Synthesis and Single-crystal Structures of Fully Dehydrated and Highly Proton-exchanged Zeolites Y, |H74Na1|[Si117Al75O384]-FAU and |H73Na2|[Si117Al75O384]-FAU

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crystal 1

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
0	2	2	598527.9	541840.3	6452.13	6	8	8	44237.04	52340.75	359.46
0	2	2	5.04	-19.81	19.81	8	8	8	152875.2	149531.3	1544.07
0	1	3	322327.3	285579.3	1762.84	1	1	9	12945.86	14131.45	119.25
0	3	3	616525.9	593834.4	3587.74	1	3	9	72094.52	60612.33	554.24
0	3	3	30313.99	34327.15	421.56	3	3	9	53.46	990.53	39.62
0	0	4	31389.05	22140.27	342.79	1	5	9	9252.89	7523.93	56.15
0	2	4	2189.79	1903.75	39.66	3	5	9	8202.82	13050.65	168.69
0	4	4	784945.8	828279.3	8697.64	5	5	9	18074.99	16701.82	139.18
0	4	4	9788.02	10379.79	99.42	1	7	9	24946.41	29664.58	945.76
0	4	4	102922.7	85657.41	901.01	3	7	9	28937.75	24187.04	140.88
0	1	5	222167.8	192455.3	1170.2	5	7	9	19679.43	16821.95	112.48
0	3	5	10366.34	10173.89	70.32	7	7	9	93903.57	98291.63	604
0	3	5	699909.6	705162.1	3895.52	1	9	9	4430.32	6185.86	79.31
0	5	5	96164.3	77193.77	489.99	3	9	9	35179.13	30759.29	239.22
0	5	5	12250.34	12407.11	119.3	5	9	9	232351.6	239707.1	1338
0	5	5	2199513	2516046	46596.16	7	9	9	11871.6	11591.49	119.09
0	2	6	94895.62	79646.77	798.85	9	9	9	99689.59	130114.7	1347.19
0	2	6	537.69	891.63	79.26	0	2	10	156.97	827.91	79.24
0	4	6	295530.1	292516.9	1163.16	2	2	10	32761.73	42204.58	319.28
0	4	6	8850.13	7546.6	79.44	2	4	10	6429.77	7921.15	218.21
0	6	6	589363.4	573306.3	4235.24	4	4	10	83.18	79.24	59.43
2	6	6	80.03	-19.81	19.81	0	6	10	42768.2	35421.74	619.35
4	6	6	488333.8	456984.4	2361.51	2	6	10	10377.1	11854.29	198.51
6	6	6	957894.4	1154013	10203.29	4	6	10	2951.79	3371.52	79.29
1	1	7	1203.74	1367.45	39.64	6	6	10	2856.98	2814.51	59.46
1	3	7	16714.08	11850.36	408.15	2	8	10	168520.4	162163.9	5254.04
3	3	7	197461.5	165620.6	960.72	4	8	10	2580.17	2061.21	42.04
1	5	7	39695.66	33198.37	460.44	6	8	10	18299.51	21890.66	268.25
3	5	7	51937.2	46752.25	233.84	8	8	10	13154.3	14114.09	138.96
5	5	7	44093.29	28818.7	220.14	0	10	10	434058.8	462480.5	3348.08
1	7	7	6781.57	6091.4	79.37	2	10	10	2743.47	2338.68	59.46
3	7	7	147.43	257.54	39.62	4	10	10	11151.26	10756.4	119.07
5	7	7	99949.02	92877.09	566.2	6	10	10	21597.47	23811.46	218.64
7	7	7	2558.22	2259.5	99.1	8	10	10	101544.6	102758.5	643.25
0	0	8	719.56	317.03	79.26	10	10	10	43.7	237.73	118.86
2	2	8	105702.5	107752.3	713.05	1	1	11	119913.3	90752.41	527.87
0	4	8	209946.6	196965.8	11545.27	1	3	11	12434.7	10755.18	89.37
2	4	8	10400.43	10682.41	76.29	3	3	11	123805.8	146693	913.03
4	4	8	50953.54	38612.14	280.67	1	5	11	15230.71	12915.55	119.21
2	6	8	18570.62	10533.85	70.34	3	5	11	807.77	1262.03	32.97
4	6	8	32304.65	32824.13	458.81	5	5	11	8977.17	8234.52	99.21
6	6	8	6096.45	5791.68	79.34	1	7	11	11093.01	11718.89	297.75
0	8	8	203570.2	268620	2041.72	3	7	11	23017.39	24488.82	318.24
2	8	8	11.81	257.54	39.62	5	7	11	65783.1	61402.28	981.38
4	8	8	219763.8	222470.1	1238.35	7	7	11	46420.79	41768.27	299.34

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
1	9	11	2438.93	1705.3	42.04	5	9	13	24799.2	25220.18	208.75
3	9	11	345427.6	346277.4	1285.06	7	9	13	3061.29	3478.22	56.06
5	9	11	1585.06	1942.1	42.03	9	9	13	62780.2	65691.22	459.38
7	9	11	36967.92	39309.53	203.87	1	11	13	34163.34	34318.61	338.38
9	9	11	54608.2	55036.5	379.29	3	11	13	21356.34	21006.45	337.76
1	11	11	511301.9	509567.2	2661.2	5	11	13	12145.22	12472.08	109.14
3	11	11	781.2	1624.64	59.44	7	11	13	771.81	792.99	42.03
5	11	11	266953.6	262257.4	1398.27	9	11	13	34062.46	33561.39	566.99
7	11	11	5616.25	6939.06	99.13	11	11	13	48860.29	50889.25	378.58
9	11	11	16097.75	17410.81	158.82	1	13	13	2941.22	6282.3	118.91
11	11	11	852435.8	889060.4	7423.21	3	13	13	71635.07	69571.83	479.81
0	0	12	375050.2	303914.9	3159.59	5	13	13	4.01	118.86	59.43
2	2	12	952.04	2536.19	59.44	7	13	13	6303.96	5689.97	99.13
0	4	12	11932.5	11654.23	198.54	9	13	13	20503.18	22320.72	198.58
2	4	12	27174.88	32522.06	228.95	11	13	13	25.02	851.85	79.24
4	4	12	12527.42	11177.89	138.98	13	13	13	29842.45	31024.09	417.36
2	6	12	24012.49	21046.2	133.07	0	2	14	97655.27	89265.57	540.87
4	6	12	2066.4	1714.71	42.04	2	2	14	18.54	-59.43	79.24
6	6	12	35393.66	33130.89	258.99	2	4	14	4057.53	3384.07	218.06
0	8	12	10921.26	10004.72	158.77	4	4	14	22243.18	21986.25	218.67
2	8	12	38461.46	38626.4	218.13	0	6	14	171.54	219.85	99.05
4	8	12	87852.6	87105.49	823.38	2	6	14	83882.26	86953.95	1203.84
6	8	12	589.52	545.01	42.03	4	6	14	62421.71	59995.36	311.05
8	8	12	231081.6	240214.8	1309.3	6	6	14	2.68	-39.62	39.62
2	10	12	2697.02	3886.94	99.09	2	8	14	8012.24	7774.93	188.42
4	10	12	14.51	-32.97	32.97	4	8	14	251.43	307.39	42.03
6	10	12	149267.9	150443.7	2609.07	6	8	14	152678.6	160140.9	3610
8	10	12	535.9	703.46	42.03	8	8	14	218.7	515.09	59.43
10	10	12	121115.8	120604.5	704.11	0	10	14	23653.14	24032.36	566.44
0	12	12	949058.6	1150653	7689	2	10	14	7138.59	7317.26	70.11
2	12	12	1380.07	1089.78	59.44	4	10	14	12265.41	11783.76	90.4
4	12	12	1974.17	2239.18	79.26	6	10	14	403.37	443.19	47.55
6	12	12	6595.48	7653.5	99.14	8	10	14	48177.02	48564.52	986.57
8	12	12	31561.15	30053.88	258.57	10	10	14	8398.53	7892.55	118.98
10	12	12	4355.47	3587.59	79.28	2	12	14	110427.4	109555.4	483.01
12	12	12	285663.9	323740.3	3027.91	4	12	14	1685.26	1863.42	56.04
1	1	13	999.48	990.7	39.63	6	12	14	3795.87	3671.1	61.91
1	3	13	31042.6	27640.55	153.01	8	12	14	12008.11	12044.32	158.71
3	3	13	14871.87	15114.11	158.89	10	12	14	18886.2	20439.84	140.39
1	5	13	26086.12	23092.1	189.02	12	12	14	1581.89	1545.48	79.26
3	5	13	129.25	164.43	59.43	0	14	14	78913.23	82438.35	779.98
5	5	13	117.26	416.03	59.43	2	14	14	1153.69	1228.42	79.25
1	7	13	38.7	145.28	32.97	4	14	14	44493.24	41762.61	318.65
3	7	13	14690.01	15806.87	158.85	6	14	14	226347.2	228771.1	1240.01
5	7	13	18272.83	19126.48	556.22	8	14	14	1525.16	1644.55	79.26
7	7	13	12100.52	15697.49	158.76	10	14	14	518.78	237.74	79.25
1	9	13	25525.97	24548.6	377.83	12	14	14	52937.52	56118.29	378.5
3	9	13	37661.73	36603.25	197.2	14	14	14	1147.65	812.32	138.69

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
1	1	15	141.96	237.73	39.62	8	8	16	136808	141264	866.03
1	3	15	22989.43	22345.55	140.58	2	10	16	14859.75	15728.97	118.67
3	3	15	31112.32	38573.09	298.55	4	10	16	1132.08	1478.92	47.55
1	5	15	9918.02	12166.4	238.08	6	10	16	23443.87	24764.16	154.53
3	5	15	96135.27	91840.33	733.23	8	10	16	3521.45	3507.9	61.9
5	5	15	51828.81	50031.38	379.18	10	10	16	15172.79	15062.02	158.76
1	7	15	1897.95	2190.76	49.54	0	12	16	32691.03	30185.31	259.88
3	7	15	25657.27	23580.64	154.65	2	12	16	111.99	436.74	42.02
5	7	15	190.57	546.63	79.24	4	12	16	26353.24	25772.67	377.57
7	7	15	977.83	1723.73	79.25	6	12	16	12626.83	11079.48	317.43
1	9	15	16555.86	16027.18	118.72	8	12	16	2160.2	5811	683.63
3	9	15	1168.54	1861.05	59.44	10	12	16	971.97	906.23	47.55
5	9	15	49695.32	48099.15	877.33	12	12	16	13851.95	14800.12	158.71
7	9	15	16220.04	16906.72	258.07	2	14	16	33322.88	34391.82	196.85
9	9	15	6702.01	7375.51	118.96	4	14	16	3.89	16.98	49.53
1	11	15	4373.51	4922.39	178.39	6	14	16	5253.71	5593.22	138.75
3	11	15	88887.06	87790.48	3045.03	8	14	16	3779.51	3904.64	70.07
5	11	15	10539.5	11006.81	287.63	10	14	16	3205.09	3329.38	56.05
7	11	15	48890.32	49871.8	1345.1	12	14	16	184.08	219.5	56.03
9	11	15	2800.12	2973.06	56.05	14	14	16	31089.13	33442.29	258.32
11	11	15	877.57	1763.3	79.25	0	16	16	47919.48	48288.52	477.91
1	13	15	4914.28	6465.02	138.76	2	16	16	39.42	-79.24	99.05
3	13	15	1624.71	1575.8	56.04	4	16	16	28846.21	28634.53	238.46
5	13	15	62995.52	64591.4	310.46	6	16	16	3233.13	3586.9	99.09
7	13	15	124.67	1698.51	89.15	8	16	16	1874.56	3368.42	99.07
9	13	15	6013.63	6096.19	70.09	10	16	16	3584.62	3884.23	99.09
11	13	15	7011.62	7211.45	188.34	12	16	16	7558.43	7573.15	118.95
13	13	15	3425.41	3487.87	79.27	14	16	16	312.01	297.16	99.05
1	15	15	9879.24	9638.72	119	16	16	16	87888.54	93196.13	978.49
3	15	15	16303.94	17822.6	178.62	1	1	17	75973.89	76212.12	480.45
5	15	15	7299.33	7197.04	99.13	1	3	17	2561.25	2511.4	47.56
7	15	15	34412.02	32491.77	258.5	3	3	17	8881.52	7001.51	99.17
9	15	15	14366.43	16666.17	178.57	1	5	17	6303.96	6587.46	178.44
11	15	15	9205.49	9081.78	118.98	3	5	17	239.03	537.83	42.03
13	15	15	3627	3448.26	99.09	5	5	17	467817.1	475497.3	2643.4
15	15	15	2245.31	2357.95	158.52	1	7	17	702.05	679.7	47.55
0	0	16	336616.8	359391.6	3614.48	3	7	17	11425.5	11473.94	277.75
2	2	16	5412.54	6621.89	99.13	5	7	17	153881.1	155954.9	1918.1
0	4	16	32956.7	40744.68	1124.58	7	7	17	19553.02	19023.7	198.58
2	4	16	10195.41	8967.37	84.17	1	9	17	10620.09	10515.97	90.37
4	4	16	4236.22	10902.18	158.58	3	9	17	194483.8	200920.5	3650.49
2	6	16	9963	11380.71	208.3	5	9	17	579.16	2348.41	108.96
4	6	16	270.29	155.66	47.55	7	9	17	28198.24	27047.76	556.54
6	6	16	825431.3	906643.6	4612.46	9	9	17	10358.24	10234.26	138.84
0	8	16	15443.19	15996.8	357.32	1	11	17	38429.36	37593.35	211.08
2	8	16	17814.21	19337.7	327.64	3	11	17	1038.78	1912.14	138.69
4	8	16	73272.35	72193.76	769.95	5	11	17	138214.3	137020.3	3401.26
6	8	16	358.3	670.92	69.34	7	11	17	11978.63	14381.32	198.37

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
9	11	17	4079.96	3904.8	70.07	10	12	18	173.77	198.11	56.03
11	11	17	1341.15	1525.62	59.44	12	12	18	3628.08	3329.36	99.09
1	13	17	16002.42	16562.27	426.7	0	14	18	10140.17	9025.12	126.21
3	13	17	10901.99	12353.4	109.09	2	14	18	1064.99	961.02	56.04
5	13	17	1199.61	1110.95	56.04	4	14	18	40284.65	43790.01	706.27
7	13	17	287.73	352.08	47.55	6	14	18	1429.4	1228.27	108.97
9	13	17	28452.02	29020.84	175.21	8	14	18	32904.18	38663.98	357.79
11	13	17	8172.69	8392.5	218.1	10	14	18	962.4	941.53	61.88
13	13	17	15043.84	15752.94	158.72	12	14	18	1536.95	1456.21	168.41
1	15	17	235.56	99.05	69.34	14	14	18	1506.16	1743.56	99.07
3	15	17	27116.26	27308.51	161.1	2	16	18	6453.42	6126.82	76.14
5	15	17	25311.38	25564.18	154.5	4	16	18	14.93	82.07	47.55
7	15	17	0.13	640.45	99.05	6	16	18	100149	102900.8	1170.46
9	15	17	6598.4	6988.19	84.1	8	16	18	87.24	55.03	61.88
11	15	17	9045.04	9854.92	98.14	10	16	18	1073.97	1197	99.06
13	15	17	2748.1	3201.73	70.06	12	16	18	1819.81	1783.24	70.05
15	15	17	445.77	435.85	99.06	14	16	18	8778.69	9745.42	98.13
1	17	17	11585.45	11761.53	138.84	16	16	18	4916.89	4816.03	118.91
3	17	17	76.86	336.78	79.24	0	18	18	21629.89	25013.94	297.79
5	17	17	110747.1	115836.7	681.04	2	18	18	160.79	118.86	79.24
7	17	17	80150.73	84002.99	519.15	4	18	18	4131.44	4201.49	99.09
9	17	17	245.88	237.73	79.24	6	18	18	2955.67	2417.55	99.08
11	17	17	693.74	891.53	79.25	8	18	18	7650.6	7216.19	118.95
13	17	17	17.18	297.16	99.05	10	18	18	249.02	257.54	99.05
15	17	17	5980.35	6104.89	138.75	12	18	18	5683.99	6184.02	118.92
17	17	17	203386.7	208612.3	1753.89	14	18	18	1575.59	1703.93	99.07
0	2	18	336.83	462.99	47.55	16	18	18	23889.98	22272.96	218.36
2	2	18	4549.53	3508.53	79.29	18	18	18	1038.35	1406.66	217.93
2	4	18	10678.9	14358.26	605.05	1	1	19	13415.68	13791.46	138.91
4	4	18	8200	7139.17	118.99	1	3	19	22459.41	22850.84	148.99
0	6	18	63164.34	64095.99	465.3	3	3	19	19172.18	17057.37	178.72
2	6	18	5927.51	5663.11	76.15	1	5	19	1188.61	1420.42	208.04
4	6	18	36175.04	35828.15	211.06	3	5	19	103475.2	101960.8	474.96
6	6	18	2842.12	2893.31	99.09	5	5	19	2213.07	3170.5	99.08
2	8	18	51753.81	53524.9	281.92	1	7	19	14350.09	14231.89	248.05
4	8	18	6630.78	7216.78	84.12	3	7	19	45186.1	49064.49	308.69
6	8	18	22.55	128.77	56.03	5	7	19	909.96	943.7	56.04
8	8	18	7189.27	5987.65	118.96	7	7	19	746.29	1367.03	79.25
0	10	18	164.81	252.59	80.6	1	9	19	86781.91	83302.94	2130.79
2	10	18	1511.42	3850.43	158.51	3	9	19	2090.63	2179.84	56.05
4	10	18	76.55	1330.94	208.01	5	9	19	5788.6	6884.4	198.23
6	10	18	4768.75	4093.27	70.08	7	9	19	10127.79	10312.93	98.17
8	10	18	302.62	618.11	118.87	9	9	19	92.78	-19.81	99.05
10	10	18	452.08	99.06	79.25	1	11	19	1886.4	2072.84	61.89
2	12	18	3798.12	3791.92	69.37	3	11	19	2617.73	2965.9	198.16
4	12	18	1174.33	969.21	49.53	5	11	19	4488.83	5143.48	70.07
6	12	18	35662.11	39928.04	785.54	7	11	19	6074.11	6117.4	109.03
8	12	18	794.47	594.36	56.04	9	11	19	8381	8403.2	228.02

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
11	11	19	382.48	1188.67	99.06	4	10	20	253.33	334.38	56.03
1	13	19	13705.41	13806.15	495.98	6	10	20	9384.99	10807.41	327.2
3	13	19	19.07	577.24	56.03	8	10	20	815.24	788.61	61.88
5	13	19	11228.66	10707.6	247.92	10	10	20	5124.18	5232.66	118.92
7	13	19	612.28	797.62	79.25	0	12	20	93.79	84.65	76.09
9	13	19	3295.47	3202.32	76.12	2	12	20	2018.08	1977.3	61.89
11	13	19	8709.37	9282.59	178.45	4	12	20	6675.34	8291.97	90.31
13	13	19	3605.86	4121.98	118.9	6	12	20	556.06	568.97	56.04
1	15	19	4882.76	5004.64	70.08	8	12	20	9282.29	8952.84	98.15
3	15	19	16796.81	16821.45	118.65	10	12	20	59.93	118.86	70.04
5	15	19	1396.09	1836.61	89.16	12	12	20	110.19	79.24	99.05
7	15	19	15032.51	15358.85	158.72	2	14	20	20048.81	19563.43	456.56
9	15	19	1903.29	2040.85	61.89	4	14	20	0.18	103.45	61.88
11	15	19	13814.03	13007.42	1110.83	6	14	20	34047.86	36604.81	308.09
13	15	19	880.82	912.29	148.59	8	14	20	471.97	428.02	70.04
15	15	19	4512.14	3745.68	99.09	10	14	20	26682.31	27710.21	357.49
1	17	19	121.1	178.3	56.03	12	14	20	168.68	188.2	70.04
3	17	19	2547.62	2912.99	70.06	14	14	20	1977.15	2556	118.88
5	17	19	6512.31	6492.72	84.1	0	16	20	366.34	714.2	90.25
7	17	19	416.91	432.36	61.88	2	16	20	684.88	638.62	61.88
9	17	19	8297.83	7953.29	158.61	4	16	20	9763.25	10471.71	208.21
11	17	19	3343.72	3542.84	76.12	6	16	20	29.41	-70.44	99.05
13	17	19	1196.35	1644.44	84.06	8	16	20	14312.09	15363.99	912.5
15	17	19	5721.27	5450.87	84.09	10	16	20	24.22	36.57	84
17	17	19	6102.17	6084.95	138.74	12	16	20	1.74	286.35	76.09
1	19	19	241.68	416.03	79.24	14	16	20	2109.62	2249.29	84.06
3	19	19	8462.08	7970.07	118.96	16	16	20	3425.37	3111.15	138.71
5	19	19	11996.85	10808.65	138.83	2	18	20	4487.94	4627.69	84.08
7	19	19	15391.25	15295.29	198.38	4	18	20	355.47	227.83	70.04
9	19	19	863.75	1069.84	99.06	6	18	20	9029.94	8505.76	98.14
11	19	19	8746.22	7117.43	138.78	8	18	20	101.23	168.39	70.04
13	19	19	1.14	178.29	118.86	10	18	20	25.76	325.66	76.09
15	19	19	9190.57	9100.05	158.61	12	18	20	0.74	-35.66	98.9
17	19	19	6153.32	5827.23	138.74	14	18	20	14773.06	14046.49	158.68
0	0	20	16064.66	13854.41	297.73	16	18	20	39.31	7.62	90.25
2	2	20	61632.57	63000.19	439.03	18	18	20	4692.56	4023.06	158.54
0	4	20	18046.23	18320.19	873.52	0	20	20	1765.27	2338	158.51
2	4	20	2090.55	1999.77	128.8	2	20	20	146.01	0	118.86
4	4	20	68671.84	72664.28	499.2	4	20	20	5817.52	5985.85	138.74
2	6	20	99211.04	101703.5	481.7	6	20	20	384.23	594.33	99.06
4	6	20	299.29	388.6	56.03	8	20	20	283.21	851.87	118.87
6	6	20	74.68	178.3	79.24	10	20	20	1703.96	1783.2	138.69
0	8	20	367739	365274.6	2556.41	12	20	20	35722.41	35786.46	258.31
2	8	20	1373.76	1138.72	69.35	14	20	20	135.27	217.92	138.67
4	8	20	21470.03	23226.64	377.3	16	20	20	13572.79	12216.72	178.49
6	8	20	3668	3597.71	70.07	1	1	21	33363.32	33528.43	278.41
8	8	20	5436.44	5649.24	118.93	1	3	21	19809.91	19209.23	168.77
2	10	20	29186.18	31581.96	894.3	3	3	21	29504.46	31067.08	258.4

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
1	5	21	25809.28	25873.46	377.49	13	19	21	2285.19	2333.27	108.98
3	5	21	5500.49	4996	70.08	15	19	21	149.03	-39.62	104.35
5	5	21	14266.44	15099.38	158.73	1	21	21	2670.22	2635.39	118.89
1	7	21	1597.22	1538.85	108.98	3	21	21	12305.64	12097.21	158.65
3	7	21	5676.36	5682.13	128.85	5	21	21	4408.02	3606.86	138.73
5	7	21	283.67	408.3	56.03	7	21	21	0.16	0	118.86
7	7	21	181.72	-39.62	138.68	9	21	21	2825.55	2853.38	138.71
1	9	21	19561.3	19574.54	387.11	11	21	21	835.79	911.34	158.49
3	9	21	13330.58	14898.95	126.25	13	21	21	1764.79	1367.11	158.51
5	9	21	6965.38	7008.79	84.11	0	2	22	47553.56	48125.06	418.2
7	9	21	25.03	4.95	80.6	2	2	22	1.58	-19.81	138.67
9	9	21	13179.12	16107.42	178.53	2	4	22	31163.78	31436.3	516.81
1	11	21	46728.36	46843.26	266.33	4	4	22	346.81	435.85	79.24
3	11	21	9934.29	10170.56	104.47	0	6	22	101604.8	102657.9	2613.32
5	11	21	4079.93	3937.02	109	2	6	22	24.72	99.05	59.43
7	11	21	7.9	229.01	56.03	4	6	22	17267.67	19124.96	228.24
9	11	21	94.87	138.67	70.04	6	6	22	29930.67	30821.8	278.21
11	11	21	56724.59	59534.52	398.36	2	8	22	17457.2	17807.37	297.7
1	13	21	2190.55	2179.62	61.89	4	8	22	1343.29	1217.33	237.76
3	13	21	21704.41	21770.34	943.03	6	8	22	2126.43	2616.14	70.06
5	13	21	3821.79	4328.44	76.12	8	8	22	947.75	851.93	99.06
7	13	21	697.04	1109.46	70.05	0	10	22	205960.8	220003.6	4560.36
9	13	21	6804.75	6813.36	90.31	2	10	22	16.41	-52.23	99.05
11	13	21	282.96	605.69	70.04	4	10	22	733.64	1066.53	108.97
13	13	21	7013.16	7770.64	138.76	6	10	22	206.89	167.29	61.88
1	15	21	1975.33	1882.56	70.05	8	10	22	12271.09	13093.7	158.67
3	15	21	164.48	445.96	56.03	10	10	22	3443.68	3487.78	118.9
5	15	21	1096.85	1031.77	70.05	2	12	22	8507.29	9482.85	118.96
7	15	21	74.66	-48.43	79.24	4	12	22	52.61	45.28	47.55
9	15	21	1812.98	2270.27	168.42	6	12	22	16549.66	17292.53	132.74
11	15	21	316.35	364.29	76.1	8	12	22	44.83	29.72	70.04
13	15	21	481.66	459.1	84.05	10	12	22	58633.75	59918.95	458.13
15	15	21	1332.01	1842.58	118.88	12	12	22	674.62	792.47	118.87
1	17	21	4183.34	4340.99	84.08	0	14	22	88.3	216.39	108.96
3	17	21	2552.69	2348.47	70.06	2	14	22	3032.18	2845.86	128.81
5	17	21	391.66	546.43	70.04	4	14	22	5728.36	6047.42	267.59
7	17	21	95.43	318.21	70.04	6	14	22	512.5	640.78	148.59
9	17	21	5531.92	5569.55	84.09	8	14	22	27634.22	26654.11	168.53
11	17	21	3765.55	3828.38	227.9	10	14	22	3.39	49.53	70.04
13	17	21	9844.48	10389.5	112.16	12	14	22	447.76	833.96	84.05
15	17	21	387.32	377.45	84.05	14	14	22	20986.46	21275.54	198.47
17	17	21	980.6	1267.97	138.68	2	16	22	2123.72	2004.38	79.26
1	19	21	550.54	609.51	76.1	4	16	22	10.44	0	108.96
3	19	21	2600.29	2235.69	76.11	6	16	22	12579.68	12822.48	112.19
5	19	21	2090.96	2093.87	76.11	8	16	22	15.8	-19.81	104.35
7	19	21	0.9	217.91	84.05	10	16	22	8054.51	7689.33	104.44
9	19	21	1965.36	1954.12	84.06	12	16	22	1326.13	1554.53	118.88
11	19	21	6876.49	6779.37	112.13	14	16	22	659.82	736.58	90.25

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
16	16	22	8.69	99.05	118.86	1	15	23	86.06	726.48	70.04
0	18	22	1246.44	1353.05	118.47	3	15	23	6397.46	5912.35	178.4
2	18	22	32.82	29.72	168.39	5	15	23	746.29	1134.83	79.25
4	18	22	11914.33	12091.67	337.13	7	15	23	3941.65	4005.57	99.09
6	18	22	19.67	-28.62	61.88	9	15	23	7427.53	7622.75	98.12
8	18	22	4017.23	4298.59	90.28	11	15	23	350.76	713.75	84.05
10	18	22	692.83	1000.48	99.06	13	15	23	8298.18	8142.66	128.86
12	18	22	5447.92	5088.97	277.47	15	15	23	1954.92	1783.23	138.7
14	18	22	638.67	527.06	99.06	1	17	23	6201.92	6366.46	118.93
2	20	22	22517.5	21259.13	426.75	3	17	23	447.43	744.11	84.05
4	20	22	874.32	901.55	84.05	5	17	23	3438.67	3432.36	118.9
6	20	22	816.03	699.19	90.25	7	17	23	2912.6	2982.42	297.23
8	20	22	390.07	469.81	99.06	9	17	23	1634.56	1988.45	118.88
10	20	22	1186.84	1139.12	148.59	11	17	23	25021.04	23025.6	148.89
12	20	22	1.35	150.56	122.1	13	17	23	4047.74	3469.01	98.09
0	22	22	126701.5	127549.2	1001.01	15	17	23	1010.89	1058.83	277.37
2	22	22	113.75	79.24	118.86	1	19	23	3584.07	3885.94	158.53
4	22	22	1467.85	1069.89	138.69	3	19	23	19320.47	17807.56	565.54
6	22	22	4232.04	3745.48	178.36	5	19	23	642.67	709.07	90.25
8	22	22	1797.1	1545.44	158.51	7	19	23	4150.32	3983.29	104.4
1	1	23	71988.57	72760.21	479.08	9	19	23	1972.6	1834.49	118.88
1	3	23	11155.12	11717.05	327.26	11	19	23	189.28	326.88	98.06
3	3	23	86227.11	80516.35	519.72	13	19	23	3929.66	2769.72	160.69
1	5	23	26477.95	26202.36	175.16	1	21	23	7841.06	7154.94	247.79
3	5	23	711.7	741.61	79.25	3	21	23	3493.2	2982.37	98.09
5	5	23	1217.49	1050.08	79.25	5	21	23	5662.55	5146.45	128.83
1	7	23	1477.26	1720.79	108.97	7	21	23	263.84	297.16	118.87
3	7	23	4199.91	4677.26	84.08	9	21	23	1762.33	1311.87	158.51
5	7	23	17826.63	17732.46	140.33	1	23	23	16299.06	14242.76	238.04
7	7	23	6185.04	6600.91	118.94	0	0	24	147891.2	127534.3	1447.88
1	9	23	223.36	356.82	79.24	2	2	24	55514.93	58472.68	438.3
3	9	23	2783.67	3270.71	70.06	0	4	24	544.44	482.91	84.05
5	9	23	227.34	255.34	61.88	2	4	24	259.32	148.58	56.03
7	9	23	1349.07	1724.64	70.05	4	4	24	90.97	277.35	59.43
9	9	23	28264.11	28027.79	238.37	2	6	24	17393.78	16140.44	416.74
1	11	23	98763.9	103092.5	1990.08	4	6	24	202.66	156.29	61.88
3	11	23	227.33	428.11	118.87	6	6	24	1069.11	2456.75	99.06
5	11	23	4319.16	4559.7	208.1	0	8	24	23758.89	22617.22	259.47
7	11	23	1535.66	1864.35	70.05	2	8	24	357.89	297.17	61.88
9	11	23	1529.48	1749.19	99.07	4	8	24	805.8	823.27	70.05
11	11	23	56779.1	56353.68	378.35	6	8	24	1859.76	2170.03	70.05
1	13	23	7359.79	7818.66	104.43	8	8	24	6673.74	7175.9	138.76
3	13	23	4793.38	5365.85	90.29	2	10	24	6885.54	6866.94	168.5
5	13	23	2789.1	2783.12	89.17	4	10	24	20.38	138.67	70.04
7	13	23	961.73	1152.18	70.05	6	10	24	14626.68	14686.77	317.4
9	13	23	2955.65	3141.08	84.07	8	10	24	520.84	612.2	70.04
11	13	23	13077.39	13593.38	317.34	10	10	24	2.06	574.5	99.05
13	13	23	2549.68	2892.96	118.89	0	12	24	66816.86	72740.84	520.97

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
2	12	24	4395.87	4232.4	84.08	3	11	25	48797.29	46949.12	298.49
4	12	24	3525.69	3076.66	99.08	5	11	25	1.63	46.22	80.6
6	12	24	11.78	30.82	61.88	7	11	25	1823.53	1640.51	76.11
8	12	24	6326.18	6051.96	90.3	9	11	25	1015.97	1150.57	76.1
10	12	24	0.35	-50.94	95.09	11	11	25	274.84	475.46	118.87
12	12	24	17293.16	17935.7	198.4	1	13	25	11984.58	12329.71	228.07
2	14	24	18552.74	19166.8	406.8	3	13	25	7313.3	7376.44	158.59
4	14	24	2434.77	2063.78	84.07	5	13	25	12495.03	11697.28	118.58
6	14	24	7485.68	6748.03	346.91	7	13	25	173.92	203.51	76.1
8	14	24	204.05	287.26	84.05	9	13	25	7941.22	8020.33	112.14
10	14	24	13881.68	14318.37	132.69	11	13	25	5209.57	4716.98	90.29
12	14	24	20.43	-16.51	116.99	13	13	25	3358.07	3309.27	138.71
14	14	24	13659.59	11939.55	178.5	1	15	25	4289.54	4078.85	257.63
0	16	24	2231.65	2272.32	123.78	3	15	25	3024.43	2578.47	84.07
2	16	24	1128.88	1317.6	84.06	5	15	25	582.69	457.37	90.25
4	16	24	1873.83	2110.57	84.06	7	15	25	7540.6	7493.68	98.12
6	16	24	138.73	287.25	84.05	9	15	25	283.23	270.39	108.96
8	16	24	841.87	931.58	84.05	11	15	25	1406.69	1758.58	208.03
10	16	24	3.13	-80.28	128.17	13	15	25	1456.37	1036.36	98.07
12	16	24	4264.74	3762.79	104.4	1	17	25	2421.13	2586.14	98.08
14	16	24	136.38	178.3	98.06	3	17	25	33527.39	32495.45	367.54
2	18	24	1033.14	897.87	90.26	5	17	25	139.77	287.25	84.05
4	18	24	823.17	858.87	108.96	7	17	25	4117.47	4210.61	198.17
6	18	24	175.95	842.07	98.06	9	17	25	427.86	566.1	104.37
8	18	24	517.2	416.5	98.06	11	17	25	615.92	435.85	112.07
10	18	24	1332.22	1060.07	112.08	1	19	25	2565.34	2251.1	98.08
12	18	24	7.54	29.72	98.06	3	19	25	581.07	631.76	98.06
0	20	24	2242.66	2077.07	132.55	5	19	25	1513.98	1595.56	138.69
2	20	24	35.12	138.67	90.25	7	19	25	4957.94	4332.17	140.14
4	20	24	1334.94	1092.94	98.07	0	2	26	7773	7069.06	386.59
6	20	24	430.18	366.51	112.07	2	2	26	250.63	138.68	79.24
8	20	24	4945.01	5589.92	126.12	2	4	26	6215.82	5897.83	148.67
1	1	25	1416.19	1545.43	79.25	4	4	26	371.64	217.92	99.06
1	3	25	7114.15	7355.04	98.13	0	6	26	9199.88	8699.38	208.19
3	3	25	10.61	-138.67	138.67	2	6	26	500.24	664.3	138.68
1	5	25	1672.51	1704.2	70.05	4	6	26	352.41	1281.27	247.64
3	5	25	9857.67	10244.09	148.72	6	6	26	731.05	792.47	99.06
5	5	25	1068.32	832.12	79.25	2	8	26	29.73	75.64	76.09
1	7	25	1324.56	1326.57	108.97	4	8	26	412.45	445.97	70.04
3	7	25	5899.9	6159.56	366.7	6	8	26	24187.99	24125.83	238.25
5	7	25	4457.64	4826.38	84.08	8	8	26	9	19.81	99.05
7	7	25	14644.54	14977.37	178.54	0	10	26	1656.6	2035.52	118.47
1	9	25	17223.41	16862.69	327.4	2	10	26	375.07	307.07	84.05
3	9	25	3554.61	3651.61	138.72	4	10	26	3261.18	3592.11	138.71
5	9	25	27397.85	28130.21	863.95	6	10	26	69.31	-51.27	118.45
7	9	25	3796.87	3806.53	76.12	8	10	26	2016.77	1672.55	76.11
9	9	25	9686.64	9398.38	158.62	10	10	26	192.12	416.03	118.86
1	11	25	442.15	687.08	84.05	2	12	26	17313.91	16788.28	218.25

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
4	12	26	473.96	521.57	76.1	1	15	27	265.71	96.01	90.25
6	12	26	80.13	29.72	84.05	3	15	27	5680.24	5936.2	112.12
8	12	26	1142.7	1150.48	84.06	5	15	27	1101.46	1251	98.07
10	12	26	1364.54	1640.11	158.5	7	15	27	25.47	51.27	113.61
12	12	26	129.04	138.67	118.86	9	15	27	1966.72	1467.91	138.01
0	14	26	25740.73	27441.78	476.52	1	17	27	4531.03	4320.28	104.4
2	14	26	880.39	816.64	84.05	3	17	27	334.1	544.98	98.06
4	14	26	9172.03	7938.34	104.44	5	17	27	26632.91	23669.74	317.66
6	14	26	6500.27	6585.56	178.39	0	0	28	5528.53	5173.11	297.31
8	14	26	5368.79	4806.42	227.92	2	2	28	28580.94	27547.99	238.34
10	14	26	231.86	178.3	84.05	0	4	28	12560.17	11042.67	634.65
12	14	26	5566.74	4752.36	118.51	2	4	28	143.25	101.88	95.09
2	16	26	12538.2	11895.1	436.29	4	4	28	10.62	79.24	99.05
4	16	26	1107.88	1009	108.97	2	6	28	127.41	237.73	84.05
6	16	26	3576.1	3864.71	104.39	4	6	28	317.03	289.67	89.15
8	16	26	1342.65	1231.33	104.37	6	6	28	173231.1	176442.2	945.15
10	16	26	46.44	136.79	146.59	0	8	28	2931.82	3141.54	126.11
0	18	26	4838.61	4105.85	154.15	2	8	28	543.82	470.84	84.05
2	18	26	0.06	108.96	98.06	4	8	28	6888.97	7182.32	218.05
4	18	26	4847.26	4420.29	112.11	6	8	28	17.62	111.43	109.46
6	18	26	468.61	243.02	104.37	8	8	28	1035.01	891.55	138.69
1	1	27	129.33	257.54	79.24	2	10	28	9074.46	8007.16	465.91
1	3	27	184.54	156.68	76.1	4	10	28	4.42	-43.58	104.36
3	3	27	19095.98	16451.82	178.61	6	10	28	1879.35	1946.79	99.07
1	5	27	3143.73	3063.17	84.07	8	10	28	416.31	241.23	118.46
3	5	27	1348.11	1066.68	76.1	10	10	28	4632.01	4637.43	237.82
5	5	27	33728.57	32449.59	298.07	0	12	28	39003.71	35051.25	824.86
1	7	27	2631.72	3121.67	84.07	2	12	28	110.4	25.09	104.36
3	7	27	6800.47	6631.87	98.12	4	12	28	1671.08	2258.88	98.07
5	7	27	14551.78	13621.98	257.87	6	12	28	486.13	416.04	90.25
7	7	27	785.21	891.53	118.87	8	12	28	32.8	83.9	118.45
1	9	27	86.16	72.04	79.24	10	12	28	0.4	198.1	154.09
3	9	27	7595.42	7437.6	104.43	2	14	28	12024.42	11782.23	132.66
5	9	27	1899.63	1851.72	118.88	4	14	28	204.9	168.39	98.06
7	9	27	1898.75	1754.02	84.06	6	14	28	184.47	339.42	104.36
9	9	27	30.52	732.99	118.86	8	14	28	18.37	112.86	230.82
1	11	27	5201.71	5143.17	98.1	0	16	28	26436.45	21898.3	1042.3
3	11	27	1338.9	1476.65	84.06	2	16	28	207.04	178.3	98.06
5	11	27	7481.01	7380.19	118.94	4	16	28	14472.51	11977.59	307.42
7	11	27	1587.66	1734.16	98.07	1	1	29	277.37	257.54	138.68
9	11	27	1.72	-69.86	128.17	1	3	29	334.22	397.21	84.05
11	11	27	1804.15	1921.9	138.69	3	3	29	22748.3	20227.06	238.2
1	13	27	185.57	337.85	84.05	1	5	29	4237.12	3565.64	90.28
3	13	27	1268.06	1407.81	98.07	3	5	29	174.71	267.44	84.05
5	13	27	247.95	677.16	90.25	5	5	29	37729.96	32734.14	298.13
7	13	27	1458.59	1916.1	98.07	1	7	29	1091.42	1241.21	118.87
9	13	27	1122.74	1106.03	168.4	3	7	29	4457.3	4484.48	104.4
11	13	27	222.32	316.97	112.07	5	7	29	9582.12	9021.7	307.31

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	
7	7	29	989.46	851.92	118.87	2	4	32	96.01	57.35	132.53	2
1	9	29	1210.7	1525.82	98.07	4	4	32	278.77	118.87	277.35	4
3	9	29	2996.93	2726.28	104.39							
5	9	29	2507.98	2675.56	98.08							
7	9	29	556.75	769.29	104.37							
9	9	29	1292.46	1505.75	198.13							
1	11	29	4850.62	4419.61	112.11							
3	11	29	2911.99	2879.47	104.39							
5	11	29	3021.9	2864.56	178.34							
7	11	29	3613.25	3537.27	198.16							
9	11	29	76.41	140.87	179.57							
1	13	29	1312.36	1153.94	104.37							
3	13	29	1914.36	2080.42	112.08							
5	13	29	33.45	118.86	112.06							
7	13	29	411.58	555.68	284.88							
0	2	30	3651.5	3307.78	160.69							
2	2	30	14.62	138.67	138.67							
2	4	30	2869.94	2697.21	98.08							
4	4	30	427.22	495.28	138.68							
0	6	30	6186.01	5976.86	160.72							
2	6	30	53.96	-49.53	148.58							
4	6	30	129.91	126.48	90.25							
6	6	30	96.41	138.67	138.67							
2	8	30	1535.92	1612.73	168.41							
4	8	30	0.6	-63.39	131.87							
6	8	30	12261.08	10952.55	257.8							
8	8	30	0	217.91	158.48							
0	10	30	252.49	318.86	168.39							
2	10	30	216.82	128.77	168.39							
4	10	30	1802.97	1661.45	123.77							
6	10	30	224.17	198.11	154.09							
2	12	30	10011.41	8582.18	247.83							
4	12	30	142.45	69.34	168.39							
1	1	31	436.47	1010.37	138.68							
1	3	31	2995.74	2903.26	126.1							
3	3	31	159.92	79.24	138.67							
1	5	31	208.82	117.54	104.36							
3	5	31	2798.53	2544.66	118.48							
5	5	31	28.57	217.91	158.48							
1	7	31	228.26	118.86	112.07							
3	7	31	4451.13	3937.15	132.57							
5	7	31	1997.78	1600.12	118.47							
7	7	31	5166.59	4558.31	198.19							
1	9	31	4214.97	3680.69	544.97							
3	9	31	405.02	319.06	132.53							
0	0	32	17958.87	19185.01	436.47							
2	2	32	6640.23	5807.62	178.39							
0	4	32	226.15	908	604.23							

crystal 2

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
2	2	2	918.55	12643.82	255.34	1	3	9	53151.2	51509.99	211.41
1	1	3	295759	340273.8	2254.05	3	3	9	0.47	493.07	44.02
1	3	3	599480.5	572546.8	4252.76	1	5	9	8583.33	5913.77	123.27
3	3	3	28713.63	38424.54	493.07	3	5	9	6515.76	8278.31	65.15
0	0	4	33891.42	26467.5	378.61	5	5	9	10187.4	11402.33	105.66
2	2	4	1589.12	774.83	52.83	1	7	9	17248.23	20560.25	149.68
2	4	4	10297.3	18463.86	158.49	3	7	9	19639.6	18681.18	264.15
4	4	4	99454.47	123964.1	1303.12	5	7	9	12044.68	9830.66	68.49
1	1	5	204615.9	216820.4	1153.44	7	7	9	56271.16	57962.59	334.59
1	3	5	7361.45	9474.46	68.49	1	9	9	2327.35	3328.25	70.44
3	3	5	633634.3	707534.6	22522.91	3	9	9	20744.09	19494.03	132.07
1	5	5	84290.28	61607.82	369.81	5	9	9	137473.1	138932.4	713.2
3	5	5	10699.32	13876.51	123.27	7	9	9	6783.3	6841.4	88.05
0	2	6	81905.63	86740.11	503.84	9	9	9	53426.84	55946.28	545.9
2	2	6	105.17	2544.61	79.24	0	2	10	258.77	540.83	57.23
2	4	6	250387.1	280540.1	2667.89	2	2	10	26869.15	34347.88	211.32
4	4	6	6282.41	5793.62	88.05	2	4	10	4650.54	5256.89	49.81
0	6	6	477454.5	416999.6	3187.37	4	4	10	97.98	220.12	61.63
2	6	6	1.94	-44.02	44.02	0	6	10	33019.28	30627.38	506.28
4	6	6	367346.3	329910.5	1769.78	2	6	10	7915.88	8514.78	62.26
6	6	6	705409.4	790582.4	11067.75	4	6	10	2331.31	2386.26	49.81
1	1	7	747.12	1206.27	52.83	6	6	10	1415.95	1241.49	70.44
1	3	7	12618.86	9599.95	158.49	2	8	10	101989.5	97209.76	629.55
3	3	7	157078.1	154156.1	845.27	4	8	10	1227.78	552.66	61.63
1	5	7	29921.27	24223.63	374.21	6	8	10	11084.97	12991.19	83.88
3	5	7	39359.72	38309.7	202.51	8	8	10	7100.43	7528.18	96.85
5	5	7	31088.83	22813.47	158.49	0	10	10	241068.9	256407.2	1831.42
1	7	7	6189.29	4235.15	70.44	2	10	10	1883.91	757.22	61.63
3	7	7	488.58	-70.44	70.44	4	10	10	6314.63	6568.45	79.24
5	7	7	75429.9	72288.16	413.83	6	10	10	10992.49	11736.92	114.46
7	7	7	541.72	730.81	96.85	8	10	10	46632.62	44491.11	290.56
0	0	8	1228.42	871.68	114.46	10	10	10	64.79	79.24	105.66
2	2	8	85423.94	91562.06	501.88	1	1	11	82997.38	67859.3	369.81
0	4	8	154311.2	150350.3	4001.82	1	3	11	9365.46	7654.38	149.68
2	4	8	8420.91	6955.86	52.65	3	3	11	87861.36	97082.73	528.29
4	4	8	34960.95	31090.07	202.51	1	5	11	11102.06	10636.28	215.72
2	6	8	14248.66	9035.5	123.27	3	5	11	719.23	855.47	88.05
4	6	8	20299.35	23988.14	189.3	5	5	11	5881.63	5238.91	88.05
6	6	8	5847.28	5890.47	79.24	1	7	11	5908.22	5953.43	58.9
0	8	8	133550.5	167645.1	1241.49	3	7	11	14783.66	14096.63	86.5
2	8	8	72.03	96.85	52.83	5	7	11	36288.36	32908.92	155.65
4	8	8	145920.6	139258.2	704.39	7	7	11	24720.14	21175.76	158.49
6	8	8	28653.76	31178.12	202.51	1	9	11	1333.71	1188.99	74.84
8	8	8	83296.56	83672.88	827.66	3	9	11	186199.5	180910.9	823.26
1	1	9	11761.13	11296.67	96.85	5	9	11	662.05	251.16	43.96

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
7	9	11	16862.7	16869.25	242.13	5	11	13	4496.36	4699.45	215.72
9	9	11	23030.3	23130.45	167.29	7	11	13	262.46	144.08	67.64
1	11	11	248608.5	258177	1303.12	9	11	13	12191.36	10904.21	356.6
3	11	11	456.43	713.2	70.44	11	11	13	14187.2	13964.56	140.88
5	11	11	125204.3	120098.7	625.15	1	13	13	939.69	2958.44	96.85
7	11	11	2829.61	3064.1	79.24	3	13	13	26055.6	24812.18	202.51
9	11	11	5467.2	6172.23	123.27	5	13	13	73.45	123.27	88.05
0	0	12	244871.1	221909.7	2121.98	7	13	13	1978.79	1708.15	79.24
2	2	12	734.98	1452.81	61.63	9	13	13	5850.6	6947.06	123.27
0	4	12	6847.79	7783.53	167.29	11	13	13	45.12	-140.88	140.88
2	4	12	20443.33	21466.62	105.84	13	13	13	7413.11	7721.89	220.12
4	4	12	7387.19	6339.52	88.05	0	2	14	51338.69	48657.54	270.78
2	6	12	13571.47	13273.2	127.67	2	2	14	2.85	-105.66	105.66
4	6	12	1385.81	909.83	92.45	2	4	14	2068.16	1598.68	49.81
6	6	12	19077.58	16870.17	140.88	4	4	14	11150.82	10777.19	105.66
0	8	12	6516.66	6404.75	96.85	0	6	14	25.75	-27.12	69.07
2	8	12	18804.92	21392.1	108.82	2	6	14	41891.88	41247.45	589.93
4	8	12	46591.33	45822.97	195.45	4	6	14	32061.58	31879.2	506.28
6	8	12	215.94	-77.64	77.64	6	6	14	0.18	-88.05	88.05
8	8	12	102957.9	104690.2	563.51	2	8	14	4198.17	4284.13	68.49
2	10	12	1542.67	1968.79	52.65	4	8	14	72.06	82.49	58.9
4	10	12	79.5	-74.71	74.71	6	8	14	67435.07	71869.99	289.46
6	10	12	67498.66	67327.86	541.5	8	8	14	181.48	140.88	88.05
8	10	12	250.58	127.93	52.65	0	10	14	10237.41	10363.03	180.5
10	10	12	43274.48	43865.96	290.56	2	10	14	3442.51	3215.55	65.15
2	12	12	328.41	369.81	79.24	4	10	14	5373.85	4564.21	162.89
4	12	12	915.05	1241.49	88.05	6	10	14	279.64	422.09	140.88
6	12	12	2754.77	2553.42	88.05	8	10	14	16875.91	15760.76	105.84
8	12	12	11352.11	11287.87	140.88	10	10	14	3190.2	2350.91	96.85
10	12	12	1686.34	607.54	105.66	2	12	14	40302.62	39983.51	193.01
12	12	12	82664.63	93032.48	1012.56	4	12	14	853.06	682.87	58.9
1	1	13	709.12	924.51	61.63	6	12	14	1164.61	1541.67	71.4
1	3	13	16453.81	17444.27	176.1	8	12	14	3800.52	3493.93	158.49
3	3	13	9866.35	9808.65	96.85	10	12	14	5260.19	5347.89	268.55
1	5	13	13218.38	11770.78	189.31	12	12	14	592.43	220.12	123.27
3	5	13	226.03	322.8	180.5	0	14	14	22496.27	26458.7	290.56
5	5	13	28.8	96.85	79.24	2	14	14	343.77	501.88	79.24
1	7	13	14.45	-54.27	54.27	4	14	14	14855.69	14272.73	149.68
3	7	13	7611.92	7313.5	330.18	6	14	14	66666.05	63641.75	369.81
5	7	13	9599.37	9666.76	73.94	8	14	14	149.1	176.1	105.66
7	7	13	5651.54	8945.77	105.66	10	14	14	244.15	35.22	105.66
1	9	13	12350	12819.71	211.32	12	14	14	10778	12080.31	167.29
3	9	13	20224.94	18411.9	347.79	14	14	14	243.63	255.34	193.71
5	9	13	11605.95	12961.44	268.55	1	1	15	24.23	-52.83	52.83
7	9	13	1535.66	1458.82	62.26	1	3	15	10711.09	9537.78	140.88
9	9	13	23921.89	25393.3	202.51	3	3	15	14080.05	19599.69	140.88
1	11	13	15717.22	16823.16	154.09	1	5	15	6015.32	5912.65	62.26
3	11	13	8945.23	8162.36	77.64	3	5	15	46482.7	45009.05	409.43

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
5	5	15	23694.85	24468.79	176.1	0	12	16	10209.75	10353.54	145.28
1	7	15	1176.07	1523.45	83.65	2	12	16	0.02	40.36	162.89
3	7	15	11702.37	11786.08	127.67	4	12	16	8575.74	7688.89	281.76
5	7	15	4.04	-65.15	65.15	6	12	16	3048.11	2897.03	79.24
7	7	15	575.2	686.78	105.66	8	12	16	652.2	2436.4	71.4
1	9	15	7670.33	7987.45	294.96	10	12	16	87.38	-69.79	69.79
3	9	15	623.89	626.32	162.89	12	12	16	2931.04	2808.76	105.66
5	9	15	20573.07	20581.59	118.29	2	14	16	9083.54	9661.28	206.91
7	9	15	5600.16	5811.28	80.94	4	14	16	4.13	-73.26	73.26
9	9	15	2335.58	2553.42	105.66	6	14	16	960.15	995.18	73.94
1	11	15	1737.71	2041.63	65.15	8	14	16	774.53	689.14	66.04
3	11	15	32190.8	31819.62	361	10	14	16	682.47	594.47	132.07
5	11	15	4254.35	4051.06	145.28	12	14	16	29.53	7.4	77.64
7	11	15	15075.9	14470.95	105.84	14	14	16	5102.22	5247.71	123.27
9	11	15	633.55	651.68	62.26	0	16	16	11065.59	11367.11	167.29
11	11	15	157.21	378.61	79.24	2	16	16	4.95	-123.27	123.27
1	13	15	1212.44	1990.78	65.15	4	16	16	5586.2	5423.81	114.46
3	13	15	553.93	480.91	67.64	6	16	16	565.29	237.73	96.85
5	13	15	18513.65	17790.79	554.71	8	16	16	249.93	810.05	96.85
7	13	15	205.21	524.85	140.88	10	16	16	586.83	466.66	114.46
9	13	15	1920.37	1440.23	167.29	12	16	16	1138.4	1267.9	114.46
11	13	15	1429.3	1314.79	71.4	14	16	16	45.01	61.63	132.07
13	13	15	558.76	677.98	105.66	16	16	16	9277.61	10530.65	246.54
1	15	15	2443.99	2166	96.85	1	1	17	32993.24	31336.61	211.32
3	15	15	4467.1	4842.69	105.66	1	3	17	1084.68	1314.06	92.45
5	15	15	1787.1	1505.64	96.85	3	3	17	2773.69	2025.12	88.05
7	15	15	7569.41	7484.16	114.46	1	5	17	2701.7	2553.42	58.9
9	15	15	2984.35	3372.27	105.66	3	5	17	5.14	140.88	56.03
11	15	15	1808.68	1813.81	96.85	5	5	17	172745.4	182877.6	994.95
13	15	15	725.51	475.46	132.07	1	7	17	276.36	224.52	62.26
15	15	15	331.94	228.93	184.9	3	7	17	4285.15	4701.51	171.7
0	0	16	160283.8	156867.9	1549.66	5	7	17	53545.73	56466	242.81
2	2	16	3190.89	4604.96	96.85	7	7	17	5575.18	6304.3	132.07
0	4	16	16001.33	19309.47	146.21	1	9	17	3912.48	3663.63	140.88
2	4	16	3432.81	3190.21	88.05	3	9	17	68410.05	70270.09	704.39
4	4	16	2153.71	9702.99	105.66	5	9	17	113.44	985.38	71.4
2	6	16	3798.49	5745.22	68.49	7	9	17	8060.52	8195.53	145.28
4	6	16	235.28	-83.88	83.88	9	9	17	2575.41	2544.61	105.66
0	8	16	6921.73	7775.83	206.91	1	11	17	12187.11	11641.67	387.42
2	8	16	6646.12	6256.03	74.71	3	11	17	631.53	895.16	92.45
4	8	16	30251.69	30786.64	272.95	5	11	17	38328.36	37844.87	264.15
6	8	16	151.99	-71.4	71.4	7	11	17	3042.65	3461.74	224.52
8	8	16	45383.98	44429.48	308.17	9	11	17	878.62	530.14	62.26
2	10	16	5271.22	5707.43	246.54	11	11	17	457.33	475.46	88.05
4	10	16	716.31	725.4	74.84	1	13	17	3905.26	4155.38	202.51
6	10	16	7481.11	7617.91	83.88	3	13	17	2935.18	3339.97	281.76
8	10	16	1108.55	986.15	71.4	5	13	17	192.99	-75.89	75.89
10	10	16	4262	4516.91	105.66	7	13	17	91.59	49.38	74.84

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
9	13	17	6426.7	6086.07	132.07	8	14	18	6453.26	7100.65	206.91
11	13	17	1488.31	1456.14	101.26	10	14	18	119.37	132.07	105.66
13	13	17	2387.87	2474.17	123.27	12	14	18	245.58	94.34	105.66
1	15	17	61.76	-67.95	67.95	14	14	18	176.12	193.71	132.07
3	15	17	6333.45	5413.99	361	2	16	18	1095.94	1104.15	67.64
5	15	17	5226.4	5040.97	83.88	4	16	18	21.57	-73.94	73.94
7	15	17	5.71	60.38	101.26	6	16	18	16332.18	16811.47	594.33
9	15	17	1257.26	1156.5	77.64	8	16	18	13.97	-16.35	176.1
11	15	17	1464.76	1472.48	259.74	10	16	18	102.84	198.11	74.71
13	15	17	421.88	479.57	123.27	12	16	18	313.66	321.94	242.13
15	15	17	74.41	-114.46	149.68	14	16	18	892.73	1001.22	99.24
1	17	17	2371.64	1875.44	88.05	16	16	18	424.43	669.17	158.49
3	17	17	16.7	-140.88	140.88	0	18	18	3521.54	3786.1	167.29
5	17	17	18591.91	19687.74	167.29	2	18	18	30.89	-35.22	88.05
7	17	17	13039.34	13585.95	158.49	4	18	18	661.27	563.51	105.66
9	17	17	49.02	44.02	123.27	6	18	18	465.26	325.78	123.27
11	17	17	56.36	0	132.07	8	18	18	1079.36	977.34	114.46
13	17	17	22.16	96.85	167.29	10	18	18	74.64	167.29	132.07
15	17	17	586.73	642.76	158.49	12	18	18	699.82	686.78	272.95
17	17	17	16976.58	17451.29	431.44	14	18	18	133.23	352.2	264.15
0	2	18	133.52	180.5	87.16	16	18	18	1895.29	2236.44	211.32
2	2	18	1682.52	1461.61	88.05	18	18	18	121.42	290.56	334.59
2	4	18	3866.23	5569.1	68.49	1	1	19	5047.29	4895.52	105.66
4	4	18	2128.29	2703.1	88.05	1	3	19	7772.55	7823.17	80.94
0	6	18	21745.23	23612.32	250.94	3	3	19	5754.38	5538.28	105.66
2	6	18	1865.25	2002.67	65.15	1	5	19	282.56	355.72	62.26
4	6	18	12688.46	12687.35	171.7	3	5	19	33135.9	31250.58	330.18
6	6	18	1162.14	766.03	96.85	5	5	19	837.51	1118.22	96.85
2	8	18	17963.05	19860.44	171.7	1	7	19	3979.28	3342.44	68.49
4	8	18	2802.33	2290.09	71.4	3	7	19	14681.82	14855.22	202.51
6	8	18	0.1	13.02	96.85	5	7	19	131.47	536.34	114.46
8	8	18	1658.58	1426.39	105.66	7	7	19	41.22	361	96.85
0	10	18	102.35	490.99	118.87	1	9	19	23983.5	22998.72	338.99
2	10	18	532.06	1858.68	158.49	3	9	19	518.49	650.96	67.64
4	10	18	35.56	639.84	68.49	5	9	19	1590.73	2156.51	132.07
6	10	18	1323.22	910.95	71.4	7	9	19	2367.98	2512.16	73.94
8	10	18	46.16	-81.32	81.32	9	9	19	10.22	-70.44	70.44
10	10	18	101.11	-79.24	79.24	1	11	19	378.21	251.93	62.26
2	12	18	958.58	755.37	74.84	3	11	19	473.62	631.81	96.85
4	12	18	138.75	79.24	68.49	5	11	19	1146.43	1030.17	68.49
6	12	18	8368.68	9210.09	246.54	7	11	19	1537.33	1320.97	68.49
8	12	18	316.27	145.28	68.49	9	11	19	1596.88	1508.95	74.84
10	12	18	52.09	-90.12	90.12	11	11	19	86.15	272.95	96.85
12	12	18	520.6	572.32	105.66	1	13	19	2852.77	2665.58	74.84
0	14	18	2260.84	1446.43	83.88	3	13	19	12.92	8.8	114.46
2	14	18	249.83	51.95	96.85	5	13	19	2122.44	2000.11	74.71
4	14	18	8349.48	8882.32	198.11	7	13	19	224.24	121.67	67.64
6	14	18	242.01	156.37	92.45	9	13	19	459.42	476.81	67.64

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
11	13	19	1347.08	1229.48	77.64	6	12	20	53.65	50.99	73.94
13	13	19	565.03	598.73	114.46	8	12	20	1371.57	1562.31	71.4
1	15	19	869.58	726.64	68.49	10	12	20	6.83	-29.35	59.99
3	15	19	2529.14	2710.86	268.55	12	12	20	24.73	193.71	105.66
5	15	19	342.73	369.49	101.26	2	14	20	3755.83	3342.68	127.67
7	15	19	2519.72	2397.23	80.22	4	14	20	7.56	-66.67	88.05
9	15	19	275.65	385.49	80.94	6	14	20	5725.56	5921.88	80.22
11	15	19	1622.94	1838.52	96.35	8	14	20	111.95	106.79	92.79
13	15	19	74.94	50.51	117.8	10	14	20	3541.4	3623.85	123.27
15	15	19	409.73	396.22	149.68	12	14	20	20.58	-87.91	87.91
1	17	19	31.86	-67.64	67.64	14	14	20	261.57	149.68	140.88
3	17	19	400.26	338.66	77.64	0	16	20	86.39	8.8	105.84
5	17	19	984.87	1022.32	82.51	2	16	20	38.65	93.55	73.94
7	17	19	89.64	1.82	90.12	4	16	20	1420.78	1310.86	83.88
9	17	19	1128.5	1030.51	86.5	6	16	20	0.4	57.23	80.94
11	17	19	434.81	346.45	209.37	8	16	20	1853.51	2092.54	96.35
13	17	19	86.37	388.42	197.09	10	16	20	0.05	26.41	84.53
15	17	19	486.3	353.4	195.46	12	16	20	1.49	505.9	479.87
17	17	19	510.27	1153.44	228.93	14	16	20	213.58	189.31	186.47
1	19	19	29.67	167.29	167.29	16	16	20	278.54	316.98	369.81
3	19	19	962.76	1215.07	140.88	2	18	20	553.84	655.5	189.31
5	19	19	1303.65	1276.71	149.68	4	18	20	37.37	-1.23	132.88
7	19	19	1717.08	1743.37	149.68	6	18	20	998.61	958.57	99.03
9	19	19	52.39	123.27	572.32	8	18	20	14.24	-118.29	118.29
11	19	19	672.39	1047.78	704.39	10	18	20	2.95	-154.28	214.19
15	19	19	616.12	836.46	361	14	18	20	1092.16	942.12	422.63
17	19	19	360.63	1364.76	906.9	16	18	20	5.76	364.52	250.94
0	0	20	4061.52	3971.01	211.32	2	20	20	7.45	211.32	228.93
2	2	20	20143.53	19828.61	158.49	1	1	21	8430.41	8989.79	123.27
0	4	20	4966.95	5530.61	99.62	1	3	21	5543.11	5207.74	77.64
2	4	20	730.56	567.44	65.15	3	3	21	7461.01	7492.96	114.46
4	4	20	20189.53	20673.88	158.49	1	5	21	7160.81	6630.03	167.29
2	6	20	28565.31	28512.87	149.68	3	5	21	1443.48	1237.1	62.26
4	6	20	40.99	-48.6	145.28	5	5	21	3051.04	3284.22	105.66
6	6	20	0.3	-132.07	132.07	1	7	21	372.58	-73.94	73.94
0	8	20	94747.34	97505.75	506.7	3	7	21	1199.06	847.01	154.09
2	8	20	450.93	-96.85	96.85	5	7	21	79.98	8.8	114.46
4	8	20	5256.32	6047.57	118.87	7	7	21	8.36	26.41	96.85
6	8	20	871.09	611.59	71.4	1	9	21	3926.43	3717.43	158.49
8	8	20	838.1	1135.83	105.66	3	9	21	3141.83	3100.79	71.4
2	10	20	6636.09	7129.94	220.12	5	9	21	1376.33	1443.29	71.4
4	10	20	103.83	-92.45	92.45	7	9	21	0.3	-51.07	74.84
6	10	20	2005.34	2522.42	132.07	9	9	21	2604.34	2949.64	114.46
8	10	20	152.11	223.15	140.88	1	11	21	8576.71	8693.91	83.88
10	10	20	1000.07	801.25	105.66	3	11	21	1907.16	1981.38	162.89
0	12	20	15.32	-117.8	117.8	5	11	21	833.43	801.51	73.94
2	12	20	459.95	273.45	61.33	7	11	21	27.65	24.13	79.81
4	12	20	1276.63	1756.2	71.4	9	11	21	9.73	-61.63	61.63

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
11	11	21	7791.47	8197.35	123.27	8	12	22	4.38	-26.41	96.85
1	13	21	449.4	503.14	70.44	10	12	22	7127.88	7243.51	96.35
3	13	21	3518.28	3843.46	80.94	12	12	22	76.45	184.9	114.46
5	13	21	662.76	817.55	77.64	0	14	22	52.9	232.31	198.11
7	13	21	166.07	330.71	68.49	2	14	22	406.81	286.16	80.94
9	13	21	955.2	802.09	80.22	4	14	22	713.54	822.49	83.88
11	13	21	30.73	67.83	83.88	6	14	22	90.19	190.87	95.15
13	13	21	730.87	739.61	140.88	8	14	22	2983.66	2997.49	92.77
1	15	21	418.24	200.82	136.48	10	14	22	1.2	-49.89	102.59
3	15	21	42.27	31.13	83.65	12	14	22	53.07	95.52	99.24
5	15	21	160.61	13.21	101.26	2	16	22	239.77	154.09	99.62
7	15	21	11.04	140.88	87.16	4	16	22	0.49	94.26	100.99
9	15	21	169.22	284.21	105.66	6	16	22	1242.06	1210.38	220.12
11	15	21	59.96	4.28	107.76	8	16	22	1.74	218.43	158.67
13	15	21	74.54	165.89	136.55	10	16	22	623.24	824.34	369.81
15	15	21	116.74	343.39	766.03	0	18	22	178.39	-704.39	704.39
1	17	21	536.23	710.6	116.34	2	18	22	0	489.2	308.32
3	17	21	297.63	305.77	101.46	4	18	22	1097.96	1708.15	686.78
5	17	21	34.87	25.64	103.66	6	18	22	0.81	-220.12	554.71
7	17	21	14.02	1.87	102.59	10	18	22	95.83	-677.98	677.98
9	17	21	533.03	570.79	161.52	2	20	22	1697.62	1578.57	405.02
11	17	21	268.48	181.75	321.38	0	22	22	8131.71	6445.18	396.22
15	17	21	32.8	1127.03	915.71	1	1	23	15864.51	14924.29	140.88
1	19	21	22.23	-161.56	194.27	1	3	23	2553.69	2126.83	68.49
9	19	21	159.11	-132.07	581.12	3	3	23	18136.12	17829.9	140.88
1	21	21	226.57	361	405.02	1	5	23	5920.98	5172.97	74.71
5	21	21	332.33	501.88	589.93	3	5	23	180.71	125.12	58.9
0	2	22	11181.3	11099.47	121.29	5	5	23	213.68	52.83	96.85
2	2	22	4.03	-96.85	96.85	1	7	23	340.58	110.06	62.26
2	4	22	7274.58	6832.78	74.71	3	7	23	657.38	730.15	71.4
4	4	22	29.09	-123.27	123.27	5	7	23	3348.46	2954.52	167.29
0	6	22	24219.59	23400.32	164.9	7	7	23	1160.59	986.15	105.66
2	6	22	0.01	-73.94	73.94	1	9	23	7.87	-86.5	86.5
4	6	22	3462.2	3693.78	74.71	3	9	23	388.54	474.63	71.4
6	6	22	6048.76	5784.81	105.66	5	9	23	18.47	101.26	74.71
2	8	22	3694.06	3595.39	96.85	7	9	23	196.06	124.25	127.67
4	8	22	212.89	114.46	74.71	9	9	23	3734.71	4199.93	132.07
6	8	22	483.72	483.14	74.71	1	11	23	15155.44	15349.87	180.5
8	8	22	140.3	0	132.07	3	11	23	49.56	-76.64	83.88
0	10	22	36844.3	39646.52	462.26	5	11	23	680.47	728.12	145.28
2	10	22	58.96	-105.66	105.66	7	11	23	213.03	268.55	99.62
4	10	22	131.55	220.12	68.49	9	11	23	194.35	95.09	90.93
6	10	22	13.32	16.51	73.94	11	11	23	6114.99	5670.35	132.07
8	10	22	1802.13	1894.41	132.07	1	13	23	936.53	951.25	74.71
10	10	22	446.07	528.29	114.46	3	13	23	705.97	813.53	90.12
2	12	22	1247.48	1564.37	74.71	5	13	23	362.43	333.37	90.12
4	12	22	0.79	199.24	211.32	7	13	23	85.1	159.75	206.91
6	12	22	2722.01	2588.91	162.89	9	13	23	273.66	132.07	87.16

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
11	13	23	1184.04	1161.27	90.12	12	14	24	0.98	-140.88	598.73
13	13	23	237.11	378.61	158.49	0	16	24	174.6	70.44	519.49
1	15	23	18.99	277.65	127.67	2	16	24	111.38	1106.44	761.62
3	15	23	673.74	533.02	105.84	6	16	24	4.92	378.61	413.83
5	15	23	70.89	224.08	180.5	8	16	24	66.37	160.54	293.24
7	15	23	299.31	131.92	174.28	2	18	24	89.75	-484.27	572.32
9	15	23	670.85	738.74	111.55	4	18	24	108.66	1241.49	598.73
11	15	23	34.52	9.74	154.09	0	20	24	139.64	-195.82	276
1	17	23	625.52	774.83	484.27	2	20	24	1.6	-21.02	192.7
3	17	23	54.89	405.02	387.42	1	1	25	240.3	281.76	96.85
5	17	23	249.26	4508.1	1012.56	1	3	25	1011.99	1150.4	68.49
7	17	23	241.31	-422.63	422.63	3	3	25	0.62	-44.02	123.27
11	17	23	1798.85	2553.42	713.2	1	5	25	189.5	106.08	83.65
1	19	23	269.43	341.31	202.51	3	5	25	1506.44	1485.5	71.4
3	19	23	1380.13	1480.75	408.66	5	5	25	128.42	96.85	105.66
1	21	23	519.95	449.19	268.55	1	7	25	150.75	118.87	68.49
3	21	23	216.24	167.29	387.42	3	7	25	742.36	872.31	74.71
1	23	23	780.57	422.63	343.39	5	7	25	555.11	450.6	74.71
0	0	24	28544.55	28668.72	378.61	7	7	25	1838.47	1787.39	132.07
2	2	24	10355.21	10662.72	123.27	1	9	25	2022.05	1926.14	80.94
0	4	24	110.28	55.23	101.46	3	9	25	543.18	528.29	80.94
2	4	24	12.1	-65.15	65.15	5	9	25	3481.15	3163.79	101.46
4	4	24	2.06	-17.61	132.07	7	9	25	474.58	358.32	92.77
2	6	24	3053.99	2942.47	71.4	9	9	25	1129.81	1038.98	158.49
4	6	24	68.67	48.43	74.71	1	11	25	61.89	-90.12	90.12
6	6	24	214.55	361	96.85	3	11	25	5104.89	5080	303.77
0	8	24	3459.02	3435.66	145.28	5	11	25	5.23	-29.35	128.98
2	8	24	80.33	-51.07	76.16	7	11	25	181.58	175	193.71
4	8	24	95.72	148.92	118.87	9	11	25	71.52	237.73	105.84
6	8	24	292.2	399.49	77.64	11	11	25	4.67	-202.51	202.51
8	8	24	937.31	854.07	140.88	1	13	25	1209.29	1128.39	149.68
2	10	24	883.94	762.24	74.71	3	13	25	746.24	915.83	107.76
4	10	24	24.44	32.05	83.65	5	13	25	1148.61	808.69	160.44
6	10	24	1905.92	1851.91	193.71	7	13	25	12.06	112.95	268.55
8	10	24	78.47	185.64	107.47	9	13	25	686.35	487.57	158.55
10	10	24	0.01	-52.83	123.27	11	13	25	371.33	283.49	183.77
0	12	24	8384.21	8587.5	563.51	1	15	25	372.01	645.94	233.33
2	12	24	562.46	606.77	96.85	3	15	25	280.2	266.1	192.51
4	12	24	456.66	472.9	101.46	5	15	25	36.47	-408.47	444.87
6	12	24	0	-100.99	100.99	7	15	25	564.36	893.51	642.76
8	12	24	621.21	628.07	220.12	1	17	25	173.99	-396.22	396.22
10	12	24	1.45	-92.32	99.24	3	17	25	2545.5	5776.01	1127.03
12	12	24	1477.74	1505.64	193.71	1	19	25	145.3	-449.05	686.78
2	14	24	1987.95	1868.06	103.66	3	19	25	25.25	-255.34	625.15
4	14	24	272.92	8.56	242.13	0	2	26	1018.01	972.84	102.59
6	14	24	738.72	643.15	161.52	2	2	26	66.56	35.22	96.85
8	14	24	23.67	-154.16	154.16	2	4	26	818.42	791.42	77.64
10	14	24	1160.76	974.69	135.28	4	4	26	56.71	-8.8	132.07

h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)	h	k	l	Fcal^2	Fobs^2	σ(Fobs^2)
0	6	26	1310.84	819.4	121.29	5	13	27	5.31	1250.29	572.32
2	6	26	103.53	31.24	92.79	1	15	27	12.95	-62.61	330.02
4	6	26	41.83	218.36	92.77	3	15	27	374.75	184.9	836.46
6	6	26	65.25	-26.41	158.49	5	15	27	81.24	722	607.54
2	8	26	1.06	-98.54	98.54	1	17	27	232.09	801.25	651.56
4	8	26	67.08	0.5	107.76	3	17	27	13.13	1488.03	827.66
6	8	26	2748.72	2396.89	96.35	0	0	28	546.4	915.71	528.29
8	8	26	4.16	-105.66	220.12	2	2	28	3079.39	3662.83	431.44
0	10	26	201.75	257.59	141.5	2	4	28	14.46	-213.17	213.17
2	10	26	14.71	-81.2	171.7	4	4	28	2.35	-158.49	158.49
4	10	26	311.63	220.12	117.22	2	6	28	1.62	94.28	275.75
6	10	26	6.23	-30.13	139.98	4	6	28	33.19	-69.34	158.55
8	10	26	143.93	50.68	139.98	6	6	28	14240.13	13128.09	220.12
10	10	26	51.92	396.22	378.61	2	8	28	54.55	-52.03	205.18
2	12	26	1495.88	1502.08	140.88	4	8	28	600.32	631.15	143.3
4	12	26	22.32	65.34	117.8	6	8	28	2.74	212.73	149.76
6	12	26	17.79	372.46	202.51	8	8	28	119.39	334.59	220.12
8	12	26	101.38	413.83	845.27	2	10	28	644.71	366.14	221.81
0	14	26	1991.73	1504.36	444.65	4	10	28	0.86	-183.98	183.98
2	14	26	65.44	45.06	303.77	6	10	28	118.06	497.27	291.03
4	14	26	649.14	406.27	233.33	8	10	28	28.33	816.58	373.4
6	14	26	492.46	589.93	616.34	0	12	28	2730.44	2368.52	572.32
2	16	26	907.28	2210.03	510.68	2	14	28	790.76	697.25	946.53
4	16	26	90.51	783.64	757.22	2	16	28	10.31	-26.41	537.1
0	18	26	256.77	466.66	537.1	1	1	29	19.62	-387.42	387.42
2	18	26	0.78	-880.49	889.29	1	3	29	29.67	-96.85	290.56
1	1	27	6.97	26.41	96.85	3	3	29	2093.5	2315.69	422.63
1	3	27	22.01	47.69	111.55	3	5	29	13.45	-150.6	150.6
3	3	27	2338.18	1928.27	149.68	5	5	29	2763.06	2289.27	184.9
1	5	27	380.84	223.79	143.3	3	7	29	299.68	598.73	210.59
3	5	27	149.47	47.94	281.76	5	7	29	655.59	834.54	165.01
5	5	27	3442.89	3363.47	176.1	7	7	29	52.84	167.29	220.12
1	7	27	368.83	500.42	193.71	3	9	29	213.55	-88.05	369.81
3	7	27	676.96	483.25	131.17	5	9	29	158.62	118.67	343.39
5	7	27	1313.16	1156.38	107.76	7	9	29	37.81	51.34	242.13
7	7	27	55.11	8.8	158.49	0	2	30	256.15	227.48	379.17
1	9	27	30.34	-23.8	112.06	2	4	30	195.49	251.73	363.86
3	9	27	772.66	602.81	133.75	4	4	30	52.96	-61.63	308.17
5	9	27	190.45	196.72	116.34	4	6	30	8.67	183.59	197.04
7	9	27	203.99	652.66	387.42	6	6	30	9.53	-35.22	325.78
9	9	27	1.17	334.59	237.73	4	8	30	0.46	193.71	598.73
1	11	27	400.71	259.86	114.05	3	5	31	177.5	0	563.51
3	11	27	117.84	281.57	184.9						
5	11	27	616.42	564.19	202.51						
7	11	27	106.83	246.9	300.76						
9	11	27	1.52	-14.67	419.39						
1	13	27	35.8	1309	1060.99						
3	13	27	97.82	-9.8	252.78						