AM-90-429

col. 1 of 1

Crystal-structure refinement of a F-bearing spessartine garnet

Joseph R. Smyth, Robin E. Madel, Tamsin C. McCormick, James L. Munoz, George R. Rossman

For deposit: Table 5

American Mineralogist, 75, 3-4, 314-318.

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
1	1	2	76.952	75.238	0	2	2	44.025	45.625
1	2	3	58.425	62.961	2	3	3	79.852	69.086
0	0	4	383.187	415.838	0	2	4	374.906	411.570
2	2	4	193.315	200.523	1	3	4	116.558	111.303
0	4	4	154.281	151.655	4	4	4	441.584	483.177
1	2	5	167.107	165.056	2	3	5	151.340	149.941
1	4	5	15.864	14.543	3	4	5	26.766	25.575
2	5	5	113.798	112.625	1	1	6	218.729	215.148
0	2	6	48.639	42.417	1	3	6	30.628	28.629
3	3	6	75.154	69.063	0	4	6	380.803	406.368
2	4	6	321.374	332.091	1	5	6	76.869	70.427
3	5	6	12.156	7.818	5	5	6	72.519	67.264
0	6	6	49.364	47.382	4	6	6	244.003	246.011
1	2	7	47.510	46.459	2	3	7	10.957	5.891
1	4	7	63.430	62.331	3	4	7	33.834	32.973
2	5	7	9.298	3.618	4	5	7	63.486	65.451
1	6	7	21.678	21.572	3	6	7	39.689	39.902
5	6	7	80.884	77.719	2	7	7	71.808	68.559
6	7	7	19.447	16.095	0	0	8	474.345	536.145
0	2	8	44.359	44.595	2	2	8	16.575	8.673
1	3	8	6.064	7.668	0	4	8	264.775	271.919
2	4	8	265.904	278.698	4	4	8	13.021	.592
1	5	8	62.008	63.409	3	5	8	87.506	88.373
0	6	8	11.529	3.928	2	6	8	59.889	63.023
4	6	8	232.600	233.813	6	6	8	44.387	46.661
1	7	8	17.259	15.296	3	7	8	39.494	38.863
5	7	8	21.608	20.031	0	8	8	415.766	436.213
8	8	8	342.843	351.507	1	2	9	48.332	46.619
2	3	9	64.713	64.053	1	4	9	81.093	79.933
3	4	9	35.981	36.670	2	5	9	32.203	29.992
4	5	9	10.567	10.939	1	6	9	57.157	56.516
3	6	9	50.619	50.111	5	6	9	42.477	42.005
2	7	9	16.506	13.996	4	7	9	17.454	16.787
6	7	9	72.645	73.709	1	8	9	41.236	40.853
3	8	9	20.939	20.242	5	8	9	24.856	22.612
7	8	9	15.279	11.742	2	9	9	54.620	55.109
6	9	9	39.187	38.008	1	1	10	7.890	9.673
0	2	10	133.273	135.139	1	3	10	45.070	41.377
3	3	10	52.654	50.201	0	4	10	269.668	269.292
2	4	10	222.814	225.731	1	5	10	58.969	56.302
3	5	10	57.589	56.413	5	5	10	35.618	33.807
0	6	10	76.952	80.240	2	6	10	32.886	31.909
4	6	10	167.748	168.813	1	7	10	60.739	60.666
3	7	10	34.907	36.967	5	7	10	17.537	16.852
7	7	10	31.018	29.007	0	8	10	20.660	15.260
2	8	10	21.064	21.640	4	8	10	216.401	215.475

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
6	8	10	18.165	14.089	1	9	10	26.125	25.428
3	9	10	17.412	14.918	5	9	10	13.118	9.586
7	9	10	23.434	20.511	9	9	10	49.573	48.007
0	10	10	77.914	71.205	4	10	10	167.929	166.639
8	10	10	41.404	40.347	1	2	11	43.495	42.831
2	3	11	23.964	23.348	1	4	11	37.110	37.208
3	4	11	11.501	9.734	6	10	12	145.791	142.003
2	5	11	9.382	8.621	4	5	11	6.357*	1.884
1	6	11	17.663	15.403	3	6	11	88.189	87.950
5	6	11	34.503	33.727	2	7	11	46.381	45.150
4	7	11	51.371	51.032	6	7	11	26.278	25.173
1	8	11	26.975	28.052	3	8	11	20.660	21.868
5	8	11	37.640	36.674	7	8	11	20.409	20.243
2	9	11	32.384	31.366	4	9	11	23.615	21.984
6	9	11	16.882	14.174	8	9	11	9.549	5.810
1	10	11	30.223	29.123	3	10	11	10.762	4.749
5	10	11	7.667	7.401	7	10	11	24.619	24.546
9	10	11	48.737	48.444	2	11	11	23.657	22.480
6	11	11	4.238*	1.405	10	11	11	42.449	42.259
0	0	12	111.832	110.917	0	2	12	214.129	215.867
2	2	12	234.900	237.329	1	3	12	39.173	37.069
0	4	12	12.895	8.677	2	4	12	11.738	6.865
4	4	12	185.007	187.492	1	5	12	6.190*	2.155
3	5	12	33.235	32.186	0	6	12	182.288	181.214
2	6	12	138.040	135.750	4	6	12	19.615	15.841
6	6	12	150.238	144.213	1	7	12	10.219	8.687
3	7	12	39.271	38.390	5	7	12	10.595	9.785
0	8	12	156.554	146.517	2	8	12	187.669	180.330
4	8	12	50.005	49.441	6	8	12	173.924	170.843
8	8	12	140.187	129.105	1	9	12	21.399	19.910
3	9	12	20.604	18.683	5	9	12	5.632*	3.482
7	9	12	17.719	17.195	0	10	12	155.173	146.061
2	10	12	150.726	143.933	4	10	12	7.333*	2.358
8	10	12	129.272	122.907	10	10	12	70.038	67.528
1	11	12	30.056	30.361	3	11	12	10.149	8.486
5	11	12	7.528*	3.920	7	11	12	9.103	4.744
9	11	12	10.623	6.025	0	12	12	35.841	31.435
4	12	12	195.992	196.796	8	12	12	13.397	9.558
12	12	12	93.096	95.024	1	2	13	6.538*	2.832
2	3	13	42.658	42.148	1	4	13	8.908	.769
3	4	13	18.290	17.894	2	5	13	24.062	24.103
4	5	13	24.773	22.286	1	6	13	9.243	7.430
3	6	13	7.793	5.034	5	6	13	38.936	41.500
2	7	13	41.738	41.082	4	7	13	16.729	13.127
6	7	13	27.324	25.702	1	8	13	18.834	17.224
1	3	14	50.395	52.365					

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
3	8	13	27.435	27.367	5	8	13	35.381	35.551
7	8	13	30.014	29.671	2	9	13	13.773	12.195
4	9	13	10.302	6.719	6	9	13	26.641	25.873
8	9	13	17.063	15.746	1	10	13	33.262	33.453
3	10	13	23.155	23.381	5	10	13	14.847	12.627
7	10	13	12.003	11.567	9	10	13	22.333	22.834
2	11	13	37.612	37.725	4	11	13	29.345	29.250
6	11	13	7.765*	2.700	8	11	13	13.885	12.019
10	11	13	25.860	25.696	1	12	13	9.995	4.640
3	12	13	23.629	22.180	5	12	13	12.128	10.080
7	12	13	24.870	24.710	9	12	13	19.879	19.320
11	12	13	16.338	15.206	2	13	13	29.192	29.329
6	13	13	36.427	40.779	10	13	13	13.871	14.463
1	1	14	26.334	24.234	0	2	14	23.713	14.260
3	3	14	28.815	28.805	0	4	14	165.824	169.158
2	4	14	178.552	186.261	1	5	14	11.640	1.993
3	5	14	35.395	36.439	5	5	14	13.035	8.454
0	6	14	46.855	49.407	2	6	14	16.004	11.409
4	6	14	115.944	116.576	1	7	14	42.826	43.005
3	7	14	30.767	31.823	5	7	14	23.769	21.938
7	7	14	55.386	56.219	0	8	14	20.423	24.395
2	8	14	46.395	46.311	4	8	14	143.045	148.124
6	8	14	14.833	13.098	1	9	14	17.802	16.035
3	9	14	25.010	25.641	5	9	14	35.284	37.505
7	9	14	13.773	4.390	9	9	14	44.289	43.515
0	10	14	17.816	6.146	2	10	14	15.530	4.614
4	10	14	94.769	93.156	6	10	14	20.841	22.113
8	10	14	21.970	23.925	1	11	14	31.297	30.165
3	11	14	9.159	4.026	5	11	14	39.898	41.000
7	11	14	15.502	15.378	9	11	14	17.677	16.162
11	11	14	11.794	9.794	0	12	14	138.877	136.107
2	12	14	71.334	67.937	4	12	14	11.222	.449
6	12	14	112.682	110.929	8	12	14	110.647	111.328
10	12	14	86.808	84.864	1	13	14	27.142	27.032
3	13	14	27.101	32.336	5	13	14	20.116	22.092
7	13	14	23.365	24.875	9	13	14	14.484	12.451
11	13	14	19.601	23.382	13	13	14	10.246*	5.395
0	14	14	34.252	35.827	4	14	14	61.576	63.089
8	14	14	11.808	1.088	12	14	14	94.504	92.346
1	2	15	44.652	46.941	2	3	15	54.717	56.900
1	4	15	5.855*	5.372	1	4	17	20.298	20.321
3	4	15	14.875	13.725	2	5	15	13.522	11.291
4	5	15	16.255	16.942	1	6	15	12.087	4.482
3	6	15	25.302	28.357	5	6	15	17.844	15.448
2	7	15	28.313	29.646	4	7	15	4.154*	5.220
6	7	15	38.225	40.041	1	8	15	37.236	36.909

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
3	8	15	16.171	17.158	5	8	15	28.955	29.059
7	8	15	20.144	17.907	2	9	15	9.508	1.807
4	9	15	19.196	18.785	6	9	15	20.674	21.213
8	9	15	21.678	19.148	1	10	15	36.957	37.714
3	10	15	23.476	23.785	5	10	15	18.778	17.417
7	10	15	12.045	10.128	9	10	15	10.623	10.335
2	11	15	10.832	3.122	4	11	15	10.720	5.468
6	11	15	22.152	23.500	8	11	15	19.336	19.885
10	11	15	10.163	7.407	1	12	15	16.617	12.485
3	12	15	7.124*	7.721	5	12	15	17.914	15.920
7	12	15	9.884	4.829	9	12	15	4.865*	10.494
11	12	15	12.156	.326	2	13	15	8.141*	8.312
4	13	15	10.623	5.224	6	13	15	24.563	24.222
8	13	15	30.948	31.340	10	13	15	4.851*	5.853
1	14	15	11.236	7.033	3	14	15	4.684*	1.173
5	14	15	27.784	28.186	7	14	15	9.619*	4.222
9	14	15	27.129	26.714	2	15	15	8.783*	11.710
6	15	15	6.636*	3.250	0	0	16	211.340	212.423
0	2	16	24.006	20.930	2	2	16	48.974	49.229
1	3	16	17.802	15.446	0	4	16	118.217	115.059
2	4	16	161.586	164.411	4	4	16	18.039	19.556
1	5	16	15.349	13.153	4	8	8	180.434	181.805
3	5	16	12.254	10.110	0	6	16	19.545	16.215
2	6	16	39.884	40.660	4	6	16	134.151	136.352
6	6	16	17.119	16.154	1	7	16	24.076	21.448
3	7	16	23.727	23.101	5	7	16	19.029	19.583
0	8	16	267.772	264.537	2	8	16	15.432	13.999
4	8	16	107.887	106.715	6	8	16	6.942*	1.778
8	8	16	211.828	209.114	1	9	16	24.340	21.461
3	9	16	23.811	22.932	5	9	16	12.839	8.192
7	9	16	11.571	.869	0	10	16	10.428	4.575
2	10	16	13.341	1.538	4	10	16	92.789	91.303
6	10	16	14.693	13.485	8	10	16	15.586	13.363
10	10	16	56.975	57.964	1	11	16	6.399*	2.852
3	11	16	4.559*	6.849	5	11	16	12.686	11.342
7	11	16	24.703	25.019	9	11	16	17.509	13.951
0	12	16	122.441	118.013	2	12	16	114.996	112.996
4	12	16	14.875	15.001	6	12	16	100.178	100.500
8	12	16	77.385	75.025	10	12	16	114.536	113.071
1	13	16	9.995	.072	3	13	16	15.488	9.422
5	13	16	13.745	12.293	7	13	16	14.596	12.938
9	13	16	13.355	6.863	0	14	16	28.718	28.352
2	14	16	8.574*	12.669	4	14	16	91.548	94.713
6	14	16	15.167	14.530	8	14	16	11.334	9.937

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
1	15	16	6.190*	3.794	3	15	16	12.547	.371
5	15	16	11.501	11.231	7	15	16	7.319*	5.467
0	16	16	177.702	176.464	4	16	16	80.786	81.341
1	2	17	6.622*	3.273	2	3	17	11.696	11.347
3	4	17	16.534	20.467	2	5	17	11.362	7.425
4	5	17	22.444	23.072	1	6	17	7.876*	.535
3	6	17	22.221	24.327	5	6	17	13.188	14.759
2	7	17	21.831	21.190	4	7	17	23.281	24.701
6	7	17	31.659	32.653	1	8	17	7.444*	4.994
3	8	17	19.740	19.776	5	8	17	13.955	9.432
7	8	17	9.006	3.806	2	9	17	13.787	14.428
4	9	17	24.675	23.872	6	9	17	19.224	21.089
8	9	17	4.656*	2.767	1	10	17	19.154	21.035
3	10	17	22.570	24.469	5	10	17	25.971	27.717
7	10	17	14.289	12.310	9	10	17	6.942*	4.154
2	11	17	13.355	9.387	4	11	17	10.916	3.359
6	11	17	39.104	39.384	8	11	17	14.847	10.535
10	11	17	9.786	5.991	1	12	17	17.649	16.320
3	12	17	19.141	16.291	5	12	17	7.138*	5.748
7	12	17	8.323*	.715	9	12	17	11.961	.924
2	13	17	35.437	36.292	4	13	17	9.535	7.517
6	13	17	18.332	18.085	8	13	17	10.442	5.555
1	14	17	34.127	36.039	3	14	17	7.347*	3.916
5	14	17	33.904	36.257	7	14	17	6.594*	6.159
2	15	17	15.572	14.251	4	15	17	18.207	18.454
1	1	18	33.472	34.852	0	2	18	22.514	23.323
1	3	18	31.185	32.921	3	3	18	59.889	59.361
0	4	18	91.465	90.058	2	4	18	97.278	98.190
1	5	18	9.926	2.848	3	5	18	10.665	1.902
5	5	18	12.993	10.583	0	6	18	10.846	14.731
2	6	18	15.181	16.084	4	9	19	28.746	28.255
4	6	18	91.576	90.382	1	7	18	26.627	28.378
3	7	18	37.291	40.890	5	7	18	37.905	39.023
7	7	18	8.657*	12.115	0	8	18	12.965	12.836
2	8	18	16.701	20.678	4	8	18	108.458	112.317
6	8	18	13.495	11.582	1	9	18	18.722	20.329
3	9	18	16.185	16.992	5	9	18	25.999	26.338
7	9	18	31.283	32.218	9	9	18	11.613	3.172
0	10	18	11.487	9.061	2	10	18	23.337	23.597
4	10	18	76.492	73.661	6	10	18	15.837	11.538
8	10	18	20.088	24.124	1	11	18	21.301	19.926
3	11	18	25.832	26.267	5	11	18	33.137	31.897
7	11	18	10.818	10.864	9	11	18	17.189	16.781
0	12	18	117.994	118.782	2	12	18	79.657	76.219
4	12	18	10.595*	6.620	6	12	18	75.447	74.462
8	12	18	82.724	82.812	1	13	18	27.226	29.111

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
3	13	18	11.055	10.744	5	13	18	50.744	51.128
0	14	18	20.646	18.749	2	14	18	10.051	8.176
4	14	18	69.299	70.229	1	2	19	9.201	7.205
2	3	19	35.451	38.257	1	4	19	14.903	10.734
3	4	19	13.550	3.162	2	5	19	13.383	8.994
4	5	19	11.654	7.636	1	6	19	44.499	44.846
3	6	19	11.487	9.173	5	6	19	13.425	12.145
2	7	19	27.714	28.498	4	7	19	17.077	15.712
6	7	19	12.087	6.654	1	8	19	11.013	7.267
3	8	19	12.212	6.654	5	8	19	9.814	8.528
7	8	19	20.102	20.481	2	9	19	4.782*	7.279
6	9	19	11.947	13.484	8	9	19	28.035	27.605
1	10	19	10.525	.642	3	10	19	8.518*	12.254
5	10	19	20.841	22.431	7	10	19	18.945	23.136
2	11	19	14.554	13.753	4	11	19	11.696	13.095
6	11	19	12.839	1.594	1	12	19	9.800*	6.860
3	12	19	11.487	2.879	5	12	19	15.335	15.501
2	13	19	10.665*	8.109	0	0	20	126.902	127.389
0	2	20	131.488	136.758	2	2	20	114.996	110.452
1	3	20	14.624	13.812	0	4	20	16.157	9.254
2	4	20	12.658	.373	4	4	20	124.532	128.585
1	5	20	5.757*	6.158	3	5	20	10.539	6.996
0	6	20	84.731	82.154	2	6	20	94.239	90.592
4	6	20	11.640	9.109	6	6	20	88.049	87.414
1	7	20	8.267*	6.549	3	7	20	8.755*	.095
5	7	20	10.637	10.169	0	8	20	61.088	62.724
2	8	20	109.086	108.903	4	8	20	27.756	30.448
6	8	20	100.303	101.600	8	8	20	65.786	65.364
1	9	20	20.116	21.142	3	9	20	9.034*	2.706
5	9	20	10.846	7.188	7	9	20	11.543	5.918
0	10	20	94.239	92.142	2	10	20	54.480	51.401
4	10	20	16.826	18.213	6	10	20	64.517	63.258
1	11	20	16.074	14.820	3	11	20	10.888	4.381
1	2	21	4.796*	6.773	2	3	21	9.075*	10.845
1	4	21	6.455*	5.818	3	4	21	24.508	22.317
2	5	21	15.153	14.022	4	5	21	7.570*	8.703
1	6	21	32.998	32.425	3	6	21	24.814	27.513
5	6	21	4.796*	3.360	1	7	22	37.347	36.642
2	7	21	27.435	28.914	4	7	21	10.651	8.138
6	7	21	14.680	8.252	1	8	21	6.719*	5.940
3	8	21	23.588	23.663	5	8	21	13.244	7.618
2	9	21	4.865*	4.946	1	1	22	11.738	.569
0	2	22	21.929	23.818	1	3	22	22.110	23.895
3	3	22	45.600	48.005	0	4	22	68.003	66.421

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
2	4	22	53.198	52.334	1	5	22	22.082	24.383
3	5	22	19.670	21.587	5	5	22	14.010	11.591
0	6	22	12.463	4.020	2	6	22	4.963*	7.480
4	6	22	70.582	68.803	1	7	22	37.347	36.642