

Andradite, $\text{Ca}_3\text{Fe}^{3+}_2(\text{SiO}_4)_3$

Andradite

Quartieri S, Oberti R, Boiocchi M, Dalconi M C, Boscherini F, Safonova O, Woodland A B
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Site preference and local geometry of Sc in garnets: Part II.

The crystal-chemistry of octahedral Sc in the andradite- $\text{Ca}_3\text{Sc}_2\text{Si}_3\text{O}_{12}$ join

12.0578 12.0578 12.0578 90 90 90 Ia-3d

atom	x	y	z	Wyckoff
CaX	0.125	0	0.25	24c
FeY	0	0	0	16a
SiZ	0.375	0	0.25	24d
O	0.0394	0.0487	0.6554	96h

Raman Active Modes

WP	A _{1g}	A _{1u}	A _{2g}	A _{2u}	E _u	E _g	T _{2u}	T _{2g}	T _{1u}	T _{1g}
96h	3	6	.	9	.	.
24d	1	.	3	.	.
24c	1	.	2	.	.
16a

Total number of modes:

$$3A_{1g} + 8E_g + 14T_{2g} = 25$$