

## Enstatite, MgSiO<sub>3</sub>

Enstatite

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High temperature single crystal X-ray diffraction studies

of the ortho-ortho phase transition in enstatite, Mg<sub>2</sub>Si<sub>2</sub>O<sub>6</sub> at 1360 K

18.251 8.814 5.181 90 90 90 Pbcn

atom	x	y	z	Wyckoff
Mg1	0.3758	0.6537	0.8660	8c
Mg2	0.3768	0.4869	0.3590	8c
SiA	0.2717	0.3415	0.0505	8c
SiB	0.4735	0.3374	0.7983	8c
O1A	0.1834	0.3400	0.0356	8c
O1B	0.5625	0.3403	0.8002	8c
O2A	0.3108	0.5027	0.0432	8c
O2B	0.4327	0.4833	0.6896	8c
O3A	0.3032	0.2226	-0.1679	8c
O3B	0.4475	0.1955	0.6040	8c

(10 × 8c)

### Raman Active Modes

WP	A <sub>g</sub>	A <sub>u</sub>	B <sub>1g</sub>	B <sub>1u</sub>	B <sub>2g</sub>	B <sub>2u</sub>	B <sub>3g</sub>	B <sub>3u</sub>
8c	3	·	3	·	3	·	3	·

Total number of modes:

$$30A_g + 30B_{1g} + 30B_{2g} + 30B_{3g} = 120$$