

## Rutile, TiO<sub>2</sub>

Rutile

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H in rutile-type compounds: I. Single-crystal neutron and X-ray diffraction study of H in rutile

4.5922 4.5922 2.9574 90 90 90 P4<sub>2</sub>/mmm

atom	x	y	z	Wyckoff
Ti	0	0	0	2a
O	0.30496	0.30496	0	4f

### Raman Active Modes

WP	A <sub>1g</sub>	A <sub>1u</sub>	A <sub>2g</sub>	A <sub>2u</sub>	B <sub>1g</sub>	B <sub>1u</sub>	B <sub>2g</sub>	B <sub>2u</sub>	E <sub>u</sub>	E <sub>g</sub>
<b>4f</b>	<b>1</b>	.	.	.	<b>1</b>	.	<b>1</b>	.	.	<b>1</b>
<b>2a</b>	.	.	.	.	.	.	.	.	.	.

Total number of modes:

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