

Supporting Information

(Observed and Calculated Structure Factors Squared with Esds)

for

Crystal Structure of Zeolite LTA Containing Extraframework Tungsten(VI) Ions

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TABLES OF OBSERVED AND CALCULATED STRUCTURE FACTORS SQUARED WITH ESDS for $(\text{WCl})_{0.6}(\text{Ti}_7\text{Cl}_6)_{0.5}\text{Ti}_{8.5}\text{-A}$

In these tables, the Miller indices h, k, l appear in the first three columns. The fourth column is F_o^2 times the scale factor from least squares which puts the observed structure factors on an absolute scale, the fifth column is F_c^2 and the sixth column is σ_{hkl} , the estimated standard deviation of the corresponding F_o^2 , calculated from counting statistics.

Table S1. Observed and Calculated Structure Factors for $(\text{WCl})_{0.6}(\text{Tl}_7\text{Cl}_6)_{0.5}\text{Tl}_{8.5}\text{-A}$

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
0	1	1	2180.46	1918.19	22.76	5	5	5	1371.66	880.77	23.41
1	1	1	7133.89	10317.04	102.48	0	0	6	4155.7	15881.67	472.11
0	1	2	5718.23	5312.01	38.64	0	1	6	2218.24	1723.81	23.86
1	1	2	123.91	172.21	3.7	1	1	6	2043.12	2029.52	15.19
1	2	2	2751.33	3137.07	22.99	0	2	6	57189.2	47592.73	591.93
2	2	2	53536.59	22940	282.28	1	2	6	5293.54	4607.77	19.27
0	0	3	33089.39	40105.22	951.85	2	2	6	13637.34	11708.21	81.52
0	1	3	3211.26	2643.64	20.31	0	3	6	833.59	752.73	9.8
1	1	3	50335.07	69171.46	417.8	1	3	6	606.92	645.89	8.16
0	2	3	92385.82	111837.32	4806.03	2	3	6	726.13	609.46	9.14
1	2	3	3189.87	3638.63	18.26	3	3	6	37.45	32.9	6.75
2	2	3	373.7	290.04	7.59	0	4	6	3126.75	2845.96	29.66
0	3	3	946.97	1797.5	30.64	1	4	6	2831.51	3262.87	34.9
1	3	3	7217.26	10256.42	58.62	2	4	6	29999.31	25863.45	89.85
2	3	3	38868.81	45802.09	226.53	3	4	6	2435.7	1732.96	9.7
3	3	3	8000.58	13665.86	206.02	4	4	6	11566.13	9644.4	71.54
0	0	4	198969.95	195042.69	6431.17	0	5	6	17907.97	18305.27	98.75
0	1	4	63733.53	73585.62	1798.34	1	5	6	389.91	347.8	6.72
1	1	4	2872.43	5329.63	32.15	2	5	6	2668.31	2270.06	11.5
1	2	4	222.44	258.56	4.28	3	5	6	1298.28	1423.21	9.06
2	2	4	187761.44	196988.92	5514.1	4	5	6	135.41	107.58	7.21
0	3	4	353.26	560.27	9.88	5	5	6	49.94	51.73	9.52
1	3	4	54.37	84.07	4.44	0	6	6	59209.83	53521.18	377.81
2	3	4	17774.2	20192.34	74.72	1	6	6	548.18	665.3	11.51
3	3	4	7069.66	5692.11	35.56	2	6	6	5338.17	5005.51	43.01
0	4	4	156985.89	169411.72	3087.96	3	6	6	944.15	860.34	11.75
1	4	4	4340.4	5379.49	38.77	4	6	6	5944.8	5170.6	33.26
2	4	4	5178.12	4602.15	52.51	5	6	6	918.38	864.04	12.3
3	4	4	4035.21	3583.32	23.97	6	6	6	1330.43	1651.46	40.8
4	4	4	49199.46	49409.31	408.53	0	0	7	19925.26	17487.37	304.56
0	0	5	63294.71	76864.08	1819.2	0	1	7	11733.16	10351.54	139.34
0	1	5	5193.3	5783.88	41.26	1	1	7	204.66	368.81	7.66
1	1	5	269.93	604.16	7.47	0	2	7	37438.67	38909.91	403.32
0	2	5	16057.5	14317.73	81.47	1	2	7	527.84	449.71	5.13
1	2	5	1745.89	1477.58	9.14	2	2	7	17922.04	17436.47	85.91
2	2	5	21287.59	22113.7	114.95	0	3	7	4676.8	3526.02	31.79
0	3	5	9611.17	9564.51	65.4	1	3	7	5404.6	5363.9	22.66
1	3	5	6687.25	8746.5	37.65	2	3	7	1463.7	1281.96	10.44
2	3	5	2360.45	1339	11.86	3	3	7	4020.65	5764.95	39.06
3	3	5	221.74	169.85	6.66	0	4	7	3547.46	3306.33	27.65
0	4	5	4699.92	5526.21	45.09	1	4	7	92.96	67.2	5.45
1	4	5	230.03	130.59	4.61	2	4	7	3538.53	3214.49	14.56
2	4	5	4863.51	4407.34	21.75	3	4	7	4671.33	4169.5	20.05
3	4	5	3302.33	2946.47	15.61	4	4	7	4452.31	4390.64	39.89
4	4	5	29106.03	28203.38	137.4	0	5	7	10898.67	9857.86	59.39
0	5	5	63736.32	58833.14	432.79	1	5	7	67.88	117.31	6.26
1	5	5	5161.36	5242.42	31.05	2	5	7	2551.69	1847.68	11.99
2	5	5	3301.16	2956.77	27.92	3	5	7	740.87	555.78	9.74
3	5	5	4886.39	7715.03	56.2	4	5	7	6687.7	6576.3	25.77
4	5	5	632.19	855.05	14.15	5	5	7	58.67	56.77	10.99

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
0	6	7	2882.34	2190.51	17.33	7	7	8	808.03	933.38	14.98
1	6	7	63.29	56.31	6.43	0	8	8	890.47	872.36	20.4
2	6	7	1242.93	1511.35	11.84	1	8	8	350.87	345.94	15.03
3	6	7	25.81	39.42	7.22	2	8	8	7560.24	6362.66	44.79
4	6	7	6666.89	6270.85	25.82	3	8	8	2289.71	2357.49	18.88
5	6	7	150.47	118.42	7.48	4	8	8	2606.98	2447.46	22.12
6	6	7	154.41	239	11.63	5	8	8	399.07	455.17	16.73
0	7	7	1297.92	1072.66	21.72	6	8	8	1609.86	1536.75	19.06
1	7	7	16.12	49.34	10.72	7	8	8	99.33	133.4	13.58
2	7	7	942.29	1198.68	15.17	8	8	8	533.19	404.89	26.16
3	7	7	4149.76	3844.58	25.78	0	0	9	909.89	1220.46	61.22
4	7	7	2323.09	1765.13	15.93	0	1	9	80.72	197.53	14.22
5	7	7	2448.07	2084.09	18.07	1	1	9	464.4	274.68	13.11
6	7	7	740.11	885.87	17.92	0	2	9	5751.85	6630.69	58.46
7	7	7	883.24	1002.58	27.41	1	2	9	43.61	61.14	5.36
0	0	8	40974.13	37452.41	631.37	2	2	9	3044.27	2516.05	17.88
0	1	8	648.65	508.41	14.21	0	3	9	5152.46	4587.02	29.25
1	1	8	3368.86	3164.7	27.54	1	3	9	957.46	933.83	8.73
0	2	8	7564.93	7436.11	166.71	2	3	9	568.16	423.06	6.43
1	2	8	32.5	77.64	4.19	3	3	9	1154.73	1415.79	15.33
2	2	8	10654.46	8810.75	50.7	0	4	9	16412.7	14349.53	97.65
0	3	8	3064.14	2832.09	24.17	1	4	9	14.2	37.52	6.83
1	3	8	2053.3	1753.81	12.55	2	4	9	9192.67	9479.09	37.61
2	3	8	8849.21	7775.55	29.29	3	4	9	47.06	80.34	7.12
3	3	8	10549.3	8975.29	48.88	4	4	9	186.7	179.26	10.44
0	4	8	9645.37	8639.6	51.74	0	5	9	322.89	310.63	12
1	4	8	103.82	144.18	9.06	1	5	9	1505.04	1443.04	12.69
2	4	8	1459.51	1606.69	16	2	5	9	2395.72	2828.84	14.89
3	4	8	768.2	608.64	8.33	3	5	9	9.55	-7.48	7.48
4	4	8	13802.21	13193.34	76.55	4	5	9	1297.93	1174.87	10.06
0	5	8	359.14	329.79	12.16	5	5	9	21.25	18.77	11.27
1	5	8	2131.91	2047.06	12.1	0	6	9	1400.54	1646.86	22.77
2	5	8	450.44	504.09	8.37	1	6	9	366.62	355.22	7.94
3	5	8	110.36	142.96	6.95	2	6	9	2880.24	2540.4	14.21
4	5	8	346.75	436.84	8.04	3	6	9	93.71	88.18	7.95
5	5	8	3045.07	2885.98	22.14	4	6	9	1716.93	2155.25	14.33
0	6	8	1223.28	1225.88	20.72	5	6	9	67.22	92.37	8.62
1	6	8	112.25	66.6	6.89	6	6	9	588.98	601.31	13.77
2	6	8	5074.48	4392.52	21.82	0	7	9	4029.51	4428.25	36.1
3	6	8	3288.03	2970.01	15.03	1	7	9	4.96	3.29	8.23
4	6	8	3116.07	2760.69	25.45	2	7	9	2228.12	2093.85	16.78
5	6	8	1260.53	1063.62	10.36	3	7	9	50.62	52.4	8.39
6	6	8	4085.78	3716.86	28.36	4	7	9	45	93.71	8.65
0	7	8	138.86	121.69	11.81	5	7	9	8.39	2.78	8.62
1	7	8	475.62	483.21	8.43	6	7	9	369.75	463.13	10.05
2	7	8	888.12	911.83	9.64	7	7	9	13.88	31.71	14.04
3	7	8	144.36	140.66	8.17	0	8	9	1653.25	1537.55	18.36
4	7	8	2362.51	2175.54	14.14	1	8	9	349.6	338.27	9.55
5	7	8	34.07	33.33	8.72	2	8	9	829.13	852.4	10.61
6	7	8	453.26	459.74	9.28	3	8	9	321.5	305.18	9.27

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
4	8	9	291.86	306.5	9.15	0	8	10	801.86	703.29	16.31
5	8	9	77.23	107.01	9.29	1	8	10	64.18	57.38	9.46
6	8	9	581.58	686.45	10.77	2	8	10	1342.35	1421.98	12.72
7	8	9	4.42	5.88	10.06	3	8	10	153.91	152.86	9.58
8	8	9	1035.49	1137.76	18.22	4	8	10	478.62	476.33	10.63
0	9	9	880.83	993.39	25.63	5	8	10	234.62	249.38	10.42
1	9	9	85.46	91.93	13.12	6	8	10	716.2	853.94	11.89
2	9	9	260.71	421.55	13.68	7	8	10	79.87	107.81	10.74
3	9	9	5.92	-2.28	13.86	8	8	10	531.36	680.59	17.66
4	9	9	494.84	569.87	22.23	0	9	10	840.33	894.7	16.4
5	9	9	1110.71	1266.09	16.92	1	9	10	89.68	116.14	10.32
6	9	9	475.36	550.13	15.9	2	9	10	161.61	168.37	9.73
7	9	9	174.64	200.34	23.66	3	9	10	161.52	185.84	10.38
8	9	9	162.75	214.76	18.3	4	9	10	199.03	225.9	10.72
9	9	9	5.63	42.34	28.74	5	9	10	304.27	292.8	11.29
0	1	10	4.79	39.35	20.27	6	9	10	568.79	617.88	11.99
1	1	10	88.99	89.66	17.3	7	9	10	59.29	75.67	11.26
0	2	10	4195.84	3425.41	72.66	8	9	10	210.98	257.43	12.71
1	2	10	258.2	208.12	10.54	9	9	10	1.26	6.87	19.48
2	2	10	1259.37	1335.45	21.46	0	10	10	1825.78	2228.84	31.66
0	3	10	22.01	8.78	12.29	1	10	10	14.7	-0.73	15.15
1	3	10	961.33	933.29	14.98	2	10	10	450.28	445.82	15.9
2	3	10	7.92	-5.64	5.64	3	10	10	246.79	282.83	15.53
3	3	10	731.61	610.77	12.29	4	10	10	75.38	121.32	15.89
0	4	10	5087.56	4786.09	39.92	5	10	10	536.52	701.98	17.93
1	4	10	1628.28	1504.92	12.05	6	10	10	670.59	785.25	19.97
2	4	10	3239.72	2837.66	17.23	7	10	10	7.35	8.03	17.67
3	4	10	14.99	-7.42	7.42	8	10	10	247.21	271.39	17.54
4	4	10	808.62	780.94	15.79	9	10	10	7.12	26.01	18.76
0	5	10	176.18	140.51	11.07	10	10	10	21.04	53.31	32.35
1	5	10	561.38	499.83	8.82	0	0	11	26013.51	25801.24	396.04
2	5	10	1003.23	894.7	9.87	0	1	11	248.66	216.77	15.3
3	5	10	257.43	284.45	8.13	1	1	11	11.01	29.52	13.95
4	5	10	113.74	123.5	8.97	0	2	11	1857.17	1818.22	21.46
5	5	10	1103.88	1062.08	14.89	1	2	11	21.44	19.75	9.37
0	6	10	2667.02	2266.55	22.78	2	2	11	3344.84	3659.07	29.65
1	6	10	1402.66	1384.23	11.25	0	3	11	724.06	712.42	16.41
2	6	10	2690.83	2512.67	17.64	1	3	11	2.05	2.16	7.77
3	6	10	279.9	263.79	8.69	2	3	11	1270.53	1326.05	16.77
4	6	10	1591.62	1505.08	13.31	3	3	11	261.27	211.84	9.78
5	6	10	16.03	27.18	9.34	0	4	11	2249.83	2087.5	50.14
6	6	10	458.39	406.78	23.01	1	4	11	1125.46	1017.92	15.52
0	7	10	1389.95	1420.91	17.92	2	4	11	3792.38	3503.62	45.49
1	7	10	133.59	136.13	8.8	3	4	11	45.95	43.62	7.91
2	7	10	239.21	228.51	9.01	4	4	11	1139.73	1244.62	16.46
3	7	10	693.72	666.3	10.39	0	5	11	129.28	55.57	13.2
4	7	10	222.31	221.24	9.73	1	5	11	19.57	2.17	7.97
5	7	10	10.61	3.99	11.92	2	5	11	446.08	503.69	9.07
6	7	10	110.66	142.14	10.02	3	5	11	27.06	10.19	8.69
7	7	10	0.06	7.18	15.24	4	5	11	232.83	284.52	9.73

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
5	5	11	2039.75	2194.34	40.96	4	11	11	94.53	111.48	20.65
0	6	11	191	176.02	13.76	5	11	11	61.14	98.51	19.39
1	6	11	2.39	12.59	8.97	6	11	11	21.44	45.42	17.65
2	6	11	1708.14	1758.75	12.85	7	11	11	12.29	21.52	19.41
3	6	11	34.61	22.24	8.91	8	11	11	299.44	380.12	20.71
4	6	11	827.34	854.98	10.65	9	11	11	11.8	44.7	16.82
5	6	11	2257.47	2313.15	15.12	10	11	11	1.84	19.26	12.21
6	6	11	3018.64	3345.15	27.22	11	11	11	306.31	372.36	24.45
0	7	11	108.95	181.03	13.22	0	0	12	2777.9	2423.22	68.88
1	7	11	579.91	532	9.86	0	1	12	249.48	282.1	15.48
2	7	11	1096.79	1205.83	11.6	1	1	12	97.01	98.62	14.5
3	7	11	1.66	-9.45	9.5	0	2	12	865.31	760.41	36.1
4	7	11	81.28	139.83	10.08	1	2	12	10.26	2.19	10.84
5	7	11	129.8	120.9	10.85	2	2	12	2215.89	1896.11	25.91
6	7	11	271.6	279.42	10.9	0	3	12	57.59	82.81	20.83
7	7	11	40.14	32.68	14.94	1	3	12	298.29	408.98	13.12
0	8	11	2054.65	1885.29	20.82	2	3	12	38.02	28.2	15.09
1	8	11	106.73	92.48	10.16	3	3	12	371.98	373.31	12.66
2	8	11	893.29	902.94	11.64	0	4	12	109.44	87.45	35.29
3	8	11	29.81	25.77	9.99	1	4	12	769.3	616.55	18.16
4	8	11	689.48	778.44	11.7	2	4	12	644.61	462.06	10.64
5	8	11	61.79	100.02	10.9	3	4	12	305.68	222.6	7.66
6	8	11	133.2	161.75	11.5	4	4	12	934.13	853.84	15.63
7	8	11	59.68	81.08	11.99	0	5	12	205.22	180.29	22.75
8	8	11	74.87	100.22	15.98	1	5	12	68.21	52.35	7.7
0	9	11	363.71	388.37	17.38	2	5	12	5.44	-10.11	10.11
1	9	11	28	22.43	11.19	3	5	12	374.57	423.46	9.21
2	9	11	179.76	257.68	12.45	4	5	12	283.78	306.6	12.11
3	9	11	323.83	333.5	11.26	5	5	12	193.41	202.12	14.79
4	9	11	837.32	927.1	12.97	0	6	12	1195.93	1044.75	17.66
5	9	11	10.75	19.29	11.47	1	6	12	435.25	454.35	9.83
6	9	11	43.69	61.49	14.36	2	6	12	463.55	428.57	9.87
7	9	11	402.59	476.14	13.19	3	6	12	2.58	7.7	9.4
8	9	11	199.05	228.48	13.74	4	6	12	861.44	822.48	11.74
9	9	11	3.68	13.14	18.15	5	6	12	132.58	113.45	10.48
0	10	11	4.48	15.13	21.57	6	6	12	354.86	417.55	21.18
1	10	11	15.19	12.55	13.28	0	7	12	57.4	92.45	15.26
2	10	11	304.89	323.71	12.94	1	7	12	7.31	14.58	10.7
3	10	11	1.19	-3.86	12.63	2	7	12	55.52	51.78	10.72
4	10	11	820.49	997	16.1	3	7	12	158.88	221.89	10.02
5	10	11	15.35	21.38	11.66	4	7	12	53.92	55.43	9.83
6	10	11	141.92	162.86	12.77	5	7	12	50.14	14.74	10.49
7	10	11	188.54	245.34	14.21	6	7	12	405.44	461.89	12.05
8	10	11	49.8	98.98	13.32	7	7	12	18.73	32.58	16.17
9	10	11	44.96	59.29	12.2	0	8	12	759.46	852.39	18.92
10	10	11	85.6	100.75	26.01	1	8	12	161.78	164.58	11.5
0	11	11	2785.51	3274.23	48.7	2	8	12	155.02	165.28	11.2
1	11	11	101.69	187.93	18.1	3	8	12	0.45	2.73	11.62
2	11	11	104.8	73.24	18.3	4	8	12	483.32	646.49	12.58
3	11	11	62.17	101.36	18.93	5	8	12	11.9	3.87	11.66

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
6	8	12	227.8	309.5	12.26	1	1	13	8.42	22.34	30.85
7	8	12	184.84	216.45	12.27	0	2	13	1384.93	1372.49	45.32
8	8	12	211.69	267.04	18.48	1	2	13	5.96	16.04	17.99
0	9	12	199	217.11	33.46	2	2	13	1335.06	1294.67	24.6
1	9	12	109.37	129.49	14.07	0	3	13	394.69	409.38	36.87
2	9	12	536.2	476.07	12.97	1	3	13	14.53	40.35	17.47
3	9	12	35.19	69.59	11.94	2	3	13	3.43	5.04	12.01
4	9	12	86.48	107.19	11.79	3	3	13	111.79	90.73	16.73
5	9	12	1.96	2.04	12.1	0	4	13	1272.13	1226.21	36.63
6	9	12	19.54	9.62	15.34	1	4	13	38.22	32.38	15.84
7	9	12	0.74	-6.68	13.72	2	4	13	2241.74	2234.44	19.07
8	9	12	2.42	11.77	13.55	3	4	13	24.38	23.9	9.86
9	9	12	118.58	122.36	16.79	4	4	13	347.82	312.49	23.27
0	10	12	350.4	372.55	23.11	0	5	13	227.69	272.87	15.61
1	10	12	33.31	16.94	13.98	1	5	13	57.99	35.24	9.68
2	10	12	181.06	311.63	13.42	2	5	13	464.67	415.43	20.78
3	10	12	7.6	19.35	13.09	3	5	13	12.65	3.08	9.32
4	10	12	563.33	658.95	15.01	4	5	13	16.59	24.37	9.83
5	10	12	33.86	26.03	12.82	5	5	13	153.93	136.82	18.43
6	10	12	2.76	26.3	12.31	0	6	13	1387.74	1440.13	22.38
7	10	12	117.65	149.3	13.51	1	6	13	16.23	15.25	9.26
8	10	12	17.08	43.88	13.76	2	6	13	921.82	846.49	21.67
9	10	12	45.94	54.27	11.65	3	6	13	96.02	95.53	9.82
10	10	12	6.63	22.62	13.46	4	6	13	843.18	898.31	11.9
0	11	12	381.84	412.37	20.51	5	6	13	87.71	98.89	11.6
1	11	12	2.35	19.45	12.89	6	6	13	296.6	288.49	19.09
2	11	12	150.88	218.63	12.37	0	7	13	329.07	292.33	18.65
3	11	12	15.92	12.4	12.56	1	7	13	43.15	78.46	11.78
4	11	12	5.3	4.22	13.75	2	7	13	511.29	572.28	12.06
5	11	12	10.68	2.62	15.49	3	7	13	7.37	8.51	11.04
6	11	12	72.54	134.68	14.86	4	7	13	24.27	21.57	11.29
7	11	12	1.59	1.6	11.59	5	7	13	8	20.49	11.58
8	11	12	92.07	133.48	18.45	6	7	13	82.9	91.89	11.96
9	11	12	10.59	25.34	14.53	7	7	13	4.6	4.54	18.02
10	11	12	30.22	34.78	9.06	0	8	13	824.96	839.68	40.67
11	11	12	39.85	32.45	11.27	1	8	13	68.07	66.69	12.11
0	12	12	18.07	61.43	35.29	2	8	13	304.05	291.63	12.25
1	12	12	47.81	49.86	24.01	3	8	13	482.56	573.14	13.51
2	12	12	69.77	142.53	21.2	4	8	13	336.76	391.28	12.43
3	12	12	64.68	68.91	19.48	5	8	13	4.12	-2.16	12.01
4	12	12	19.67	33.07	17.19	6	8	13	119.35	140.69	12.61
5	12	12	38.21	74.24	18.48	7	8	13	30.96	26.73	12.77
6	12	12	91.11	118.18	27.97	8	8	13	401.99	527.63	19.59
7	12	12	1.12	14.25	14.81	0	9	13	56.04	64	20.47
8	12	12	51.25	53.51	16.6	1	9	13	3.58	6.68	13.76
9	12	12	1.69	8.23	10.98	2	9	13	119.97	98.36	13.01
10	12	12	43.8	14	9.51	3	9	13	1.6	11.89	13.46
11	12	12	1.52	11.63	20.26	4	9	13	379.22	457	13.83
12	12	12	0.72	0.79	26.32	5	9	13	68.62	71.08	12.8
0	1	13	36.8	84.26	65.64	6	9	13	136.58	164.68	12.54

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
7	9	13	83.04	71.33	12.58	0	1	14	35.4	77.46	52.28
8	9	13	44.6	58.43	12.73	1	1	14	154.34	125.79	32.42
9	9	13	19.48	34.69	16.07	0	2	14	71.36	87.3	24
0	10	13	284.08	295.58	19.39	1	2	14	2.47	-17.4	17.4
1	10	13	4.21	13.21	13.8	2	2	14	592.66	411.47	24.5
2	10	13	127.67	155.33	12.53	0	3	14	255.55	285.6	20.95
3	10	13	57.92	44.47	12.38	1	3	14	39.63	39.42	15.32
4	10	13	298.87	354.97	13.59	2	3	14	338.45	409.39	17.21
5	10	13	18.32	36.13	13.97	3	3	14	542.46	539.25	24.3
6	10	13	85.94	120.1	12.66	0	4	14	52.41	48.61	19.87
7	10	13	93.24	107.33	16.94	1	4	14	175.39	203.49	13.59
8	10	13	108.21	122.56	10.5	2	4	14	544.04	697.08	15.81
9	10	13	6.46	15.42	9.66	3	4	14	37.96	26.22	14.98
10	10	13	10.49	15.19	9.83	4	4	14	90.76	76.4	25.23
0	11	13	131.48	71.29	21.79	0	5	14	527.09	473.09	24.85
1	11	13	8.42	32.57	14.79	1	5	14	278.29	312.57	14.87
2	11	13	47.96	45.45	13.58	2	5	14	51.63	57.97	12.36
3	11	13	83.13	84.56	12.84	3	5	14	16.04	24.86	10.85
4	11	13	229.57	233.8	17.38	4	5	14	0.16	15.9	11.98
5	11	13	5.14	5.6	11.33	5	5	14	3.2	18.85	15.06
6	11	13	101.1	119.49	15.28	0	6	14	818.7	843	25.56
7	11	13	51.22	52.95	11.54	1	6	14	26.92	27.1	13.47
8	11	13	79.78	58.14	8.06	2	6	14	278.28	185.55	14.23
9	11	13	3.25	19.89	7.68	3	6	14	10.26	18.65	11.18
10	11	13	17.51	9.72	6.23	4	6	14	131.9	128.45	10.37
11	11	13	17.59	-0.55	11.26	5	6	14	18.76	33.17	10.84
0	12	13	141.17	231.98	76.86	6	6	14	87.22	90.24	16.73
1	12	13	0.16	2.29	17.09	0	7	14	29.09	40.79	18.66
2	12	13	114.97	78.25	14.7	1	7	14	147.41	127.9	12.41
3	12	13	6.96	11.78	13.33	2	7	14	106.25	86.31	15.36
4	12	13	23.45	20.87	10.13	3	7	14	1.4	-3.44	11.28
5	12	13	10.65	31.32	8.96	4	7	14	4.23	15.99	11.37
6	12	13	65.08	51.08	8.13	5	7	14	2.76	6.64	11.86
7	12	13	1.32	6.53	7.61	6	7	14	17.82	16.17	13.78
8	12	13	19.27	18.67	8	7	7	14	21.76	40.17	16.99
9	12	13	25.63	3.91	6.08	0	8	14	435.47	414.81	29.02
10	12	13	9.68	14.47	16.98	1	8	14	2.52	8.56	13.33
11	12	13	18.57	26.08	21.96	2	8	14	6.14	29.14	13.25
12	12	13	2.79	36.63	43.13	3	8	14	580.75	635.29	13.92
0	13	13	67.69	23.27	18.56	4	8	14	121.95	144.14	12.53
1	13	13	0.86	30.41	12.06	5	8	14	0.61	32.32	12.27
2	13	13	115.05	53.42	11.95	6	8	14	11.38	17.57	12.23
3	13	13	2.32	11.71	11.73	7	8	14	24.08	54.37	11.38
4	13	13	157.72	101.4	43.27	8	8	14	340.48	355.87	22.35
5	13	13	23.07	15.63	11.76	0	9	14	11.14	51.63	19.73
6	13	13	32.46	13.74	15.16	1	9	14	2.17	3.77	13.08
7	13	13	30.03	5.93	10.6	2	9	14	91.03	125.05	14.74
8	13	13	6.28	4.91	12.49	3	9	14	30.86	32.11	12.73
9	13	13	11.1	154.42	108.61	4	9	14	143.92	221.5	19.73
10	13	13	8.57	-1.95	22.7	5	9	14	0.44	27.29	13.36

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
6	9	14	26.58	38.68	17.13	2	14	14	36.49	12.2	16.14
7	9	14	41.23	31.12	13.7	3	14	14	28.8	17.14	22.18
8	9	14	2.47	15.99	11.43	4	14	14	3.14	19.38	14.99
9	9	14	21.76	39.14	23.13	5	14	14	9.08	-6.85	20.02
0	10	14	45.72	74.79	21.51	6	14	14	10.69	-7.06	26.4
1	10	14	1.61	18.24	14.1	7	14	14	0.71	6.25	34.91
2	10	14	56.19	67.28	12.64	0	0	15	278.71	252.56	54.12
3	10	14	4.43	5.19	12.21	0	1	15	567.68	590.86	50.34
4	10	14	167.48	276.57	12.22	1	1	15	171.17	165.54	22.04
5	10	14	10.3	48.92	12.37	0	2	15	1386.96	1411.57	69.72
6	10	14	3.62	6.14	10.02	1	2	15	36.91	8.78	18.9
7	10	14	54.95	65.06	10.03	2	2	15	1981.74	1915.59	51.95
8	10	14	16.79	18.92	8.67	0	3	15	3.21	11.24	26.8
9	10	14	8.64	8.49	7.37	1	3	15	49.37	64.1	16.51
10	10	14	5.01	4.13	13.59	2	3	15	12.56	48.45	19.72
0	11	14	17.37	32.65	23.79	3	3	15	9.96	29.11	23.4
1	11	14	2.98	10.85	13.39	0	4	15	425.61	449.86	33.21
2	11	14	8.28	18.68	12.37	1	4	15	3.11	33.54	16.28
3	11	14	28.34	65.44	12.88	2	4	15	169.44	193.52	14.62
4	11	14	22.06	37.29	11.71	3	4	15	157.85	167.56	14.64
5	11	14	61.28	60.44	9.37	4	4	15	536.53	522.76	23.38
6	11	14	81.74	70.28	11.76	0	5	15	95.31	39.71	36.29
7	11	14	1.32	32.63	10.45	1	5	15	10.66	13.09	17.02
8	11	14	29.49	25.89	6.97	2	5	15	119.35	147.19	14.35
9	11	14	0.27	35.16	14.64	3	5	15	7.72	14.87	14.02
10	11	14	5.29	11.54	9.19	4	5	15	335.15	374.15	15.24
11	11	14	1.12	-3	21.32	5	5	15	56.71	78.07	15.85
0	12	14	37.1	65.28	31.76	0	6	15	477.25	440.15	28.96
1	12	14	3.79	13.76	7.35	1	6	15	11.09	25.09	16.27
2	12	14	33.37	47.1	9.66	2	6	15	488.66	501.88	16.24
3	12	14	0.04	10.62	9.16	3	6	15	24.57	18.9	11.86
4	12	14	1.22	25.44	14.34	4	6	15	795.94	779.52	15.06
5	12	14	18.35	26.81	8.62	5	6	15	10.25	15.3	12.36
6	12	14	32.82	16.13	7.1	6	6	15	55.19	26.17	15.33
7	12	14	1.68	2.61	6.24	0	7	15	21.58	43.3	27.6
8	12	14	5.46	11.7	7.22	1	7	15	3.18	-1.92	15.23
9	12	14	6.61	1.59	11.33	2	7	15	12.17	6.47	14.28
10	12	14	2.99	15.96	17.06	3	7	15	51.02	46.63	12.59
0	13	14	13.68	5.09	10.83	4	7	15	69.29	61.71	12.2
1	13	14	0.69	4.08	7.52	5	7	15	141.76	123.83	10.63
2	13	14	55.9	29.6	7.08	6	7	15	186.58	161	10.75
3	13	14	6.95	18.17	8.11	7	7	15	16.03	9.39	14.59
4	13	14	36.47	60.07	16.53	0	8	15	289.41	211.56	29.54
5	13	14	7.81	20.23	13.51	1	8	15	43.42	41.16	14
6	13	14	13.34	43.01	13.79	2	8	15	66.28	84.52	12.09
7	13	14	9.54	49.13	14.88	3	8	15	38.47	37.63	10.67
8	13	14	1.93	62.53	34.18	4	8	15	437.75	390.1	12.14
9	13	14	6.01	11.3	21.8	5	8	15	3.5	9.81	11.94
0	14	14	4.17	-6.54	34.24	6	8	15	77.32	64.02	14.26
1	14	14	1.35	-4.24	14.57	7	8	15	131.78	127.18	9.55

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
8	8	15	144.07	116.55	27.45	7	13	15	2.77	-9.14	22.94
0	9	15	336.64	254.55	22.75	8	13	15	11.4	16.21	58.29
1	9	15	0.64	6.49	12.57	1	14	15	7.38	28.38	27.05
2	9	15	227.42	213.32	11.05	2	14	15	32.67	137.78	135.8
3	9	15	1.28	22.01	10.5	3	14	15	0.06	3.76	65.48
4	9	15	18.8	10.66	11.12	4	14	15	3.92	18.44	30.9
5	9	15	8.39	10.47	11.65	5	14	15	0.49	-15.95	44.44
6	9	15	58.81	84.15	11.66	0	1	16	3.3	-2.59	27.86
7	9	15	0.73	15.15	9.87	1	1	16	44.54	74.24	33.04
8	9	15	3.14	17.61	8.58	0	2	16	89.77	61.62	40.65
9	9	15	26.3	5.23	11.52	1	2	16	40.42	54.21	15.61
0	10	15	432.69	399.62	54.25	2	2	16	7.58	30.35	18.39
1	10	15	36.9	48.26	11.65	0	3	16	106.1	88.54	35.45
2	10	15	121.78	105.98	11.47	1	3	16	39.45	62.35	25.73
3	10	15	0.3	7.49	10.99	2	3	16	62.11	117.7	15.23
4	10	15	83.24	67.05	9.6	3	3	16	23.19	37.93	22.36
5	10	15	8.86	13.64	9.9	0	4	16	171.03	220.52	42.22
6	10	15	35.86	26.14	8.77	1	4	16	15.33	36.81	18.46
7	10	15	16.04	15.54	6.18	2	4	16	113.09	97.49	15.51
8	10	15	12.47	11.02	6.78	3	4	16	1.77	8.52	14.73
9	10	15	7.77	22.74	11.24	4	4	16	1.2	15.06	20.78
10	10	15	0.78	117.35	67.44	0	5	16	247.5	244.52	76.21
0	11	15	14.43	-1.26	13.31	1	5	16	57.09	63.8	17.08
1	11	15	54.54	33.45	10.83	2	5	16	17.07	-2.82	16.23
2	11	15	125.45	93.4	15.09	3	5	16	13.88	41.58	14.53
3	11	15	0.59	20.89	9.88	4	5	16	53.43	88.45	15.55
4	11	15	39.83	35.89	10.13	5	5	16	60.59	40.71	23
5	11	15	4.06	15.37	7.92	0	6	16	140.17	219.29	37.91
6	11	15	50.08	19.57	6.19	1	6	16	23.35	29.85	18.46
7	11	15	0.99	17.36	17.12	2	6	16	59.94	102.68	16.78
8	11	15	25.53	27.53	21.42	3	6	16	1.5	16.85	13.74
9	11	15	41.78	-1.77	16.5	4	6	16	123.53	159.54	13.98
10	11	15	42.82	1.31	63.52	5	6	16	35.58	27.22	12.12
0	12	15	3.79	38.43	13.93	6	6	16	88.16	78.22	14.14
1	12	15	9.91	10.29	10.51	0	7	16	26.5	89.08	38.56
2	12	15	18.69	4.68	11.82	1	7	16	11.22	10.31	19.64
3	12	15	27.01	29.5	11.96	2	7	16	61.32	75.65	12.74
4	12	15	51.19	104.68	44.52	3	7	16	0.32	11.93	13.29
5	12	15	5.15	44.23	10.89	4	7	16	9.5	7.57	12.45
6	12	15	38.2	33.66	22	5	7	16	16.52	26.64	10.25
7	12	15	6.75	5.11	11.79	6	7	16	21.63	30.51	12.98
8	12	15	35.32	31.35	19.96	7	7	16	5.3	13.13	15.29
9	12	15	5.14	-0.26	28.75	0	8	16	80.85	110.64	28.49
0	13	15	93.17	0.57	22.58	1	8	16	1.25	9.31	13.49
1	13	15	0.8	29.24	23.66	2	8	16	109.31	112.2	11.42
2	13	15	88.99	27.13	10.89	3	8	16	10.71	35.21	16.56
3	13	15	0.25	34.17	15.7	4	8	16	14.87	25.62	11.05
4	13	15	16.64	138.29	97.95	5	8	16	1.94	9.29	10.34
5	13	15	2.18	3.32	19.13	6	8	16	1.2	6.04	8.31
6	13	15	22.31	41.79	30	7	8	16	0.91	16.27	8.86

h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$	h	k	l	Fcal ²	Fobs ²	$\sigma(\text{Fobs}^2)$
8	8	16	2.01	26.53	16.47	2	3	17	26.16	40.4	14.83
0	9	16	15.37	10.92	13.61	3	3	17	1.52	-2.66	17.18
1	9	16	5.68	9.32	11.44	0	4	17	315.92	307.61	72.68
2	9	16	0.49	10.89	10.59	1	4	17	2.21	34.28	20.42
3	9	16	2.01	11.26	9.42	2	4	17	305.13	297.42	19.77
4	9	16	15.85	35.34	9.41	3	4	17	12.34	19.6	14.3
5	9	16	7.58	24.54	9.19	4	4	17	400.56	455.25	23.29
6	9	16	20.59	36.43	14.1	0	5	17	158.21	142.39	27.76
7	9	16	2.33	1.63	5.91	1	5	17	0.48	-2.85	17.21
8	9	16	10.44	9.24	9.47	2	5	17	33.22	10.19	14.56
9	9	16	0.04	10.12	23.83	3	5	17	3.18	16.64	15.88
0	10	16	6.44	11.22	16.6	4	5	17	0.97	9.73	15.21
1	10	16	8.79	18.98	10.46	5	5	17	2.69	-6.37	20.05
2	10	16	4.3	18.6	8.78	0	6	17	535.22	470.64	55.82
3	10	16	4.16	7.15	8.12	1	6	17	0.04	7.93	12.64
4	10	16	9.24	17.71	7.01	2	6	17	172.1	144.32	21.51
5	10	16	27	12.91	7.54	3	6	17	26.85	20.15	13.67
6	10	16	33.52	18.69	15.81	4	6	17	62.15	68.08	18.3
7	10	16	3.84	4.61	11.52	5	6	17	17.5	28.75	13.81
8	10	16	2.21	8.25	18.49	6	6	17	74.8	33.89	11.48
0	11	16	85.51	67.49	58.16	0	7	17	54.49	32.75	22.45
1	11	16	0.19	49.91	23.58	1	7	17	5.57	-6.05	14.21
2	11	16	11.08	39.6	19.62	2	7	17	42.31	17.1	10.42
3	11	16	10.59	16.66	11.59	3	7	17	2.48	11.13	10.63
4	11	16	15.9	5.03	12.72	4	7	17	61.69	36.05	8.23
5	11	16	45.18	42.5	23.32	5	7	17	0.73	2.51	7.95
6	11	16	11.47	68.77	36.67	6	7	17	17.26	16.77	8.46
7	11	16	0.67	109.36	57.84	7	7	17	9.72	6.79	9.77
8	11	16	7	-5.17	19.59	0	8	17	82.23	60.73	19.21
0	12	16	3.53	181.15	45.75	1	8	17	1.89	-8.79	13.31
1	12	16	7.55	73.17	93.77	2	8	17	96.74	74.21	15.65
2	12	16	13.96	33.58	22.15	3	8	17	1.67	6.75	7.99
3	12	16	0.36	17.98	18.19	4	8	17	49.23	19.2	9.61
4	12	16	0.5	-4.4	13.59	5	8	17	39.9	17.91	9.81
5	12	16	0	87.24	73.12	6	8	17	120.65	110.58	13.13
6	12	16	3.73	64.09	41.99	7	8	17	6.7	21.57	18.68
7	12	16	1.19	-13.63	26.02	1	9	17	14.65	-6.92	19.78
0	13	16	1.73	3.45	25.21	2	9	17	71.62	13.28	12.1
1	13	16	0.27	25.42	41.3	3	9	17	3.74	-5.11	10.82
2	13	16	3	49.46	40.22	4	9	17	30.42	8.46	8.83
3	13	16	1.53	29.26	25.84	5	9	17	8.73	-0.83	10.8
4	13	16	6.26	3.08	26.68	6	9	17	18.76	3.4	11.71
5	13	16	1.65	-16.74	28.46	7	9	17	4.51	5.13	18.39
0	1	17	3.72	14.43	39.6	0	10	17	49.83	275	85.22
1	1	17	72.29	25.04	22.48	1	10	17	16.38	-6.63	12.09
0	2	17	349.16	254.91	43.92	2	10	17	70.14	82.8	43.73
1	2	17	15.8	12.31	19.7	3	10	17	17.01	14.66	9.96
2	2	17	359.61	354.14	26.92	4	10	17	31.55	22.64	15.39
0	3	17	9.48	20.25	27.63	5	10	17	2.9	-3.68	13.4
1	3	17	37.86	77.58	17.73	6	10	17	19.69	18.99	15.97

h	k	l	Fcal ²	Fobs ²	σ(Fobs ²)	h	k	l	Fcal ²	Fobs ²	σ(Fobs ²)
1	11	17	0.01	-2.02	26.61	2	11	18	0.3	-4.71	29.28
2	11	17	38.45	27.28	18.11	0	2	19	186.96	94.47	35.03
3	11	17	0.92	29.73	23.24	1	2	19	8.39	5.83	8.14
4	11	17	26.43	17.77	19.24	2	2	19	110.75	32.62	9.47
5	11	17	30.64	-0.21	23.12	2	3	19	49.62	13.87	15.93
1	12	17	1.21	-2.32	23.62						
2	12	17	19.06	23.48	17.46						
3	12	17	0.18	5.97	22.6						
4	12	17	34.1	25.08	36.26						
1	13	17	0.16	6.01	39.73						
1	2	18	2.33	8.71	25.86						
2	2	18	0.92	9.27	17.96						
0	3	18	11.4	31.22	26.13						
1	3	18	15.13	34.26	20.56						
2	3	18	4.16	21.59	13.85						
3	3	18	2.93	8.43	12.76						
0	4	18	62.8	34.56	25.99						
1	4	18	0.02	3.63	19.29						
2	4	18	56.36	86.53	22.56						
3	4	18	2.4	13.93	9.61						
4	4	18	0.84	-8.41	13.06						
0	5	18	2.78	42.77	37.9						
1	5	18	2.45	1.68	12.03						
2	5	18	1.56	14.86	7.95						
3	5	18	0.01	11.52	11.17						
4	5	18	0.11	-0.43	9.49						
5	5	18	0.24	28.48	10.49						
0	6	18	0.62	-9.43	21.65						
1	6	18	9.54	11.12	9.51						
2	6	18	13.8	10.98	7.86						
3	6	18	0.79	12.68	7.55						
4	6	18	0.54	10.59	8.14						
5	6	18	6.39	1.52	9.15						
1	7	18	0.73	6.54	32.94						
2	7	18	8.2	28.52	21.79						
3	7	18	2.77	8.41	8.43						
4	7	18	0.1	-1.81	10.45						
5	7	18	1.91	16.48	35.63						
0	8	18	9.86	245.2	54.89						
1	8	18	4.65	8.1	33.2						
2	8	18	12.54	8.59	10.03						
3	8	18	0.08	20.17	17.48						
4	8	18	2.72	33.03	15.3						
0	9	18	0.11	-6.8	50.97						
1	9	18	1.92	13.18	32.13						
2	9	18	1.44	16.32	18.45						
3	9	18	5.9	-1.22	23.19						
2	10	18	1.77	27.71	56.72						
3	10	18	1.94	-7.53	25.82						
1	11	18	1.5	296.43	64.83						