

Zircon, ZrSiO₄

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Rare-earth elements in synthetic zircon: Part 2. A single-crystal

X-ray study of xenotime substitution

6.6102 6.6102 5.986 90 90 90 *I4₁/amd

0 -.25 .125

atom	x	y	z	Wyckoff
Si	0	0.75	5/8	4b
Zr	0	0.75	1/8	4a
O	0	0.0657	0.1961	16h

Raman Active Modes

WP	A _{1g}	A _{1u}	A _{2g}	A _{2u}	B _{1g}	B _{1u}	B _{2g}	B _{2u}	E _u	E _g
16h	2	.	.	.	2	.	1	.	.	3
4b	1	1
4a	1	1

Total number of modes:

$$2A_{1g} + 4B_{1g} + 1B_{2g} + 5E_g = 12$$