Experimental Information for Thiamine Hydrochloride Dehydrate ($C_{12}H_{19}Cl_2N_4OS$)

Data Collection

A colorless needle of $C_{12}H_{19}Cl_2N_4OS$ having approximate dimensions of 0.31 × 0.20 × 0.17 mm was mounted on a glass fiber in a random orientation. Preliminary examination and data collection were performed with Mo $K\alpha$ radiation (λ = 0.71073 Å) on a Nonius KappaCCD. Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 11379 reflections in the range 4° < θ < 30°. The monoclinic cell parameters and calculated volume are: a = 7.099(1), b = 19.808(2), c = 11.638(1) Å, β = 101.53(1)°, V = 1603.6Å^3. For Z = 4 and M_r = 338.28 the calculated density is 1.40 g/cm^3. The space group was determined by the program *ABSEN* (McArdle 1996). From the systematic presences of:

$$h\,0\,l \quad h + l = 2n$$
$$0\,k\,0 \quad k = 2n$$

and from subsequent least-squares refinement, the space group was determined to be $P2_1/n$ (No. 14). The data were collected at a temperature of 263 ± 1 K. Data were collected to a maximum 2θ of 61.0°.

Data Reduction

A total of 11379 reflections were collected, of which 4074 were unique. Lorentz and polarization corrections were applied to the data. The linear absorption coefficient is 5.3 cm^{-1} for Mo $K\alpha$ radiation. An empirical absorption correction using *SCALEPACK* (Otwinowski & Minor 1996) was applied. Transmission coefficients ranged from 0.701 to 0.914 with an average value of 0.869. A secondary extinction correction was applied (Sheldrick 1997). The final coefficient, refined in least-squares, was 0.0170000 (in absolute units). Intensities of equivalent reflections were averaged. The agreement factor for the averaging was 4.5% based on intensity.

Structure Solution and Refinement

The structure was solved by direct methods using *SIR97* (Altomare *et al*. 1999). The remaining atoms were located in succeeding difference Fourier syntheses. Hydrogen atoms were included in the refinement but restrained to ride on the atom to which they are bonded. The structure was refined in full-matrix least-squares where the function minimized was $\Sigma w(|F_o|^2 - |F_c|^2)^2$ and the weight w is defined as

$$w = 1/[\sigma^2(F_o^2) + (0.1024P)^2 + 0.5044P]$$

where $P = \frac{1}{3}(F_o^2 + 2F_c^2)$. Scattering factors were taken from the "International Tables for Crystallography" (Hahn 1992). 4074 reflections were used in the refinements. However, only reflections with $F_o^2 > 2\sigma(F_o^2)$ were used in calculating R. The final cycle of refinement included 197 variable parameters and converged (largest parameter shift was 0.01 times its esd) with unweighted and weighted agreement factors of:

$$R_1 = \Sigma\,|F_o - F_c| \,/\, \Sigma\,F_o = 0.064$$
$$R_2 = \mathrm{SQRT}\,(\Sigma\, w(\,F_o^2 - F_c^2\,)^2 \,/\, \Sigma\, w(F_o^2)^2\,) = 0.170$$

The standard deviation of an observation of unit weight was 1.05. The highest peak in the final difference Fourier had a height of 0.65 e/Å^3. The minimum negative peak had a height of –0.67 e/Å^3. Refinement was performed on a AlphaServer 2100 using *SHELX97* (Sheldrick 1997). Crystallographic drawings were done using programs *ORTEP* (Johnson 1976), *PLUTON* (Spek 1991) and/or *Xtal_GX* (Hall & duBoulay 1995).

References

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Crystallographic Data

$Cl_2SON_4C_{12}H_{19}$	formula weight 338.28
a = 7.0994(6) Å	space group $P2_1/n$ (No. 14)
b = 19.808(2) Å	T = 263 K
c = 11.6378(11) Å	λ = 0.71073 Å
β = 101.529(6)°	ρ_{calc} = 1.401 g cm^{-3}
V = 1603.6(5) Å^3	μ = 0.531 mm^{-1}
Z = 4	
transmission coefficient	0.701 – 0.914
	$R(F_o)^a$ = 0.064
	$R_w(F_o^2)^b$ = 0.170

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a $R = \Sigma\,||F_o| - |F_c||/\,\Sigma\,|F_o|$ for $F_o^2 > 2\sigma(F_o^2)$

b $R_w = [\Sigma\, w\,(|F_o^2| - |F_c^2|)^2 / \Sigma\, w\,|F_o^2|^2]^{1/2}$

Crystal Data and Data Collection Parameters

formula	$Cl_2SON_4C_{12}H_{19}$
formula weight	338.28
space group	$P2_1/n$ (No. 14)
a, Å	7.0994(6)
b, Å	19.808(2)
c, Å	11.6378(11)
β, deg	101.529(6)
V, Å^3	1603.6(5)
Z	4
D_c,g cm^{-3}	1.401
crystal dimensions, mm	0.31× 0.20× 0.17
temperature, K	263.
wavelength radiation (Å)	Mo $K\alpha$ (0.71073)
monochromator	graphite
linear abs coefficient, mm^{-1}	0.531
absorption correction applied	empirical[a]
transmission factors: min, max	0.70, 0.91
diffractometer	Nonius KappaCCD
h range	0 to 8
k range	0 to 26
l range	–15 to 15
2θ range, deg	8.00 – 60.96
programs used	*SHELXL97*
F_{000}	708.0
weighting	$w = 1/[\sigma^2(F_o^2) + (0.1024P)^2 + 0.5044P]$ where $P = (F_o^2 + 2F_c^2)/3$
data collected	11379
unique data	4074
R_{int}	0.045
data used in refinement	4074
cutoff used in R-factor calculations	$F_o^2 > 2.0\sigma(F_o^2)$
data with $I > 2.0\sigma(I)$	2622
refined extinction coefficient	0.0170
number of variables	197
largest shift/esd in final cycle	0.00
$R(F_o)$	0.064
$R_w(F_o^2)$	0.170
goodness of fit	1.054

a Otwinowski, Z.: Minor, (1996) W. *Methods Enzymol*., **276**, 307–326.

Fractional Coordinates

Atom	*x*	*y*	*z*	*U* (Å^2)
CL1	0.20911(11)	0.09548(4)	–0.07646(7)	0.0529(3)
CL2	1.07366(11)	0.07841(4)	0.36080(7)	0.0497(3)
S4	0.59291(13)	0.21891(5)	0.33944(9)	0.0592(3)
O33	1.1303(8)	0.2325(2)	0.3890(6)	0.169(2)
N1	0.6057(3)	0.11777(12)	0.2131(2)	0.0396(7)
N8	0.7158(4)	–0.01705(16)	0.3906(3)	0.0511(9)
N9	0.4319(4)	–0.07208(13)	0.3832(2)	0.0456(7)
N11	0.1824(4)	–0.05939(13)	0.2206(2)	0.0446(8)
C2	0.7317(4)	0.16356(15)	0.1779(3)	0.0428(9)
C3	0.7420(5)	0.22185(16)	0.2398(3)	0.0470(9)
C5	0.5199(4)	0.14037(17)	0.2965(3)	0.0497(9)
C6	0.5800(4)	0.04950(15)	0.1619(3)	0.0432(9)
C7	0.4647(4)	0.00284(15)	0.2220(3)	0.0410(8)
C8	0.5402(4)	–0.02859(16)	0.3325(3)	0.0427(8)
C10	0.2564(4)	–0.08560(15)	0.3257(3)	0.0435(9)
C12	0.2842(4)	–0.01476(16)	0.1695(3)	0.0451(9)
C21	0.8364(5)	0.1459(2)	0.0830(3)	0.0606(11)
C31	0.8766(5)	0.28090(17)	0.2381(4)	0.0579(10)
C32	1.0743(10)	0.2651(4)	0.3045(6)	0.167(3)
C101	0.1330(5)	–0.1322(2)	0.3788(3)	0.0597(10)
H11	-0.068(6)	0.0761(18)	-0.186(3)	0.058(10)
H12	0.2292	0.0040	0.0973	0.0590
H33	1.1227	0.1923	0.3717	0.2200
H5A	0.5478	0.1102	0.3634	0.0650
H5B	0.3818	0.1405	0.2679	0.0650
H6A	0.7057	0.0296	0.1646	0.0560
H6B	0.5173	0.0533	0.0801	0.0560
H81	0.809(6)	0.014(2)	0.368(4)	0.071(12)
H82	0.762(6)	-0.044(2)	0.463(4)	0.078(12)
H10A	0.1886	-0.1765	0.3853	0.0780
H10B	0.0069	-0.1340	0.3299	0.0780
H10C	0.1238	-0.1161	0.4553	0.0780
H21A	0.8977	0.1855	0.0602	0.0790
H21B	0.7472	0.1285	0.0167	0.0790
H21C	0.9320	0.1123	0.1112	0.0790
H31A	0.8819	0.2918	0.1575	0.0760
H31B	0.8274	0.3201	0.2726	0.0760
H32A	1.1388	0.2461	0.2459	0.2170
H32B	1.1327	0.3090	0.3234	0.2170

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i\cdot\mathbf{a}_j$

Hydrogens included in calculation of structure factors but not refined.

$B_{iso}(H) = 1.3*B_{iso}(C)$

Atomic Displacement Parameters (*U*s)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
CL1	0.0448(5)	0.0591(5)	0.0518(5)	0.0036(3)	0.0024(3)	0.0060(4)
CL2	0.0448(5)	0.0525(5)	0.0509(5)	0.0028(3)	0.0071(3)	0.0053(3)
S4	0.0634(6)	0.0485(5)	0.0738(6)	0.0027(4)	0.0334(5)	0.0106(4)
O33	0.119(3)	0.073(3)	0.269(7)	0.016(3)	0.074(4)	0.012(3)
N1	0.0360(12)	0.0407(13)	0.0413(13)	0.0021(10)	0.0059(10)	0.0010(10)
N8	0.0437(15)	0.0584(18)	0.0480(16)	0.0035(12)	0.0018(12)	0.0067(13)
N9	0.0442(14)	0.0432(14)	0.0477(14)	0.0001(11)	0.0054(11)	0.0012(11)
N11	0.0373(14)	0.0451(15)	0.0492(15)	0.0018(11)	0.0037(11)	0.0044(12)
C2	0.0429(16)	0.0424(17)	0.0442(16)	0.0025(12)	0.0114(12)	0.0065(13)
C3	0.0480(17)	0.0415(18)	0.0533(18)	0.0010(13)	0.0141(14)	0.0026(14)
C5	0.0439(16)	0.0491(19)	0.0585(19)	0.0023(13)	0.0159(14)	0.0012(15)
C6	0.0438(16)	0.0431(17)	0.0419(16)	0.0002(13)	0.0065(12)	0.0040(13)
C7	0.0415(15)	0.0402(16)	0.0406(15)	0.0011(12)	0.0062(12)	0.0020(13)
C8	0.0425(16)	0.0441(17)	0.0412(15)	0.0023(12)	0.0076(12)	0.0025(13)
C10	0.0439(16)	0.0397(16)	0.0469(17)	0.0011(12)	0.0088(13)	0.0045(13)
C12	0.0442(16)	0.0415(17)	0.0476(17)	0.0019(13)	0.0045(13)	0.0014(13)
C21	0.073(2)	0.056(2)	0.060(2)	0.0034(17)	0.0306(18)	0.0001(17)
C31	0.062(2)	0.0433(19)	0.073(2)	0.0069(15)	0.0243(18)	0.0006(17)
C32	0.141(5)	0.168(7)	0.153(6)	0.113(5)	0.064(4)	0.106(5)
C101	0.057(2)	0.063(2)	0.059(2)	0.0106(17)	0.0116(16)	0.0009(17)

The form of the anisotropic temperature factor is:

$$\exp[\, 2\pi\{h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23}\}]$$

where a^*, b^*, and c^* are reciprocal lattice constants.

Bond Distances

Atom 1	Atom 2	Distance (Å)	Atom 1	Atom 2	Distance (Å)
S4	C5	1.684(4)	N11	C12	1.352(4)
S4	C3	1.720(3)	C2	C3	1.356(4)
O33	C32	1.178(7)	C2	C21	1.491(4)
N1	C5	1.324(4)	C3	C31	1.513(4)
N1	C2	1.392(4)	C6	C7	1.497(4)
N1	C6	1.474(4)	C7	C12	1.351(4)
N8	C8	1.314(4)	C7	C8	1.433(4)
N9	C10	1.319(4)	C10	C101	1.489(5)
N9	C8	1.365(4)	C31	C32	1.494(8)
N11	C10	1.336(4)			

Numbers in parentheses are estimated standard deviations in the least significant digits.

Bond Angles

Atom 1	Atom 2	Atom 3	Angle (°)	Atom 1	Atom 2	Atom 3	Angle (°)
C5	S4	C3	91.49(16)	N1	C6	C7	114.4(2)
C5	N1	C2	114.4(3)	C12	C7	C8	116.4(3)
C5	N1	C6	124.7(3)	C12	C7	C6	120.4(3)
C2	N1	C6	120.9(2)	C8	C7	C6	123.1(3)
C10	N9	C8	117.7(3)	N8	C8	N9	116.5(3)
C10	N11	C12	120.7(3)	N8	C8	C7	122.2(3)
C3	C2	N1	111.6(3)	N9	C8	C7	121.4(3)
C3	C2	C21	127.7(3)	N9	C10	N11	123.0(3)
N1	C2	C21	120.7(3)	N9	C10	C101	119.3(3)
C2	C3	C31	128.2(3)	N11	C10	C101	117.7(3)
C2	C3	S4	110.8(2)	C7	C12	N11	120.8(3)
C31	C3	S4	120.7(3)	C32	C31	C3	111.2(3)
N1	C5	S4	111.7(2)	O33	C32	C31	132.3(6)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Torsion Angles

Atom 1	Atom 2	Atom 3	Atom 4	Angle (°)
C5	S4	C3	C2	0.09 (0.29)
C5	S4	C3	C31	174.06 (0.30)
C3	S4	C5	N1	0.84 (0.26)
C5	N1	C2	C3	1.33 (0.38)
C5	N1	C2	C21	178.82 (0.29)
C6	N1	C2	C3	176.69 (0.27)
C6	N1	C2	C21	3.16 (0.42)
C2	N1	C5	S4	1.39 (0.34)
C6	N1	C5	S4	176.54 (0.22)
C2	N1	C6	C7	170.70 (0.26)
C5	N1	C6	C7	7.11 (0.41)
C10	N9	C8	N8	178.70 (0.29)
C10	N9	C8	C7	1.62 (0.44)
C8	N9	C10	N11	0.83 (0.45)
C8	N9	C10	C101	179.29 (0.29)
C12	N11	C10	N9	2.62 (0.46)
C12	N11	C10	C101	177.50 (0.29)
C10	N11	C12	C7	1.86 (0.46)
N1	C2	C3	S4	0.64 (0.36)
N1	C2	C3	C31	172.75 (0.33)
C21	C2	C3	S4	179.51 (0.28)
C21	C2	C3	C31	7.10 (0.60)
S4	C3	C31	C32	97.21 (0.42)
C2	C3	C31	C32	75.60 (0.55)
N1	C6	C7	C8	76.11 (0.36)
N1	C6	C7	C12	107.83 (0.34)
C6	C7	C8	N8	1.88 (0.49)
C6	C7	C8	N9	178.45 (0.28)
C12	C7	C8	N8	178.09 (0.31)
C12	C7	C8	N9	2.24 (0.45)
C6	C7	C12	N11	176.80 (0.28)
C8	C7	C12	N11	0.48 (0.46)
C3	C31	C32	O33	34.34 (0.99)

Calculated Powder Diffraction Data for Thiamine Hydrochloride Dehydrate

Cu $K\alpha$ Wavelength λ = 1.54178 Å

h	*k*	*l*	*d*-Spacing (Å)	2θ (°)	Integrated Intensity	Relative Intensity
0	2	1	7.4775	11.835	311782.	21.11%
1	1	0	6.5632	13.491	245762.	16.64%
1	0	-1	6.5488	13.521	84627.2	5.73%
1	1	-1	6.2178	14.244	12421.3	0.84%
0	3	1	5.7140	15.507	25787.7	1.75%
0	0	2	5.7015	15.541	1476780.	100.00%
1	2	0	5.6924	15.566	220957.	14.96%
0	1	2	5.4790	16.176	729715.	49.41%
1	0	1	5.4721	16.197	162281.	10.99%
1	2	-1	5.4626	16.225	404532.	27.39%
1	1	1	5.2745	16.808	40.0264	0.00%
0	4	0	4.9521	17.911	49448.8	3.35%
0	2	2	4.9412	17.951	31125.8	2.11%
1	2	1	4.7896	18.524	403209.	27.30%
1	3	0	4.7889	18.527	22908.5	1.55%
1	1	-2	4.7728	18.590	2988.01	0.20%
1	3	-1	4.6497	19.087	72885.4	4.94%
0	4	1	4.5423	19.543	495779.	33.57%
1	2	-2	4.4046	20.159	1089260.	73.76%
0	3	2	4.3153	20.581	152531.	10.33%

h	k	l	d-Spacing (Å)	2θ (°)	Integrated Intensity	Relative Intensity
1	3	1	4.2132	21.085	62989.3	4.27%
1	4	0	4.0342	22.032	218430.	14.79%
1	1	2	3.9511	22.502	856723.	58.01%
1	4	-1	3.9499	22.509	1077.94	0.07%
1	3	-2	3.9440	22.543	102564.	6.95%
0	5	1	3.7423	23.776	41311.5	2.80%
0	4	2	3.7387	23.798	183555.	12.43%
1	2	2	3.7345	23.826	21190.8	1.43%
0	1	3	3.7329	23.836	96809.7	6.56%
1	4	1	3.6718	24.239	236.615	0.02%
1	0	-3	3.6572	24.337	1231.47	0.08%
1	1	-3	3.5965	24.754	791.859	0.05%
0	2	3	3.5486	25.093	89571.6	6.07%
1	4	-2	3.4894	25.526	1008410.	68.28%
2	0	0	3.4781	25.611	38811.1	2.63%
2	1	-1	3.4747	25.636	6720.24	0.46%
1	5	0	3.4425	25.880	487355.	33.00%
1	3	2	3.4412	25.890	302871.	20.51%
1	2	-3	3.4308	25.970	67435.3	4.57%
2	1	0	3.4257	26.010	509848.	34.52%
1	5	-1	3.3897	26.291	101332.	6.86%
2	2	-1	3.3246	26.815	142113.	9.62%
0	6	0	3.3014	27.007	295873.	20.04%
0	3	3	3.2942	27.067	25224.0	1.71%
2	2	0	3.2816	27.173	1698.37	0.12%
2	0	-2	3.2744	27.234	630035.	42.66%
0	5	2	3.2534	27.413	246713.	16.71%
1	5	1	3.2090	27.800	56991.8	3.86%
1	3	-3	3.1993	27.886	13732.6	0.93%
0	6	1	3.1712	28.138	11638.7	0.79%
1	4	2	3.1268	28.546	279781.	18.95%
2	1	1	3.1161	28.646	354658.	24.02%
2	3	-1	3.1127	28.679	5367.69	0.36%
2	2	-2	3.1089	28.714	27799.9	1.88%
1	0	3	3.0861	28.931	12516.3	0.85%
1	5	-2	3.0851	28.940	843877.	57.14%
2	3	0	3.0773	29.016	30254.1	2.05%
1	1	3	3.0493	29.288	26160.7	1.77%
0	4	3	3.0152	29.626	48402.5	3.28%
2	2	1	3.0065	29.714	36257.1	2.46%
1	6	0	2.9825	29.958	14483.7	0.98%
1	6	-1	2.9480	30.318	4395.72	0.30%
1	2	3	2.9463	30.335	319122.	21.61%
1	4	-3	2.9419	30.382	7687.03	0.52%
2	3	-2	2.9335	30.471	10741.8	0.73%
2	4	-1	2.8742	31.116	63735.7	4.32%
0	6	2	2.8570	31.308	1548.63	0.10%
0	0	4	2.8507	31.378	246174.	16.67%
2	3	1	2.8470	31.420	70089.7	4.75%
2	4	0	2.8462	31.429	3330.30	0.23%
2	1	-3	2.8376	31.527	1443.63	0.10%
1	6	1	2.8268	31.651	53116.0	3.60%
1	5	2	2.8259	31.661	238673.	16.16%
0	1	4	2.8217	31.710	2706.01	0.18%
1	1	-4	2.8160	31.776	112968.	7.65%
1	3	3	2.7958	32.012	169054.	11.45%
2	2	-3	2.7541	32.509	5.55562	0.00%
0	7	1	2.7465	32.602	40685.5	2.76%
0	5	3	2.7428	32.647	18544.6	1.26%
1	6	-2	2.7410	32.669	40125.9	2.72%
0	2	4	2.7395	32.687	24189.8	1.64%
2	0	2	2.7360	32.730	228646.	15.48%
1	2	-4	2.7343	32.751	15233.6	1.03%
2	4	-2	2.7313	32.788	4442.39	0.30%
2	1	2	2.7103	33.050	34517.8	2.34%
1	5	-3	2.6873	33.341	470.091	0.03%
2	4	1	2.6611	33.678	163173.	11.05%
2	2	2	2.6373	33.992	74904.9	5.07%
2	5	-1	2.6353	34.018	52463.8	3.55%
2	3	-3	2.6299	34.090	997.957	0.07%
1	7	0	2.6212	34.207	3379.32	0.23%
1	4	3	2.6191	34.235	27079.0	1.83%
0	3	4	2.6172	34.260	93669.1	6.34%
2	5	0	2.6137	34.308	200032.	13.55%
1	3	-4	2.6127	34.322	20892.6	1.41%
1	7	-1	2.5976	34.527	43356.8	2.94%
1	6	2	2.5544	35.130	531.998	0.04%
0	7	2	2.5347	35.412	238215.	16.13%
2	3	2	2.5276	35.515	13516.8	0.92%
2	5	-2	2.5239	35.569	1476.99	0.10%
1	7	1	2.5136	35.720	39308.8	2.66%
0	6	3	2.4925	36.032	62751.7	4.25%
2	4	-3	2.4813	36.201	908.057	0.06%
0	8	0	2.4760	36.280	9184.11	0.62%
0	4	4	2.4706	36.362	2807.67	0.19%
2	5	1	2.4682	36.399	24261.4	1.64%
1	4	-4	2.4668	36.421	140473.	9.51%
2	0	-4	2.4589	36.543	945.780	0.06%
1	7	-2	2.4527	36.638	59775.3	4.05%
1	1	4	2.4513	36.659	152.418	0.01%
1	6	-3	2.4506	36.670	26422.5	1.79%
2	1	-4	2.4401	36.833	290764.	19.69%
1	5	3	2.4346	36.920	8980.87	0.61%
0	8	1	2.4197	37.156	8671.44	0.59%
2	6	-1	2.4110	37.294	7862.09	0.53%
1	2	4	2.3968	37.523	15930.9	1.08%
2	4	2	2.3948	37.556	10442.1	0.71%
2	6	0	2.3945	37.561	914.009	0.06%
2	2	-4	2.3864	37.693	7765.92	0.53%
3	0	-1	2.3665	38.023	1600.99	0.11%
3	1	-1	2.3497	38.304	7106.95	0.48%
1	8	0	2.3327	38.595	37676.4	2.55%
2	1	3	2.3271	38.692	48823.2	3.31%
2	6	-2	2.3248	38.731	48996.3	3.32%
2	5	-3	2.3227	38.768	32180.9	2.18%
1	7	2	2.3163	38.879	19675.5	1.33%
1	8	-1	2.3160	38.884	11493.7	0.78%
0	5	4	2.3139	38.920	124.086	0.01%
1	3	4	2.3137	38.925	6392.84	0.43%
1	5	-4	2.3108	38.975	28478.8	1.93%
1	0	-5	2.3080	39.025	25126.3	1.70%
2	3	-4	2.3043	39.090	6887.83	0.47%
3	1	0	2.3030	39.113	66230.1	4.48%
3	1	-2	2.2998	39.169	44258.9	3.00%
1	1	-5	2.2924	39.300	16733.8	1.13%
2	6	1	2.2811	39.504	28173.2	1.91%
2	2	3	2.2803	39.518	46787.6	3.17%
0	8	2	2.2711	39.684	3309.84	0.22%
0	7	3	2.2698	39.708	83439.5	5.65%
0	1	5	2.2656	39.785	41459.7	2.81%
3	2	0	2.2577	39.931	480.553	0.03%
1	8	1	2.2559	39.964	3557.77	0.24%
3	2	-2	2.2547	39.987	23611.2	1.60%
1	6	3	2.2545	39.990	6289.26	0.43%
2	5	2	2.2513	40.048	38967.2	2.64%
1	2	-5	2.2477	40.115	23409.9	1.59%

h	*k*	*l*	*d*-Spacing (Å)	2θ (°)	Integrated Intensity	Relative Intensity
1	7	-3	2.2381	40.296	5273.25	0.36%
3	3	-1	2.2277	40.492	136640.	9.25%
0	2	5	2.2224	40.592	38313.5	2.59%
1	8	-2	2.2115	40.800	40007.7	2.71%
1	4	4	2.2105	40.820	4880.42	0.33%
2	3	3	2.2083	40.862	12124.6	0.82%
2	7	-1	2.2078	40.873	4604.99	0.31%
2	4	-4	2.2023	40.979	57306.9	3.88%
2	7	0	2.1950	41.121	117593.	7.96%
3	0	1	2.1884	41.251	1982.00	0.13%
3	3	0	2.1877	41.264	1228.71	0.08%
3	3	-2	2.1850	41.319	3067.29	0.21%
3	0	-3	2.1829	41.360	22929.9	1.55%
1	3	-5	2.1787	41.444	13180.7	0.89%
3	1	1	2.1752	41.514	106.520	0.01%
3	1	-3	2.1698	41.622	4923.54	0.33%
2	6	-3	2.1648	41.723	15001.3	1.02%
0	9	1	2.1610	41.798	9385.55	0.64%
0	6	4	2.1577	41.867	84075.8	5.69%
0	3	5	2.1556	41.908	17268.2	1.17%
1	6	-4	2.1551	41.918	564.438	0.04%
2	7	-2	2.1410	42.207	3449.39	0.23%
3	2	1	2.1369	42.293	6265.95	0.42%
3	4	-1	2.1352	42.328	363.377	0.02%
3	2	-3	2.1318	42.400	22091.5	1.50%
2	4	3	2.1181	42.686	224.586	0.02%
1	8	2	2.1100	42.859	724.062	0.05%
2	7	1	2.1067	42.929	94864.5	6.42%
2	6	2	2.1066	42.930	58838.9	3.98%
3	4	0	2.0999	43.074	7291.31	0.49%
2	1	-5	2.0985	43.105	15890.3	1.08%
1	9	0	2.0984	43.107	22074.7	1.49%
3	4	-2	2.0975	43.127	33742.0	2.28%
1	5	4	2.0962	43.155	20404.5	1.38%
1	4	-5	2.0919	43.247	16866.4	1.14%
2	5	-4	2.0892	43.307	110176.	7.46%
1	9	-1	2.0863	43.371	2628.77	0.18%
1	7	3	2.0857	43.383	11905.3	0.81%
3	3	1	2.0773	43.567	1661.94	0.11%
0	8	3	2.0747	43.625	272.036	0.02%
3	3	-3	2.0726	43.671	10965.1	0.74%
0	4	5	2.0715	43.696	2565.05	0.17%
2	2	-5	2.0640	43.862	3416.11	0.23%
0	9	2	2.0533	44.104	55315.6	3.75%
1	8	-3	2.0503	44.170	1117.74	0.08%
1	0	5	2.0492	44.195	9173.96	0.62%
1	9	1	2.0420	44.361	77581.9	5.25%
1	1	5	2.0384	44.443	575.238	0.04%
3	5	-1	2.0316	44.599	10906.1	0.74%
2	8	-1	2.0270	44.706	18445.6	1.25%
2	8	0	2.0171	44.937	303.484	0.02%
2	5	3	2.0169	44.942	5697.06	0.39%
2	0	4	2.0161	44.961	73.7327	0.00%
2	7	-3	2.0140	45.009	167.229	0.01%
2	3	-5	2.0102	45.100	1456.34	0.10%
1	9	-2	2.0089	45.130	73434.5	4.97%
0	7	4	2.0083	45.144	3012.14	0.20%
1	2	5	2.0067	45.182	502.418	0.03%
1	7	-4	2.0063	45.193	3531.99	0.24%
2	1	4	2.0057	45.206	5251.01	0.36%
3	1	2	2.0018	45.299	12127.8	0.82%
3	4	1	2.0017	45.303	16816.5	1.14%
3	5	0	2.0012	45.315	29985.5	2.03%
3	5	-2	1.9991	45.365	49227.1	3.33%
3	4	-3	1.9975	45.403	4046.97	0.27%
3	1	-4	1.9955	45.450	2271.72	0.15%
1	5	-5	1.9942	45.481	2671.94	0.18%
0	10	0	1.9808	45.806	3524.29	0.24%
1	6	4	1.9779	45.879	2370.88	0.16%
0	5	5	1.9765	45.913	15073.7	1.02%
2	2	4	1.9756	45.936	21083.2	1.43%
2	8	-2	1.9750	45.950	59112.5	4.00%
2	6	-4	1.9720	46.023	32861.4	2.23%
2	7	2	1.9670	46.148	692.362	0.05%
3	2	-4	1.9658	46.176	12.1567	0.00%
1	3	5	1.9572	46.393	157636.	10.67%
0	10	1	1.9516	46.532	4344.01	0.29%
2	8	1	1.9479	46.625	2387.63	0.16%
2	4	-5	1.9414	46.791	2438.56	0.17%
1	9	2	1.9319	47.036	2959.11	0.20%
1	8	3	1.9313	47.052	2826.77	0.19%
2	3	4	1.9282	47.131	3367.24	0.23%
1	1	-6	1.9251	47.212	40.7408	0.00%
3	3	2	1.9247	47.221	50082.3	3.39%
3	6	-1	1.9234	47.257	1061.41	0.07%
3	3	-4	1.9191	47.367	660.031	0.04%
3	5	1	1.9156	47.460	31.1557	0.00%
3	5	-3	1.9119	47.558	7695.58	0.52%
2	6	3	1.9109	47.585	5143.48	0.35%
1	10	0	1.9051	47.738	18957.7	1.28%
0	9	3	1.9047	47.749	17332.8	1.17%
0	0	6	1.9005	47.861	1623.79	0.11%
1	2	-6	1.8984	47.918	41017.3	2.78%
3	6	0	1.8975	47.942	1412.94	0.10%
1	10	-1	1.8960	47.981	3083.82	0.21%
3	6	-2	1.8957	47.990	1051.33	0.07%
1	4	5	1.8935	48.048	15010.2	1.02%
0	1	6	1.8918	48.094	10574.4	0.72%
1	6	-5	1.8916	48.101	13113.7	0.89%
1	9	-3	1.8858	48.258	59.5791	0.00%
0	6	5	1.8764	48.514	18438.3	1.25%
2	8	-3	1.8740	48.581	2642.06	0.18%
0	10	2	1.8711	48.660	2193.53	0.15%
0	8	4	1.8694	48.709	1054.28	0.07%
1	8	-4	1.8677	48.755	3762.49	0.25%
2	9	-1	1.8676	48.759	12567.6	0.85%
2	4	4	1.8673	48.767	33660.6	2.28%
0	2	6	1.8664	48.790	2035.37	0.14%
3	4	2	1.8641	48.855	1935.80	0.13%
2	5	-5	1.8626	48.898	22922.4	1.55%
1	10	1	1.8626	48.898	2555.39	0.17%
1	7	4	1.8610	48.944	14742.6	1.00%
2	9	0	1.8598	48.975	28841.3	1.95%
3	4	-4	1.8590	48.997	22830.0	1.55%
1	3	-6	1.8562	49.077	3642.01	0.25%
2	7	-4	1.8561	49.081	54358.2	3.68%
1	10	-2	1.8374	49.613	34647.9	2.35%
2	8	2	1.8359	49.657	1448.36	0.10%
2	0	-6	1.8286	49.867	71032.1	4.81%
2	9	-2	1.8266	49.925	3229.58	0.22%
0	3	6	1.8263	49.934	1106.90	0.07%
0	2	0	9.9042	8.928	333515.	22.58%
0	1	1	9.8825	8.948	257128.	17.41%