)	-5717(9)	-7753(7)	-7127(2)	30(1)
N(5A)	-5957(8)	-8277(6)	-7969(2)	28(1)
C(7B)	394(10)	-10036(7)	-2598(2)	29(1)
C(8B)	-681(10)	-10925(7)	-3320(2)	33(1)
C(9B)	-2557(10)	-9776(7)	-3715(2)	35(1)
C(10B)	-3338(9)	-7673(7)	-3375(2)	30(1)
C(11B)	-2351(10)	-6759(7)	-2649(2)	34(1)
C(12B)	-463(10)	-7963(7)	-2265(2)	32(1)
C(6B)	2553(10)	-11347(7)	-2220(2)	32(1)
N(5B)	2863(9)	-10871(6)	-1379(2)	34(1)
O(1W)	-6635(9)	-9267(6)	-9689(2)	42(1)
Cl(1B)	-5643(2)	-6153(2)	-3881(1)	50(1)

I-1235-3

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

O(12)-C(1)	1.256(5)	O(11)-C(1)	1.275(5)
C(1)-C(2)	1.521(6)	C(2)-C(3)	1.535(4)
C(3)-O(3)	1.421(4)	C(3)-C(4)	1.522(5)
C(4)-O(41)	1.241(5)	C(4)-O(42)	1.266(5)
C(7A)-C(8A)	1.398(5)	C(7A)-C(12A)	1.400(6)
C(7A)-C(6A)	1.496(6)	C(8A)-C(9A)	1.389(6)
C(9A)-C(10A)	1.386(7)	C(10A)-C(11A)	1.384(5)
C(10A)-Cl(1A)	1.741(5)	C(11A)-C(12A)	1.376(6)
C(6A)-N(5A)	1.483(5)	C(7B)-C(12B)	1.379(6)
C(7B)-C(8B)	1.382(5)	C(7B)-C(6B)	1.515(6)
C(8B)-C(9B)	1.379(6)	C(9B)-C(10B)	1.385(6)
C(10B)-C(11B)	1.378(6)	C(10B)-Cl(1B)	1.751(4)
C(11B)-C(12B)	1.392(6)	C(6B)-N(5B)	1.480(5)

O(12)-C(1)-O(11)	123.2(4)	O(12)-C(1)-C(2)	119.1(4)
O(11)-C(1)-C(2)	117.7(4)	C(1)-C(2)-C(3)	111.2(3)
O(3)-C(3)-C(4)	111.7(3)	O(3)-C(3)-C(2)	111.5(2)
C(4)-C(3)-C(2)	108.4(3)	O(41)-C(4)-O(42)	123.9(4)
O(41)-C(4)-C(3)	119.6(3)	O(42)-C(4)-C(3)	116.3(3)
C(8A)-C(7A)-C(12A)	117.8(4)	C(8A)-C(7A)-C(6A)	118.5(4)
C(12A)-C(7A)-C(6A)	123.6(3)	C(9A)-C(8A)-C(7A)	121.2(4)
C(10A)-C(9A)-C(8A)	119.4(4)	C(11A)-C(10A)-C(9A)	120.4(4)
C(11A)-C(10A)-Cl(1A)	120.2(4)	C(9A)-C(10A)-Cl(1A)	119.4(3)
C(12A)-C(11A)-C(10A)	119.8(4)	C(11A)-C(12A)-C(7A)	121.3(4)
N(5A)-C(6A)-C(7A)	114.5(3)	C(12B)-C(7B)-C(8B)	118.9(4)
C(12B)-C(7B)-C(6B)	122.9(4)	C(8B)-C(7B)-C(6B)	118.1(4)
C(9B)-C(8B)-C(7B)	121.6(4)	C(8B)-C(9B)-C(10B)	118.4(4)
C(11B)-C(10B)-C(9B)	121.6(4)	C(11B)-C(10B)-Cl(1B)	119.5(3)
C(9B)-C(10B)-Cl(1B)	118.9(3)	C(10B)-C(11B)-C(12B)	118.6(4)
C(7B)-C(12B)-C(11B)	120.9(4)	N(5B)-C(6B)-C(7B)	115.1(4)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
O(12)	35(2)	38(2)	35(1)	5(1)	-3(1)	3(1)
O(11)	40(2)	41(2)	34(2)	17(1)	-1(1)	9(2)
C(1)	30(3)	27(2)	26(2)	-2(2)	5(2)	6(2)
C(2)	32(2)	28(2)	26(2)	10(1)	-1(2)	14(2)
C(3)	17(2)	26(2)	28(2)	2(1)	2(2)	4(2)
O(3)	35(1)	23(1)	45(1)	8(1)	0(1)	12(1)
C(4)	23(2)	26(2)	20(2)	2(1)	1(2)	14(2)
O(41)	26(2)	33(1)	43(2)	2(1)	-7(1)	-4(1)
O(42)	30(2)	30(1)	39(2)	16(1)	-4(1)	0(1)
C(7A)	25(2)	28(2)	26(2)	3(2)	-1(2)	-3(2)
C(8A)	43(3)	26(2)	33(2)	3(2)	1(2)	3(2)
C(9A)	44(3)	40(2)	24(2)	3(2)	-1(2)	-1(2)
C(10A)	39(3)	32(2)	36(2)	13(2)	-7(2)	3(2)
Cl(1A)	50(1)	49(1)	51(1)	17(1)	-21(1)	6(1)
C(11A)	41(3)	27(2)	33(2)	2(2)	-5(2)	4(2)
C(12A)	32(3)	32(2)	29(2)	1(2)	-9(2)	4(2)
C(6A)	27(2)	31(2)	33(2)	5(2)	-1(2)	5(2)
N(5A)	27(2)	27(2)	31(2)	8(1)	-4(2)	6(2)
C(7B)	29(3)	30(2)	29(2)	10(2)	4(2)	3(2)
C(8B)	36(3)	33(2)	27(2)	-1(2)	2(2)	3(2)
C(9B)	40(3)	37(2)	27(2)	4(2)	-7(2)	-3(2)
C(10B)	24(2)	34(2)	32(2)	14(2)	-2(2)	-4(2)
C(11B)	34(3)	32(2)	36(2)	4(2)	-6(2)	8(2)
C(12B)	40(3)	31(2)	26(2)	-1(2)	-3(2)	7(2)
C(6B)	37(3)	33(2)	30(2)	6(2)	4(2)	9(2)
N(5B)	35(2)	36(2)	32(2)	11(2)	-2(2)	9(2)
O(1W)	33(1)	48(2)	47(1)	19(1)	1(1)	4(1)
Cl(1B)	51(1)	49(1)	51(1)	17(1)	-20(1)	8(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(21)	-1058(9)	-6343(7)	-9861(2)	33
H(22)	886(9)	-4331(7)	-10165(2)	33
H(3)	-3758(8)	-4083(6)	-9156(2)	28
H(3O)	-207(6)	-721(4)	-9394(1)	40
H(8A)	-2971(10)	-6559(7)	-5796(2)	41
H(9A)	121(11)	-8553(8)	-5109(2)	44
H(11A)	-267(10)	-13760(7)	-6866(2)	41
H(12A)	-3377(9)	-11802(7)	-7552(2)	38
H(61A)	-5306(9)	-5930(7)	-7022(2)	36
H(62A)	-7590(9)	-8189(7)	-7033(2)	36
H(51A)	-7291(8)	-7444(6)	-8166(2)	34
H(52A)	-6446(8)	-9854(6)	-8098(2)	34
H(53A)	-4283(8)	-7857(6)	-8164(2)	34
H(8B)	-80(10)	-12373(7)	-3547(2)	39
H(9B)	-3311(10)	-10426(7)	-4213(2)	42
H(11B)	-2966(10)	-5333(7)	-2410(2)	41
H(12B)	281(10)	-7337(7)	-1764(2)	39
H(61B)	4442(10)	-11022(7)	-2419(2)	39
H(62B)	2208(10)	-13101(7)	-2426(2)	39
H(51B)	4285(9)	-11768(6)	-1188(2)	40
H(52B)	1115(9)	-11323(6)	-1164(2)	40
H(53B)	3393(9)	-9211(6)	-1236(2)	40
H(1W1)	-6268(9)	-8221(6)	-10002(2)	50
H(1W2)	-4812(9)	-9321(6)	-9601(2)	50

4CLB2MAL I-1235-6

perators for generating equivalent atoms:

1	x-1, y-1, z
2	x-1, y, z
3	x, y-1, z+1
4	x+1, y, z+1
5	x+1, y-1, z+1
6	x+1, y+1, z
7	x, y-1, z
8	x-1, y+1, z
9	x, y+1, z
10	x+1, y-1, z

elected torsion angles

95.75	(0.38)	O11 - C1 - C2 - C3
-82.71	(0.42)	O12 - C1 - C2 - C3
173.42	(0.37)	C1 - C2 - C3 - C4
-62.94	(0.37)	C1 - C2 - C3 - O3
89.45	(0.37)	C2 - C3 - C4 - O41
-86.86	(0.36)	C2 - C3 - C4 - O42
-33.86	(0.50)	O3 - C3 - C4 - O41
149.83	(0.31)	O3 - C3 - C4 - O42

istance N-N

2.814	(0.005)	N5A - O42
2.806	(0.004)	N5A - O41_$1
2.776	(0.005)	N5A - O42_$2
2.808	(0.005)	N5B - O11_$3
2.948	(0.005)	N5B - O12_$4
2.748	(0.005)	N5B - O11_$5

istance NH-N

1.905	(0.005)	H51A - O42
1.837	(0.004)	H52A - O41_$1
1.830	(0.005)	H53A - O42_$2
1.919	(0.005)	H51B - O11_$3
2.048	(0.005)	H52B - O12_$4
1.846	(0.005)	H53B - O11_$5

ngle NHN

158.20	(0.12)	N5A - H51A - O42
164.67	(0.13)	N5A - H52A - O41_$1
152.52	(0.13)	N5A - H53A - O42_$2
163.57	(0.14)	N5B - H51B - O11_$3
170.01	(0.14)	N5B - H52B - O12_$4
142.08	(0.15)	N5B - H53B - O11_$5

istance O-O

2.839	(0.005)	O3 - O1W_$6
2.882	(0.004)	O1W - O12
2.769	(0.005)	O1W - O3_$7

istance OH-O

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(1)

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    1.966 (0.005)  H3O - O1W_$6
    2.013 (0.004)  H1W1 - O12
    1.985 (0.004)  H1W2 - O3_$7


Angle OHO

  174.06 ( 0.13)  O3 - H3O - O1W_$6
  175.42 ( 0.15)  O1W - H1W1 - O12
  145.79 ( 0.14)  O1W - H1W2 - O3_$7


Distance C-CL

    4.140 (0.005)  C8A - Cl1A_$8
    3.689 (0.004)  C8A - Cl1A_$9
    4.109 (0.005)  C8B - Cl1B_$10
    3.682 (0.005)  C8B - Cl1B_$7


Distance H-CL

    3.270 (0.005)  H8A - Cl1A_$8
    3.229 (0.005)  H8A - Cl1A_$9
    3.221 (0.005)  H8B - Cl1B_$10
    3.285 (0.005)  H8B - Cl1B_$7


Angle CHCL

  151.59 ( 0.08)  C8A - H8A - Cl1A_$8
  111.39 ( 0.09)  C8A - H8A - Cl1A_$9
  154.61 ( 0.08)  C8B - H8B - Cl1B_$10
  106.97 ( 0.08)  C8B - H8B - Cl1B_$7
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Table 1. Crystal data and structure refinement for .2

Identification code	edammal
Empirical formula	$C_6H_{14}N_2O_5$
Formula weight	194.19
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 5.9800(10) Å α = 90° b = 8.5690(10) Å β = 90° c = 17.8770(10) Å γ = 90°
Volume	916.1(2) $Å^3$
Z	4
Density (calculated)	1.408 Mg/m^3
Absorption coefficient	0.122 mm^{-1}
F(000)	416
Crystal size	0.72 x 0.51 x 0.18 mm
θ range for data collection	2.28 to 24.98°
Index ranges	$-7 \le h \le 0$, $0 \le k \le 10$, $-21 \le \ell \le 21$
Reflections collected	1884
Independent reflections	1612 (R_{int} = 0.0109)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1612 / 0 / 118
Goodness-of-fit on F^2	1.077
Final R indices [I>2σ(I)]	R1 = 0.0316, wR2 = 0.0858
R indices (all data)	R1 = 0.0333, wR2 = 0.0872
Absolute structure parameter	−0.6(14)
Largest diff. peak and hole	0.348 and −0.273 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 2 U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(11)	9392(2)	11017(2)	721(1)	20(1)
O(12)	9020(2)	8458(2)	774(1)	21(1)
C(1)	8591(3)	9807(2)	1011(1)	14(1)
C(2)	7016(3)	10032(2)	1674(1)	17(1)
C(3)	5584(3)	8640(2)	1892(1)	16(1)
O(3)	4195(2)	8164(2)	1283(1)	20(1)
C(4)	4141(3)	9100(2)	2568(1)	16(1)
O(41)	2148(2)	9432(2)	2435(1)	27(1)
O(42)	5047(2)	9127(2)	3198(1)	19(1)
N(5)	9415(3)	8724(2)	3614(1)	16(1)
C(6)	9244(3)	9753(2)	4280(1)	17(1)
C(7)	11311(3)	9744(2)	4763(1)	17(1)
N(8)	13171(3)	10687(2)	4447(1)	15(1)

Table 3. Bond lengths [Å] and angles [°] for 2

O(11)-C(1)	1.253(2)	O(12)-C(1)	1.258(2)
C(1)-C(2)	1.528(3)	C(2)-C(3)	1.518(3)
C(3)-O(3)	1.428(2)	C(3)-C(4)	1.537(3)
C(4)-O(41)	1.248(2)	C(4)-O(42)	1.251(2)
N(5)-C(6)	1.486(2)	C(6)-C(7)	1.508(3)
C(7)-N(8)	1.487(2)		

O(11)-C(1)-O(12)	122.9(2)	O(11)-C(1)-C(2)	116.9(2)
O(12)-C(1)-C(2)	120.2(2)	C(3)-C(2)-C(1)	116.6(2)
O(3)-C(3)-C(2)	111.0(2)	O(3)-C(3)-C(4)	110.2(2)
C(2)-C(3)-C(4)	108.4(2)	O(41)-C(4)-O(42)	125.5(2)
O(41)-C(4)-C(3)	116.4(2)	O(42)-C(4)-C(3)	118.0(2)
N(5)-C(6)-C(7)	113.6(2)	N(8)-C(7)-C(6)	113.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 2

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(11)	24(1)	18(1)	19(1)	2(1)	6(1)	-4(1)
O(12)	21(1)	18(1)	26(1)	-5(1)	10(1)	-1(1)
C(1)	11(1)	20(1)	13(1)	-1(1)	-2(1)	-1(1)
C(2)	16(1)	19(1)	14(1)	-4(1)	2(1)	-1(1)
C(3)	15(1)	20(1)	13(1)	-2(1)	0(1)	1(1)
O(3)	15(1)	29(1)	16(1)	-4(1)	-1(1)	-1(1)
C(4)	15(1)	20(1)	14(1)	0(1)	1(1)	-1(1)
O(41)	14(1)	50(1)	17(1)	4(1)	3(1)	6(1)
O(42)	15(1)	29(1)	14(1)	-3(1)	1(1)	1(1)
N(5)	13(1)	20(1)	14(1)	-2(1)	0(1)	1(1)
C(6)	15(1)	18(1)	17(1)	-2(1)	3(1)	2(1)
C(7)	20(1)	20(1)	12(1)	0(1)	0(1)	-2(1)
N(8)	13(1)	17(1)	15(1)	-1(1)	0(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 \times 10^3$) for 2

	x	y	z	U(eq)
H(21)	6100(3)	10953(2)	1591(1)	20
H(22)	7881(3)	10284(2)	1978(1)	20
H(3)	6625(3)	7735(2)	1982(1)	19
H(30)	2851(2)	8405(2)	1418(1)	24
H(51)	10653(3)	9102(2)	3330(1)	23
H(52)	9748(3)	7701(2)	3602(1)	23
H(53)	8094(3)	8721(2)	3386(1)	23
H(61)	8861(3)	10671(2)	4188(1)	20
H(62)	8164(3)	9359(2)	4582(1)	20
H(71)	10956(3)	10215(2)	5206(1)	21
H(72)	11810(3)	8672(2)	4819(1)	21
H(81)	14140(3)	10835(2)	4808(1)	23
H(82)	12790(3)	11531(2)	4423(1)	23
H(83)	13857(3)	10286(2)	4013(1)	23

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(2)

ED AMMVAL

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Operators for generating equivalent atoms:

$1 x+1, y, z
$2 -x+2, y-1/2, -z+1/2
$3 -x+5/2, -y+2, z+1/2
$4 -x+2, y+1/2, -z+1/2

Selected torsion angles

164.34 (0.16) O11 - C1 - C2 - C3
-15.11 (0.26) O12 - C1 - C2 - C3
179.71 (0.15) C1 - C2 - C3 - C4
-59.11 (0.20) C1 - C2 - C3 - O3
101.51 (0.19) C2 - C3 - C4 - O41
-77.80 (0.21) C2 - C3 - C4 - O42
-20.13 (0.23) O3 - C3 - C4 - O41
160.56 (0.16) O3 - C3 - C4 - O42

Distance N-O

2.735 (0.002) N5 - O41_$1
2.702 (0.002) N5 - O11_$2
2.737 (0.002) N5 - O42
2.997 (0.002) N8 - O12_$3
2.740 (0.002) N8 - O12_$4
2.834 (0.002) N8 - O42_$1

Distance NH-O

1.854 (0.002) H51 - O41_$1
1.952 (0.002) H52 - O11_$2
1.885 (0.002) H53 - O42
2.135 (0.002) H81 - O12_$3
2.005 (0.002) H82 - O12_$4
1.901 (0.002) H83 - O42_$1

Angle NHO

152.21 (0.06) N5 - H51 - O41_$1
139.92 (0.06) N5 - H52 - O11_$2
160.05 (0.06) N5 - H53 - O42
167.72 (0.06) N8 - H81 - O12_$3
162.92 (0.06) N8 - H82 - O12_$4
169.73 (0.06) N8 - H83 - O42_$1

Distance O-O

2.630 (0.002) O3 - O41

Distance OH-O

2.063 (0.002) H3O - O41

Angle OHO

122.54 (0.06) O3 - H3O - O41

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Table 1. Crystal data and structure refinement for 3

Identification code	pipmal
Empirical formula	$C_8H_{18}N_2O_6$
Formula weight	238.24
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 6.7110(10) Å $\alpha = 90^\circ$ b = 10.4370(10) Å $\beta = 90^\circ$ c = 15.577(2) Å $\gamma = 90^\circ$
Volume	1091.1(2) $Å^3$
Z	4
Density (calculated)	1.450 Mg/m^3
Absorption coefficient	0.124 mm^{-1}
F(000)	512
Crystal size	0.64 x 0.54 x 0.32 mm
θ range for data collection	2.35 to 24.99°
Index ranges	$-7 \le h \le 7$, $0 \le k \le 12$, $0 \le \ell \le 18$
Reflections collected	2084
Independent reflections	1912 (R_{int} = 0.0173)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1912 / 0 / 145
Goodness-of-fit on F^2	1.104
Final R indices [$I>2\sigma(I)$]	R1 = 0.0299, wR2 = 0.0804
R indices (all data)	R1 = 0.0313, wR2 = 0.0819
Absolute structure parameter	−0.6(11)
Largest diff. peak and hole	0.204 and −0.288 $eÅ^{-3}$

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 3 U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(11)	4848(2)	41(1)	6441(1)	22(1)
O(12)	4095(2)	1956(1)	5925(1)	16(1)
C(1)	3936(3)	1075(2)	6490(1)	13(1)
C(2)	2542(3)	1316(2)	7244(1)	14(1)
C(3)	2891(3)	2637(2)	7636(1)	13(1)
O(3)	4925(2)	2705(1)	7861(1)	16(1)
C(4)	1496(3)	2827(2)	8408(1)	13(1)
O(41)	2117(2)	2445(1)	9134(1)	15(1)
O(42)	-161(2)	3334(1)	8277(1)	18(1)
N(5)	9495(2)	-1167(1)	4549(1)	12(1)
C(6)	7827(3)	-821(2)	3964(1)	16(1)
C(7)	6262(3)	-75(2)	4453(1)	15(1)
N(8)	7137(2)	1081(1)	4878(1)	14(1)
C(9)	8874(3)	746(2)	5436(1)	14(1)
C(10)	10428(3)	-4(2)	4935(1)	15(1)
O(1W)	-1837(2)	3263(1)	6648(1)	20(1)

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

O(11)-C(1)	1.243(2)	O(12)-C(1)	1.278(2)
C(1)-C(2)	1.522(2)	C(2)-C(3)	1.526(2)
C(3)-O(3)	1.411(2)	C(3)-C(4)	1.536(2)
C(4)-O(42)	1.248(2)	C(4)-O(41)	1.270(2)
N(5)-C(6)	1.488(2)	N(5)-C(10)	1.493(2)
C(6)-C(7)	1.513(3)	C(7)-N(8)	1.497(2)
N(8)-C(9)	1.495(2)	C(9)-C(10)	1.520(3)

O(11)-C(1)-O(12)	122.8(2)	O(11)-C(1)-C(2)	119.6(2)
O(12)-C(1)-C(2)	117.7(2)	C(1)-C(2)-C(3)	111.35(14)
O(3)-C(3)-C(2)	107.0(2)	O(3)-C(3)-C(4)	112.91(14)
C(2)-C(3)-C(4)	109.68(14)	O(42)-C(4)-O(41)	124.8(2)
O(42)-C(4)-C(3)	118.1(2)	O(41)-C(4)-C(3)	117.1(2)
C(6)-N(5)-C(10)	111.39(14)	N(5)-C(6)-C(7)	109.80(14)
N(8)-C(7)-C(6)	111.4(2)	C(9)-N(8)-C(7)	112.05(14)
N(8)-C(9)-C(10)	110.87(14)	N(5)-C(10)-C(9)	109.75(14)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 3

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(11)	25(1)	14(1)	27(1)	6(1)	10(1)	8(1)
O(12)	20(1)	14(1)	14(1)	4(1)	3(1)	5(1)
C(1)	12(1)	14(1)	14(1)	-2(1)	-2(1)	1(1)
C(2)	17(1)	11(1)	13(1)	0(1)	1(1)	-2(1)
C(3)	14(1)	12(1)	14(1)	1(1)	0(1)	0(1)
O(3)	14(1)	16(1)	19(1)	-5(1)	1(1)	-2(1)
C(4)	15(1)	9(1)	13(1)	-2(1)	-1(1)	-1(1)
O(41)	16(1)	16(1)	13(1)	0(1)	2(1)	4(1)
O(42)	14(1)	22(1)	16(1)	-1(1)	-1(1)	5(1)
N(5)	12(1)	11(1)	14(1)	2(1)	3(1)	2(1)
C(6)	18(1)	16(1)	14(1)	1(1)	-2(1)	1(1)
C(7)	14(1)	14(1)	18(1)	1(1)	0(1)	-2(1)
N(8)	15(1)	12(1)	14(1)	1(1)	3(1)	3(1)
C(9)	17(1)	10(1)	15(1)	1(1)	0(1)	-2(1)
C(10)	12(1)	16(1)	17(1)	1(1)	0(1)	-2(1)
O(1W)	19(1)	24(1)	16(1)	1(1)	2(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 \times 10^3$) for 3

	x	y	z	U(eq)
H(21)	2617(3)	765(2)	7624(1)	16
H(22)	1083(3)	1227(2)	7015(1)	16
H(3)	2451(3)	3275(2)	7224(1)	16
H(30)	5121(2)	3454(1)	8200(1)	20
H(51)	9051(2)	-1693(1)	4982(1)	15
H(52)	10428(2)	-1628(1)	4395(1)	15
H(61)	7282(3)	-1634(2)	3777(1)	19
H(62)	8382(3)	-383(2)	3580(1)	19
H(71)	5271(3)	221(2)	3998(1)	18
H(72)	5724(3)	-575(2)	4793(1)	18
H(81)	7548(2)	1672(1)	4372(1)	16
H(82)	6217(2)	1397(1)	5183(1)	16
H(91)	8362(3)	247(2)	5780(1)	17
H(92)	9431(3)	1457(2)	5587(1)	17
H(101)	11013(3)	464(2)	4411(1)	18
H(102)	11533(3)	-336(2)	5213(1)	18
H(1W1)	-1375(2)	3283(1)	7182(1)	24
H(1W2)	-2882(2)	2951(1)	6778(1)	24

(3)

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Operators for generating equivalent atoms:

$1 -x+1, y-1/2, -z+3/2
$2 -x+3/2, -y, z-1/2
$3 x+1/2, -y+1/2, -z+1
$4 x-1, y, z
$5 -x+1, y+1/2, -z+3/2

Selected torsion angles

133.16 (0.18) O11 - C1 - C2 - C3
-47.60 (0.21) O12 - C1 - C2 - C3
-178.54 (0.14) C1 - C2 - C3 - C4
-55.74 (0.18) C1 - C2 - C3 - O3
87.94 (0.19) C2 - C3 - C4 - O41
-91.57 (0.18) C2 - C3 - C4 - O42
-31.32 (0.22) O3 - C3 - C4 - O41
149.18 (0.16) O3 - C3 - C4 - O42

Distance N-N

2.734 (0.002) N5 - O41_$1
2.715 (0.002) N5 - O41_$2
2.737 (0.002) N8 - O12_$3
2.768 (0.002) N8 - O12

Distance NH-N

1.822 (0.002) H51 - O41_$1
1.900 (0.002) H52 - O41_$2
1.828 (0.002) H81 - O12_$3
1.925 (0.002) H82 - O12

Angle NHN

171.43 (0.06) N5 - H51 - O41_$1
169.19 (0.06) N5 - H52 - O41_$2
143.87 (0.06) N8 - H81 - O12_$3
174.51 (0.06) N8 - H82 - O12

Distance O-O

2.777 (0.002) O1W - O42
2.938 (0.002) O1W - O3_$4
2.674 (0.002) O3 - O11_$5

Distance OH-O

1.891 (0.002) H1W1 - O42
2.253 (0.002) H1W2 - O3_$4
1.748 (0.002) H3O - O11_$5

Angle OHO

174.85 (0.06) O1W - H1W1 - O42
144.03 (0.05) O1W - H1W2 - O3_$4
163.07 (0.06) O3 - H3O - O11_$5

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Table 1. Crystal data and structure refinement for 4

Identification code	3mebzmal
Empirical formula	$C_{20}H_{28}N_2O_5$
Formula weight	376.44
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 10.011(2) Å α = 90° b = 8.381(2) Å β = 107.27(2)° c = 12.779(4) Å γ = 90°
Volume	1023.8(5) $Å^3$
Z	2
Density (calculated)	1.221 Mg/m^3
Absorption coefficient	0.088 mm^{-1}
F(000)	404
Crystal size	0.61 x 0.36 x 0.33 mm
θ range for data collection	1.67 to 25.00°
Index ranges	$-11 \le h \le 3$, $-1 \le k \le 9$, $-15 \le \ell \le 14$
Reflections collected	2872
Independent reflections	2191 (R_{int} = 0.0206)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2191 / 1 / 244
Goodness-of-fit on F^2	1.108
Final R indices [I>2σ(I)]	R1 = 0.0387, wR2 = 0.1119
R indices (all data)	R1 = 0.0449, wR2 = 0.1252
Absolute structure parameter	-1(2)
Largest diff. peak and hole	0.575 and -0.203 $eÅ^{-3}$

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for ⅓U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(11)	5226(2)	2100(3)	5870(2)	25(1)
O(12)	4460(2)	2394(3)	7327(2)	26(1)
C(1)	4920(3)	1548(4)	6695(2)	20(1)
C(2)	5087(4)	-249(4)	6901(3)	22(1)
C(3)	5076(3)	-702(4)	8044(3)	19(1)
O(3)	3795(2)	-316(3)	8250(2)	32(1)
C(4)	5388(3)	-2464(4)	8322(2)	18(1)
O(41)	5143(2)	-2955(3)	9193(2)	25(1)
O(42)	5882(2)	-3313(3)	7729(2)	23(1)
N(5A)	5660(3)	307(4)	4202(2)	22(1)
C(6A)	7097(3)	474(5)	4105(3)	28(1)
C(7A)	8213(3)	-198(5)	5085(3)	28(1)
C(8A)	8073(4)	-1674(5)	5522(3)	28(1)
C(9A)	9152(4)	-2347(6)	6371(3)	35(1)
C(91A)	8958(5)	-3916(6)	6842(4)	52(1)
C(10A)	10397(4)	-1484(7)	6755(3)	45(1)
C(11A)	10538(4)	-2(7)	6328(3)	47(1)
C(12A)	9457(4)	659(6)	5506(3)	38(1)
N(5B)	4169(3)	-1111(3)	10614(2)	20(1)
C(6B)	2610(3)	-1177(4)	10327(3)	26(1)
C(7B)	2115(3)	-2863(4)	10373(3)	23(1)
C(8B)	2146(3)	-3944(5)	9561(3)	24(1)
C(9B)	1738(3)	-5531(5)	9601(3)	27(1)
C(91B)	1828(4)	-6701(5)	8742(3)	36(1)
C(10B)	1277(3)	-6010(5)	10488(3)	32(1)
C(11B)	1240(4)	-4940(5)	11302(3)	35(1)
C(12B)	1660(3)	-3355(5)	11251(3)	30(1)

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Table 3. Bond lengths [Å] and angles [°] for 4

O(11)-C(1)	1.269(4)	O(12)-C(1)	1.260(4)
C(1)-C(2)	1.530(5)	C(2)-C(3)	1.512(4)
C(3)-O(3)	1.420(4)	C(3)-C(4)	1.528(5)
C(4)-O(42)	1.245(4)	C(4)-O(41)	1.277(4)
N(5A)-C(6A)	1.486(4)	C(6A)-C(7A)	1.517(5)
C(7A)-C(8A)	1.382(6)	C(7A)-C(12A)	1.400(5)
C(8A)-C(9A)	1.402(5)	C(9A)-C(10A)	1.398(6)
C(9A)-C(91A)	1.483(7)	C(10A)-C(11A)	1.381(8)
C(11A)-C(12A)	1.380(6)	N(5B)-C(6B)	1.495(4)
C(6B)-C(7B)	1.504(5)	C(7B)-C(8B)	1.385(5)
C(7B)-C(12B)	1.393(5)	C(8B)-C(9B)	1.397(5)
C(9B)-C(10B)	1.404(5)	C(9B)-C(91B)	1.494(5)
C(10B)-C(11B)	1.381(6)	C(11B)-C(12B)	1.401(6)

O(12)-C(1)-O(11)	123.5(3)	O(12)-C(1)-C(2)	119.0(3)
O(11)-C(1)-C(2)	117.4(3)	C(3)-C(2)-C(1)	112.5(3)
O(3)-C(3)-C(2)	112.8(3)	O(3)-C(3)-C(4)	108.1(3)
C(2)-C(3)-C(4)	114.0(3)	O(42)-C(4)-O(41)	124.1(3)
O(42)-C(4)-C(3)	120.1(3)	O(41)-C(4)-C(3)	115.8(3)
N(5A)-C(6A)-C(7A)	113.0(3)	C(8A)-C(7A)-C(12A)	119.3(3)
C(8A)-C(7A)-C(6A)	121.9(3)	C(12A)-C(7A)-C(6A)	118.7(4)
C(7A)-C(8A)-C(9A)	121.7(4)	C(10A)-C(9A)-C(8A)	117.8(4)
C(10A)-C(9A)-C(91A)	121.7(4)	C(8A)-C(9A)-C(91A)	120.5(4)
C(11A)-C(10A)-C(9A)	120.8(4)	C(12A)-C(11A)-C(10A)	120.8(4)
C(11A)-C(12A)-C(7A)	119.6(4)	N(5B)-C(6B)-C(7B)	110.9(3)
C(8B)-C(7B)-C(12B)	119.7(4)	C(8B)-C(7B)-C(6B)	120.3(3)
C(12B)-C(7B)-C(6B)	120.0(3)	C(7B)-C(8B)-C(9B)	121.6(3)
C(8B)-C(9B)-C(10B)	118.1(4)	C(8B)-C(9B)-C(91B)	121.0(3)
C(10B)-C(9B)-C(91B)	120.8(4)	C(11B)-C(10B)-C(9B)	120.7(4)
C(10B)-C(11B)-C(12B)	120.4(3)	C(7B)-C(12B)-C(11B)	119.5(4)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 4

The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
O(11)	38(1)	20(1)	21(1)	0(1)	13(1)	1(1)
O(12)	40(1)	20(1)	19(1)	-2(1)	12(1)	6(1)
C(1)	24(2)	17(2)	15(1)	-1(1)	1(1)	-2(1)
C(2)	33(2)	16(2)	19(2)	-1(1)	10(1)	1(2)
C(3)	21(2)	18(2)	18(1)	-4(1)	6(1)	0(1)
O(3)	30(1)	31(2)	39(1)	9(1)	16(1)	2(1)
C(4)	17(1)	19(2)	16(1)	-2(1)	1(1)	-3(1)
O(41)	37(1)	16(1)	27(1)	1(1)	18(1)	2(1)
O(42)	31(1)	20(1)	20(1)	-2(1)	9(1)	3(1)
N(5A)	29(1)	20(2)	15(1)	-1(1)	4(1)	0(1)
C(6A)	30(2)	30(2)	26(2)	3(2)	11(1)	0(2)
C(7A)	28(2)	38(2)	19(2)	-6(2)	11(1)	1(2)
C(8A)	29(2)	34(2)	23(2)	-2(2)	7(1)	6(2)
C(9A)	35(2)	47(3)	25(2)	-3(2)	12(1)	16(2)
C(91A)	57(3)	49(3)	47(2)	10(2)	11(2)	22(2)
C(10A)	29(2)	79(4)	24(2)	-6(2)	5(1)	15(2)
C(11A)	30(2)	81(4)	32(2)	-11(2)	13(2)	-12(2)
C(12A)	30(2)	57(3)	30(2)	-9(2)	12(2)	-10(2)
N(5B)	29(1)	14(1)	19(1)	1(1)	10(1)	0(1)
C(6B)	27(2)	21(2)	30(2)	4(2)	6(1)	5(2)
C(7B)	17(2)	24(2)	28(2)	9(2)	5(1)	5(1)
C(8B)	17(2)	27(2)	24(2)	6(2)	1(1)	1(1)
C(9B)	18(2)	27(2)	32(2)	4(2)	1(1)	-1(2)
C(91B)	38(2)	22(2)	44(2)	-3(2)	4(2)	-3(2)
C(10B)	19(2)	27(2)	46(2)	11(2)	6(2)	-5(2)
C(11B)	25(2)	42(2)	41(2)	15(2)	15(2)	-4(2)
C(12B)	22(2)	37(2)	32(2)	5(2)	10(1)	6(2)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 4

	x	y	z	U(eq)
H(22)	4333(4)	-791(4)	6380(3)	27
H(21)	5971(4)	-553(4)	6773(3)	27
H(3)	5801(3)	-14(4)	8600(3)	23
H(3O)	3611(2)	768(3)	8060(2)	39
H(53A)	5218(3)	720(4)	3632(2)	32
H(52A)	5619(3)	765(4)	4808(2)	32
H(51A)	5382(3)	-721(4)	4169(2)	32
H(62A)	7407(3)	1690(5)	4057(3)	34
H(61A)	6989(3)	-107(5)	3420(3)	34
H(8A)	7191(4)	-2453(5)	5212(3)	34
H(93A)	9817(5)	-4245(6)	7366(4)	78
H(92A)	8616(5)	-4681(6)	6431(4)	78
H(91A)	8205(5)	-3916(6)	7189(4)	78
H(10A)	11181(4)	-1931(7)	7389(3)	54
H(11A)	11400(4)	693(7)	6581(3)	56
H(12A)	9613(4)	1771(6)	5137(3)	46
H(53B)	4366(3)	-1511(3)	11231(2)	30
H(52B)	4360(3)	-94(3)	10675(2)	30
H(51B)	4567(3)	-1576(3)	10203(2)	30
H(62B)	2170(3)	-786(4)	9589(3)	32
H(61B)	2367(3)	-494(4)	10807(3)	32
H(8B)	2583(3)	-3634(5)	8950(3)	28
H(93B)	1996(4)	-7781(5)	8997(3)	55
H(92B)	2404(4)	-6341(5)	8213(3)	55
H(91B)	1204(4)	-6588(5)	7892(3)	55
H(10B)	1021(3)	-7152(5)	10501(3)	38
H(11B)	1019(4)	-5324(5)	11972(3)	42
H(12B)	1775(3)	-2570(5)	11826(3)	36

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3MeBzMAL I-1235-21

(4)

Operators for generating equivalent atoms:

$1 -x+1, y+1/2, -z+1
$2 -x+1, y-1/2, -z+1
$3 -x+1, y-1/2, -z+2
$4 -x+1, y+1/2, -z+2

Selected torsion angles

164.54	(0.26)	O11 - C1 - C2 - C3
-17.16	(0.44)	O12 - C1 - C2 - C3
-174.15	(0.28)	C1 - C2 - C3 - C4
62.11	(0.38)	C1 - C2 - C3 - O3
-167.88	(0.27)	C2 - C3 - C4 - O41
13.89	(0.41)	C2 - C3 - C4 - O42
-41.64	(0.35)	O3 - C3 - C4 - O41
140.13	(0.29)	O3 - C3 - C4 - O42

Distance N-O

2.748	(0.003)	N5A - O42_$1
2.745	(0.003)	N5A - O11
2.824	(0.004)	N5A - O11_$2
2.869	(0.004)	N5B - O12_$3
2.726	(0.004)	N5B - O41_$4
2.773	(0.003)	N5B - O41

Distance NH-O

1.938	(0.003)	H53A - O42_$1
1.889	(0.003)	H52A - O11
1.921	(0.004)	H51A - O11_$2
2.081	(0.003)	H53B - O12_$3
1.855	(0.004)	H52B - O41_$4
1.943	(0.003)	H51B - O41

Angle NHO

178.59	(0.11)	N5A - H53A - O42_$1
165.79	(0.11)	N5A - H52A - O11
178.49	(0.10)	N5A - H51A - O11_$2
159.57	(0.09)	N5B - H53B - O12_$3
177.15	(0.10)	N5B - H52B - O41_$4
167.75	(0.11)	N5B - H51B - O41

Distance O-O

2.731	(0.004)	O3 - O12

Distance OH-O

1.982	(0.003)	H3O - O12

Angle OHO

134.77	(0.10)	O3 - H3O - O12

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Table 1. Crystal data and structure refinement for 5

Identification code	bz3clmal
Empirical formula	$C_{18}H_{24}Cl_2N_2O_6$
Formula weight	435.29
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 4.8460(10) Å α = 90° b = 35.267(6) Å β = 95.69(2)° c = 5.7530(10) Å γ = 90°
Volume	978.4(3) $Å^3$
Z	2
Density (calculated)	1.478 Mg/m^3
Absorption coefficient	0.370 mm^{-1}
F(000)	456
Crystal size	0.88 x 0.18 x 0.16 mm
θ range for data collection	2.31 to 24.99°
Index ranges	$0 \le h \le 5$, $0 \le k \le 41$, $-6 \le \ell \le 6$
Reflections collected	1952
Independent reflections	1748 (R_{int} = 0.0278)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1748 / 1 / 253
Goodness-of-fit on F^2	1.056
Final R indices [$I>2\sigma(I)$]	R1 = 0.0423, wR2 = 0.0811
R indices (all data)	R1 = 0.0715, wR2 = 0.0939
Absolute structure parameter	0.0(2)
Largest diff. peak and hole	0.180 and −0.185 $eÅ^{-3}$

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(11)	3038(12)	4586(2)	5513(10)	39(2)
O(12)	5897(13)	4442(1)	8635(10)	40(1)
C(1)	3710(17)	4385(2)	7310(13)	28(2)
C(2)	1886(16)	4061(2)	7856(14)	32(2)
C(3)	2915(16)	3690(2)	6881(12)	24(2)
O(3)	2820(8)	3695(1)	4394(6)	37(1)
C(4)	1109(15)	3363(2)	7692(13)	23(2)
O(41)	-1036(11)	3268(2)	6477(9)	38(1)
O(42)	1892(11)	3226(2)	9687(9)	32(1)
N(5A)	7196(14)	3058(2)	1901(10)	29(2)
C(6A)	7111(18)	2640(2)	1681(15)	29(2)
C(7A)	5046(17)	2446(2)	3024(13)	24(2)
C(8A)	4031(17)	2095(2)	2278(13)	29(2)
C(9A)	2217(19)	1904(2)	3534(15)	34(2)
Cl(9A)	862(6)	1473(1)	2466(4)	54(1)
C(10A)	1325(18)	2049(3)	5537(16)	39(2)
C(11A)	2295(20)	2401(2)	6316(15)	36(2)
C(12A)	4139(17)	2601(2)	5054(13)	31(2)
N(5B)	2276(16)	-253(2)	-3355(12)	36(2)
C(6B)	2234(20)	168(2)	-3508(15)	36(2)
C(7B)	127(18)	347(2)	-2063(14)	30(2)
C(8B)	-903(17)	702(3)	-2799(15)	35(2)
C(9B)	-2787(18)	886(2)	-1504(14)	33(2)
Cl(9B)	-4189(6)	1316(1)	-2506(4)	53(1)
C(10B)	-3617(18)	727(2)	541(16)	37(2)
C(11B)	-2582(21)	374(2)	1214(15)	38(2)
C(12B)	-719(18)	190(2)	-52(14)	35(2)
O(1W)	7523(17)	3912(2)	2318(13)	47(1)

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Table 3. Bond lengths [Å] and angles [°] for 5

O(11)-C(1)	1.269(9)	O(12)-C(1)	1.259(9)
C(1)-C(2)	1.496(11)	C(2)-C(3)	1.526(7)
C(3)-O(3)	1.427(7)	C(3)-C(4)	1.549(10)
C(4)-O(41)	1.240(9)	C(4)-O(42)	1.268(9)
N(5A)-C(6A)	1.480(9)	C(6A)-C(7A)	1.490(11)
C(7A)-C(8A)	1.384(11)	C(7A)-C(12A)	1.400(10)
C(8A)-C(9A)	1.369(11)	C(9A)-C(10A)	1.369(12)
C(9A)-Cl(9A)	1.743(8)	C(10A)-C(11A)	1.386(12)
C(11A)-C(12A)	1.398(12)	N(5B)-C(6B)	1.485(9)
C(6B)-C(7B)	1.517(12)	C(7B)-C(12B)	1.381(11)
C(7B)-C(8B)	1.397(12)	C(8B)-C(9B)	1.395(12)
C(9B)-C(10B)	1.398(12)	C(9B)-Cl(9B)	1.737(9)
C(10B)-C(11B)	1.384(12)	C(11B)-C(12B)	1.377(13)

O(12)-C(1)-O(11)	122.4(8)	O(12)-C(1)-C(2)	118.4(7)
O(11)-C(1)-C(2)	119.2(7)	C(1)-C(2)-C(3)	110.8(5)
O(3)-C(3)-C(2)	112.3(4)	O(3)-C(3)-C(4)	110.3(6)
C(2)-C(3)-C(4)	108.2(5)	O(41)-C(4)-O(42)	124.5(7)
O(41)-C(4)-C(3)	119.9(7)	O(42)-C(4)-C(3)	115.5(6)
N(5A)-C(6A)-C(7A)	115.3(7)	C(8A)-C(7A)-C(12A)	118.6(7)
C(8A)-C(7A)-C(6A)	119.1(7)	C(12A)-C(7A)-C(6A)	122.3(7)
C(9A)-C(8A)-C(7A)	120.2(7)	C(10A)-C(9A)-C(8A)	122.2(8)
C(10A)-C(9A)-Cl(9A)	118.9(7)	C(8A)-C(9A)-Cl(9A)	118.8(7)
C(9A)-C(10A)-C(11A)	118.8(8)	C(10A)-C(11A)-C(12A)	119.9(8)
C(11A)-C(12A)-C(7A)	120.3(8)	N(5B)-C(6B)-C(7B)	112.9(7)
C(12B)-C(7B)-C(8B)	119.1(8)	C(12B)-C(7B)-C(6B)	124.3(8)
C(8B)-C(7B)-C(6B)	116.5(7)	C(9B)-C(8B)-C(7B)	119.2(8)
C(8B)-C(9B)-C(10B)	121.4(8)	C(8B)-C(9B)-Cl(9B)	119.0(7)
C(10B)-C(9B)-Cl(9B)	119.6(6)	C(11B)-C(10B)-C(9B)	118.0(8)
C(12B)-C(11B)-C(10B)	120.9(8)	C(11B)-C(12B)-C(7B)	121.2(8)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 5

The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
O(11)	43(4)	39(3)	34(3)	10(3)	-2(3)	-4(3)
O(12)	37(3)	33(3)	49(3)	-1(2)	2(3)	-7(2)
C(1)	30(4)	27(4)	27(4)	-6(3)	2(4)	3(3)
C(2)	20(4)	44(4)	33(4)	5(4)	11(3)	-4(3)
C(3)	30(4)	21(3)	21(3)	3(3)	0(3)	2(3)
O(3)	41(2)	45(3)	26(2)	2(2)	7(2)	-5(2)
C(4)	18(4)	24(4)	28(4)	-3(3)	10(3)	-3(3)
O(41)	26(3)	49(3)	35(3)	1(2)	-9(2)	-13(2)
O(42)	30(3)	34(3)	33(3)	10(3)	3(2)	-5(3)
N(5A)	29(4)	31(4)	27(3)	8(3)	5(3)	-4(3)
C(6A)	25(4)	32(5)	31(4)	-1(3)	4(3)	5(4)
C(7A)	19(4)	32(5)	20(4)	4(3)	0(3)	0(3)
C(8A)	37(5)	20(4)	29(4)	-1(3)	-1(4)	4(4)
C(9A)	45(5)	15(4)	41(5)	1(4)	-8(4)	-8(4)
Cl(9A)	66(2)	33(1)	62(2)	-7(1)	0(1)	-18(1)
C(10A)	42(6)	37(6)	38(5)	6(4)	1(5)	-5(4)
C(11A)	38(5)	41(5)	30(5)	-3(4)	5(4)	-11(4)
C(12A)	34(5)	30(5)	30(4)	-2(4)	8(4)	-7(4)
N(5B)	39(4)	31(4)	37(4)	0(3)	6(3)	7(3)
C(6B)	40(5)	36(5)	32(4)	-3(4)	7(4)	9(4)
C(7B)	28(4)	28(5)	33(5)	0(4)	-2(4)	-2(4)
C(8B)	35(5)	37(5)	33(5)	-1(4)	3(4)	-3(4)
C(9B)	29(5)	35(5)	34(5)	0(4)	-5(4)	-2(4)
Cl(9B)	60(2)	34(1)	63(2)	6(1)	3(1)	15(1)
C(10B)	39(6)	36(6)	36(5)	-12(4)	4(5)	4(4)
C(11B)	47(5)	36(5)	34(5)	-1(4)	12(5)	-2(5)
C(12B)	43(5)	25(5)	37(5)	4(4)	5(4)	6(4)
O(1W)	37(2)	54(2)	50(3)	13(2)	6(2)	-1(2)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5

	x	y	z	U(eq)
H(21)	-92(16)	4122(2)	7196(14)	48
H(22)	1526(16)	4068(2)	9586(14)	48
H(3)	5189(16)	3663(2)	7808(12)	37
H(3O)	1204(8)	3691(1)	3797(6)	56
H(51A)	8721(14)	3134(2)	1062(10)	43
H(52A)	5728(14)	3200(2)	1250(10)	43
H(53A)	7900(14)	3104(2)	3651(10)	43
H(61A)	6770(18)	2599(2)	45(15)	44
H(62A)	8983(18)	2534(2)	2051(15)	44
H(8A)	4687(17)	1967(2)	828(13)	43
H(10A)	35(18)	1937(3)	6569(16)	59
H(11A)	1537(20)	2536(2)	7811(15)	54
H(12A)	4808(17)	2851(2)	5631(13)	47
H(51B)	3768(16)	-370(2)	-4231(12)	54
H(52B)	2684(16)	-333(2)	-1633(12)	54
H(53B)	518(16)	-360(2)	-3839(12)	54
H(61B)	1725(20)	224(2)	-5177(15)	54
H(62B)	4097(20)	220(2)	-2372(15)	54
H(8B)	-275(17)	807(3)	-4126(15)	53
H(10B)	-5036(18)	866(2)	1396(16)	55
H(11B)	-3339(21)	276(2)	2779(15)	58
H(12B)	-21(18)	-64(2)	400(14)	52
H(1W1)	5750(17)	3873(2)	3002(13)	70
H(1W2)	6581(17)	4073(2)	1202(13)	70

(3)

perators for generating equivalent atoms for bz3clmal:

1 x+1, y, z-1
2 x, y, z-1
3 x+1, y, z
4 -x+1, y-1/2, -z
5 -x+1, y-1/2, -z+1
6 -x, y-1/2, -z
7 x-1, y, z
8 x, y, z+1
9 x+1, y, z+1

elected torsion angles

95.12	(0.75)	O11 - C1 - C2 - C3
-83.45	(0.80)	O12 - C1 - C2 - C3
174.96	(0.83)	C1 - C2 - C3 - C4
-62.97	(0.69)	C1 - C2 - C3 - O3
89.75	(0.71)	C2 - C3 - C4 - O41
-85.92	(0.70)	C2 - C3 - C4 - O42
-33.54	(0.93)	O3 - C3 - C4 - O41
150.79	(0.60)	O3 - C3 - C4 - O42

istance N-O

2.779	(0.009)	N5A - O42_$1
2.816	(0.009)	N5A - O42_$2
2.787	(0.008)	N5A - O41_$3
2.754	(0.010)	N5B - O11_$4
2.973	(0.009)	N5B - O12_$5
2.804	(0.010)	N5B - O11_$6

istance NH-O

1.826	(0.009)	H51A - O42_$1
1.986	(0.009)	H52A - O42_$2
1.754	(0.008)	H53A - O41_$3
1.786	(0.010)	H51B - O11_$4
1.960	(0.009)	H52B - O12_$5
1.899	(0.010)	H53B - O11_$6

ngle NHO

172.05	(0.27)	N5A - H51A - O42_$1
149.60	(0.22)	N5A - H52A - O42_$2
169.54	(0.27)	N5A - H53A - O41_$3
159.14	(0.28)	N5B - H51B - O11_$4
167.00	(0.26)	N5B - H52B - O12_$5
158.88	(0.27)	N5B - H53B - O11_$6

istance O-O

2.783	(0.009)	O1W - O3
2.878	(0.009)	O1W - O12_$2
2.764	(0.007)	O3 - O41
2.827	(0.009)	O3 - O1W_$7

istance OH-O

(5)

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1.810 (0.008) H1W1 - O3
1.972 (0.009) H1W2 - O12_$2
2.051 (0.009) H3O - O1W_$7
2.473 (0.007) H3O - O41

ngle OHO

166.87 (0.27) O1W - H1W1 - O3
160.72 (0.30) O1W - H1W2 - O12_$2
156.73 (0.23) O3 - H3O - O1W_$7
101.99 (0.16) O3 - H3O - O41

istance C-CL

4.040 (0.008) C8A - Cl9B_$3
3.960 (0.009) C10A - Cl9B_$8
3.425 (0.009) C9A - Cl9B_$9
3.490 (0.009) C10A - Cl9B_$9
4.001 (0.009) C8B - Cl9A_$2
3.986 (0.009) C10B - Cl9A_$7
3.439 (0.009) C9B - Cl9A
3.518 (0.009) C10B - Cl9A

istance HCL

3.073 (0.008) H8A - Cl9B_$3
3.078 (0.009) H10A - Cl9B_$8
3.143 (0.009) H8B - Cl9A_$2
3.025 (0.009) H10B - Cl9A_$7

ngle CHCL

157.56 (0.16) C8A - H8A - Cl9B_$3
149.41 (0.18) C10A - H10A - Cl9B_$8
154.81 (0.16) C8B - H8B - Cl9A_$2
159.14 (0.18) C10B - H10B - Cl9A_$7

istance CLCL

3.618 (0.005) Cl9A - Cl9B
3.949 (0.005) Cl9A - Cl9B_$3

Table 1. Crystal data and structure refinement for 6

Identification code	hexanmal
Empirical formula	$C_{10}H_{24}N_2O_6$
Formula weight	268.31
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 8.7860(10) Å α = 62.150(10)°
	b = 9.6790(10) Å β = 78.900(10)°
	c = 9.9110(10) Å γ = 67.100(10)°
Volume	686.41(13) $Å^3$
Z	2
Density (calculated)	1.298 Mg/m^3
Absorption coefficient	0.106 mm^{-1}
F(000)	292
Crystal size	0.33 x 0.32 x 0.11 mm
θ range for data collection	2.32 to 27.49°
Index ranges	$-10 \le h \le 11$, $-10 \le k \le 11$, $-12 \le \ell \le 12$
Reflections collected	5599
Independent reflections	5599 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5599 / 3 / 325
Goodness-of-fit on F^2	1.026
Final R indices [I>2σ(I)]	R1 = 0.0592, wR2 = 0.1140
R indices (all data)	R1 = 0.1124, wR2 = 0.1377
Absolute structure parameter	1(2)
Largest diff. peak and hole	0.264 and −0.215 $eÅ^{-3}$

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for (U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(11A)	8448(5)	5689(5)	-2624(4)	50(1)
O(12A)	10189(4)	4383(5)	-720(4)	45(1)
C(1A)	8813(6)	4792(6)	-1262(6)	30(1)
C(2A)	7521(6)	4125(7)	-148(6)	38(1)
C(3A)	7471(6)	2585(6)	-189(5)	31(1)
O(3A)	6963(3)	2989(4)	-1656(3)	42(1)
C(4A)	6226(7)	1939(7)	1041(6)	31(1)
O(41A)	4871(4)	2179(5)	605(4)	35(1)
O(42A)	6679(5)	1245(5)	2386(4)	49(1)
N(5A)	6576(5)	6191(6)	14968(4)	38(1)
C(6A)	7704(7)	6464(7)	13612(6)	44(2)
C(7A)	6780(7)	7436(7)	12160(5)	37(1)
C(8A)	7911(6)	7778(7)	10792(6)	37(1)
C(9A)	7024(6)	8785(7)	9283(6)	40(1)
C(10A)	8185(6)	9181(7)	7893(5)	31(1)
C(11A)	7187(7)	10300(7)	6432(6)	41(1)
N(12A)	8250(5)	10668(6)	5058(4)	40(1)
O(11B)	-531(5)	2667(5)	6160(6)	67(1)
O(12B)	1276(5)	1211(6)	5054(4)	58(1)
C(1B)	863(7)	2208(7)	5644(5)	34(1)
C(2B)	2180(6)	2797(7)	5766(5)	30(1)
C(3B)	2605(6)	4048(7)	4210(6)	33(1)
O(3B)	3126(4)	3370(4)	3143(3)	50(1)
C(4B)	3955(7)	4589(7)	4363(5)	32(1)
O(41B)	5358(5)	4064(5)	3874(5)	56(1)
O(42B)	3537(5)	5529(5)	5035(4)	49(1)
N(5B)	1882(5)	1797(5)	1936(4)	31(1)
C(6B)	1811(6)	237(7)	2075(5)	32(1)
C(7B)	2293(6)	65(7)	597(5)	32(1)
C(8B)	2303(7)	-1588(7)	758(5)	38(1)
C(9B)	2641(6)	-1731(6)	-739(5)	34(1)
C(10B)	2669(6)	-3354(7)	-591(5)	32(1)
C(11B)	3140(7)	-3502(7)	-2079(6)	36(1)
N(12B)	3122(5)	-5091(5)	-1942(4)	33(1)
O(1WA)	4761(5)	9431(5)	4630(4)	57(1)
O(1WB)	182(5)	7486(5)	5208(4)	54(1)

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

O(11A)-C(1A)	1.239(6)	O(12A)-C(1A)	1.259(6)
C(1A)-C(2A)	1.532(7)	C(2A)-C(3A)	1.527(5)
C(3A)-O(3A)	1.431(6)	C(3A)-C(4A)	1.543(6)
C(4A)-O(42A)	1.243(6)	C(4A)-O(41A)	1.244(6)
N(5A)-C(6A)	1.489(6)	C(6A)-C(7A)	1.484(7)
C(7A)-C(8A)	1.501(6)	C(8A)-C(9A)	1.513(5)
C(9A)-C(10A)	1.535(6)	C(10A)-C(11A)	1.524(7)
C(11A)-N(12A)	1.473(6)	O(11B)-C(1B)	1.227(6)
O(12B)-C(1B)	1.257(7)	C(1B)-C(2B)	1.521(7)
C(2B)-C(3B)	1.539(4)	C(3B)-O(3B)	1.410(5)
C(3B)-C(4B)	1.527(7)	C(4B)-O(41B)	1.235(6)
C(4B)-O(42B)	1.272(6)	N(5B)-C(6B)	1.476(6)
C(6B)-C(7B)	1.512(6)	C(7B)-C(8B)	1.528(7)
C(8B)-C(9B)	1.516(4)	C(9B)-C(10B)	1.499(7)
C(10B)-C(11B)	1.511(6)	C(11B)-N(12B)	1.485(7)

O(11A)-C(1A)-O(12A)	124.3(5)	O(11A)-C(1A)-C(2A)	118.6(5)
O(12A)-C(1A)-C(2A)	117.1(5)	C(3A)-C(2A)-C(1A)	112.1(4)
O(3A)-C(3A)-C(2A)	110.6(3)	O(3A)-C(3A)-C(4A)	109.5(4)
C(2A)-C(3A)-C(4A)	108.2(4)	O(42A)-C(4A)-O(41A)	126.4(5)
O(42A)-C(4A)-C(3A)	116.0(5)	O(41A)-C(4A)-C(3A)	117.7(4)
C(7A)-C(6A)-N(5A)	111.9(4)	C(6A)-C(7A)-C(8A)	111.9(5)
C(7A)-C(8A)-C(9A)	113.9(4)	C(8A)-C(9A)-C(10A)	113.6(3)
C(11A)-C(10A)-C(9A)	110.2(4)	N(12A)-C(11A)-C(10A)	112.2(5)
O(11B)-C(1B)-O(12B)	122.5(5)	O(11B)-C(1B)-C(2B)	119.8(5)
O(12B)-C(1B)-C(2B)	117.7(5)	C(1B)-C(2B)-C(3B)	112.3(3)
O(3B)-C(3B)-C(4B)	109.1(4)	O(3B)-C(3B)-C(2B)	111.4(3)
C(4B)-C(3B)-C(2B)	111.1(3)	O(41B)-C(4B)-O(42B)	125.0(5)
O(41B)-C(4B)-C(3B)	118.9(5)	O(42B)-C(4B)-C(3B)	116.1(5)
N(5B)-C(6B)-C(7B)	111.8(4)	C(6B)-C(7B)-C(8B)	112.0(4)
C(9B)-C(8B)-C(7B)	113.0(3)	C(10B)-C(9B)-C(8B)	113.5(3)
C(9B)-C(10B)-C(11B)	111.9(4)	N(12B)-C(11B)-C(10B)	111.8(4)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 6

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(11A)	56(3)	59(3)	33(2)	-3(2)	-8(2)	-35(2)
O(12A)	33(2)	54(3)	44(2)	-9(2)	-5(2)	-24(2)
C(1A)	32(3)	25(3)	38(3)	-14(2)	-4(2)	-12(2)
C(2A)	34(3)	47(3)	44(3)	-28(3)	6(2)	-18(3)
C(3A)	25(3)	31(3)	38(3)	-14(2)	0(2)	-11(2)
O(3A)	42(2)	59(2)	36(2)	-27(2)	11(1)	-27(2)
C(4A)	33(3)	33(3)	32(3)	-14(2)	4(2)	-17(2)
O(41A)	25(2)	48(2)	34(2)	-14(2)	2(1)	-19(2)
O(42A)	53(2)	65(3)	31(2)	-9(2)	-7(2)	-33(2)
N(5A)	37(2)	45(3)	28(2)	-4(2)	-6(2)	-21(2)
C(6A)	29(3)	56(4)	37(3)	-18(3)	-2(2)	-8(3)
C(7A)	32(3)	44(3)	32(3)	-10(2)	-3(2)	-16(3)
C(8A)	32(3)	45(3)	35(3)	-20(3)	3(2)	-10(3)
C(9A)	29(3)	56(4)	35(3)	-19(3)	6(2)	-20(3)
C(10A)	29(3)	34(3)	34(3)	-15(2)	0(2)	-13(2)
C(11A)	35(3)	47(4)	34(3)	-6(3)	-3(2)	-20(3)
N(12A)	39(3)	48(3)	32(2)	-7(2)	-7(2)	-26(2)
O(11B)	36(3)	61(3)	112(4)	-46(3)	17(2)	-21(2)
O(12B)	81(3)	88(3)	52(2)	-48(2)	31(2)	-69(3)
C(1B)	43(4)	37(3)	24(2)	-4(2)	-1(2)	-25(3)
C(2B)	35(3)	30(3)	29(2)	-17(2)	2(2)	-13(2)
C(3B)	34(3)	47(3)	32(3)	-17(2)	4(2)	-28(3)
O(3B)	74(2)	74(2)	38(2)	-37(2)	19(2)	-52(2)
C(4B)	38(3)	33(3)	25(2)	-6(2)	-2(2)	-21(3)
O(41B)	33(2)	47(3)	81(3)	-19(2)	3(2)	-19(2)
O(42B)	69(3)	64(3)	36(2)	-27(2)	8(2)	-43(2)
N(5B)	29(2)	42(3)	27(2)	-16(2)	2(2)	-16(2)
C(6B)	31(3)	42(4)	29(3)	-15(2)	3(2)	-20(3)
C(7B)	32(3)	39(3)	30(3)	-17(2)	1(2)	-14(3)
C(8B)	48(3)	46(4)	29(3)	-16(2)	4(2)	-28(3)
C(9B)	34(3)	31(3)	38(3)	-15(2)	-6(2)	-11(2)
C(10B)	30(3)	39(4)	33(3)	-20(3)	5(2)	-15(3)
C(11B)	51(4)	34(3)	30(3)	-14(2)	4(2)	-24(3)
N(12B)	33(2)	40(3)	32(2)	-19(2)	5(2)	-17(2)
O(1WA)	59(3)	47(3)	56(2)	-17(2)	0(2)	-14(2)
O(1WB)	59(3)	44(3)	55(2)	-20(2)	13(2)	-24(2)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 6

	x	y	z	U(eq)
H(21A)	6411(6)	5052(7)	-221(6)	57
H(22A)	7776(6)	3981(7)	773(6)	57
H(3A)	8553(6)	1576(6)	220(5)	47
H(30A)	7804(3)	3189(4)	-2408(3)	63
H(51A)	5985(5)	5510(6)	14964(4)	57
H(52A)	5612(5)	7000(6)	14963(4)	57
H(53A)	7165(5)	5522(6)	15767(4)	57
H(61A)	8486(7)	5229(7)	13831(6)	66
H(62A)	8262(7)	7100(7)	13631(6)	66
H(71A)	6015(7)	8585(7)	12004(5)	56
H(72A)	5999(7)	7125(7)	12004(5)	56
H(81A)	8713(6)	6792(7)	10604(6)	56
H(82A)	8587(6)	8495(7)	10804(6)	56
H(91A)	6211(6)	9945(7)	9188(6)	60
H(92A)	6384(6)	8207(7)	8989(6)	60
H(10A)	8947(6)	8126(7)	7806(5)	47
H(10B)	8818(6)	9865(7)	7806(5)	47
H(11A)	6430(7)	11483(7)	6218(6)	62
H(11B)	6636(7)	9607(7)	6418(6)	62
H(12A)	7696(5)	11256(6)	4189(4)	59
H(12B)	9068(5)	10913(6)	4995(4)	59
H(12C)	8978(5)	9518(6)	4995(4)	59
H(21B)	3262(6)	1757(7)	6178(5)	44
H(22B)	1472(6)	3582(7)	6177(5)	44
H(3B)	1546(6)	5142(7)	3599(6)	50
H(30B)	4371(4)	3064(4)	2833(3)	76
H(51B)	1114(5)	2789(5)	1194(4)	46
H(52B)	2786(5)	1886(5)	1597(4)	46
H(53B)	1561(5)	1912(5)	2794(4)	46
H(61B)	2618(6)	-696(7)	2782(5)	49
H(62B)	673(6)	215(7)	2379(5)	49
H(71B)	3363(6)	188(7)	199(5)	49
H(72B)	1517(6)	1028(7)	-203(5)	49
H(81B)	1289(7)	-1722(7)	1170(5)	56
H(82B)	3101(7)	-2629(7)	1573(5)	56
H(91B)	3773(6)	-1582(6)	-1209(5)	50
H(92B)	1801(6)	-734(6)	-1612(5)	50
H(10C)	1606(6)	-3593(7)	-219(5)	48
H(10D)	3423(6)	-4295(7)	183(5)	48
H(11C)	4263(7)	-3453(7)	-2399(6)	54
H(11D)	2426(7)	-2571(7)	-3001(6)	54
H(12D)	3392(5)	-5298(5)	-2798(4)	50
H(12E)	2150(5)	-5191(5)	-1600(4)	50
H(12F)	3842(5)	-5996(5)	-1397(4)	50
H(1WA)	3628(5)	9979(5)	5015(4)	86
H(2WA)	5352(5)	10051(5)	3817(4)	86
H(1WB)	1422(5)	6786(5)	4993(4)	81
H(2WB)	-417(5)	6631(5)	6209(4)	81

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Table 6. Observed and calculated structure factors for 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
0	-1	-20	24	28	4	0	4	-17	59	57	2	2	-4	-14	54	54	2	1	3	-13	84	82	1	4	-2	-11	38	34	2
1	-1	-20	33	27	2	1	4	-17	75	73	1	-1	-3	-14	44	40	2	2	3	-13	0	8	1	-1	-1	-11	33	33	2
-1	0	-20	56	54	2	-1	-3	-16	26	21	3	0	-3	-14	71	69	1	3	3	-13	12	15	12	0	-1	-11	176	170	1
0	0	-20	8	16	7	0	-3	-16	17	22	6	1	-3	-14	90	92	1	-1	4	-13	26	22	3	1	-1	-11	72	73	1
1	0	-20	63	62	1	1	-3	-16	15	12	6	2	-3	-14	2	12	2	0	4	-13	46	40	2	2	-1	-11	49	49	1
-1	1	-20	22	17	4	2	-3	-16	56	61	2	3	-3	-14	43	42	2	1	4	-13	31	32	2	3	-1	-11	54	52	1
0	1	-20	23	19	4	-1	-2	-16	71	73	1	-1	-2	-14	55	54	1	2	4	-13	72	71	1	4	-1	-11	14	13	5
1	1	-20	53	55	2	0	-2	-16	53	49	1	0	-2	-14	51	52	1	3	4	-13	20	28	5	-1	0	-11	86	85	1
-1	2	-20	67	68	1	1	-2	-16	4	17	4	1	-2	-14	129	128	1	-1	5	-13	31	21	2	0	0	-11	47	47	1
0	2	-20	88	84	1	2	-2	-16	17	10	5	2	-2	-14	151	151	1	0	5	-13	27	19	3	1	0	-11	56	56	1
1	2	-20	0	19	1	3	-2	-16	24	30	4	3	-2	-14	33	31	2	1	5	-13	55	50	1	2	0	-11	29	31	2
0	-2	-19	31	30	3	-1	-1	-16	43	43	2	4	-2	-14	18	14	4	2	5	-13	33	32	3	3	0	-11	55	57	1
1	-2	-19	39	39	2	0	-1	-16	65	63	1	-1	-1	-14	128	135	1	0	-5	-12	14	15	9	4	0	-11	14	5	4
-1	-1	-19	27	28	3	1	-1	-16	39	42	2	0	-1	-14	34	36	2	1	-5	-12	25	18	3	5	0	-11	31	31	2
0	-1	-19	0	11	1	2	-1	-16	17	14	4	1	-1	-14	61	60	1	-1	-4	-12	30	31	3	-1	1	-11	117	115	1
1	-1	-19	39	47	2	3	-1	-16	59	61	1	2	-1	-14	102	95	1	0	-4	-12	26	17	3	0	1	-11	110	109	1
2	-1	-19	36	35	2	-1	0	-16	0	15	1	3	-1	-14	50	48	1	1	-4	-12	42	38	2	1	1	-11	58	60	1
-1	0	-19	62	58	1	0	0	-16	33	38	2	4	-1	-14	15	7	4	2	-4	-12	48	48	2	2	1	-11	87	85	1
0	0	-19	83	79	1	1	0	-16	93	97	1	-1	0	-14	34	32	2	3	-4	-12	33	35	2	3	1	-11	72	76	1
1	0	-19	11	19	10	2	0	-16	55	53	1	0	0	-14	42	42	2	-1	-3	-12	0	7	1	4	1	-11	33	29	2
2	0	-19	23	22	3	3	0	-16	32	30	2	1	0	-14	69	71	1	0	-3	-12	56	53	1	-1	2	-11	65	64	1
-1	1	-19	30	20	3	-1	1	-16	117	116	1	2	0	-14	41	40	2	1	-3	-12	48	51	2	0	2	-11	15	16	4
0	1	-19	39	38	2	0	1	-16	98	103	1	3	0	-14	52	49	1	2	-3	-12	33	40	2	1	2	-11	97	97	1
1	1	-19	66	62	1	1	1	-16	81	78	1	4	0	-14	17	11	5	3	-3	-12	0	1	1	2	2	-11	121	121	1
2	1	-19	35	39	2	2	1	-16	19	20	4	-1	1	-14	49	51	2	4	-3	-12	7	13	6	3	2	-11	31	30	2
-1	2	-19	24	27	4	3	1	-16	57	55	1	0	1	-14	37	34	2	-1	-2	-12	22	24	4	4	2	-11	49	42	2
0	2	-19	13	23	12	-1	2	-16	71	73	1	1	1	-14	9	12	9	0	-2	-12	73	73	1	-1	3	-11	93	97	1
1	2	-19	57	55	1	0	2	-16	252	258	1	2	1	-14	45	44	2	1	-2	-12	147	146	1	0	3	-11	189	189	1
2	2	-19	36	36	2	1	2	-16	14	10	7	3	1	-14	17	17	4	2	-2	-12	110	111	1	1	3	-11	66	63	1
-1	3	-19	94	95	1	2	2	-16	29	30	3	4	1	-14	27	25	3	3	-2	-12	15	3	4	2	3	-11	26	21	2
0	3	-19	34	38	3	3	2	-16	43	41	2	-1	2	-14	61	59	1	4	-2	-12	30	27	2	3	3	-11	0	8	1
1	3	-19	117	114	1	-1	3	-16	0	15	1	0	2	-14	79	79	1	-1	-1	-12	55	58	1	4	3	-11	152	153	1
-1	-2	-18	28	28	3	0	3	-16	42	42	2	1	2	-14	13	17	8	0	-1	-12	127	130	1	-1	4	-11	58	57	1
0	-2	-18	35	34	2	1	3	-16	25	26	3	2	2	-14	66	69	1	1	-1	-12	64	61	1	0	4	-11	125	124	1
1	-2	-18	22	24	4	2	3	-16	103	100	1	3	2	-14	49	50	2	2	-1	-12	152	150	1	1	4	-11	91	91	1
2	-2	-18	39	36	2	3	3	-16	22	25	4	4	2	-14	76	69	1	3	-1	-12	73	74	1	2	4	-11	54	55	2
-1	-1	-18	58	60	2	-1	4	-16	36	40	2	-1	3	-14	50	47	1	4	-1	-12	27	20	2	3	4	-11	22	23	4
0	-1	-18	48	50	2	0	4	-16	0	8	1	0	3	-14	234	238	1	-1	0	-12	258	256	1	-1	5	-11	61	66	2
1	-1	-18	24	17	3	1	4	-16	70	70	1	1	3	-14	92	90	1	0	0	-12	39	31	1	0	5	-11	16	19	6
2	-1	-18	29	28	2	2	4	-16	18	21	6	2	3	-14	70	66	1	1	0	-12	241	234	1	1	5	-11	17	21	6
-1	0	-18	25	24	3	0	-4	-15	17	13	6	3	3	-14	57	53	2	2	0	-12	38	40	1	2	5	-11	80	81	1
0	0	-18	77	77	1	1	-4	-15	18	15	5	-1	4	-14	152	154	1	3	0	-12	84	81	1	-1	6	-11	27	25	3
1	0	-18	56	58	1	-1	-3	-15	14	25	11	0	4	-14	22	22	3	4	0	-12	80	77	1	0	6	-11	26	20	3
2	0	-18	19	23	5	0	-3	-15	13	18	12	1	4	-14	49	50	2	-1	1	-12	75	76	1	-1	-5	-10	75	73	1
3	0	-18	29	28	3	1	-3	-15	53	53	1	2	4	-14	101	103	1	0	1	-12	54	57	1	0	-5	-10	75	72	1
-1	1	-18	24	25	4	2	-3	-15	38	37	2	-1	5	-14	27	33	3	1	1	-12	79	78	1	1	-5	-10	14	14	7
0	1	-18	83	80	1	3	-3	-15	21	25	4	0	5	-14	87	86	1	2	1	-12	47	47	1	2	-5	-10	36	36	2
1	1	-18	26	26	3	-1	-2	-15	18	24	5	1	5	-14	32	35	3	3	1	-12	32	35	2	-1	-4	-10	73	74	1
2	1	-18	62	57	1	0	-2	-15	15	10	6	-1	-4	-13	99	94	1	4	1	-12	21	18	3	0	-4	-10	146	141	1
3	1	-18	0	9	1	1	-2	-15	24	26	3	0	-4	-13	61	59	1	-1	2	-12	106	101	1	1	-4	-10	68	65	1
-1	2	-18	42	40	2	2	-2	-15	84	84	1	1	-4	-13	17	21	5	0	2	-12	113	114	1	2	-4	-10	57	53	1
0	2	-18	75	72	1	3	-2	-15	27	30	3	2	-4	-13	0	8	1	1	2	-12	22	23	3	3	-4	-10	109	110	1
1	2	-18	0	8	1	-1	-1	-15	146	147	1	3	-4	-13	51	54	2	2	2	-12	30	30	2	-1	-3	-10	65	63	1
2	2	-18	58	55	1	0	-1	-15	44	46	2	-1	-3	-13	99	99	1	3	2	-12	15	15	5	0	-3	-10	173	177	1
-1	3	-18	34	36	2	1	-1	-15	26	30	3	0	-3	-13	22	25	4	4	2	-12	32	34	3	1	-3	-10	39	36	2
0	3	-18	0	5	1	2	-1	-15	81	79	1	1	-3	-13	128	127	1	-1	3	-12	60	53	1	2	-3	-10	25	25	3
1	3	-18	48	46	2	3	-1	-15	66	68	1	2	-3	-13	29	30	2	0	3	-12	38	36	2	3	-3	-10	58	56	1
2	3	-18	26	28	3	4	-1	-15	14	17	8	3	-3	-13	38	37	2	1	3	-12	43	44	2	4	-3	-10	3	15	3
0	4	-18	39	39	2	-1	0	-15	11	24	10	-1	-2	-13	46	48	2	2	3	-12	61	60	1	-1	-2	-10	70	68	1
0	-3	-17	47	47	2	0	0	-15	116	116	1	0	-2	-13	22	24	3	3	3	-12	36	35	2	0	-2	-10	73	73	1
1	-3	-17	0	3	1	1	0	-15	40	37	2	1	-2	-13	42	42	2	4	3	-12	23	23	4	1	-2	-10	104	105	1
-1	-2	-17	72	77	1	2	0	-15	30	32	2	2	-2	-13	91	85	1	-1	4	-12	70	71	1	2	-2	-10	62	59	1
0	-2	-17	0	16	1	3	0	-15	87	81	1	3	-2	-13	0	11	1	0	4	-12	67	70	1	3	-2	-10	70	75	1
1	-2	-17	22	20	4	4	0	-15	0	6	1	4	-2	-13	10	6	10	1	4	-12	94	95	1	4	-2	-10	21	22	3
2	-2	-17	66	68	1	-1	1	-15	205	203	1	-1	-1	-13	25	27	3	2	4	-12	27	18	3	-1	-1	-10	86	80	1
-1	-1	-17	26	27	3	0	1	-15	30	32	3	0	-1	-13	96	97	1	3	4	-12	20	19	4	0	-1	-10	184	184	1
0	-1	-17	56	57	1	1	1	-15	4	9	3	1	-1	-13	63	64	1	-1	5	-12	71	70	1	1	-1	-10	196	196	1
1	-1	-17	68	68	1	2	1	-15	48	46	1	2	-1	-13	63	62	1	0	5	-12	18	14	5	2	-1	-10	93	92	1
2	-1	-17	27	23	3	3	1	-15	49	45	1	3	-1	-13	21	22	3	1	5	-12	48	48	2	3	-1	-10	26	27	2
3	-1	-17	110	105	1	4	1	-15	0	6	1	4	-1	-13	0	5	1	2	5	-12	36	40	2	4	-1	-10	15	20	5
-1	0	-17	82	86	1	-1	2	-15	11	14	10	-1	0	-13	69	73	1	-1	-5	-11	16	9	7	5	-1	-10	50	52	1
0	0	-17	43	48	2	0	2	-15	62	59	1	0	0	-13	160	162	1	0	-5	-11	0	3	1	-1	0	-10	202	206	1
1	0	-17	34	36	2	1	2	-15	65	64	1	1	0	-13	30	31	2	1	-5	-11	30	27	3	0	0	-10	38	43	1
2	0	-17	41	44	2	2	2	-15	0	6	1	2	0	-13	24	21	3	2	-5	-11	18	11	4	1	0	-10	141	138	1
3	0	-17	7	8	6	3	2	-15	30	27	2	3	0	-13	111	114	1	-1	-4	-11	49	45	2	2	0	-10	174	178	1
-1	1	-17	72	67	1	-1	3	-15	96	94	1	4	0	-13	53	54	1	0	-4	-11	72	74	1	3	0	-10	88	90	1
0	1	-17	41	43	2	0	3	-15	91	90	1	-1	1	-13	137	138	1	1	-4	-11	34	37	2	4	0	-10	37	38	2
1	1	-17	102	98	1	1	3	-15	83	82	1	0	1	-13	148	148	1	2	-4	-11	12	4	9	5	0	-10	0	5	1
2	1	-17	45	45	1	2	3	-15	38	39	2	1	1	-13	145	149	1	3	-4	-11	43	43	2	-1	1	-10	220	218	1
3	1	-17	10	7	10	3	3	-15	24	18	3	2	1	-13	194	191	1	-1	-3	-11	34	31	2	0	1	-10	192	196	1
-1	2	-17	22	21	4	-1	4	-15	8	7	7	3	1	-13	34	32	2	0	-3	-11	168	167	1	1	1	-10	234	230	1
0	2	-17	53	54	2	0	4	-15	21	16	4	4	1	-13	71	67	1	1	-3	-11	144	144	1	2	1	-10	84	87	1
1	2	-17	98	99	1	1	4	-15	88	88	1	-1	2	-13	333	340	1	2	-3	-11	25	20	3	3	1	-10	37	36	1
2	2	-17	15	17	6	2	4	-15	21	19	4	0	2	-13	89	93	1	3	-3	-11	21	22	3	4	1	-10	116	114	1
3	2	-17	48	47	2	-1	5	-15	92	90	1	1	2	-13	57	54	1	4	-3	-11	118	116	1	5	1	-10	24	14	3
-1	3	-17	44	41	2	0	5	-15	80	76	1	2	2	-13	72	69	1	-1	-2	-11	88	86	1	-1	2	-10	14	15	6
0	3	-17	99	101	1	1	5	-15	47	40	2	3	2	-13	80	80	1	0	-2	-11	55	54	1	0	2	-10	213	207	1
1	3	-17	102	105	1	-1	-4	-14	38	28	2	4	2	-13	48	44	2	1	-2	-11	195	190	1	1	2	-10	155	156	1
2	3	-17	15	12	7	0	-4	-14	23	21	4	-1	3	-13	97	100	1	2	-2	-11	82	83	1	2	2	-10	41	41	1
-1	4	-17	91	87	1	1	-4	-14	6	12	6	0	3	-13	72	71	1	3	-2	-11	50	47	1	3	2	-10	172	172	1

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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	h	k	l	10Fo	10Fc	10s
4	2	-10	89	86	1	0	-5	-8	23	13	3	5	-3	-7	17	12	5	4	-1	-6	13	15	5	2	1	-5	65	71	1
-1	3	-10	150	154	1	1	-5	-8	43	43	2	-1	-2	-7	85	85	1	5	-1	-6	37	32	2	3	1	-5	25	26	2
0	3	-10	82	81	1	2	-5	-8	45	50	2	0	-2	-7	32	29	1	-1	0	-6	241	244	1	4	1	-5	25	20	2
1	3	-10	113	115	1	3	-5	-8	13	11	10	1	-2	-7	43	42	1	0	0	-6	234	235	1	5	1	-5	25	17	3
2	3	-10	29	28	2	-1	-4	-8	201	198	1	2	-2	-7	208	204	1	1	0	-6	102	99	1	-1	2	-5	15	16	4
3	3	-10	34	32	2	0	-4	-8	60	60	1	3	-2	-7	18	21	3	2	0	-6	49	44	1	0	2	-5	80	75	1
4	3	-10	35	37	2	1	-4	-8	106	99	1	4	-2	-7	8	5	8	3	0	-6	230	223	1	1	2	-5	54	55	1
-1	4	-10	214	211	1	2	-4	-8	21	19	3	5	-2	-7	0	5	1	4	0	-6	22	26	2	2	2	-5	167	179	1
0	4	-10	56	58	1	3	-4	-8	41	44	2	-1	-1	-7	125	128	1	5	0	-6	81	77	1	3	2	-5	55	55	1
1	4	-10	128	130	1	4	-4	-8	14	9	6	0	-1	-7	57	58	1	-1	1	-6	526	503	1	4	2	-5	28	30	2
2	4	-10	82	87	1	-1	-3	-8	78	77	1	1	-1	-7	161	155	1	0	1	-6	179	186	1	5	2	-5	46	45	2
3	4	-10	70	71	1	0	-3	-8	126	125	1	2	-1	-7	267	261	1	1	1	-6	213	214	1	-1	3	-5	149	143	1
-1	5	-10	102	100	1	1	-3	-8	85	82	1	3	-1	-7	17	22	3	2	1	-6	279	285	1	0	3	-5	78	74	1
0	5	-10	29	34	3	2	-3	-8	44	45	1	4	-1	-7	145	143	1	3	1	-6	25	24	2	1	3	-5	110	114	1
1	5	-10	136	135	1	3	-3	-8	143	145	1	5	-1	-7	41	41	2	4	1	-6	24	29	2	2	3	-5	69	70	1
2	5	-10	35	33	2	4	-3	-8	19	21	4	-1	0	-7	71	66	1	5	1	-6	12	8	11	3	3	-5	14	17	11
-1	6	-10	56	53	2	-1	-2	-8	170	159	1	0	0	-7	514	520	1	-1	2	-6	328	311	1	4	3	-5	53	46	2
0	6	-10	18	17	5	0	-2	-8	74	72	1	1	0	-7	344	343	1	0	2	-6	71	70	1	-1	4	-5	132	130	1
1	6	-10	27	26	4	1	-2	-8	44	47	1	2	0	-7	128	131	1	1	2	-6	154	159	1	0	4	-5	91	94	1
-1	5	-9	65	62	1	2	-2	-8	21	20	2	3	0	-7	64	63	1	2	2	-6	98	105	1	1	4	-5	52	55	1
0	5	-9	34	23	2	3	-2	-8	64	63	1	4	0	-7	34	35	2	3	2	-6	169	182	1	2	4	-5	37	35	2
1	5	-9	12	14	12	4	-2	-8	28	23	2	5	0	-7	20	20	4	4	2	-6	26	26	3	3	4	-5	63	60	1
2	5	-9	22	18	3	5	-2	-8	73	66	1	-1	1	-7	298	292	1	5	2	-6	0	10	1	4	4	-5	56	56	2
3	5	-9	9	10	8	-1	-1	-8	43	40	1	0	1	-7	22	15	2	-1	3	-6	125	127	1	-1	5	-5	232	230	1
-1	4	-9	0	11	1	0	-1	-8	121	126	1	1	1	-7	65	66	1	0	3	-6	124	124	1	0	5	-5	131	132	1
0	4	-9	59	58	1	1	-1	-8	53	45	1	2	1	-7	298	299	1	1	3	-6	26	29	2	1	5	-5	47	45	2
1	4	-9	31	31	2	2	-1	-8	216	205	1	3	1	-7	35	30	1	2	3	-6	21	27	3	2	5	-5	14	11	7
2	4	-9	22	19	3	3	-1	-8	98	94	1	4	1	-7	23	17	2	3	3	-6	61	67	1	3	5	-5	117	117	1
3	4	-9	70	73	1	4	-1	-8	59	60	1	5	1	-7	6	5	5	4	3	-6	19	21	5	-1	6	-5	22	19	4
4	4	-9	12	10	12	5	-1	-8	18	14	4	-1	2	-7	325	304	1	-1	4	-6	73	71	1	0	6	-5	99	105	1
-1	3	-9	60	58	1	-1	0	-8	139	134	1	0	2	-7	89	91	1	0	4	-6	85	88	1	1	6	-5	56	55	2
0	3	-9	176	178	1	0	0	-8	150	144	1	1	2	-7	67	65	1	1	4	-6	83	86	1	2	6	-5	11	7	11
1	3	-9	51	54	1	1	0	-8	55	58	1	2	2	-7	56	60	1	2	4	-6	57	61	1	-1	-6	-4	22	18	4
2	3	-9	138	138	1	2	0	-8	41	34	1	3	2	-7	230	243	1	3	4	-6	51	56	2	0	-6	-4	92	90	1
3	3	-9	40	44	2	3	0	-8	19	13	3	4	2	-7	79	73	1	4	4	-6	24	21	4	1	-6	-4	61	66	1
4	3	-9	17	10	4	4	0	-8	26	18	2	5	2	-7	7	7	6	-1	5	-6	76	78	1	2	-6	-4	17	18	5
-1	2	-9	91	86	1	5	0	-8	35	35	2	-1	3	-7	52	58	1	0	5	-6	28	25	3	-1	-5	-4	38	39	2
0	2	-9	166	165	1	-1	1	-8	50	49	1	0	3	-7	390	389	1	1	5	-6	102	105	1	0	-5	-4	101	99	1
1	2	-9	129	125	1	0	1	-8	29	35	1	1	3	-7	82	87	1	2	5	-6	20	17	4	1	-5	-4	86	88	1
2	2	-9	113	111	1	1	1	-8	115	115	1	2	3	-7	73	77	1	3	5	-6	44	44	2	2	-5	-4	35	35	2
3	2	-9	9	11	8	2	1	-8	69	68	1	3	3	-7	112	115	1	-1	6	-6	46	45	2	3	-5	-4	28	34	3
4	2	-9	93	92	1	3	1	-8	93	96	1	4	3	-7	103	111	1	0	6	-6	122	122	1	4	-5	-4	50	50	2
5	2	-9	7	8	6	4	1	-8	49	45	1	-1	4	-7	80	80	1	1	6	-6	7	22	7	-1	-4	-4	32	32	2
-1	1	-9	81	89	1	5	1	-8	63	55	1	0	4	-7	41	41	2	2	6	-6	27	35	4	0	-4	-4	45	40	1
0	1	-9	338	325	1	-1	2	-8	213	210	1	1	4	-7	89	88	1	-1	-6	-5	25	22	4	1	-4	-4	41	38	1
1	1	-9	90	90	1	0	2	-8	96	98	1	2	4	-7	78	83	1	0	-6	-5	28	24	3	2	-4	-4	123	125	1
2	1	-9	79	79	1	1	2	-8	215	215	1	3	4	-7	67	66	1	1	-6	-5	17	16	6	3	-4	-4	44	39	1
3	1	-9	55	51	1	2	2	-8	82	84	1	4	4	-7	21	12	4	2	-6	-5	44	45	2	4	-4	-4	25	22	3
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5	1	-9	9	7	9	4	2	-8	39	39	2	0	5	-7	116	120	1	0	-5	-5	60	60	1	0	-3	-4	107	101	1
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0	0	-9	115	110	1	-1	3	-8	109	110	1	2	5	-7	57	58	1	2	-5	-5	48	49	1	2	-3	-4	21	22	2
1	0	-9	237	234	1	0	3	-8	63	60	1	3	5	-7	26	28	3	3	-5	-5	9	4	9	3	-3	-4	99	105	1
2	0	-9	6	7	6	1	3	-8	82	82	1	-1	6	-7	21	26	5	-1	-4	-5	112	107	1	4	-3	-4	144	144	1
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0	1	-9	56	54	1	0	4	-8	32	35	2	1	-6	-6	38	34	2	4	-4	-5	20	18	3	2	-2	-4	198	199	1
1	1	-9	43	44	1	1	4	-8	75	75	1	2	-6	-6	40	35	2	-1	-3	-5	124	124	1	3	-2	-4	57	59	1
2	1	-9	23	26	2	2	4	-8	19	16	4	-1	-5	-6	71	68	1	0	-3	-5	86	81	1	4	-2	-4	16	19	5
3	1	-9	49	42	1	3	4	-8	62	62	2	0	-5	-6	57	58	1	1	-3	-5	49	43	1	5	-2	-4	29	31	3
4	1	-9	23	15	2	4	4	-8	72	73	2	1	-5	-6	28	25	3	2	-3	-5	54	53	1	-1	-1	-4	48	48	1
5	1	-9	39	42	2	-1	5	-8	79	77	1	2	-5	-6	68	68	1	3	-3	-5	30	31	2	0	-1	-4	278	269	1
-1	2	-9	85	86	1	0	5	-8	120	118	1	3	-5	-6	5	1	5	4	-3	-5	82	84	1	1	-1	-4	248	245	1
0	2	-9	188	187	1	1	5	-8	65	64	1	-1	-4	-6	100	97	1	5	-3	-5	24	28	3	2	-1	-4	104	115	1
1	2	-9	90	84	1	2	5	-8	16	19	5	0	-4	-6	51	49	1	-1	-2	-5	62	60	1	3	-1	-4	73	78	1
2	2	-9	13	12	5	3	5	-8	29	32	3	1	-4	-6	51	47	1	0	-2	-5	72	75	1	4	-1	-4	32	36	2
3	2	-9	28	30	2	-1	6	-8	81	82	1	2	-4	-6	101	101	1	1	-2	-5	83	79	1	5	-1	-4	0	16	1
4	2	-9	37	46	2	0	6	-8	87	92	1	3	-4	-6	40	40	2	2	-2	-5	126	121	1	-1	0	-4	161	164	1
-1	3	-9	152	151	1	1	6	-8	108	111	1	4	-4	-6	9	11	8	3	-2	-5	58	58	1	0	0	-4	287	289	1
0	3	-9	80	83	1	0	-6	-7	40	38	2	-1	-3	-6	203	198	1	4	-2	-5	7	7	7	1	0	-4	257	252	1
1	3	-9	97	98	1	1	-6	-7	78	75	1	0	-3	-6	38	43	1	5	-2	-5	90	89	1	2	0	-4	80	81	1
2	3	-9	151	156	1	-1	-5	-7	14	4	9	1	-3	-6	101	97	1	-1	-1	-5	196	184	1	3	0	-4	78	87	1
3	3	-9	42	49	2	0	-5	-7	31	27	2	2	-3	-6	70	72	1	0	-1	-5	492	489	1	4	0	-4	115	111	1
4	3	-9	59	56	2	1	-5	-7	27	24	3	3	-3	-6	96	95	1	1	-1	-5	185	174	1	5	0	-4	22	23	3
-1	4	-9	27	17	3	2	-5	-7	106	107	1	4	-3	-6	49	53	2	2	-1	-5	318	309	1	-1	1	-4	227	214	1
0	4	-9	141	145	1	3	-5	-7	28	26	3	5	-3	-6	25	20	3	3	-1	-5	43	40	1	0	1	-4	164	163	1
1	4	-9	46	49	2	-1	-4	-7	176	171	1	-1	-2	-6	190	181	1	4	-1	-5	58	58	1	2	1	-4	200	208	1
2	4	-9	20	21	4	0	-4	-7	53	54	1	0	-2	-6	134	131	1	5	-1	-5	66	59	1	3	1	-4	25	14	2
3	4	-9	5	8	5	1	-4	-7	40	39	2	1	-2	-6	439	424	1	-1	0	-5	123	123	1	4	1	-4	46	47	1
-1	5	-9	39	40	2	2	-4	-7	81	86	1	2	-2	-6	13	11	4	0	0	-5	116	125	1	5	1	-4	113	114	1
0	5	-9	137	139	1	3	-4	-7	85	88	1	3	-2	-6	68	72	1	1	0	-5	311	309	1	-1	2	-4	226	211	1
1	5	-9	33	34	2	4	-4	-7	36	37	2	4	-2	-6	44	42	1	2	0	-5	39	36	1	0	2	-4	75	89	1
2	5	-9	13	16	8	-1	-3	-7	87	87	1	5	-2	-6	93	95	1	3	0	-5	45	45	1	1	2	-4	99	113	1
3	5	-9	11	16	10	0	-3	-7	222	220	1	-1	-1	-6	374	360	1	4	0	-5	34	32	2	2	2	-4	372	396	1
-1	6	-9	22	17	4	1	-3	-7	42	43	1	0	-1	-6	141	146	1	5	0	-5	11	14	11	3	2	-4	12	15	7
0	6	-9	0	11	1	2	-3	-7	145	141	1	1	-1	-6	199	191	1	-1	1	-5	167	159	1	4	2	-4	26	22	2
1	6	-9	82	81	1	3	-3	-7	11	11	11	2	-1	-6	62	62	1	0	1	-5	140	134	1	5	2	-4	38	41	2
-1	5	-8	53	55	2	4	-3	-7	0	5	1	3	-1	-6	53	53	1	1	1	-5	44	47	1	-1	3	-4	184	179	1

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Table 6. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	3	-4	186	191	1	-1	5	-3	135	137	1	0	-6	-1	33	32	3	0	-4	0	144	142	1	5	-3	1	84	83	1
1	3	-4	82	84	1	0	5	-3	124	126	1	1	-6	-1	24	17	3	1	-4	0	41	37	1	-1	-2	1	340	340	1
2	3	-4	14	19	5	1	5	-3	100	100	1	2	-6	-1	16	17	6	2	-4	0	46	45	1	0	-2	1	459	458	1
3	3	-4	198	204	1	2	5	-3	0	11	1	3	-6	-1	30	23	2	3	-4	0	99	101	1	1	-2	1	386	376	1
4	3	-4	105	105	1	3	5	-3	23	26	4	-1	-5	-1	41	41	2	4	-4	0	35	37	2	2	-2	1	160	157	1
-1	4	-4	204	207	1	-1	6	-3	83	87	1	0	-5	-1	21	24	4	-1	-3	0	136	137	1	3	-2	1	136	139	1
0	4	-4	220	222	1	0	6	-3	48	48	2	1	-5	-1	74	74	1	0	-3	0	84	87	1	4	-2	1	22	22	3
1	4	-4	28	28	2	1	6	-3	95	95	1	2	-5	-1	82	81	1	1	-3	0	214	203	1	5	-2	1	53	50	1
2	4	-4	214	221	1	2	6	-3	16	13	7	3	-5	-1	46	47	2	2	-3	0	96	103	1	-1	-1	1	826	880	1
3	4	-4	62	62	1	-1	-6	-2	52	52	2	4	-5	-1	45	43	2	3	-3	0	103	107	1	0	-1	1	280	263	1
4	4	-4	40	37	2	0	-6	-2	37	37	2	-1	-4	-1	197	192	1	4	-3	0	23	25	3	1	-1	1	83	85	1
-1	5	-4	51	57	2	1	-6	-2	31	30	3	0	-4	-1	48	50	1	5	-3	0	35	37	2	2	-1	1	186	182	1
0	5	-4	10	16	10	2	-6	-2	65	64	1	1	-4	-1	143	144	1	-1	-2	0	54	54	1	3	-1	1	229	236	1
1	5	-4	51	52	2	3	-6	-2	7	13	6	2	-4	-1	42	43	1	0	-2	0	160	150	1	4	-1	1	36	36	2
2	5	-4	42	41	2	-1	-5	-2	11	11	11	3	-4	-1	89	91	1	1	-2	0	132	126	1	5	-1	1	45	43	2
3	5	-4	9	21	8	0	-5	-2	87	84	1	4	-4	-1	66	70	1	2	-2	0	267	275	1	-1	0	1	158	162	1
-1	6	-4	15	23	7	1	-5	-2	56	61	1	-1	-3	-1	96	92	1	3	-2	0	41	43	1	1	0	1	15	18	2
0	6	-4	18	23	6	2	-5	-2	27	20	2	0	-3	-1	221	210	1	4	-2	0	54	58	1	2	0	1	114	106	1
1	6	-4	30	33	3	3	-5	-2	32	29	2	1	-3	-1	92	91	1	5	-2	0	77	80	1	3	0	1	37	36	1
2	6	-4	51	54	2	4	-5	-2	28	29	3	2	-3	-1	99	98	1	-1	-1	0	319	321	1	4	0	1	43	40	1
-1	-6	-3	61	59	2	-1	-4	-2	9	16	9	3	-3	-1	195	205	1	0	-1	0	115	117	1	5	0	1	9	3	8
0	-6	-3	0	8	1	0	-4	-2	46	47	1	4	-3	-1	72	72	1	1	-1	0	340	352	1	-1	1	1	408	414	1
1	-6	-3	45	49	2	1	-4	-2	39	42	2	5	-3	-1	25	28	3	2	-1	0	327	332	1	0	1	1	106	105	1
2	-6	-3	19	17	4	2	-4	-2	35	36	2	-1	-2	-1	240	245	1	3	-1	0	268	276	1	1	1	1	233	254	1
-1	-5	-3	107	101	1	3	-4	-2	152	157	1	0	-2	-1	96	95	1	4	-1	0	191	198	1	2	1	1	49	48	1
0	-5	-3	29	25	2	4	-4	-2	59	63	1	1	-2	-1	111	110	1	5	-1	0	30	26	2	3	1	1	32	31	1
1	-5	-3	77	78	1	-1	-3	-2	132	132	1	2	-2	-1	55	58	1	-1	0	0	124	122	1	4	1	1	44	40	1
2	-5	-3	67	65	1	0	-3	-2	264	257	1	3	-2	-1	187	193	1	1	0	0	121	122	1	5	1	1	26	24	3
3	-5	-3	53	58	1	1	-3	-2	81	85	1	4	-2	-1	37	36	2	2	0	0	315	323	1	-1	2	1	114	107	1
4	-5	-3	66	66	1	2	-3	-2	73	72	1	5	-2	-1	102	100	1	3	0	0	70	71	1	0	2	1	96	95	1
-1	-4	-3	118	117	1	3	-3	-2	97	97	1	-1	-1	-1	242	256	1	4	0	0	176	167	1	1	2	1	230	246	1
0	-4	-3	99	98	1	4	-3	-2	72	74	1	0	-1	-1	109	103	1	5	0	0	50	48	1	2	2	1	78	85	1
1	-4	-3	221	217	1	5	-3	-2	29	37	3	1	-1	-1	400	414	1	-1	1	0	343	352	1	3	2	1	34	35	2
2	-4	-3	37	35	2	-1	-2	-2	62	67	1	2	-1	-1	109	112	1	0	1	0	114	115	1	4	2	1	15	14	5
3	-4	-3	65	67	1	0	-2	-2	286	275	1	3	-1	-1	42	46	1	1	1	0	301	323	1	5	2	1	28	24	3
4	-4	-3	54	56	1	1	-2	-2	391	360	1	4	-1	-1	52	56	1	2	1	0	263	281	1	-1	3	1	89	93	1
-1	-3	-3	188	188	1	2	-2	-2	27	31	1	5	-1	-1	59	59	1	3	1	0	42	38	1	0	3	1	217	210	1
0	-3	-3	48	40	1	3	-2	-2	43	41	1	-1	0	-1	19	19	2	4	1	0	74	70	1	1	3	1	94	92	1
1	-3	-3	10	9	9	4	-2	-2	178	185	1	1	0	-1	155	163	1	5	1	0	36	37	2	2	3	1	15	12	4
2	-3	-3	157	159	1	5	-2	-2	64	67	1	2	0	-1	131	126	1	-1	2	0	127	129	1	3	3	1	139	140	1
3	-3	-3	92	96	1	-1	-1	-2	207	212	1	3	0	-1	114	113	1	0	2	0	157	150	1	4	3	1	30	32	3
4	-3	-3	80	83	1	0	-1	-2	500	498	1	4	0	-1	118	121	1	1	2	0	48	53	1	-1	4	1	142	144	1
5	-3	-3	67	64	1	1	-1	-2	39	37	1	5	0	-1	74	70	1	2	2	0	121	132	1	0	4	1	51	47	1
-1	-2	-3	115	117	1	2	-1	-2	77	81	1	-1	1	-1	80	88	1	3	2	0	114	124	1	1	4	1	191	193	1
0	-2	-3	149	150	1	3	-1	-2	17	17	3	0	1	-1	275	264	1	4	2	0	58	59	1	2	4	1	44	41	2
1	-2	-3	91	87	1	4	-1	-2	75	80	1	1	1	-1	782	880	1	5	2	0	25	23	3	3	4	1	33	37	2
2	-2	-3	159	161	1	5	-1	-2	0	9	1	2	1	-1	55	57	1	-1	3	0	214	203	1	4	4	1	6	20	5
3	-2	-3	74	80	1	-1	0	-2	51	43	1	3	1	-1	233	241	1	0	3	0	82	87	1	-1	5	1	70	74	1
4	-2	-3	135	134	1	0	0	-2	52	61	1	4	1	-1	130	125	1	1	3	0	133	136	1	0	5	1	14	23	8
5	-2	-3	12	17	12	1	0	-2	75	68	1	5	1	-1	37	29	2	2	3	0	29	22	2	1	5	1	38	40	2
-1	-1	-3	262	255	1	2	0	-2	252	260	1	-1	2	-1	382	376	1	3	3	0	34	34	2	2	5	1	80	84	1
0	-1	-3	527	510	1	3	0	-2	25	25	2	0	2	-1	449	458	1	4	3	0	75	77	1	3	5	1	98	100	1
1	-1	-3	419	422	1	4	0	-2	106	111	1	1	2	-1	326	339	1	-1	4	0	38	37	2	-1	6	1	20	18	5
2	-1	-3	61	48	1	5	0	-2	46	46	2	2	2	-1	38	40	1	0	4	0	138	143	1	0	6	1	28	32	3
3	-1	-3	41	39	1	-1	1	-2	107	97	1	3	2	-1	76	80	1	1	4	0	114	118	1	1	6	1	30	27	3
4	-1	-3	77	78	1	0	1	-2	54	54	1	4	2	-1	45	45	2	2	4	0	118	128	1	2	6	1	22	14	4
5	-1	-3	133	133	1	1	1	-2	189	211	1	5	2	-1	91	89	1	3	4	0	13	19	11	-1	-6	2	0	22	1
-1	0	-3	183	173	1	2	1	-2	41	43	1	-1	3	-1	85	80	1	4	4	0	35	36	2	0	-6	2	14	11	8
0	0	-3	162	170	1	3	1	-2	97	100	1	0	3	-1	16	19	3	-1	5	0	64	61	1	1	-6	2	36	40	2
1	0	-3	804	832	1	4	1	-2	13	9	9	1	3	-1	216	234	1	0	5	0	29	31	3	2	-6	2	65	61	1
2	0	-3	112	109	1	5	1	-2	37	36	2	2	3	-1	98	100	1	1	5	0	23	23	3	3	-6	2	30	31	3
3	0	-3	152	157	1	-1	2	-2	69	71	1	3	3	-1	131	137	1	2	5	0	106	104	1	-1	-5	2	30	29	3
4	0	-3	65	71	1	0	2	-2	31	30	1	4	3	-1	32	36	2	3	5	0	60	63	2	0	-5	2	103	101	1
5	0	-3	58	59	1	1	2	-2	93	86	1	-1	4	-1	124	120	1	-1	6	0	29	30	3	1	-5	2	134	133	1
-1	1	-3	440	438	1	2	2	-2	101	97	1	0	4	-1	67	67	1	0	6	0	155	157	1	2	-5	2	133	130	1
0	1	-3	85	94	1	3	2	-2	87	91	1	1	4	-1	91	94	1	1	6	0	25	18	3	3	-5	2	68	70	1
1	1	-3	490	536	1	4	2	-2	13	10	6	2	4	-1	86	85	1	2	6	0	3	13	2	4	-5	2	75	76	1
2	1	-3	301	320	1	5	2	-2	42	47	3	3	4	-1	72	74	1	-1	-6	1	87	86	1	-1	-4	2	29	28	2
3	1	-3	147	153	1	-1	3	-2	276	267	1	4	4	-1	50	50	2	0	-6	1	0	14	1	0	-4	2	116	112	1
4	1	-3	46	47	1	0	3	-2	27	34	2	-1	5	-1	83	83	1	1	-6	1	60	57	1	1	-4	2	8	12	7
5	1	-3	90	90	1	1	3	-2	272	285	1	0	5	-1	39	44	2	2	-6	1	20	10	4	2	-4	2	277	274	1
-1	2	-3	265	257	1	2	3	-2	64	66	1	1	5	-1	41	43	2	3	-6	1	42	38	2	3	-4	2	51	54	1
0	2	-3	294	291	1	3	3	-2	57	56	1	2	5	-1	0	12	1	-1	-5	1	39	43	2	4	-4	2	72	70	1
1	2	-3	159	165	1	4	3	-2	0	12	1	3	5	-1	33	34	3	0	-5	1	47	46	2	-1	-3	2	279	285	1
2	2	-3	196	206	1	-1	4	-2	14	14	6	-1	6	-1	55	58	2	1	-5	1	82	83	1	0	-3	2	27	35	2
3	2	-3	32	39	2	0	4	-2	114	111	1	0	6	-1	0	12	1	2	-5	1	51	54	2	1	-3	2	279	267	1
4	2	-3	39	38	2	1	4	-2	23	28	3	1	6	-1	87	86	1	3	-5	1	35	29	2	2	-3	2	53	54	1
5	2	-3	34	39	3	2	4	-2	64	64	1	2	6	-1	8	16	7	4	-5	1	38	34	2	3	-3	2	23	27	3
-1	3	-3	214	203	1	3	4	-2	38	35	2	-1	-6	0	14	20	13	-1	-4	1	97	94	1	4	-3	2	80	84	1
0	3	-3	170	167	1	4	4	-2	84	81	1	0	-6	0	158	156	1	0	-4	1	69	67	1	5	-3	2	7	19	7
1	3	-3	60	57	1	-1	5	-2	132	133	1	1	-6	0	32	31	2	1	-4	1	128	120	1	-1	-2	2	96	85	1
2	3	-3	101	112	1	0	5	-2	99	102	1	2	-6	0	69	67	1	2	-4	1	203	202	1	0	-2	2	32	33	1
3	3	-3	8	15	8	1	5	-2	30	30	3	3	-6	0	25	25	3	3	-4	1	103	104	1	1	-2	2	73	69	1
4	3	-3	42	44	2	2	5	-2	91	95	1	-1	-5	0	28	23	3	4	-4	1	46	48	1	2	-2	2	137	142	1
-1	4	-3	106	102	1	3	5	-2	30	31	3	0	-5	0	30	30	2	-1	-3	1	225	233	1	3	-2	2	50	50	1
0	4	-3	85	86	1	-1	6	-2	35	40	2	1	-5	0	62	62	1	0	-3	1	18	20	2	4	-2	2	23	27	3
1	4	-3	45	49	2	0	6	-2	0	10	1	2	-5	0	156	153	1	1	-3	1	87	80	1	5	-2	2	21	26	4
2	4	-3	185	192	1	1	6	-2	27	21	3	3	-5	0	90	88	1	2	-3	1	39	37	1	-1	-1	2	199	211	1
3	4	-3	39	40	2	2	6	-2	24	26	4	4	-5	0	32	36	2	3	-3	1	274	279	1	0	-1	2	58	51	1
4	4	-3	53	51	2	-1	-6	-1	32	26	3	-1	-4	0	116	119	1	4	-3	1	23	25	3	1	-1	2	101	102	1

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Table 6. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	-1	2	233	234	1	-1	1	3	422	422	1	3	2	4	32	32	2	3	4	5	32	35	3	2	-5	7	150	149	1
3	-1	2	32	39	2	0	1	3	526	510	1	4	2	4	20	18	3	-1	5	5	71	73	1	3	-5	7	16	7	5
4	-1	2	37	33	1	1	1	3	256	254	1	5	2	4	54	47	2	0	5	5	60	62	1	-1	-4	7	92	88	1
5	-1	2	19	22	5	2	1	3	77	78	1	-1	3	4	98	90	1	1	5	5	32	29	3	0	-4	7	41	40	2
-1	0	2	73	71	1	3	1	3	74	72	1	0	3	4	103	101	1	2	5	5	101	99	1	1	-4	7	81	80	1
0	0	2	56	58	1	4	1	3	70	66	1	1	3	4	80	84	1	-1	6	5	19	15	6	2	-4	7	201	200	1
1	0	2	49	43	1	5	1	3	89	82	1	2	3	4	78	81	1	0	6	5	23	24	4	3	-4	7	35	32	2
2	0	2	59	59	1	-1	2	3	91	88	1	3	3	4	51	53	1	1	6	5	26	21	3	4	-4	7	139	137	1
3	0	2	142	131	1	0	2	3	151	149	1	4	3	4	29	28	2	-1	-6	6	18	22	6	-1	-3	7	86	86	1
4	0	2	50	49	1	1	2	3	112	119	1	-1	4	4	34	39	2	0	-6	6	124	122	1	0	-3	7	399	389	1
5	0	2	71	71	1	2	2	3	192	192	1	0	4	4	43	40	1	1	-6	6	45	44	2	1	-3	7	52	57	1
-1	1	2	37	40	1	3	2	3	30	23	2	1	4	4	35	32	2	2	-6	6	50	46	2	2	-3	7	62	63	1
0	1	2	498	498	1	4	2	3	57	56	1	2	4	4	144	144	1	-1	-5	6	104	104	1	3	-3	7	64	70	1
1	1	2	194	213	1	5	2	3	33	27	2	3	4	4	0	9	1	0	-5	6	30	25	2	4	-3	7	60	53	1
2	1	2	48	46	1	-1	3	3	0	11	1	-1	5	4	80	89	1	1	-5	6	77	80	1	5	-3	7	45	46	2
3	1	2	98	93	1	0	3	3	49	40	1	0	5	4	95	98	1	2	-5	6	43	39	1	-1	-2	7	70	65	1
4	1	2	63	61	1	1	3	3	184	188	1	1	5	4	36	40	2	3	-5	6	101	103	1	0	-2	7	94	88	1
5	1	2	132	127	1	2	3	3	107	109	1	2	5	4	91	92	1	4	-5	6	41	36	2	1	-2	7	325	304	1
-1	2	2	386	360	1	3	3	3	167	167	1	3	5	4	56	58	2	-1	-4	6	87	86	1	2	-2	7	71	77	1
0	2	2	283	275	1	4	3	3	28	31	2	-1	6	4	60	66	2	0	-4	6	89	89	1	3	-2	7	29	31	2
1	2	2	65	63	1	-1	4	3	218	216	1	0	6	4	88	90	1	1	-4	6	73	70	1	4	-2	7	56	64	1
2	2	2	279	294	1	0	4	3	98	98	1	1	6	4	15	19	8	2	-4	6	42	40	1	5	-2	7	55	53	1
3	2	2	57	55	1	1	4	3	115	117	1	-1	-6	5	55	55	2	3	-4	6	101	107	1	-1	-1	7	66	63	1
4	2	2	107	107	1	2	4	3	23	15	3	0	-6	5	106	105	1	4	-4	6	47	48	2	0	-1	7	19	16	2
5	2	2	58	54	2	3	4	3	60	58	1	1	-6	5	21	21	4	-1	-3	6	24	31	2	1	-1	7	297	292	1
-1	3	2	83	83	1	4	4	3	17	17	5	2	-6	5	65	65	1	0	-3	6	128	123	1	2	-1	7	139	138	1
0	3	2	261	257	1	-1	5	3	77	78	1	3	-6	5	26	24	3	1	-3	6	125	126	1	3	-1	7	236	239	1
1	3	2	129	132	1	0	5	3	32	27	2	-1	-5	5	43	46	2	2	-3	6	110	110	1	4	-1	7	80	82	1
2	3	2	29	26	2	1	5	3	103	100	1	0	-5	5	132	132	1	3	-3	6	37	35	2	5	-1	7	26	20	3
3	3	2	39	38	2	2	5	3	84	81	1	1	-5	5	235	230	1	4	-3	6	36	33	2	-1	0	7	346	344	1
4	3	2	67	59	1	3	5	3	52	50	2	2	-5	5	48	48	1	5	-3	6	96	93	1	0	0	7	515	520	1
-1	4	2	41	41	2	-1	6	3	49	49	2	3	-5	5	88	85	1	-1	-2	6	162	159	1	1	0	7	64	69	1
0	4	2	40	48	2	0	6	3	15	8	7	4	-5	5	94	92	1	0	-2	6	72	71	1	2	0	7	125	128	1
1	4	2	16	14	5	1	6	3	59	59	2	-1	-4	5	56	56	1	1	-2	6	328	311	1	3	0	7	96	99	1
2	4	2	90	94	1	-1	-6	4	36	34	3	0	-4	5	95	93	1	2	-2	6	199	196	1	4	0	7	104	106	1
3	4	2	0	14	1	0	-6	4	22	23	4	1	-4	5	132	130	1	3	-2	6	219	216	1	5	0	7	40	37	2
4	4	2	67	63	1	1	-6	4	22	22	4	2	-4	5	59	59	1	4	-2	6	33	33	2	-1	1	7	162	155	1
-1	5	2	58	61	1	2	-6	4	51	52	2	3	-4	5	21	12	3	5	-2	6	71	70	1	0	1	7	56	58	1
0	5	2	84	83	1	3	-6	4	21	27	4	4	-4	5	49	51	1	-1	-1	6	220	215	1	1	1	7	125	126	1
1	5	2	4	13	4	-1	-5	4	51	52	2	-1	-3	5	117	114	1	0	-1	6	183	185	1	2	1	7	183	186	1
2	5	2	79	77	1	0	-5	4	12	17	11	0	-3	5	77	76	1	1	-1	6	524	503	1	3	1	7	12	12	7
3	5	2	66	63	2	1	-5	4	54	57	2	1	-3	5	153	144	1	2	-1	6	218	207	1	4	1	7	27	21	2
-1	6	2	31	29	3	2	-5	4	76	76	1	2	-3	5	87	89	1	3	-1	6	46	42	1	5	1	7	9	16	8
0	6	2	39	37	2	3	-5	4	55	50	1	3	-3	5	108	107	1	4	-1	6	107	105	1	-1	2	7	41	43	1
1	6	2	53	52	2	4	-5	4	68	65	1	4	-3	5	22	16	2	5	-1	6	47	41	2	0	2	7	33	30	1
-1	-6	3	96	95	1	-1	-4	4	29	27	2	5	-3	5	18	12	4	-1	0	6	104	97	1	1	2	7	85	84	1
0	-6	3	51	48	2	0	-4	4	226	223	1	-1	-2	5	57	56	1	0	0	6	236	235	1	2	2	7	117	120	1
1	-6	3	87	87	1	1	-4	4	210	206	1	0	-2	5	83	75	1	1	0	6	240	243	1	3	2	7	53	52	1
2	-6	3	30	31	3	2	-4	4	150	144	1	1	-2	5	14	17	3	2	0	6	32	32	1	4	2	7	55	53	1
3	-6	3	98	98	1	3	-4	4	6	14	5	2	-2	5	14	12	3	3	0	6	172	179	1	-1	3	7	43	40	1
-1	-5	3	103	101	1	4	-4	4	78	77	1	3	-2	5	58	60	1	4	0	6	226	227	1	0	3	7	219	221	1
0	-5	3	127	126	1	-1	-3	4	84	84	1	4	-2	5	37	43	2	5	0	6	26	28	3	1	3	7	84	86	1
1	-5	3	137	137	1	0	-3	4	191	190	1	5	-2	5	15	22	6	-1	1	6	199	190	1	2	3	7	36	34	2
2	-5	3	99	95	1	1	-3	4	186	179	1	-1	-1	5	54	42	1	0	1	6	140	146	1	3	3	7	27	27	2
3	-5	3	40	45	2	2	-3	4	283	276	1	0	-1	5	142	137	1	1	1	6	368	360	1	4	3	7	61	56	2
4	-5	3	6	7	6	3	-3	4	39	39	1	1	-1	5	167	157	1	2	1	6	123	125	1	-1	4	7	39	40	2
-1	-4	3	50	49	1	4	-3	4	24	22	2	2	-1	5	99	107	1	3	1	6	192	193	1	0	4	7	49	53	1
0	-4	3	87	85	1	5	-3	4	10	3	10	3	-1	5	179	171	1	4	1	6	116	116	1	1	4	7	173	172	1
1	-4	3	103	103	1	-1	-2	4	103	113	1	4	-1	5	24	20	2	5	1	6	58	58	1	2	4	7	20	16	3
2	-4	3	102	100	1	0	-2	4	79	88	1	5	-1	5	72	68	1	-1	2	6	432	424	1	3	4	7	41	41	2
3	-4	3	30	32	2	1	-2	4	230	211	1	-1	0	5	315	309	1	0	2	6	133	131	1	-1	5	7	18	23	6
4	-4	3	22	24	4	2	-2	4	305	294	1	0	0	5	119	125	1	1	2	6	186	181	1	0	5	7	27	27	3
-1	-3	3	63	57	1	3	-2	4	48	51	1	1	0	5	117	126	1	2	2	6	61	56	1	1	5	7	0	4	1
0	-3	3	174	167	1	4	-2	4	168	165	1	2	0	5	346	344	1	3	2	6	111	105	1	2	5	7	123	119	1
1	-3	3	215	203	1	5	-2	4	21	28	4	3	0	5	27	28	2	4	2	6	67	66	1	-1	6	7	75	75	1
2	-3	3	114	113	1	-1	-1	4	568	577	1	4	0	5	85	88	1	-1	3	6	96	98	1	0	6	7	39	39	2
3	-3	3	125	129	1	0	-1	4	171	161	1	5	0	5	14	16	6	0	3	6	42	41	1	-1	-6	8	115	111	1
4	-3	3	25	29	2	1	-1	4	227	216	1	-1	1	5	184	175	1	1	3	6	196	198	1	0	-6	8	88	92	1
5	-3	3	34	31	2	2	-1	4	113	102	1	0	1	5	493	489	1	2	3	6	85	82	1	1	-6	8	80	82	1
-1	-2	3	164	166	1	3	-1	4	69	72	1	1	1	5	192	184	1	3	3	6	34	35	2	2	-6	8	51	54	2
0	-2	3	303	291	1	4	-1	4	97	97	1	2	1	5	104	94	1	4	3	6	29	30	3	-1	-5	8	66	65	1
1	-2	3	268	257	1	5	-1	4	14	10	7	3	1	5	29	25	2	-1	4	6	49	48	1	0	-5	8	123	118	1
2	-2	3	111	103	1	-1	0	4	261	252	1	4	1	5	165	160	1	0	4	6	45	50	2	1	-5	8	77	79	1
3	-2	3	164	164	1	0	0	4	293	289	1	5	1	5	84	81	1	1	4	6	99	97	1	2	-5	8	11	12	11
4	-2	3	91	93	1	1	0	4	164	162	1	-1	2	5	81	82	1	2	4	6	45	43	2	3	-5	8	65	60	1
5	-2	3	80	78	1	2	0	4	28	32	1	0	2	5	74	73	1	3	4	6	77	73	1	-1	-4	8	74	75	1
-1	-1	3	515	536	1	3	0	4	112	116	1	1	2	5	58	61	1	-1	5	6	26	26	3	0	-4	8	38	34	2
0	-1	3	84	96	1	4	0	4	98	96	1	2	2	5	77	67	1	0	5	6	60	57	1	1	-4	8	159	157	1
1	-1	3	450	436	1	5	0	4	17	15	4	3	2	5	22	24	3	1	5	6	67	68	1	2	-4	8	29	26	2
2	-1	3	480	469	1	-1	1	4	247	245	1	4	2	5	39	41	2	2	5	6	96	92	1	3	-4	8	86	84	1
3	-1	3	75	71	1	0	1	4	278	269	1	-1	3	5	52	43	1	-1	6	6	35	34	3	4	-4	8	0	3	1
4	-1	3	50	47	1	1	1	4	46	49	1	0	3	5	83	81	1	0	6	6	25	25	4	-1	-3	8	85	82	1
5	-1	3	155	148	1	2	1	4	261	253	1	1	3	5	121	123	1	1	6	6	56	58	2	0	-3	8	64	59	1
-1	0	3	826	832	3	3	1	4	131	131	1	2	3	5	93	91	1	-1	-6	7	40	41	3	1	-3	8	108	111	1
0	0	3	165	170	1	4	1	4	61	61	1	3	3	5	53	51	1	0	-6	7	60	61	2	2	-3	8	40	38	1
1	0	3	182	173	1	5	1	4	42	40	2	4	3	5	41	42	2	1	-6	7	27	27	3	3	-3	8	152	163	1
2	0	3	166	166	1	-1	2	4	288	281	1	-1	4	5	95	96	1	2	-6	7	37	41	2	4	-3	8	46	46	1
3	0	3	257	252	1	0	2	4	210	213	1	0	4	5	21	23	3	-1	-5	7	53	50	2	-1	-2	8	227	215	1
4	0	3	191	188	1	1	2	4	241	242	1	1	4	5	111	107	1	0	-5	7	120	120	1	0	-2	8	95	100	1
5	0	3	36	37	2	2	2	4	37	33	1	2	4	5	97	98	1	1	-5	7	36	35	2	1	-2	8	209	210	1

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Table 6. Observed and calculated structure factors for 1 Page 5

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	-2	8	93	93	1	3	1	9	53	52	1	3	-5	11	62	61	1	2	1	12	54	55	1	0	-1	14	36	34	2
3	-2	8	52	53	1	4	1	9	192	188	1	-1	-4	11	92	92	1	3	1	12	129	128	1	1	-1	14	48	51	1
4	-2	8	21	15	3	-1	2	9	130	125	1	0	-4	11	128	125	1	4	1	12	91	86	1	2	-1	14	34	35	2
5	-2	8	41	40	2	0	2	9	163	165	1	1	-4	11	57	59	1	-1	2	12	144	146	1	3	-1	14	60	64	1
-1	-1	8	116	115	1	1	2	9	87	86	1	2	-4	11	48	50	1	0	2	12	70	74	1	4	-1	14	43	42	2
0	-1	8	32	34	1	2	2	9	176	178	1	3	-4	11	25	22	3	1	2	12	24	24	3	-1	0	14	73	70	1
1	-1	8	51	49	1	3	2	9	138	138	1	-1	-3	11	65	63	1	2	2	12	114	118	1	0	0	14	39	45	2
2	-1	8	110	110	1	4	2	9	44	43	2	0	-3	11	190	189	1	3	2	12	61	61	1	1	0	14	33	31	2
3	-1	8	53	56	1	-1	3	9	55	53	1	1	-3	11	96	97	1	-1	3	12	47	51	2	2	0	14	78	85	1
4	-1	8	46	47	1	0	3	9	172	179	1	2	-3	11	138	141	1	0	3	12	52	52	2	3	0	14	46	42	1
5	-1	8	38	39	2	1	3	9	58	58	1	3	-3	11	63	66	1	1	3	12	0	7	1	4	0	14	35	34	2
-1	0	8	55	58	1	2	3	9	0	3	1	4	-3	11	28	25	3	2	3	12	89	88	1	-1	1	14	61	60	1
0	0	8	148	145	1	3	3	9	51	48	1	-1	-2	11	99	98	1	3	3	12	4	13	3	0	1	14	36	37	2
1	0	8	138	134	1	-1	4	9	24	31	3	0	-2	11	16	16	4	-1	4	12	41	38	2	1	1	14	126	135	1
2	0	8	31	29	1	0	4	9	57	57	1	1	-2	11	65	63	1	0	4	12	19	17	5	2	1	14	38	32	2
3	0	8	146	146	1	1	4	9	15	11	7	2	-2	11	114	115	1	1	4	12	31	32	3	3	1	14	13	13	8
4	0	8	61	64	1	2	4	9	41	47	2	3	-2	11	69	69	1	2	4	12	44	39	2	-1	2	14	126	128	1
5	0	8	70	68	1	3	4	9	41	41	2	4	-2	11	110	111	1	-1	5	12	30	19	3	0	2	14	48	52	1
-1	1	8	51	47	1	-1	5	9	12	14	12	-1	-1	11	59	58	1	0	5	12	23	15	4	1	2	14	55	54	1
0	1	8	121	125	1	0	5	9	15	23	8	0	-1	11	108	111	1	-1	-5	13	50	50	2	2	2	14	116	121	1
1	1	8	39	44	1	1	5	9	59	62	2	1	-1	11	113	115	1	0	-5	13	16	20	6	3	2	14	16	12	6
2	1	8	38	34	1	2	5	9	55	53	2	2	-1	11	28	26	2	1	-5	13	16	24	6	-1	3	14	89	93	1
3	1	8	53	55	1	-1	-6	10	23	26	5	3	-1	11	92	92	1	2	-5	13	84	84	1	0	3	14	67	69	1
4	1	8	78	77	1	0	-6	10	17	17	6	4	-1	11	47	47	2	-1	-4	13	29	33	3	1	3	14	39	40	2
-1	2	8	45	47	1	1	-6	10	55	53	2	-1	0	11	53	56	1	0	-4	13	45	40	2	2	3	14	60	59	1
0	2	8	72	72	1	-1	-5	10	135	135	1	0	0	11	46	47	1	1	-4	13	25	22	3	-1	4	14	11	12	11
1	2	8	166	159	1	0	-5	10	31	32	2	1	0	11	87	83	1	2	-4	13	13	20	9	0	4	14	19	20	5
2	2	8	47	45	1	1	-5	10	102	100	1	2	0	11	127	131	1	3	-4	13	94	96	1	1	4	14	31	29	3
3	2	8	102	97	1	2	-5	10	12	19	11	3	0	11	117	117	1	-1	-3	13	86	82	1	-1	-5	15	43	40	2
4	2	8	34	32	2	3	-5	10	96	91	1	4	0	11	11	15	10	0	-3	13	73	70	1	0	-5	15	78	76	1
-1	3	8	84	83	1	-1	-4	10	134	130	1	-1	1	11	72	71	1	1	-3	13	99	99	1	1	-5	15	93	90	1
0	3	8	124	125	1	0	-4	10	57	56	1	0	1	11	171	170	1	2	-3	13	63	67	1	-1	-4	15	88	88	1
1	3	8	79	77	1	1	-4	10	217	211	1	1	1	11	32	33	2	3	-3	13	16	9	5	0	-4	15	16	16	6
2	3	8	27	20	2	2	-4	10	36	37	2	2	1	11	191	197	1	-1	-2	13	59	54	1	1	-4	15	10	9	10
3	3	8	22	25	3	3	-4	10	63	69	1	3	1	11	62	61	1	0	-2	13	88	94	1	2	-4	15	34	32	2
4	3	8	99	93	1	4	-4	10	41	42	2	4	1	11	39	42	2	1	-2	13	332	340	1	-1	-3	15	81	82	1
-1	4	8	98	99	1	-1	-3	10	117	115	1	-1	2	11	191	190	1	2	-2	13	78	77	1	0	-3	15	90	90	1
0	4	8	57	60	1	0	-3	10	84	81	1	0	2	11	52	54	1	3	-2	13	139	147	1	1	-3	15	97	94	1
1	4	8	195	198	1	1	-3	10	151	154	1	1	2	11	85	86	1	4	-2	13	61	55	1	2	-3	15	28	31	3
2	4	8	0	12	1	2	-3	10	121	128	1	2	2	11	22	29	3	-1	-1	13	146	149	1	3	-3	15	75	72	1
3	4	8	75	70	1	3	-3	10	68	62	1	3	2	11	33	36	2	0	-1	13	149	148	1	-1	-2	15	65	65	1
-1	5	8	37	43	2	4	-3	10	53	54	1	4	2	11	37	33	2	1	-1	13	136	138	1	0	-2	15	60	61	1
0	5	8	15	13	7	-1	-2	10	156	156	1	-1	3	11	141	144	1	2	-1	13	180	180	1	1	-2	15	16	12	4
1	5	8	53	55	2	0	-2	10	211	207	1	0	3	11	164	167	1	3	-1	13	48	51	1	2	-2	15	57	59	1
2	5	8	14	13	8	1	-2	10	21	13	2	1	3	11	24	32	3	4	-1	13	119	117	1	3	-2	15	16	16	5
-1	-6	9	84	81	1	2	-2	10	121	123	1	2	3	11	29	29	3	-1	0	13	31	30	2	-1	-1	15	0	9	1
0	-6	9	8	11	8	3	-2	10	144	148	1	3	3	11	110	109	1	0	0	13	160	161	1	0	-1	15	34	32	2
1	-6	9	14	16	8	4	-2	10	80	85	1	-1	4	11	37	38	2	1	0	13	72	73	1	1	-1	15	202	204	1
2	-6	9	21	17	3	-1	-1	10	237	230	1	0	4	11	67	74	1	2	0	13	107	109	1	2	-1	15	27	26	2
-1	-5	9	31	33	3	0	-1	10	193	195	1	1	4	11	45	45	2	3	0	13	11	15	11	3	-1	15	87	88	1
0	-5	9	138	140	1	1	-1	10	218	218	1	2	4	11	28	29	3	4	0	13	64	64	1	-1	0	15	34	39	2
1	-5	9	40	38	2	2	-1	10	242	248	1	-1	5	11	27	27	3	-1	1	13	62	64	1	0	0	15	118	116	1
2	-5	9	51	52	1	3	-1	10	86	85	1	0	5	11	15	2	7	0	1	13	97	96	1	1	0	15	19	24	4
3	-5	9	28	28	3	4	-1	10	21	19	3	1	5	11	5	11	5	1	1	13	22	28	3	2	0	15	45	51	2
-1	-4	9	46	49	2	-1	0	10	138	138	1	-1	-5	12	49	49	2	2	1	13	121	120	1	3	0	15	99	94	1
0	-4	9	144	145	1	0	0	10	39	43	1	0	-5	12	13	14	9	3	1	13	58	59	1	-1	1	15	28	32	3
1	-4	9	24	21	3	1	0	10	199	206	1	1	-5	12	70	69	1	4	1	13	8	7	7	0	1	15	48	46	1
2	-4	9	225	228	1	2	0	10	90	88	1	2	-5	12	57	55	1	-1	2	13	38	41	2	1	1	15	140	148	1
3	-4	9	55	55	1	3	0	10	244	248	1	-1	-4	12	99	95	1	0	2	13	27	22	3	2	1	15	27	24	3
4	-4	9	45	47	2	4	0	10	43	44	1	0	-4	12	65	70	1	1	2	13	49	48	1	3	1	15	76	75	1
-1	-3	9	99	98	1	-1	1	10	192	197	1	1	-4	12	73	70	1	2	2	13	110	117	1	-1	2	15	24	26	3
0	-3	9	80	84	1	0	1	10	183	184	1	2	-4	12	60	64	1	3	2	13	44	45	2	0	2	15	11	11	10
1	-3	9	150	152	1	1	1	10	82	81	1	3	-4	12	44	47	2	-1	3	13	125	127	1	1	2	15	13	24	12
2	-3	9	119	121	1	2	1	10	71	69	1	-1	-3	12	43	45	2	0	3	13	25	24	3	2	2	15	40	37	2
3	-3	9	23	22	2	3	1	10	118	118	1	0	-3	12	34	38	2	1	3	13	96	99	1	-1	3	15	48	53	2
4	-3	9	132	136	1	4	1	10	13	13	9	1	-3	12	55	54	1	2	3	13	6	7	5	0	3	15	21	18	4
-1	-2	9	90	85	1	-1	2	10	101	104	1	2	-3	12	127	124	1	-1	4	13	22	21	4	1	3	15	18	25	5
0	-2	9	190	186	1	0	2	10	74	71	1	3	-3	12	61	62	1	0	4	13	60	59	1	2	3	15	13	11	13
1	-2	9	85	85	1	1	2	10	69	68	1	4	-3	12	22	16	4	1	4	13	95	94	1	-1	4	15	17	15	6
2	-2	9	71	68	1	2	2	10	44	40	1	-1	-2	12	27	22	2	-1	-5	14	34	35	3	0	4	15	11	13	10
3	-2	9	0	9	1	3	2	10	76	78	1	0	-2	12	114	114	1	0	-5	14	90	85	1	-1	-4	16	73	70	1
4	-2	9	38	36	2	4	2	10	29	30	3	1	-2	12	101	102	1	1	-5	14	28	31	3	0	-4	16	11	8	10
-1	-1	9	43	44	1	-1	3	10	40	36	2	2	-2	12	68	65	1	2	-5	14	84	86	1	1	-4	16	45	40	2
0	-1	9	53	57	1	0	3	10	171	177	1	3	-2	12	63	65	1	-1	-4	14	49	49	2	2	-4	16	117	116	1
1	-1	9	135	133	1	1	3	10	66	63	1	4	-2	12	43	46	2	0	-4	14	22	22	3	-1	-3	16	25	26	3
2	-1	9	239	240	1	2	3	10	103	101	1	-1	-1	12	78	78	1	1	-4	14	152	154	1	0	-3	16	43	42	2
3	-1	9	42	38	1	3	3	10	68	71	1	0	-1	12	54	55	1	2	-4	14	95	93	1	1	-3	16	0	13	1
4	-1	9	42	44	2	-1	4	10	64	65	1	1	-1	12	76	75	1	3	-4	14	85	85	1	2	-3	16	105	104	1
5	-1	9	15	11	6	0	4	10	139	141	1	2	-1	12	195	195	1	-1	-3	14	92	90	1	3	-3	16	115	110	1
-1	0	9	237	234	1	1	4	10	69	73	1	3	-1	12	30	31	2	0	-3	14	236	238	1	-1	-2	16	11	9	11
0	0	9	118	109	1	2	4	10	62	60	1	4	-1	12	69	71	1	1	-3	14	48	48	1	0	-2	16	255	258	1
1	0	9	50	50	1	-1	5	10	13	15	12	-1	0	12	239	234	1	2	-3	14	64	68	1	1	-2	16	69	72	1
2	0	9	91	89	1	0	5	10	73	72	1	0	0	12	31	34	2	3	-3	14	35	42	2	2	-2	16	56	59	1
3	0	9	222	227	1	1	5	10	74	74	1	1	0	12	254	256	1	-1	-2	14	24	16	3	3	-2	16	20	22	3
4	0	9	32	32	2	0	-6	11	22	19	4	2	0	12	182	182	1	0	-2	14	81	77	1	-1	-1	16	79	78	1
5	0	9	54	51	2	1	-6	11	22	25	5	3	0	12	38	40	2	1	-2	14	62	60	1	0	-1	16	99	103	1
-1	1	9	91	89	1	-1	-5	11	17	19	6	4	0	12	31	32	2	2	-2	14	82	85	1	1	-1	16	117	116	1
0	1	9	333	326	1	0	-5	11	16	20	6	-1	1	12	62	62	1	3	-2	14	41	37	2	2	-1	16	102	104	1
1	1	9	81	86	1	1	-5	11	65	66	1	0	1	12	125	130	1	4	-2	14	0	7	1	3	-1	16	44	41	2
2	1	9	68	67	1	2	-5	11	51	47	2	1	1	12	56	57	1	-1	-1	14	10	12	10	-1	0	16	93	96	1

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Table 6. Observed and calculated structure factors for 1 Page 6

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	0	16	38	38	2	1	-3	17	44	42	2	-1	2	17	21	19	4	1	0	18	18	24	5	0	0	19	84	79	1
1	0	16	10	15	9	2	-3	17	61	62	1	0	2	17	19	15	5	2	0	18	91	87	1	1	0	19	60	58	1
2	0	16	72	70	1	-1	-2	17	98	98	1	1	2	17	71	77	1	-1	1	18	21	17	4	2	0	19	53	55	2
3	0	16	59	58	1	0	-2	17	51	54	2	2	2	17	15	16	8	0	1	18	44	50	2	-1	1	19	47	47	2
-1	1	16	40	41	2	1	-2	17	22	21	3	-1	3	17	9	3	9	1	1	18	55	60	2	0	1	19	20	11	4
0	1	16	65	63	1	2	-2	17	29	28	3	0	3	17	50	47	2	2	1	18	34	31	2	1	1	19	25	29	4
1	1	16	42	42	2	3	-2	17	64	69	1	0	-4	18	39	41	2	-1	2	18	24	25	3	-1	2	19	37	39	2
2	1	16	14	11	7	-1	-1	17	102	98	1	-1	-3	18	48	46	2	0	2	18	37	34	2	0	2	19	33	31	3
3	1	16	40	43	2	0	-1	17	40	41	2	0	-3	18	0	5	1	1	2	18	30	29	3	-1	-2	20	21	19	4
-1	2	16	16	17	6	1	-1	17	70	67	1	1	-3	18	35	36	2	-1	-3	19	114	115	1	0	-2	20	86	84	1
0	2	16	50	49	2	2	-1	17	13	12	8	2	-3	18	61	58	1	0	-3	19	38	38	2	1	-2	20	69	67	1
1	2	16	72	73	1	3	-1	17	4	13	4	-1	-2	18	0	7	1	1	-3	19	97	96	1	-1	-1	20	54	54	2
2	2	16	78	75	1	-1	0	17	36	37	2	0	-2	18	71	72	1	-1	-2	19	56	55	2	0	-1	20	18	19	5
-1	3	16	17	11	6	0	0	17	41	48	2	1	-2	18	38	40	2	0	-2	19	23	23	4	1	-1	20	29	17	3
0	3	16	12	22	12	1	0	17	81	85	1	2	-2	18	76	78	1	1	-2	19	28	27	3	-1	0	20	65	62	1
1	3	16	21	20	4	2	0	17	65	64	1	-1	-1	18	26	27	3	2	-2	19	32	31	2	0	0	20	16	15	6
-1	-4	17	78	72	1	3	0	17	55	55	2	0	-1	18	84	81	1	-1	-1	19	63	62	1	1	0	20	55	54	2
0	-4	17	61	57	1	-1	1	17	67	69	1	1	-1	18	24	25	3	0	-1	19	34	37	2	-1	1	20	26	27	4
1	-4	17	91	87	1	0	1	17	56	57	1	2	-1	18	16	13	5	1	-1	19	28	20	3	0	1	20	22	28	4
-1	-3	17	104	105	1	1	1	17	21	27	4	-1	0	18	57	58	2	2	-1	19	58	58	2						
0	-3	17	96	101	1	2	1	17	19	18	5	0	0	18	74	77	1	-1	0	19	23	19	4						

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Table 1. Observed and calculated structure factors for 2

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	-1	0	386	389	1	6	7	0	128	121	2	-4	2	1	138	144	1	3	6	1	62	63	2	-10	1	2	38	31	4
2	-1	0	482	476	5	7	7	0	0	12	1	-3	2	1	168	159	1	4	6	1	50	49	3	-9	1	2	122	124	2
3	-1	0	398	384	8	8	7	0	34	37	5	-2	2	1	132	139	4	5	6	1	21	24	8	-8	1	2	96	99	2
4	-1	0	281	272	1	0	8	0	60	66	2	-1	2	1	276	280	2	6	6	1	64	64	2	-7	1	2	115	110	1
5	-1	0	110	98	1	1	8	0	16	15	9	0	2	1	389	410	2	7	6	1	33	40	5	-6	1	2	147	141	1
6	-1	0	207	205	1	2	8	0	24	28	4	1	2	1	187	200	3	8	6	1	55	55	3	-5	1	2	76	62	1
7	-1	0	173	175	1	3	8	0	86	81	2	2	2	1	301	322	6	-8	7	1	36	37	5	-4	1	2	169	175	1
8	-1	0	74	78	2	4	8	0	68	65	2	3	2	1	212	212	1	-7	7	1	54	58	3	-3	1	2	135	145	1
9	-1	0	52	45	3	5	8	0	49	49	3	4	2	1	146	137	1	-6	7	1	99	101	2	-2	1	2	456	442	1
10	-1	0	50	51	4	6	8	0	135	125	2	5	2	1	160	147	1	-5	7	1	71	73	2	-1	1	2	611	625	3
11	-1	0	36	29	5	1	9	0	36	41	3	6	2	1	64	58	2	-4	7	1	80	71	2	0	1	2	130	119	3
1	0	0	471	486	4	2	9	0	29	25	4	7	2	1	108	114	1	-3	7	1	81	83	2	1	1	2	886	892	13
2	0	0	621	610	1	3	9	0	0	16	1	8	2	1	138	134	1	-2	7	1	110	111	2	2	1	2	689	680	8
3	0	0	1032	1033	1	4	9	0	41	35	4	9	2	1	46	51	4	-1	7	1	230	239	2	3	1	2	359	343	1
4	0	0	190	174	1	-11	-1	1	84	85	2	10	2	1	55	49	3	0	7	1	76	82	4	4	1	2	509	508	1
5	0	0	15	19	11	-10	-1	1	90	87	2	-11	3	1	22	22	10	1	7	1	93	92	1	5	1	2	429	428	1
6	0	0	0	17	1	-9	-1	1	155	164	1	-10	3	1	45	48	4	2	7	1	22	19	5	6	1	2	140	146	1
7	0	0	70	65	2	-8	-1	1	158	157	1	-9	3	1	66	67	2	3	7	1	80	83	2	7	1	2	175	177	1
8	0	0	62	62	3	-7	-1	1	193	192	1	-8	3	1	77	85	2	4	7	1	71	69	2	8	1	2	186	186	1
9	0	0	126	120	2	-6	-1	1	115	121	1	-7	3	1	25	27	6	5	7	1	141	142	2	9	1	2	43	38	4
10	0	0	62	63	3	-5	-1	1	141	135	1	-6	3	1	27	29	5	6	7	1	53	55	3	10	1	2	28	30	7
11	0	0	27	32	7	-4	-1	1	147	146	1	-5	3	1	61	59	2	7	7	1	21	25	10	-11	2	2	38	44	5
1	1	0	385	389	2	-3	-1	1	76	56	1	-4	3	1	215	214	1	-6	8	1	110	108	2	-10	2	2	91	87	2
2	1	0	480	476	1	-2	-1	1	318	325	2	-3	3	1	136	122	1	-5	8	1	60	62	3	-9	2	2	51	55	3
3	1	0	392	384	1	-1	-1	1	343	360	5	-2	3	1	127	126	2	-4	8	1	67	71	2	-8	2	2	141	146	1
4	1	0	274	272	1	0	-1	1	343	338	3	-1	3	1	165	148	1	-3	8	1	40	44	4	-7	2	2	161	169	1
5	1	0	108	98	1	1	-1	1	170	184	1	0	3	1	346	331	3	-2	8	1	21	24	5	-6	2	2	232	234	1
6	1	0	209	205	1	2	-1	1	801	829	1	1	3	1	269	260	2	-1	8	1	78	76	1	-5	2	2	298	290	1
7	1	0	181	175	1	3	-1	1	367	361	4	2	3	1	242	241	6	0	8	1	37	34	5	-4	2	2	61	51	1
8	1	0	79	78	2	4	-1	1	57	66	2	3	3	1	92	93	1	1	8	1	39	43	2	-3	2	2	77	58	1
9	1	0	42	45	4	5	-1	1	269	271	1	4	3	1	162	170	1	2	8	1	57	66	4	-2	2	2	201	196	3
10	1	0	58	51	3	6	-1	1	263	255	1	5	3	1	120	122	1	3	8	1	83	85	2	-1	2	2	197	181	13
11	1	0	25	29	8	7	-1	1	149	155	1	6	3	1	135	136	1	4	8	1	21	21	10	0	2	2	235	224	1
0	2	0	107	115	1	8	-1	1	70	60	2	7	3	1	49	50	3	5	8	1	26	26	7	1	2	2	87	82	6
1	2	0	296	271	5	9	-1	1	101	99	2	8	3	1	72	72	2	6	8	1	52	51	3	2	2	2	166	162	1
2	2	0	233	219	7	10	-1	1	42	38	4	9	3	1	40	40	4	-5	9	1	29	32	6	3	2	2	200	188	1
3	2	0	240	247	1	11	-1	1	0	19	1	10	3	1	40	46	5	-4	9	1	72	67	2	4	2	2	362	353	1
4	2	0	247	258	1	-11	0	1	18	6	18	-10	4	1	3	17	3	-3	9	1	54	51	3	5	2	2	68	64	2
5	2	0	114	96	1	-10	0	1	24	18	8	-9	4	1	79	80	2	-2	9	1	41	41	2	6	2	2	62	47	2
6	2	0	30	21	4	-9	0	1	58	52	3	-8	4	1	42	42	3	-1	9	1	5	16	4	7	2	2	264	260	1
7	2	0	70	77	2	-8	0	1	68	75	2	-7	4	1	71	73	2	0	9	1	22	32	6	8	2	2	142	139	1
8	2	0	40	43	4	-7	0	1	25	29	6	-6	4	1	76	77	2	1	9	1	19	18	7	9	2	2	82	79	2
9	2	0	98	95	2	-6	0	1	154	154	1	-5	4	1	89	93	1	2	9	1	22	32	5	10	2	2	108	111	2
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