

Diopside, $\text{CaMgSi}_2\text{O}_6$

Diopside

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Mossbauer spectroscopy and Rietveld refinement on synthetic ferri-Tschermak's molecule $\text{CaFe}_3+(\text{Fe}_3+\text{Si})\text{O}_6$ substituted diopside

9.7483 8.9246 5.2505 90 105.882 90 C2/c

atom	x	y	z	Wyckoff
MgM1	0	0.9078	0.25	4e
CaM2	0	0.3014	0.25	4e
SiT	0.286	0.0916	0.2302	8f
O1	0.1184	0.0871	0.1432	8f
O2	0.3623	0.2498	0.3175	8f
O3	0.3487	0.0201	0.9983	8f

$(4 \times 8f) + (2 \times 4e)$

Raman Active Modes

WP	A_g	A_u	B_g	B_u
8f	3	.	3	.
4e	1	.	2	.

Total number of modes:

$$14A_g + 16B_g = 30$$