

Supplementary Table OM1. Results of the curve-fitting analysis for the spectrum of almandine

FR-3 (Fig. 1a). Letter and symbol designations of the different spin-forbidden bands follow Moore and White (1972) and Taran et al. (Part II - in press) in this table and those following. FWHM is full width at half maximum. (This and all following supplementary Tables are for the online version only).

Band	Almandine FR-3		
	Intensity (cm ⁻¹)	Energy (cm ⁻¹)	FWHM (cm ⁻¹)
d	2.8	14317	2062
e	5.5	16007	1812
f	12.6	17610	1868
g	6.10	18915	1235
h	11.9	19795	1756
i	1.9	19846	553
IVCT	42.4	21389	5794
k	2.7	21294	1666
l	4.1	23030	689
m	3.8	23476	1061
m'	2.9	24310	1078
q	4.3	25237	1289
??	11.8	26480	974
r	36.0	27030	568

Supplementary Table OM2. Results of the curve-fitting analysis for the spectrum of almandine JF-1 (Fig. 1b).

Band	Almandine JF-1		
	Intensity (cm ⁻¹)	Energy (cm ⁻¹)	FWHM (cm ⁻¹)
d	2.01	14450	2290
e	2.51	16240	1054
f	5.26	17376	1087
g	6.45	19077	1828
h	2.26	19742	392
i	2.16	20109	557
j	1.35	20772	1041
IVCT	14.26	21638	6434
k	0.65	21647	560
l	1.05	23030	703
m	2.24	23426	1002
m'	1.56	24164	840
q	3.82	25025	1078
“??”	6.62	26370	1305
r	9.64	27055	718

Supplementary Table OM3. Results of the curve-fitting analysis for the spectrum of the intermediate almandine-pyrope garnet GTF 90-33 (Fig. 2).

Band	Almandine-Pyrope GTF 90-33		
	Intensity (cm ⁻¹)	Energy (cm ⁻¹)	FWHM (cm ⁻¹)
d	1.83	14826	2917
e	1.93	16265	1169
f	4.19	17409	1263
g	5.24	19010	1920
h	1.79	19879	567
i	0.90	20317	445
j	0.85	20737	768
k	0.25	21429	786
IVCT	12.80	21816	5265
l	1.30	23039	760
m	1.82	23438	908
q	4.37	24287	1341
“?”	8.54	25553	1552
“??”	9.72	26503	1040
r	15.22	27193	799

Supplementary Table OM4. Results of the curve-fitting analysis for the spectrum of almandine-bearing spessartine 316306 (Fig. 3a).

Band	Spessartine 316306		
	Intensity (cm ⁻¹)	Energy (cm ⁻¹)	FWHM (cm ⁻¹)
-	0.30	18891	598
IVCT	6.30	20547	5560
-	0.89	20585	618
-	0.73	21602	844
-	8.10	22872	594
n'	7.64	23220	436
n	12.34	23684	512
o	13.58	24182	431
p	14.42	24438	437

Supplementary Table OM5. Results of the curve-fitting analysis for the spectrum of the almandine-bearing spessartine 200924241653 (Fig. 3b).

Band	Spessartine 200924241653		
	Intensity (cm ⁻¹)	Energy (cm ⁻¹)	FWHM (cm ⁻¹)
IVCT	13.87	20880	6140
-	8.14	22872	519
n'	8.25	23258	378
n	10.96	23702	496
o	13.00	24192	348
p	15.84	24450	267
*	8.99	25815	338

* It cannot be determined if this band is real or an experimental artifact.

Supplementary Table OM6. Results of the curve-fitting analysis for the spectrum of grossular SGM-1 (Fig. 4a).

Band	Grossular SGM-1		
	Intensity (cm ⁻¹)	Energy (cm ⁻¹)	FWHM (cm ⁻¹)
IVCT	4.06	22712	8694
m	0.46	23119	816
“??”	1.57	26235	909
r	3.18	26984	670

Supplementary Table OM7. Results of the curve-fitting analysis for the spectrum of grossular GR 10074 (Fig. 4b).

Band	Grossular GR 10074		
	Intensity (cm ⁻¹)	Energy (cm ⁻¹)	FWHM (cm ⁻¹)
d*	0.11	14431	4162
-	0.10	17738	2305
h	0.04	19835	263
IVCT	0.54	21190	5904
n'	0.20	23122	1381
n	0.18	23837	987
p	0.29	24580	1007
??	0.50	25942	1697
r	0.44	26966	877

* Probably represents the overlapping bands e, f and g relating to {Fe²⁺}.