

Topaz, Al₂SiO₄F₂

Topaz

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New insight into crystal chemistry of topaz: a multi-methodological study

4.6601 8.8260 8.3778 90 90 90 Pbnm

atom	x	y	z	Wyckoff
Al	0.9053	0.13131	0.0816	8d
Si	0.39976	0.94088	0.25	4c
O1	0.7064	0.0311	0.25	4c
O2	0.4516	0.7564	0.25	4c
O3	0.2114	0.98979	0.09284	8d
F	0.5982	0.25263	0.05988	8d

$(3 \times 8d) + (3 \times 4c)$

Raman Active Modes

WP	A _g	A _u	B _{1g}	B _{1u}	B _{2g}	B _{2u}	B _{3g}	B _{3u}
8d	3	.	3	.	3	.	3	.
4c	2	.	1	.	2	.	1	.

Total number of modes:

$$15A_g + 12B_{1g} + 15B_{2g} + 12B_{3g} = 54$$