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

Data Collection

A colorless needle of $Cl_2H_{20}Cl_2N_4O_2S$ 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 11310 reflections in the range 4° < θ < 30°. The monoclinic cell parameters and calculated volume are: *a* = 6.993(0), *b* = 20.663(1), *c* = 11.769(1) Å, β = 98.70(0)°, *V* = 1681.0 Å^3. For *Z* = 4 and M_r = 355.29 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 296 ± 1 K. Data were collected to a maximum 2θ of 61.0°.

Data Reduction

A total of 11310 reflections were collected, of which 4307 were unique. Lorentz and polarization corrections were applied to the data. The linear absorption coefficient is 5.1 cm^{-1} for Mo $K\alpha$ radiation. An empirical absorption correction using *SCALEPACK* (Otwinowski & Minor 1996) was applied. Transmission coefficients ranged from 0.757 to 0.914 with an average value of 0.892. A secondary extinction correction was applied (Sheldrick 1997). The final coefficient, refined in least-squares, was 0.0120000 (in absolute units). Intensities of equivalent reflections were averaged. The agreement factor for the averaging was 4.1% 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). 4307 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 206 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 1.04. The highest peak in the final difference Fourier had a height of 0.55 e/Å^3. The minimum negative peak had a height of –0.36 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

$Cl_2SO_2N_4Cl_2H_{20}$	formula weight 355.29
a = 6.9928(2) Å	space group $P2_1/n$ (No. 14)
b = 20.6631(10) Å	*T* = 296 K
c = 11.7695(5) Å	λ = 0.71073 Å
β = 98.699(2)°	ρ_{calc} = 1.404 g cm^{-3}
V = 1681.0(2) Å^3	μ = 0.514 mm^{-1}
Z = 4	
transmission coefficient	0.757 – 0.914
	$R(F_o)^a$ = 0.049
	$R_w(F_o^2)^b$ = 0.138

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	$Cl_2SO_2N_4C_{l2}H_{20}$
formula weight	355.29
space group	$P2_1/n$ (No. 14)
a, Å	6.9928(2)
b, Å	20.6631(10)
c, Å	11.7695(5)
β, deg	98.699(2)
V, Å^3	1681.0(2)
Z	4
D_c,g cm^{-3}	1.404
crystal dimensions, mm	0.31× 0.20× 0.17
temperature, K	296
wavelength radiation (Å)	Mo $K\alpha$ (0.71073)
monochromator	graphite
linear abs coefficient, mm^{-1}	0.514
absorption correction applied	empirical[a]
transmission factors: min, max	0.76, 0.91
diffractometer	Nonius KappaCCD
h range	0 to 8
k range	0 to 28
l range	–15 to 15
2θ range, deg	8.00 – 61.02
programs used	*SHELXL97*
F_{000}	744.0
weighting	$w = 1/[\sigma^2(F_o^2) + (0.0911P)^2 + 0.1219P]$ where $P = (F_o^2 + 2F_c^2)/3$
data collected	11310
unique data	4307
R_{int}	0.041
data used in refinement	4307
cutoff used in R-factor calculations	$F_o^2 > 2.0\sigma(F_o^2)$
data with $I > 2.0\sigma(I)$	2767
refined extinction coefficient	0.0120
number of variables	206
largest shift/esd in final cycle	0.01
$R(F_o)$	0.049
$R_w(F_o^2)$	0.138
goodness of fit	1.042

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

Fractional Coordinates

Atom	*x*	*y*	*z*	*U* (Å^2)
CL1	0.58096(9)	0.08138(3)	0.87142(6)	0.0454(2)
CL2	0.29549(9)	–0.08429(3)	0.58094(6)	0.0477(2)
S4	0.08694(9)	0.21095(4)	0.85394(6)	0.0474(2)
O1W	–0.1703(4)	0.20795(13)	0.5692(2)	0.0756(8)
O33	0.5919(3)	0.23338(12)	0.9237(2)	0.0670(8)
N1	0.1173(3)	0.11732(10)	0.72389(17)	0.0347(5)
N8	0.2188(3)	–0.01480(13)	0.8890(2)	0.0483(7)
N9	–0.0658(3)	–0.07081(11)	0.87562(18)	0.0411(6)
N11	–0.3075(3)	–0.05532(11)	0.71950(19)	0.0407(6)
C2	0.2458(3)	0.16354(12)	0.6926(2)	0.0367(7)
C3	0.2474(3)	0.21781(13)	0.7573(2)	0.0404(7)
C5	0.0216(3)	0.13650(14)	0.8067(2)	0.0418(7)
C6	0.0964(4)	0.05300(13)	0.6678(2)	0.0399(7)
C7	–0.0236(3)	0.00599(13)	0.7243(2)	0.0366(7)
C8	0.0460(3)	–0.02632(12)	0.8298(2)	0.0368(7)
C10	–0.2387(4)	–0.08365(12)	0.8198(2)	0.0385(7)
C12	–0.2029(3)	–0.01031(13)	0.6724(2)	0.0402(7)
C21	0.3585(4)	0.15016(15)	0.5982(2)	0.0504(8)
C31	0.3775(4)	0.27615(14)	0.7575(3)	0.0501(9)
C32	0.5826(5)	0.26036(17)	0.8128(3)	0.0615(10)
C101	–0.3655(4)	–0.13087(17)	0.8678(3)	0.0534(9)
H5	–0.071	0.112	0.835	0.054
H12	–0.255	0.010	0.604	0.052
H33	0.575	0.194	0.918	0.087
H6A	0.224	0.035	0.668	0.052
H6B	0.038	0.059	0.588	0.052
H81	0.317(5)	0.013(2)	0.860(3)	0.086
H82	0.254(5)	–0.0366(17)	0.952(3)	0.060
H1OA	–0.309	–0.173	0.868	0.069
H1OB	–0.491	–0.131	0.821	0.069
H1OC	–0.378	–0.119	0.945	0.069
H111	–0.417(5)	–0.0601(16)	0.693(3)	0.054
H21A	0.424	0.189	0.580	0.066
H21B	0.273	0.136	0.531	0.066
H21C	0.452	0.117	0.622	0.066
H31A	0.327	0.311	0.799	0.065
H31B	0.378	0.290	0.679	0.065
H32A	0.639	0.230	0.764	0.080
H32B	0.660	0.300	0.818	0.080

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

Hydrogens included in calculation of structure factors but not refined.

$B_{iso}(H) = I.3*B_{iso}(C)$

Atomic Displacement Parameters (*U*s)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
CL1	0.0371(4)	0.0526(4)	0.0467(4)	0.0005(3)	0.0070(3)	0.0070(3)
CL2	0.0466(4)	0.0485(4)	0.0462(4)	–0.0052(3)	0.0015(3)	–0.0002(3)
S4	0.0421(4)	0.0499(5)	0.0529(4)	–0.0009(3)	0.0159(3)	–0.0097(3)
O1W	0.0879(17)	0.0698(17)	0.0661(15)	0.0023(13)	0.0023(13)	–0.0043(12)
O33	0.0675(14)	0.0610(15)	0.0705(15)	–0.0076(12)	0.0035(11)	–0.0028(12)
N1	0.0310(10)	0.0378(12)	0.0356(10)	0.0026(8)	0.0061(8)	0.0026(8)
N8	0.0382(12)	0.0587(17)	0.0455(13)	–0.0053(11)	–0.0018(10)	0.0119(12)
N9	0.0381(11)	0.0442(13)	0.0407(11)	–0.0013(9)	0.0052(9)	0.0048(9)
N11	0.0348(12)	0.0431(14)	0.0429(12)	–0.0019(9)	0.0017(9)	0.0001(10)
C2	0.0307(11)	0.0387(14)	0.0417(13)	0.0025(10)	0.0084(9)	0.0074(10)
C3	0.0317(12)	0.0406(15)	0.0494(15)	0.0023(10)	0.0074(10)	0.0027(12)
C5	0.0351(12)	0.0503(17)	0.0421(14)	–0.0020(11)	0.0124(10)	–0.0033(12)
C6	0.0425(13)	0.0397(15)	0.0387(13)	–0.0020(11)	0.0098(10)	0.0002(11)
C7	0.0360(12)	0.0354(14)	0.0384(13)	–0.0007(10)	0.0061(10)	–0.0001(10)
C8	0.0337(12)	0.0392(15)	0.0371(12)	0.0005(10)	0.0040(9)	0.0003(10)
C10	0.0396(13)	0.0355(14)	0.0416(14)	0.0027(10)	0.0096(10)	–0.0011(10)
C12	0.0426(13)	0.0404(15)	0.0366(13)	0.0004(11)	0.0032(10)	0.0023(11)
C21	0.0531(15)	0.0530(18)	0.0496(15)	–0.0030(13)	0.0220(12)	0.0016(13)
C31	0.0525(16)	0.0374(16)	0.0623(18)	–0.0035(12)	0.0151(13)	0.0020(13)
C32	0.0532(17)	0.061(2)	0.071(2)	–0.0139(15)	0.0121(15)	0.0025(17)
C101	0.0526(16)	0.0543(19)	0.0546(17)	–0.0116(13)	0.0126(13)	0.0043(14)

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	1.676(3)	N11	H111	0.79(3)
S4	C3	1.720(3)	N11	C10	1.340(3)
O33	C32	1.411(4)	N11	C12	1.353(3)
N1	C5	1.324(3)	C2	C3	1.355(4)
N1	C2	1.398(3)	C2	C21	1.482(3)
N1	C6	1.481(3)	C3	C31	1.510(4)
N8	H82	0.87(4)	C6	C7	1.503(3)
N8	H81	0.99(4)	C7	C12	1.352(3)
N8	C8	1.322(3)	C7	C8	1.429(4)
N9	C10	1.313(3)	C10	C101	1.486(4)
N9	C8	1.369(3)	C31	C32	1.518(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	91.66(12)	C31	C3	S4	121.2(2)
C5	N1	C2	114.0(2)	N1	C5	S4	112.09(19)
C5	N1	C6	124.8(2)	N1	C6	C7	114.0(2)
C2	N1	C6	121.27(19)	C12	C7	C8	116.6(2)
H82	N8	H81	118(3)	C12	C7	C6	120.2(2)
H82	N8	C8	118(2)	C8	C7	C6	123.1(2)
H81	N8	C8	123(2)	N8	C8	N9	116.4(2)
C10	N9	C8	118.4(2)	N8	C8	C7	122.5(2)
H111	N11	C10	119(2)	N9	C8	C7	121.1(2)
H111	N11	C12	119(2)	N9	C10	N11	122.3(2)
C10	N11	C12	121.1(2)	N9	C10	C101	120.0(2)
C3	C2	N1	111.6(2)	N11	C10	C101	117.8(2)
C3	C2	C21	128.0(2)	C7	C12	N11	120.5(2)
N1	C2	C21	120.4(2)	C3	C31	C32	111.0(2)
C2	C3	C31	128.0(2)	O33	C32	C31	112.9(3)
C2	C3	S4	110.65(19)				

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	0.05(0.24)
C5	S4	C3	C31	–175.60(0.22)
C3	S4	C5	N1	0.92(0.19)
C5	N1	C2	C3	1.71(0.29)
C5	N1	C2	C21	–177.82(0.22)
C6	N1	C2	C3	–177.71(0.21)
C6	N1	C2	C21	2.76(0.33)
C2	N1	C5	S4	–1.67(0.26)
C6	N1	C5	S4	177.73(0.18)
C2	N1	C6	C7	170.87(0.21)
C5	N1	C6	C7	–8.48(0.34)
C10	N9	C8	N8	179.86(0.25)
C10	N9	C8	C7	0.56(0.36)
C8	N9	C10	N11	0.80(0.37)
C8	N9	C10	C101	–179.00(0.24)
C12	NII	C10	N9	–1.97(0.39)
C12	NII	C10	C101	177.84(0.25)
C10	NII	C12	C7	1.70(0.38)
N1	C2	C3	S4	–0.96(0.25)
N1	C2	C3	C31	174.32(0.24)
C21	C2	C3	S4	178.53(0.21)
C21	C2	C3	C31	–6.20(0.42)
S4	C3	C31	C32	103.13(0.26)
C2	C3	C31	C32	–71.70(0.37)
N1	C6	C7	C8	–75.75(0.31)
N1	C6	C7	C12	107.90(0.27)
C6	C7	C8	N8	3.50(0.39)
C6	C7	C8	N9	–177.25(0.23)
C12	C7	C8	N8	179.97(0.23)
C12	C7	C8	N9	–0.77(0.36)
C6	C7	C12	N11	176.24(0.23)
C8	C7	C12	N11	–0.35(0.36)
C3	C31	C32	033	–53.59(0.36)

Calculated Powder Diffraction Data for Thiamine Hydrochloride Monohydrate

Cu $K\alpha$ Wavelength λ = 1.54178 Å

h	*k*	*l*	*d*-Spacing (Å)	2θ (°)	Integrated Intensity	Relative Intensity
0	2	0	10.3316	8.558	163288.	12.89%
0	1	1	10.1377	8.722	121246.	9.57%
0	2	1	7.7252	11.454	653851.	51.62%
1	1	0	6.5553	13.507	337311.	26.63%
1	0	-1	6.3815	13.877	167184.	13.20%
1	1	-1	6.0973	14.527	235794.	18.62%
0	3	1	5.9269	14.947	14118.5	1.11%
0	0	2	5.8171	15.231	1156070.	91.28%
1	2	0	5.7451	15.423	167753.	13.24%
0	1	2	5.5994	15.826	473746.	37.40%
1	0	1	5.5833	15.872	32735.5	2.58%
1	2	-1	5.4293	16.326	446070.	35.22%
1	1	1	5.3900	16.445	30416.9	2.40%
0	4	0	5.1658	17.165	83583.1	6.60%
0	2	2	5.0688	17.495	23570.8	1.86%
1	2	1	4.9120	18.059	175506.	13.86%
1	3	0	4.8790	18.182	1732.94	0.14%
0	4	1	4.7213	18.795	948428.	74.88%
1	1	-2	4.6984	18.887	1289.22	0.10%
1	3	-1	4.6811	18.957	17945.0	1.42%
0	3	2	4.4442	19.978	50345.0	3.97%
1	2	-2	4.3716	20.314	1266550.	100.00%
1	3	1	4.3373	20.476	14911.0	1.18%
1	4	0	4.1379	21.474	142695.	11.27%
1	1	2	4.0708	21.832	832381.	65.72%

h	k	l	d-Spacing (Å)	2θ (°)	Integrated Intensity	Relative Intensity
1	4	-1	4.0151	22.139	1435.62	0.11%
1	3	-2	3.9517	22.499	63023.3	4.98%
0	5	1	3.8942	22.835	8534.01	0.67%
0	4	2	3.8626	23.025	47330.9	3.74%
1	2	2	3.8526	23.085	111940.	8.84%
0	1	3	3.8115	23.338	146390.	11.56%
1	4	1	3.7918	23.461	10448.7	0.82%
0	2	3	3.6307	24.517	18195.9	1.44%
1	0	-3	3.6241	24.563	1391.72	0.11%
1	1	-3	3.5696	24.944	1757.95	0.14%
1	3	2	3.5560	25.041	120199.	9.49%
1	5	0	3.5470	25.105	579695.	45.77%
1	4	-2	3.5260	25.257	973640.	76.87%
1	5	-1	3.4688	25.681	104134.	8.22%
2	0	0	3.4562	25.776	12513.2	0.99%
0	6	0	3.4439	25.870	288108.	22.75%
1	2	-3	3.4198	26.055	113310.	8.95%
2	1	-1	3.4115	26.120	289.944	0.02%
2	1	0	3.4088	26.140	240357.	18.98%
0	3	3	3.3792	26.374	56088.8	4.43%
0	5	2	3.3690	26.455	241740.	19.09%
1	5	1	3.3217	26.839	146747.	11.59%
0	6	1	3.3022	27.000	1400.73	0.11%
2	2	-1	3.2800	27.186	282955.	22.34%
2	2	0	3.2776	27.206	17404.2	1.37%
1	4	2	3.2363	27.561	380461.	30.04%
1	3	-3	3.2072	27.816	28980.3	2.29%
2	0	-2	3.1908	27.962	600491.	47.41%
1	0	3	3.1829	28.032	87.6701	0.01%
2	1	-2	3.1534	28.300	44948.7	3.55%
2	1	1	3.1471	28.358	473111.	37.35%
1	1	3	3.1458	28.370	9155.14	0.72%
1	5	-2	3.1386	28.436	912731.	72.06%
0	4	3	3.1014	28.785	125058.	9.87%
2	3	-1	3.0911	28.883	299.511	0.02%
2	3	0	3.0891	28.902	77218.9	6.10%
1	6	0	3.0825	28.965	4860.54	0.38%
2	2	-2	3.0487	29.294	23512.2	1.86%
2	2	1	3.0430	29.350	15310.9	1.21%
1	2	3	3.0419	29.361	492288.	38.87%
1	6	-1	3.0307	29.471	520.126	0.04%
1	4	-3	2.9668	30.121	1482.13	0.12%
0	6	2	2.9635	30.156	10425.9	0.82%
1	6	1	2.9311	30.497	116995.	9.24%
1	5	2	2.9291	30.518	412059.	32.53%
0	0	4	2.9085	30.739	249291.	19.68%
2	3	-2	2.8952	30.884	61756.7	4.88%
2	3	1	2.8903	30.938	97597.2	7.71%
1	3	3	2.8893	30.948	243710.	19.24%
0	1	4	2.8801	31.050	3451.98	0.27%
2	4	-1	2.8741	31.116	17960.9	1.42%
2	4	0	2.8725	31.134	8247.97	0.65%
0	7	1	2.8612	31.260	11332.3	0.89%
0	5	3	2.8279	31.638	13788.8	1.09%
1	1	-4	2.8123	31.818	93691.1	7.40%
1	6	-2	2.8030	31.926	113661.	8.97%
0	2	4	2.7997	31.965	37130.8	2.93%
2	0	2	2.7917	32.060	234940.	18.55%
2	1	-3	2.7737	32.273	5544.85	0.44%
2	1	2	2.7665	32.359	103471.	8.17%
1	2	-4	2.7373	32.714	2990.70	0.24%
1	5	-3	2.7248	32.869	1834.85	0.14%
1	7	0	2.7147	32.994	1100.88	0.09%
2	4	-2	2.7147	32.995	6503.55	0.51%
2	4	1	2.7106	33.045	273024.	21.56%
1	4	3	2.7098	33.055	33100.9	2.61%
2	2	-3	2.7016	33.159	1365.13	0.11%
2	2	2	2.6950	33.242	94997.6	7.50%
0	3	4	2.6794	33.441	173243.	13.68%
1	7	-1	2.6791	33.445	2676.36	0.21%
2	5	-1	2.6525	33.791	13005.5	1.03%
2	5	0	2.6512	33.808	148203.	11.70%
1	6	2	2.6507	33.814	1391.28	0.11%
0	7	2	2.6323	34.058	151396.	11.95%
1	3	-4	2.6246	34.162	3414.93	0.27%
1	7	1	2.6096	34.364	40520.7	3.20%
2	3	-3	2.5931	34.590	796.191	0.06%
2	3	2	2.5872	34.670	46011.6	3.63%
0	8	0	2.5829	34.730	2761.97	0.22%
0	6	3	2.5751	34.839	117828.	9.30%
0	4	4	2.5344	35.416	8016.04	0.63%
1	1	4	2.5276	35.515	153.023	0.01%
2	5	-2	2.5256	35.544	2077.92	0.16%
2	5	1	2.5223	35.592	11366.9	0.90%
1	5	3	2.5217	35.601	10789.4	0.85%
0	8	1	2.5215	35.604	27492.7	2.17%
1	7	-2	2.5180	35.655	40916.3	3.23%
1	6	-3	2.4965	35.973	22449.0	1.77%
1	4	-4	2.4878	36.102	225943.	17.84%
1	2	4	2.4727	36.331	31354.9	2.48%
2	4	-3	2.4610	36.510	5238.66	0.41%
2	4	2	2.4560	36.587	8677.41	0.69%
2	6	-1	2.4405	36.827	46341.5	3.66%
2	6	0	2.4395	36.843	524.625	0.04%
1	8	0	2.4195	37.158	67539.3	5.33%
2	0	-4	2.4124	37.272	50873.2	4.02%
1	7	2	2.4059	37.377	16363.7	1.29%
2	1	-4	2.3961	37.535	130201.	10.28%
1	8	-1	2.3942	37.565	10294.0	0.81%
2	1	3	2.3896	37.640	58592.4	4.63%
1	3	4	2.3887	37.656	20539.0	1.62%
0	5	4	2.3785	37.823	5122.49	0.40%
0	8	2	2.3606	38.120	13322.7	1.05%
2	2	-4	2.3492	38.313	14977.9	1.18%
0	7	3	2.3488	38.319	95517.6	7.54%
1	8	1	2.3442	38.398	919.167	0.07%
2	2	3	2.3431	38.417	61057.9	4.82%
2	6	-2	2.3406	38.460	15796.8	1.25%
1	5	-4	2.3399	38.472	82738.2	6.53%
2	6	1	2.3380	38.504	35311.4	2.79%
1	6	3	2.3375	38.513	19260.7	1.52%
3	0	-1	2.3283	38.670	550.726	0.04%
2	5	-3	2.3175	38.858	15034.2	1.19%
3	1	-1	2.3137	38.925	24709.1	1.95%
1	0	-5	2.3136	38.927	9487.50	0.75%
2	5	2	2.3133	38.931	37505.4	2.96%
0	1	5	2.3122	38.951	31675.9	2.50%
1	1	-5	2.2992	39.180	39062.5	3.08%
3	1	0	2.2899	39.345	36442.0	2.88%
1	7	-3	2.2887	39.366	24901.7	1.97%
1	4	4	2.2842	39.448	212.024	0.02%
1	8	-2	2.2771	39.576	70796.7	5.59%
2	3	-4	2.2768	39.582	36497.0	2.88%
3	2	-1	2.2714	39.680	6748.94	0.53%
2	3	3	2.2712	39.683	22533.7	1.78%
0	2	5	2.2700	39.706	15310.8	1.21%
1	2	-5	2.2577	39.931	27330.5	2.16%
0	9	1	2.2525	40.027	13710.6	1.08%
3	1	-2	2.2491	40.089	22670.3	1.79%
3	2	0	2.2489	40.094	5177.54	0.41%
2	7	-1	2.2454	40.159	5692.75	0.45%
2	7	0	2.2446	40.173	66654.0	5.26%
0	6	4	2.2221	40.598	40199.9	3.17%
3	2	-2	2.2102	40.827	23480.6	1.85%

h	*k*	*l*	*d*-Spacing (Å)	2θ (°)	Integrated Intensity	Relative Intensity
3	3	-1	2.2057	40.913	102372.	8.08%
0	3	5	2.2044	40.938	18427.1	1.45%
3	0	1	2.1978	41.068	2526.45	0.20%
1	3	-5	2.1932	41.158	39134.0	3.09%
1	8	2	2.1932	41.158	2293.56	0.18%
1	6	-4	2.1905	41.210	1550.92	0.12%
2	4	-4	2.1858	41.303	7495.59	0.59%
3	1	1	2.1854	41.310	792.304	0.06%
3	3	0	2.1851	41.317	252.638	0.02%
2	4	3	2.1809	41.400	3085.29	0.24%
1	9	0	2.1789	41.440	45053.7	3.56%
2	6	-3	2.1721	41.576	3322.98	0.26%
2	6	2	2.1686	41.645	15395.3	1.22%
1	5	4	2.1681	41.656	29531.3	2.33%
2	7	-2	2.1668	41.681	575.941	0.05%
2	7	1	2.1648	41.723	170785.	13.48%
1	7	3	2.1644	41.731	2387.38	0.19%
1	9	-1	2.1603	41.812	61116.9	4.83%
0	8	3	2.1497	42.028	12670.2	1.00%
3	2	1	2.1497	42.030	21411.8	1.69%
3	3	-2	2.1495	42.032	10053.2	0.79%
0	9	2	2.1356	42.320	103295.	8.16%
3	0	-3	2.1272	42.496	31609.0	2.50%
1	9	1	2.1234	42.575	79812.0	6.30%
3	4	-1	2.1227	42.590	894.495	0.07%
0	4	5	2.1215	42.614	9574.63	0.76%
3	1	-3	2.1160	42.731	34018.0	2.69%
1	4	-5	2.1115	42.827	16238.5	1.28%
1	0	5	2.1108	42.841	4377.02	0.35%
3	4	0	2.1043	42.980	4150.20	0.33%
1	8	-3	2.1034	43.000	12810.9	1.01%
1	1	5	2.0999	43.075	755.656	0.06%
3	3	1	2.0938	43.207	1282.47	0.10%
3	2	-3	2.0835	43.432	27161.8	2.14%
2	5	-4	2.0834	43.433	58874.8	4.65%
2	5	3	2.0791	43.527	2126.09	0.17%
2	0	4	2.0761	43.594	1618.70	0.13%
1	9	-2	2.0731	43.659	112863.	8.91%
3	4	-2	2.0725	43.674	14890.8	1.18%
0	7	4	2.0718	43.689	10748.1	0.85%
2	1	-5	2.0710	43.706	6924.03	0.55%
2	8	-1	2.0696	43.738	73933.7	5.84%
2	8	0	2.0690	43.752	6873.21	0.54%
1	2	5	2.0681	43.771	7272.80	0.57%
0	10	0	2.0663	43.811	18084.0	1.43%
2	1	4	2.0657	43.825	5890.94	0.47%
1	6	4	2.0476	44.231	7185.02	0.57%
1	7	-4	2.0461	44.266	6.15867	0.00%
2	2	-5	2.0405	44.394	19169.9	1.51%
2	2	4	2.0354	44.512	12619.7	1.00%
0	10	1	2.0345	44.533	4779.14	0.38%
3	3	-3	2.0324	44.580	29700.2	2.34%
2	7	-3	2.0311	44.611	57.6857	0.00%
3	1	2	2.0293	44.651	22022.2	1.74%
3	5	-1	2.0285	44.670	44699.6	3.53%
2	7	2	2.0283	44.676	460.283	0.04%
0	5	5	2.0275	44.693	11900.5	0.94%
3	4	1	2.0223	44.814	11435.5	0.90%
1	5	-5	2.0187	44.899	173.317	0.01%
1	3	5	2.0182	44.912	140297.	11.08%
3	5	0	2.0125	45.046	38176.8	3.01%
1	9	2	2.0092	45.124	212.798	0.02%
2	8	-2	2.0076	45.162	10807.8	0.85%
2	8	1	2.0059	45.201	5651.71	0.45%
1	8	3	2.0056	45.209	239.532	0.02%
3	2	2	2.0006	45.328	101.254	0.01%
2	3	-5	1.9925	45.523	1342.27	0.11%
2	3	4	1.9877	45.638	7410.64	0.59%
3	5	-2	1.9846	45.715	59934.7	4.73%
1	10	0	1.9797	45.833	11843.2	0.94%
2	6	-4	1.9758	45.929	73820.9	5.83%
0	9	3	1.9756	45.934	14040.2	1.11%
2	6	3	1.9722	46.018	16288.7	1.29%
3	4	-3	1.9669	46.149	1637.05	0.13%
1	10	-1	1.9658	46.176	1097.20	0.09%
3	3	2	1.9553	46.439	29413.3	2.32%
1	4	5	1.9540	46.472	35503.8	2.80%
0	10	2	1.9471	46.646	1626.46	0.13%
3	1	-4	1.9471	46.647	1505.54	0.12%
3	5	1	1.9404	46.816	2087.94	0.16%
1	9	-3	1.9395	46.841	672.092	0.05%
0	0	6	1.9390	46.852	6139.76	0.48%
1	10	1	1.9379	46.882	5103.39	0.40%
1	1	-6	1.9365	46.918	1985.93	0.16%
0	8	4	1.9313	47.051	21632.9	1.71%
2	4	-5	1.9307	47.067	21168.4	1.67%
0	1	6	1.9305	47.071	4983.59	0.39%
3	6	-1	1.9289	47.114	2239.84	0.18%
1	7	4	1.9283	47.129	20485.1	1.62%
0	6	5	1.9280	47.136	7598.37	0.60%
2	4	4	1.9263	47.180	4968.31	0.39%
3	2	-4	1.9216	47.302	266.086	0.02%
1	6	-5	1.9204	47.333	12538.4	0.99%
3	6	0	1.9150	47.475	316.901	0.03%
2	9	-1	1.9129	47.532	6191.36	0.49%
2	9	0	1.9124	47.544	57951.5	4.58%
1	2	-6	1.9114	47.570	42966.8	3.39%
1	8	-4	1.9104	47.596	12303.2	0.97%
0	2	6	1.9057	47.721	2758.01	0.22%
1	10	-2	1.8994	47.889	45983.5	3.63%
2	8	-3	1.8982	47.922	493.320	0.04%
3	4	2	1.8968	47.961	24.5653	0.00%
2	8	2	1.8959	47.984	465.111	0.04%
3	5	-3	1.8913	48.107	1484.66	0.12%
3	6	-2	1.8910	48.117	11879.4	0.94%
3	3	-4	1.8814	48.377	347.649	0.03%
1	5	5	1.8798	48.421	5940.85	0.47%
1	3	-6	1.8718	48.641	1699.57	0.13%
2	7	-4	1.8679	48.749	21986.1	1.74%
0	3	6	1.8665	48.789	71.8415	0.01%
2	7	3	1.8649	48.834	1345.87	0.11%
2	9	-2	1.8636	48.869	33.6197	0.00%
2	9	1	1.8623	48.906	9840.90	0.78%
1	9	3	1.8620	48.913	11501.0	0.91%
3	0	3	1.8611	48.939	41910.5	3.31%
2	5	-5	1.8590	48.998	25327.1	2.00%
2	5	4	1.8551	49.107	103187.	8.15%
0	11	1	1.8544	49.127	4406.30	0.35%
3	1	3	1.8536	49.150	1263.59	0.10%
3	6	1	1.8527	49.177	27230.9	2.15%
1	10	2	1.8499	49.255	35649.9	2.81%
3	2	3	1.8316	49.780	33973.2	2.68%
3	4	-4	1.8291	49.854	24108.7	1.90%
3	5	2	1.8287	49.865	1536.77	0.12%
3	7	-1	1.8281	49.883	22444.2	1.77%
0	7	5	1.8274	49.904	3.03482	0.00%