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AM-88-346

AN exploratory examination of the electron density and electrostatic potential of phenakite

Downs and Gibbs

To be depoasited: Table 6

AMerican Mineralogist, 72, 7-8, 769-777

Table 6. Observed and calculated structure factor moduli and extinction coefficients from multipole model.

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite

H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y
1	1	0	69.19	65.41	0.84	4	1	0	58.99	50.70	0.97	7	1	0	132.78	132.89	0.86
10	1	0	39.65	41.01	0.99	13	1	0	82.68	82.93	0.97	16	1	0	66.49	66.94	0.98
2	2	0	165.09	163.08	0.57	5	2	0	136.71	134.01	0.81	11	2	0	65.65	65.80	0.98
14	2	0	93.64	93.73	0.97	17	2	0	41.56	41.61	0.99	0	3	0	99.24	96.26	0.80
3	3	0	184.75	179.34	0.65	6	3	0	67.17	66.87	0.96	9	3	0	26.63	27.56	1.00
12	3	0	80.43	81.16	0.97	15	3	0	46.03	46.06	0.99	18	3	0	37.08	37.18	0.99
1	4	0	166.43	166.25	0.65	7	4	0	32.54	35.97	0.99	10	4	0	81.49	82.08	0.97
16	4	0	38.31	37.63	0.99	2	5	0	53.25	50.13	0.97	5	5	0	60.13	62.75	0.97
8	5	0	111.32	111.78	0.93	11	5	0	83.13	83.09	0.97	14	5	0	35.30	34.97	0.99
17	5	0	60.73	60.37	0.98	0	6	0	71.27	70.58	0.94	3	6	0	71.74	68.16	0.97
6	6	0	60.78	63.59	0.97	1	7	0	142.20	141.79	0.84	4	7	0	52.68	55.69	0.98
10	7	0	63.58	63.06	0.98	13	7	0	37.41	36.64	0.99	2	8	0	35.06	36.63	0.99
5	8	0	70.59	71.89	0.97	8	8	0	73.71	73.00	0.97	11	8	0	25.23	25.96	1.00
14	8	0	21.48	20.42	1.00	0	9	0	186.59	194.06	0.77	3	9	0	15.39	17.09	1.00
6	9	0	133.66	135.27	0.92	9	9	0	21.69	18.26	1.00	12	9	0	36.35	37.37	0.99
15	9	0	74.64	75.05	0.98	1	10	0	72.05	71.41	0.97	4	10	0	40.77	41.30	0.99
7	10	0	21.38	19.72	1.00	13	10	0	28.30	28.50	1.00	2	11	0	107.37	107.40	0.94
5	11	0	63.18	62.82	0.98	8	11	0	23.52	21.15	1.00	11	11	0	61.33	61.49	0.98
0	12	0	50.65	51.46	0.99	3	12	0	20.76	21.94	1.00	6	12	0	19.62	18.97	1.00
12	12	0	28.45	28.04	1.00	1	13	0	74.10	74.96	0.97	4	13	0	70.61	71.26	0.98
7	13	0	51.75	51.30	0.99	2	14	0	115.76	116.84	0.95	8	14	0	48.83	48.77	0.99
0	15	0	90.75	91.49	0.97	3	15	0	29.55	30.34	1.00	6	15	0	38.02	38.16	0.99
1	16	0	34.21	34.92	0.99	7	16	0	48.93	48.03	0.99	2	17	0	33.66	33.37	1.00
3	18	0	69.86	69.68	0.98	1	19	0	23.11	23.11	1.00	4	19	0	18.26	18.77	1.00
7	0	1	47.36	46.06	0.98	13	0	1	35.90	36.97	0.99	16	0	1	19.77	18.15	1.00
2	1	1	111.42	108.14	0.76	5	1	1	14.22	13.04	1.00	8	1	1	39.60	39.39	0.99
11	1	1	39.68	39.28	0.99	14	1	1	28.23	29.70	1.00	17	1	1	31.82	32.32	1.00
0	2	1	21.15	20.54	0.99	6	2	1	53.24	54.95	0.97	9	2	1	69.15	68.84	0.97
12	2	1	18.62	18.82	1.00	18	2	1	24.71	23.43	1.00	-2	3	1	86.69	86.98	0.83
1	3	1	46.49	45.73	0.97	4	3	1	91.14	89.88	0.91	7	3	1	17.48	18.04	1.00
10	3	1	15.21	11.82	1.00	13	3	1	32.88	33.16	1.00	-1	4	1	68.27	67.94	0.93
2	4	1	32.09	32.53	0.99	3	5	1	44.82	44.97	0.98	6	5	1	13.98	14.70	1.00
9	5	1	16.41	16.54	1.00	12	5	1	39.77	39.85	0.99	18	5	1	26.67	24.38	1.00
-2	6	1	79.08	79.27	0.93	1	6	1	30.93	32.13	0.99	7	6	1	65.45	65.60	0.98
10	6	1	28.55	28.73	1.00	-4	7	1	48.41	47.98	0.97	-1	7	1	57.90	58.77	0.97
2	7	1	61.58	61.42	0.97	5	7	1	43.52	43.46	0.99	8	7	1	19.41	18.34	1.00
14	7	1	31.57	32.65	1.00	-6	8	1	87.83	89.21	0.93	-3	8	1	24.37	24.23	1.00
0	8	1	42.30	41.57	0.99	3	8	1	50.84	50.10	0.99	9	8	1	33.57	33.33	0.99
-8	9	1	12.20	9.50	1.00	-5	9	1	26.61	24.80	0.99	-2	9	1	42.23	43.12	0.99
-1	10	1	23.51	22.83	1.00	2	10	1	29.72	30.69	0.99	8	10	1	43.94	43.10	0.99
-6	11	1	25.12	24.75	1.00	-3	11	1	62.52	61.97	0.97	0	11	1	23.90	22.61	1.00
3	11	1	51.04	51.14	0.99	-8	12	1	66.56	66.40	0.97	-5	12	1	45.31	44.51	0.99
-2	12	1	20.60	21.21	1.00	4	12	1	43.76	43.42	0.99	10	12	1	26.62	26.78	1.00
-10	13	1	47.78	47.61	0.99	-7	13	1	18.75	17.80	1.00	-1	13	1	58.46	58.12	0.98
5	13	1	23.33	23.17	1.00	-12	14	1	31.85	32.02	1.00	-6	14	1	35.92	34.71	0.99

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite--cont.

H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y
-2	15	1	33.37	33.64	0.99	4	15	1	24.52	25.79	1.00	-13	16	1	25.44	25.28	1.00
-7	16	1	52.74	52.46	0.99	2	16	1	25.15	25.43	1.00	5	16	1	23.79	23.01	1.00
-15	17	1	21.44	21.64	1.00	-12	17	1	42.04	41.71	0.99	-3	17	1	27.71	28.71	1.00
0	17	1	40.26	39.85	0.99	-11	18	1	36.41	36.40	0.99	-5	18	1	39.31	39.04	0.99
-16	19	1	35.59	34.29	1.00	-6	20	1	20.76	20.60	1.00	-17	21	1	22.80	24.64	1.00
-11	21	1	25.09	25.49	1.00	-2	21	1	28.61	28.23	1.00	-10	22	1	26.71	24.74	1.00
-7	22	1	24.32	21.86	1.00	-15	23	1	30.05	29.68	1.00	2	0	2	35.27	34.48	0.98
5	0	2	107.48	109.01	0.87	8	0	2	18.22	16.45	1.00	11	0	2	15.49	15.63	1.00
14	0	2	22.30	21.11	1.00	17	0	2	21.14	21.11	1.00	0	1	2	79.25	78.60	0.86
3	1	2	21.93	20.75	0.99	6	1	2	31.07	30.57	0.99	12	1	2	35.09	34.73	0.99
1	2	2	59.53	58.20	0.94	4	2	2	33.43	35.68	0.99	7	2	2	31.00	31.36	0.99
10	2	2	27.30	27.49	1.00	13	2	2	22.64	22.00	1.00	-1	3	2	68.11	67.32	0.93
8	3	2	33.05	33.80	0.99	11	3	2	48.02	47.82	0.99	-3	4	2	14.92	13.11	1.00
0	4	2	70.49	70.37	0.94	3	4	2	36.79	38.44	0.99	6	4	2	84.11	83.31	0.95
15	4	2	36.92	36.89	0.99	-2	5	2	37.96	38.75	0.98	1	5	2	75.50	75.20	0.94
4	5	2	30.96	32.49	0.99	7	5	2	20.33	18.76	1.00	10	5	2	35.60	36.64	0.99
13	5	2	21.82	20.10	1.00	-4	6	2	21.79	22.41	0.99	-1	6	2	27.90	27.62	0.99
2	6	2	51.23	50.68	0.98	8	6	2	29.00	29.16	1.00	11	6	2	20.27	20.91	1.00
-3	7	2	46.13	48.14	0.98	0	7	2	34.77	35.54	0.99	3	7	2	32.47	33.57	0.99
6	7	2	15.75	14.80	1.00	9	7	2	32.25	33.00	0.99	-5	8	2	37.68	37.34	0.99
-2	8	2	32.05	30.54	0.99	1	8	2	27.57	27.56	1.00	4	8	2	38.85	39.66	0.99
7	8	2	31.20	30.10	1.00	16	8	2	30.09	31.08	1.00	-7	9	2	30.98	30.21	0.99
-4	9	2	77.34	78.78	0.95	-1	9	2	20.88	20.04	1.00	2	9	2	37.97	36.54	0.99
5	9	2	48.09	48.28	0.99	11	9	2	40.16	39.62	0.99	-9	10	2	86.59	86.67	0.96
0	10	2	67.45	67.40	0.98	3	10	2	31.29	31.71	0.99	6	10	2	26.67	27.70	1.00
-8	11	2	21.84	22.72	1.00	-5	11	2	41.83	42.09	0.99	-2	11	2	38.73	38.96	0.99
7	11	2	22.85	23.15	1.00	-7	12	2	30.56	29.51	1.00	-4	12	2	31.18	30.91	1.00
-1	12	2	27.45	27.07	1.00	5	12	2	26.77	27.24	1.00	-12	13	2	19.42	20.23	1.00
-9	13	2	14.72	14.72	1.00	-6	13	2	36.41	36.60	0.99	-3	13	2	19.45	19.77	1.00
0	13	2	16.55	16.01	1.00	6	13	2	28.09	28.67	1.00	-11	14	2	31.53	31.23	1.00
-8	14	2	43.43	43.11	0.99	-5	14	2	16.40	16.90	1.00	1	14	2	57.13	57.54	0.99
7	14	2	22.81	22.25	1.00	-13	15	2	35.84	34.87	0.99	-10	15	2	39.12	38.70	0.99
-7	15	2	17.58	16.98	1.00	-4	15	2	57.62	58.16	0.99	-15	16	2	33.45	33.49	1.00
-12	16	2	25.02	24.90	1.00	-9	16	2	21.81	21.92	1.00	-3	16	2	19.26	19.95	1.00
3	16	2	21.50	18.73	1.00	-8	17	2	24.44	23.62	1.00	-5	17	2	21.28	20.78	1.00
-10	18	2	23.44	23.53	1.00	-1	18	2	19.37	14.41	1.00	2	18	2	27.53	26.96	1.00
-18	19	2	21.06	17.76	1.00	-9	19	2	33.86	33.88	1.00	-6	19	2	22.43	17.94	1.00
-3	19	2	37.89	37.61	0.99	-14	20	2	41.06	40.81	0.99	-8	20	2	24.58	25.04	1.00
-19	21	2	29.32	28.26	1.00	-13	24	2	28.95	29.76	1.00	3	0	3	169.32	155.43	0.71
6	0	3	151.98	150.77	0.81	12	0	3	65.41	65.83	0.98	18	0	3	19.37	15.89	1.00
21	0	3	50.34	49.66	0.99	1	1	3	148.27	142.54	0.72	4	1	3	12.72	11.85	1.00
7	1	3	221.18	223.79	0.67	16	1	3	90.13	90.96	0.97	-1	2	3	149.79	142.58	0.72
5	2	3	15.21	16.11	1.00	8	2	3	95.71	96.19	0.95	11	2	3	41.62	41.49	0.99
14	2	3	59.48	60.21	0.98	20	2	3	62.81	62.79	0.98	0	3	3	169.28	155.14	0.71
3	3	3	138.86	133.22	0.83	6	3	3	55.26	55.82	0.98	9	3	3	48.98	47.84	0.99

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite--cont.

H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y
12	3	3	42.90	42.33	0.99	1	4	3	105.97	100.26	0.90	4	4	3	45.27	45.24	0.98
10	4	3	64.71	64.13	0.98	13	4	3	44.89	44.61	0.99	-4	5	3	104.84	100.15	0.89
-1	5	3	15.08	11.88	1.00	5	5	3	116.56	119.47	0.91	8	5	3	124.92	125.08	0.93
14	5	3	54.52	54.73	0.99	17	5	3	61.83	61.99	0.98	-3	6	3	133.59	133.90	0.83
0	6	3	156.03	151.64	0.81	3	6	3	177.16	177.77	0.80	6	6	3	36.16	37.07	0.99
9	6	3	43.79	44.24	0.99	12	6	3	75.25	75.78	0.98	15	6	3	64.63	64.26	0.98
-5	7	3	12.00	11.57	1.00	-2	7	3	15.44	16.33	1.00	1	7	3	136.06	135.22	0.87
4	7	3	47.30	46.50	0.99	7	7	3	61.27	62.15	0.98	10	7	3	46.38	47.25	0.99
16	7	3	27.24	28.67	1.00	-7	8	3	133.84	134.73	0.87	-4	8	3	45.80	45.34	0.98
-1	8	3	224.45	225.22	0.68	2	8	3	40.52	39.42	0.99	5	8	3	77.55	78.33	0.97
8	8	3	138.90	139.86	0.92	11	8	3	35.90	35.74	0.99	14	8	3	37.74	38.43	0.99
-6	9	3	171.20	176.13	0.78	-3	9	3	54.29	54.95	0.98	3	9	3	71.75	71.40	0.97
6	9	3	17.33	18.38	1.00	12	9	3	28.43	28.39	1.00	-8	10	3	40.33	39.90	0.99
-5	10	3	114.61	119.55	0.91	-2	10	3	96.48	96.77	0.95	1	10	3	17.61	16.95	1.00
4	10	3	94.33	94.55	0.96	7	10	3	77.26	78.06	0.98	13	10	3	64.27	64.60	0.98
-10	11	3	17.76	17.03	1.00	-7	11	3	47.15	46.91	0.99	8	11	3	30.53	30.07	1.00
11	11	3	72.40	72.84	0.98	-9	12	3	71.20	71.11	0.97	-6	12	3	35.56	36.50	0.99
-3	12	3	48.76	47.41	0.99	0	12	3	65.80	65.79	0.98	3	12	3	24.36	24.57	1.00
9	12	3	62.06	61.94	0.98	-8	13	3	77.67	78.32	0.97	-5	13	3	123.12	125.04	0.93
-2	13	3	41.43	41.12	0.99	1	13	3	22.16	21.68	1.00	4	13	3	59.50	60.63	0.99
7	13	3	31.26	30.87	1.00	-13	14	3	21.57	21.85	1.00	-10	14	3	94.08	94.66	0.96
-7	14	3	61.37	62.28	0.98	-4	14	3	64.44	64.45	0.98	2	14	3	23.05	22.19	1.00
5	14	3	65.34	65.79	0.98	8	14	3	48.24	48.25	0.99	-12	15	3	24.04	24.55	1.00
-9	15	3	17.36	18.84	1.00	-6	15	3	43.35	44.25	0.99	-3	15	3	42.52	42.42	0.99
3	15	3	47.47	48.25	0.99	9	15	3	38.09	38.74	0.99	-14	16	3	22.29	22.31	1.00
-8	16	3	137.17	139.69	0.92	-2	16	3	59.79	60.31	0.99	1	16	3	36.55	36.43	0.99
7	16	3	47.53	46.97	0.99	-16	17	3	36.06	36.27	0.99	-13	17	3	59.77	60.65	0.98
-10	17	3	76.84	77.66	0.98	-7	17	3	46.58	47.10	0.99	-4	17	3	44.77	44.25	0.99
-1	17	3	90.26	91.09	0.97	2	17	3	44.50	44.54	0.99	5	17	3	68.29	68.47	0.98
-15	18	3	47.63	48.26	0.99	-6	18	3	75.08	75.96	0.97	-17	19	3	44.73	44.94	0.99
-14	19	3	65.72	65.55	0.98	-11	19	3	30.56	29.78	1.00	-8	19	3	36.02	36.25	0.99
-5	19	3	55.47	54.71	0.99	-13	20	3	30.67	31.30	1.00	-1	20	3	23.86	21.22	1.00
2	20	3	33.16	32.91	1.00	-12	21	3	62.04	61.88	0.98	-9	21	3	28.19	28.35	1.00
-6	21	3	64.81	64.47	0.98	0	21	3	49.86	49.55	0.99	-20	22	3	32.83	32.96	1.00
-17	22	3	69.10	68.82	0.98	-14	22	3	47.86	48.23	0.99	-11	22	3	72.94	72.73	0.98
-8	22	3	38.30	38.65	0.99	-5	22	3	61.38	61.98	0.98	-2	22	3	62.09	62.52	0.98
-16	23	3	49.03	46.97	0.99	-10	23	3	64.98	64.60	0.98	-7	23	3	28.07	28.81	1.00
-15	24	3	38.67	38.72	0.99	1	0	4	59.40	60.53	0.95	4	0	4	67.62	64.57	0.96
7	0	4	29.43	29.91	0.99	10	0	4	59.24	58.90	0.98	2	1	4	52.50	52.78	0.97
5	1	4	26.65	26.62	0.99	8	1	4	20.95	20.85	1.00	11	1	4	24.04	23.79	1.00
0	2	4	26.58	27.54	0.99	3	2	4	35.35	35.25	0.99	6	2	4	25.99	25.52	1.00
9	2	4	39.07	37.94	0.99	-2	3	4	46.94	46.33	0.98	1	3	4	14.12	12.22	1.00
4	3	4	45.53	46.62	0.98	10	3	4	19.50	18.26	1.00	13	3	4	19.16	18.97	1.00
16	3	4	34.99	34.61	0.99	-1	4	4	14.26	15.65	1.00	5	4	4	73.22	73.51	0.97
8	4	4	26.90	26.58	1.00	11	4	4	50.89	51.64	0.99	0	5	4	100.77	100.37	0.92

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite--cont.

H	K	L	|FO|	|FC|	Y
3	5	4	34.81	34.17	0.99
12	5	4	21.96	20.93	1.00
7	6	4	33.77	33.72	0.99
2	7	4	24.43	25.03	1.00
3	8	4	20.31	20.15	1.00
12	8	4	23.60	24.01	1.00
-2	9	4	28.57	29.14	1.00
-7	10	4	27.86	28.67	0.99
8	10	4	22.88	23.04	1.00
3	11	4	26.91	27.09	1.00
-2	12	4	24.70	24.73	1.00
-10	13	4	29.22	28.43	1.00
2	13	4	29.99	29.45	1.00
-6	14	4	25.82	26.00	1.00
6	14	4	38.83	39.09	0.99
-5	15	4	33.90	32.90	1.00
-12	17	4	24.13	23.82	1.00
-11	18	4	22.57	22.97	1.00
-4	19	4	34.94	34.80	0.99
-9	20	4	38.46	37.96	0.99
11	0	5	19.79	20.34	1.00
6	1	5	55.20	54.46	0.98
1	2	5	71.61	70.97	0.96
10	2	5	19.59	18.94	1.00
-1	3	5	84.69	85.06	0.93
14	3	5	24.64	24.73	1.00
18	4	5	22.44	19.95	1.00
7	5	5	40.23	40.46	0.99
2	6	5	78.51	79.73	0.96
14	6	5	19.72	20.23	1.00
0	7	5	42.35	42.23	0.99
15	7	5	21.84	20.27	1.00
4	8	5	58.10	58.26	0.98
-3	10	5	17.72	16.97	1.00
12	10	5	24.01	21.94	1.00
7	11	5	34.04	33.17	1.00
-7	12	5	39.43	38.47	0.99
5	12	5	36.93	37.58	0.99
3	13	5	24.05	22.70	1.00
-7	15	5	20.06	18.04	1.00
8	15	5	27.02	28.44	1.00
-3	16	5	29.94	29.67	1.00
-5	17	5	34.92	35.76	1.00
-13	18	5	21.46	22.25	1.00
-15	19	5	21.22	22.34	1.00

H	K	L	|FO|	|FC|	Y
6	5	4	39.89	39.17	0.99
-5	6	4	65.47	66.20	0.97
-4	7	4	39.31	39.41	0.99
5	7	4	31.04	30.57	1.00
6	8	4	37.70	37.71	0.99
-8	9	4	25.63	25.37	1.00
1	9	4	78.97	78.26	0.96
-4	10	4	77.10	77.13	0.96
-9	11	4	35.47	34.40	0.99
-8	12	4	37.09	37.56	0.99
1	12	4	20.15	18.56	1.00
-7	13	4	16.74	16.51	1.00
11	13	4	27.31	27.41	1.00
-3	14	4	45.19	44.20	0.99
-14	15	4	51.27	50.83	0.99
-2	15	4	17.84	19.39	1.00
-6	17	4	20.32	20.25	1.00
-5	18	4	19.51	19.19	1.00
2	19	4	26.96	26.97	1.00
-14	21	4	23.03	21.64	1.00
17	0	5	36.17	36.19	0.99
9	1	5	19.74	19.69	1.00
4	2	5	64.83	64.87	0.97
13	2	5	30.46	30.45	1.00
5	3	5	20.21	21.85	1.00
-3	4	5	39.45	38.83	0.99
-2	5	5	13.85	11.95	1.00
13	5	5	35.57	35.10	0.99
5	6	5	22.44	22.27	1.00
-6	7	5	27.23	26.75	1.00
6	7	5	17.50	15.90	1.00
-5	8	5	39.08	39.20	0.99
-7	9	5	57.43	57.22	0.98
3	10	5	40.62	40.48	0.99
-8	11	5	43.66	42.89	0.99
10	11	5	23.72	24.32	1.00
-1	12	5	33.31	33.09	1.00
-6	13	5	58.46	58.15	0.98
-11	14	5	45.18	44.90	0.99
-1	15	5	25.95	26.22	1.00
-12	16	5	38.11	38.53	0.99
3	16	5	31.70	31.85	1.00
4	17	5	24.00	22.84	1.00
-10	18	5	39.78	38.70	0.99
-2	20	5	21.75	22.13	1.00

H	K	L	|FO|	|FC|	Y
9	5	4	15.70	16.83	1.00
-2	6	4	32.00	32.61	0.99
-1	7	4	23.83	24.43	1.00
-6	8	4	45.29	44.85	0.99
9	8	4	21.33	20.62	1.00
-5	9	4	29.78	30.58	0.99
10	9	4	32.86	31.72	1.00
5	10	4	36.94	36.50	0.99
-3	11	4	30.27	30.50	1.00
-5	12	4	16.24	16.64	1.00
4	12	4	21.43	22.55	1.00
-1	13	4	30.19	30.91	1.00
-9	14	4	43.46	43.71	0.99
0	14	4	19.52	18.75	1.00
-8	15	4	28.74	27.97	1.00
1	15	4	29.56	29.72	1.00
0	17	4	20.33	18.78	1.00
-13	19	4	27.19	26.46	1.00
-18	20	4	26.27	25.55	1.00
8	0	5	36.66	36.77	0.99
3	1	5	47.75	49.13	0.98
12	1	5	48.75	48.98	0.99
7	2	5	36.88	36.98	0.99
19	2	5	26.17	26.24	1.00
8	3	5	54.70	54.07	0.99
3	4	5	41.19	40.35	0.99
4	5	5	19.25	20.46	1.00
-4	6	5	26.70	26.79	1.00
8	6	5	31.68	31.15	1.00
-3	7	5	77.46	77.64	0.96
9	7	5	49.42	49.18	0.99
-2	8	5	48.46	48.40	0.99
-1	9	5	34.37	34.08	0.99
9	10	5	19.47	16.08	1.00
-2	11	5	60.35	60.52	0.98
-10	12	5	24.97	24.70	1.00
2	12	5	28.74	27.65	1.00
0	13	5	31.89	31.64	1.00
-5	14	5	17.69	16.25	1.00
2	15	5	19.11	20.00	1.00
-6	16	5	26.60	26.56	1.00
-8	17	5	32.33	31.47	1.00
-16	18	5	24.87	24.91	1.00
-1	18	5	30.72	29.94	1.00
-16	21	5	21.21	21.74	1.00

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite--cont.

H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y
-7	21	5	28.89	30.47	1.00	-14	23	5	18.83	15.75	1.00	-11	23	5	19.14	19.40	1.00
0	0	6	301.01	295.61	0.50	3	0	6	55.79	57.33	0.97	6	0	6	55.76	55.89	0.98
9	0	6	153.55	153.71	0.89	12	0	6	42.28	41.84	0.99	15	0	6	78.07	77.92	0.97
1	1	6	32.82	32.23	0.99	7	1	6	102.35	101.91	0.94	10	1	6	32.61	31.89	1.00
13	1	6	69.55	70.15	0.98	16	1	6	57.68	58.37	0.99	-1	2	6	33.75	33.01	0.99
2	2	6	114.15	114.37	0.91	5	2	6	95.02	96.63	0.95	11	2	6	54.49	53.90	0.99
14	2	6	80.26	80.71	0.97	17	2	6	37.13	37.29	0.99	0	3	6	57.07	58.83	0.97
3	3	6	93.62	94.94	0.95	6	3	6	51.94	53.88	0.98	9	3	6	23.65	23.76	1.00
12	3	6	68.82	68.47	0.98	15	3	6	38.59	38.71	0.99	18	3	6	35.39	35.10	0.99
-2	4	6	115.34	114.79	0.92	1	4	6	131.69	135.26	0.88	7	4	6	24.00	23.67	1.00
10	4	6	67.52	66.84	0.98	16	4	6	31.57	31.37	1.00	-4	5	6	131.31	135.43	0.89
2	5	6	22.38	25.60	1.00	5	5	6	58.38	58.72	0.98	8	5	6	91.20	90.95	0.96
11	5	6	72.14	72.24	0.98	14	5	6	31.73	31.76	1.00	17	5	6	55.06	53.97	0.99
-3	6	6	94.70	95.01	0.94	0	6	6	56.60	56.47	0.98	3	6	6	54.86	55.12	0.98
6	6	6	46.84	46.90	0.99	-5	7	6	23.44	25.27	1.00	-2	7	6	93.76	95.69	0.94
1	7	6	104.08	104.72	0.94	4	7	6	45.63	45.43	0.99	10	7	6	54.12	53.44	0.99
13	7	6	31.81	32.62	1.00	-7	8	6	104.73	104.92	0.94	-1	8	6	102.61	102.57	0.95
2	8	6	22.66	22.49	1.00	5	8	6	57.78	58.12	0.99	8	8	6	62.22	62.48	0.98
-6	9	6	54.13	54.60	0.98	-3	9	6	52.12	53.18	0.98	0	9	6	155.18	154.19	0.89
3	9	6	15.25	14.35	1.00	6	9	6	112.53	111.89	0.95	12	9	6	31.72	32.55	1.00
-8	10	6	21.64	21.76	1.00	-5	10	6	58.33	58.72	0.98	1	10	6	60.24	59.54	0.98
4	10	6	34.39	33.92	1.00	7	10	6	18.69	16.05	1.00	13	10	6	23.14	23.94	1.00
-10	11	6	59.32	59.10	0.98	-7	11	6	44.98	44.64	0.99	-4	11	6	24.53	24.28	1.00
-1	11	6	32.54	31.67	0.99	2	11	6	88.99	88.32	0.96	5	11	6	54.72	54.99	0.99
8	11	6	21.16	21.47	1.00	11	11	6	56.56	55.00	0.99	-9	12	6	17.10	15.55	1.00
-6	12	6	46.55	46.83	0.99	-3	12	6	23.84	23.28	1.00	0	12	6	43.01	43.07	0.99
3	12	6	19.73	19.39	1.00	6	12	6	20.72	17.31	1.00	-11	13	6	88.33	88.78	0.96
-8	13	6	57.41	58.26	0.98	-5	13	6	90.36	90.94	0.96	-2	13	6	54.79	54.04	0.99
1	13	6	63.33	63.34	0.98	4	13	6	60.31	60.53	0.98	7	13	6	42.50	43.17	0.99
-13	14	6	63.06	63.56	0.98	-10	14	6	33.98	34.40	0.99	-4	14	6	67.18	67.05	0.98
-1	14	6	70.76	70.05	0.98	2	14	6	100.11	100.78	0.96	8	14	6	43.59	43.97	0.99
-12	15	6	19.94	19.72	1.00	-9	15	6	111.17	112.28	0.94	-3	15	6	68.44	68.63	0.98
0	15	6	78.28	78.26	0.97	3	15	6	25.29	25.44	1.00	6	15	6	32.14	32.83	1.00
-14	16	6	100.02	100.49	0.96	-11	16	6	54.19	53.82	0.99	-8	16	6	62.92	62.73	0.98
-5	16	6	72.08	72.15	0.98	-2	16	6	80.45	79.89	0.97	1	16	6	31.31	30.94	1.00
-16	17	6	29.75	30.32	1.00	-13	17	6	60.75	61.19	0.98	-7	17	6	53.86	53.58	0.99
-1	17	6	57.95	58.32	0.99	2	17	6	30.99	30.70	1.00	-15	18	6	23.41	25.76	1.00
-12	18	6	18.70	17.29	1.00	-3	18	6	38.32	38.25	0.99	3	18	6	62.17	62.79	0.98
-17	19	6	30.60	29.87	1.00	-11	19	6	22.62	21.82	1.00	-8	19	6	19.85	19.39	1.00
-5	19	6	31.26	31.73	1.00	-2	19	6	38.87	37.79	0.99	1	19	6	20.86	18.28	1.00
-13	20	6	43.77	43.18	0.99	-7	20	6	31.69	31.94	1.00	-4	20	6	31.15	30.87	1.00
-18	21	6	62.92	62.61	0.98	-15	21	6	32.95	33.08	1.00	-9	21	6	33.10	32.01	1.00
-3	21	6	35.01	34.91	0.99	-14	22	6	43.72	44.04	0.99	-11	22	6	56.02	55.17	0.99
-5	22	6	55.24	53.83	0.99	7	0	7	30.32	30.13	1.00	13	0	7	27.98	29.02	1.00
2	1	7	75.53	75.50	0.97	8	1	7	28.46	28.22	1.00	11	1	7	31.16	30.44	1.00

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite--cont.

H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y
14	1	7	21.66	23.44	1.00	17	1	7	24.93	25.98	1.00	0	2	7	14.38	13.99	1.00
6	2	7	37.72	38.42	0.99	9	2	7	50.94	50.22	0.99	18	2	7	20.32	18.90	1.00
-2	3	7	54.48	55.05	0.98	1	3	7	27.06	26.88	1.00	4	3	7	63.38	63.21	0.98
13	3	7	25.15	25.79	1.00	-1	4	7	46.66	46.96	0.99	2	4	7	20.82	21.92	1.00
3	5	7	31.40	31.08	0.99	12	5	7	31.83	31.26	1.00	-2	6	7	54.62	55.48	0.98
1	6	7	23.19	23.63	1.00	7	6	7	48.57	48.32	0.99	10	6	7	22.37	21.34	1.00
-4	7	7	34.21	34.14	0.99	-1	7	7	38.47	38.37	0.99	2	7	7	42.07	41.41	0.99
5	7	7	31.84	31.40	1.00	-6	8	7	61.69	62.35	0.98	0	8	7	28.97	29.11	1.00
3	8	7	37.81	37.24	0.99	9	8	7	24.63	24.32	1.00	-5	9	7	19.10	17.81	1.00
-2	9	7	30.71	31.28	0.99	-1	10	7	19.38	16.68	1.00	2	10	7	25.56	24.63	1.00
8	10	7	35.45	34.14	0.99	-6	11	7	18.56	17.18	1.00	-3	11	7	45.52	45.62	0.99
0	11	7	17.29	16.31	1.00	3	11	7	39.51	39.14	0.99	-8	12	7	48.93	49.00	0.99
-5	12	7	31.79	31.46	1.00	4	12	7	33.57	34.02	1.00	-10	13	7	37.30	36.76	0.99
-1	13	7	45.85	46.07	0.99	-12	14	7	23.01	24.86	1.00	-6	14	7	26.67	25.34	1.00
-2	15	7	25.85	25.58	1.00	4	15	7	22.04	22.23	1.00	-7	16	7	38.23	38.21	0.99
-12	17	7	33.50	32.77	1.00	-3	17	7	23.13	23.87	1.00	0	17	7	33.35	32.28	1.00
-11	18	7	28.94	28.18	1.00	-5	18	7	31.48	31.02	1.00	-16	19	7	29.16	27.43	1.00
2	0	8	19.91	20.57	1.00	5	0	8	74.14	74.23	0.97	17	0	8	20.51	17.60	1.00
0	1	8	49.90	49.95	0.99	3	1	8	14.74	14.23	1.00	6	1	8	21.70	22.41	1.00
12	1	8	26.84	26.46	1.00	1	2	8	36.78	37.14	0.99	4	2	8	22.89	23.56	1.00
7	2	8	22.32	20.89	1.00	10	2	8	19.93	19.92	1.00	-1	3	8	43.30	43.58	0.99
8	3	8	24.40	23.92	1.00	11	3	8	34.35	35.12	0.99	0	4	8	45.18	44.85	0.99
3	4	8	22.42	23.06	1.00	6	4	8	57.93	57.97	0.99	15	4	8	28.54	28.87	1.00
-2	5	8	24.20	24.49	1.00	1	5	8	52.29	52.48	0.99	4	5	8	20.75	21.48	1.00
7	5	8	16.37	13.74	1.00	10	5	8	27.31	27.67	1.00	-4	6	8	18.24	17.72	1.00
-1	6	8	16.96	17.17	1.00	2	6	8	35.32	35.53	0.99	8	6	8	22.51	22.06	1.00
-3	7	8	30.47	30.88	1.00	0	7	8	24.99	25.35	1.00	3	7	8	24.34	24.58	1.00
9	7	8	25.87	25.66	1.00	-5	8	8	23.95	24.90	1.00	-2	8	8	22.40	22.30	1.00
1	8	8	20.17	18.77	1.00	4	8	8	26.90	27.02	1.00	7	8	8	22.51	21.97	1.00
-7	9	8	22.20	22.39	1.00	-4	9	8	53.66	53.83	0.99	2	9	8	24.58	25.07	1.00
5	9	8	35.84	35.87	0.99	11	9	8	30.94	30.62	1.00	-9	10	8	61.81	62.01	0.98
0	10	8	50.39	49.79	0.99	3	10	8	23.50	23.66	1.00	6	10	8	19.31	19.73	1.00
-8	11	8	17.86	16.48	1.00	-5	11	8	28.71	28.97	1.00	-2	11	8	25.85	25.79	1.00
-7	12	8	18.95	18.22	1.00	-4	12	8	25.36	23.30	1.00	-1	12	8	19.52	20.27	1.00
5	12	8	23.57	22.23	1.00	-6	13	8	25.18	25.92	1.00	6	13	8	23.43	22.52	1.00
-11	14	8	25.57	24.17	1.00	-8	14	8	32.87	33.03	1.00	1	14	8	46.11	45.88	0.99
-13	15	8	27.91	28.77	1.00	-10	15	8	27.19	27.79	1.00	-4	15	8	44.19	44.99	0.99
-15	16	8	26.61	26.71	1.00	-5	17	8	19.72	14.29	1.00	-9	19	8	27.88	26.25	1.00
-3	19	8	29.87	30.55	1.00	-14	20	8	32.70	31.67	1.00	-8	20	8	19.48	19.49	1.00
3	0	9	60.02	59.82	0.98	6	0	9	83.46	83.73	0.97	12	0	9	42.30	43.14	0.99
1	1	9	79.67	79.28	0.97	7	1	9	154.16	155.45	0.90	16	1	9	71.81	71.60	0.98
-1	2	9	79.67	78.93	0.97	2	2	9	37.08	36.89	0.99	8	2	9	62.30	61.41	0.98
11	2	9	32.33	33.49	1.00	14	2	9	39.63	38.96	0.99	0	3	9	58.71	58.81	0.98
3	3	9	89.05	88.66	0.97	6	3	9	31.38	30.54	1.00	9	3	9	28.73	30.49	1.00
12	3	9	31.88	31.26	1.00	-2	4	9	36.96	36.68	0.99	1	4	9	43.82	43.20	0.99

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite--cont.

H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y	H	K	L	|FO|	|FC|	Y
4	4	9	29.99	30.66	1.00	10	4	9	47.16	47.59	0.99	13	4	9	30.81	33.39	1.00
-4	5	9	43.39	43.72	0.99	2	5	9	16.97	15.32	1.00	5	5	9	73.53	73.84	0.98
8	5	9	88.33	88.77	0.97	14	5	9	47.04	46.96	0.99	-3	6	9	90.30	89.76	0.96
0	6	9	84.26	84.30	0.97	3	6	9	117.59	118.08	0.94	6	6	9	23.33	24.90	1.00
9	6	9	30.48	31.53	1.00	12	6	9	54.88	55.23	0.99	1	7	9	82.46	82.72	0.97
4	7	9	31.27	31.69	1.00	7	7	9	42.01	41.73	0.99	10	7	9	31.81	32.83	1.00
-7	8	9	82.17	82.88	0.97	-4	8	9	30.53	30.73	1.00	-1	8	9	153.29	154.02	0.89
2	8	9	26.79	25.74	1.00	5	8	9	52.76	53.23	0.99	8	8	9	107.22	107.07	0.95
11	8	9	32.47	30.23	1.00	-6	9	9	118.98	118.43	0.94	-3	9	9	28.82	28.85	1.00
3	9	9	49.02	49.79	0.99	-8	10	9	26.46	26.74	1.00	-5	10	9	73.01	73.73	0.98
-2	10	9	61.65	62.24	0.98	4	10	9	67.69	67.60	0.98	7	10	9	57.27	57.26	0.99
-10	11	9	15.11	12.95	1.00	-7	11	9	31.99	32.57	1.00	-9	12	9	48.74	49.22	0.99
-6	12	9	24.88	23.72	1.00	-3	12	9	29.72	29.65	1.00	0	12	9	42.24	43.19	0.99
3	12	9	19.96	18.47	1.00	-8	13	9	52.75	53.38	0.99	-5	13	9	87.71	88.67	0.97
-2	13	9	32.90	32.70	1.00	4	13	9	42.40	43.30	0.99	-13	14	9	21.58	16.68	1.00
-10	14	9	67.16	67.62	0.98	-7	14	9	41.31	41.90	0.99	-4	14	9	48.58	48.19	0.99
5	14	9	54.69	55.30	0.99	-9	15	9	15.13	14.89	1.00	-6	15	9	31.85	31.50	1.00
-3	15	9	31.75	31.53	1.00	3	15	9	33.75	33.56	1.00	-8	16	9	106.29	106.83	0.95
-2	16	9	39.84	39.07	0.99	1	16	9	33.48	31.94	1.00	-16	17	9	32.75	31.63	1.00
-13	17	9	43.00	43.46	0.99	-10	17	9	56.47	56.51	0.99	-7	17	9	31.71	32.48	1.00
-4	17	9	32.52	32.59	1.00	-1	17	9	72.11	71.64	0.98	-15	18	9	34.49	33.60	1.00
-6	18	9	55.62	55.73	0.99	-14	19	9	56.02	55.01	0.99	-11	19	9	20.75	19.67	1.00
-8	19	9	30.67	31.39	1.00	-5	19	9	47.33	46.92	0.99	1	0	10	31.54	31.69	1.00
4	0	10	37.82	37.77	0.99	10	0	10	34.62	34.62	0.99	2	1	10	28.54	27.76	1.00
0	2	10	16.85	14.71	1.00	3	2	10	20.54	20.33	1.00	9	2	10	24.23	25.29	1.00
-2	3	10	23.29	24.96	1.00	4	3	10	27.67	28.72	1.00	5	4	10	44.61	44.90	0.99
11	4	10	32.78	32.63	1.00	0	5	10	59.32	59.31	0.99	3	5	10	20.52	20.17	1.00
6	5	10	23.53	24.52	1.00	-5	6	10	37.43	37.77	0.99	-2	6	10	17.67	18.84	1.00
7	6	10	21.90	21.21	1.00	-4	7	10	25.27	24.81	1.00	5	7	10	22.75	21.58	1.00
-6	8	10	26.01	26.04	1.00	6	8	10	24.17	22.80	1.00	1	9	10	48.58	48.00	0.99
-4	10	10	48.57	47.81	0.99	5	10	10	24.37	24.67	1.00	-9	11	10	22.07	21.91	1.00
3	11	10	19.53	16.31	1.00	-8	12	10	24.25	24.43	1.00	-9	14	10	28.68	27.68	1.00
-3	14	10	29.16	29.26	1.00	-14	15	10	32.14	31.99	1.00	-8	15	10	18.42	18.71	1.00
-5	15	10	20.50	20.76	1.00	1	15	10	21.15	19.24	1.00	8	0	11	21.84	22.07	1.00
3	1	11	25.42	25.64	1.00	6	1	11	32.68	33.69	0.99	12	1	11	26.12	29.22	1.00
1	2	11	40.32	39.94	0.99	4	2	11	36.50	36.35	0.99	7	2	11	21.48	21.47	1.00
-1	3	11	46.76	46.63	0.99	8	3	11	32.27	32.63	1.00	-3	4	11	23.48	22.61	1.00
3	4	11	22.40	22.94	1.00	7	5	11	26.44	25.72	1.00	2	6	11	47.56	48.27	0.99
8	6	11	21.03	19.95	1.00	-3	7	11	44.10	45.40	0.99	0	7	11	25.41	26.22	1.00
9	7	11	35.48	34.60	0.99	-5	8	11	24.85	23.26	1.00	-2	8	11	29.38	28.87	1.00
4	8	11	36.35	36.07	0.99	-7	9	11	36.11	36.35	0.99	-1	9	11	21.18	20.29	1.00
3	10	11	23.32	24.17	1.00	-8	11	11	24.23	25.42	1.00	-2	11	11	36.87	37.29	0.99
-7	12	11	22.87	23.87	1.00	-1	12	11	21.18	19.41	1.00	5	12	11	27.35	25.66	1.00
-6	13	11	36.62	36.85	0.99	-11	14	11	27.86	28.64	1.00	-12	16	11	24.45	25.27	1.00
-8	17	11	24.66	22.33	1.00	-10	18	11	26.69	26.67	1.00	0	0	12	185.32	186.49	0.87

Observed ($|F_o|$) and Calculated ($|F_c|$) Structural Amplitudes for Phenacite--cont.

H	K	L	|FO|	|FC|	Y
3	0	12	30.55	30.72	1.00
12	0	12	25.17	25.48	1.00
13	1	12	47.45	47.67	0.99
11	2	12	36.46	37.32	0.99
6	3	12	28.19	28.18	1.00
1	4	12	74.81	76.50	0.98
-4	5	12	74.80	76.44	0.98
11	5	12	52.55	52.53	0.99
3	6	12	31.34	32.45	1.00
1	7	12	59.68	61.12	0.99
-1	8	12	57.59	58.25	0.99
-6	9	12	32.71	31.81	1.00
6	9	12	69.55	68.96	0.98
4	10	12	24.01	24.01	1.00
-1	11	12	21.89	23.30	1.00
-6	12	12	35.60	34.13	1.00
-8	13	12	41.70	42.47	0.99
1	13	12	43.49	43.18	0.99
-4	14	12	37.91	37.58	0.99
-3	15	12	45.73	46.34	0.99
-5	16	12	53.49	52.46	0.99
12	2	13	18.35	11.68	1.00
-1	4	13	25.33	25.38	1.00
-6	8	13	30.18	31.63	1.00
3	11	13	24.73	23.69	1.00
-1	13	13	29.84	29.29	1.00
1	2	14	19.53	19.78	1.00
1	5	14	26.02	27.85	1.00
0	10	14	30.57	29.85	1.00
1	1	15	39.12	38.75	0.99
0	3	15	38.09	38.35	0.99
1	4	15	25.20	25.14	1.00
-3	6	15	44.34	44.73	0.99
1	7	15	48.39	47.69	0.99
-1	8	15	89.13	88.70	0.97
-5	10	15	49.82	48.31	0.99

H	K	L	|FO|	|FC|	Y
6	0	12	27.35	28.44	1.00
7	1	12	57.55	57.91	0.99
2	2	12	60.03	60.00	0.99
0	3	12	31.44	32.21	1.00
12	3	12	46.03	46.08	0.99
7	4	12	19.39	17.51	1.00
5	5	12	29.20	29.37	1.00
-3	6	12	50.46	49.70	0.99
6	6	12	35.28	34.23	1.00
4	7	12	25.15	24.39	1.00
5	8	12	41.72	42.20	0.99
-3	9	12	27.48	27.33	1.00
-5	10	12	30.10	29.30	1.00
-10	11	12	30.23	30.92	1.00
2	11	12	58.10	57.67	0.99
0	12	12	26.16	27.07	1.00
-5	13	12	58.11	59.06	0.99
-13	14	12	43.06	43.50	0.99
-1	14	12	48.85	47.63	0.99
-11	16	12	40.09	38.79	0.99
2	1	13	39.42	39.40	0.99
-2	3	13	25.58	26.64	1.00
-2	6	13	28.72	29.26	1.00
3	8	13	22.78	21.24	1.00
-8	12	13	28.31	27.79	1.00
5	0	14	37.47	37.80	0.99
-1	3	14	21.80	23.30	1.00
-4	9	14	28.07	28.06	1.00
3	0	15	39.22	39.29	0.99
7	1	15	89.37	89.07	0.97
3	3	15	43.98	43.51	0.99
-4	5	15	25.96	25.58	1.00
0	6	15	51.80	51.67	0.99
-7	8	15	48.24	47.86	0.99
-6	9	15	70.05	68.86	0.98
4	0	16	22.55	19.56	1.00

H	K	L	|FO|	|FC|	Y
9	0	12	96.67	96.56	0.96
10	1	12	22.56	23.59	1.00
5	2	12	53.80	53.54	0.99
3	3	12	48.84	49.12	0.99
-2	4	12	59.80	60.15	0.98
10	4	12	36.47	37.34	0.99
8	5	12	58.54	59.07	0.99
0	6	12	28.04	29.14	1.00
-2	7	12	52.09	52.79	0.99
-7	8	12	60.37	61.04	0.99
8	8	12	44.84	44.25	0.99
0	9	12	96.79	96.37	0.96
1	10	12	30.90	31.59	1.00
-7	11	12	24.01	23.43	1.00
5	11	12	40.80	40.34	0.99
-11	13	12	58.54	58.30	0.99
-2	13	12	37.42	37.56	0.99
-10	14	12	24.41	24.63	1.00
-9	15	12	70.38	69.59	0.98
-8	16	12	45.14	44.71	0.99
9	2	13	29.95	28.04	1.00
4	3	13	32.60	32.48	1.00
7	6	13	26.68	27.51	1.00
-3	11	13	25.05	25.41	1.00
-10	13	13	21.56	22.66	1.00
0	1	14	26.37	26.81	1.00
6	4	14	29.75	31.14	1.00
-9	10	14	34.86	35.39	0.99
6	0	15	50.89	50.94	0.99
-1	2	15	38.76	38.38	0.99
6	3	15	23.99	23.58	1.00
5	5	15	49.64	48.59	0.99
3	6	15	67.84	68.34	0.98
-4	8	15	21.16	16.68	1.00
-3	9	15	23.77	21.96	1.00
0	5	16	27.97	30.37	1.00