

Petalite, LiAlSi₄O₁₀

Petalite

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Kristallographische untersuchungen eines petalits mittels neutronenbeugung und transmissionselektronenmikroskopie

11.737 5.171 7.630 90 112.54 90 P2/a

| atom | x | y | z | Wyckoff |
|------|--------|--------|--------|---------|
| Li | 0.25 | 0.2553 | 0 | 2e |
| Al | 0.25 | 0.7564 | 0 | 2e |
| Si1 | 0.9980 | 0.5128 | 0.2896 | 4g |
| Si2 | 0.1477 | 0.0099 | 0.2896 | 4g |
| O1 | 0 | 0.5 | 0.5 | 2b |
| O2 | 0.25 | 0.9654 | 0.5 | 2f |
| O3 | 0.0938 | 0.3012 | 0.2704 | 4g |
| O4 | 0.3617 | 0.5358 | 0.1342 | 4g |
| O5 | 0.0381 | 0.8011 | 0.2518 | 4g |
| O6 | 0.2076 | 0.9779 | 0.1353 | 4g |

$$(6 \times 4g) + (1 \times 2f) + (2 \times 2e) + (1 \times 2b)$$

Raman Active Modes

| WP | A _g | A _u | B _g | B _u |
|----|----------------|----------------|----------------|----------------|
| 4g | 3 | · | 3 | · |
| 2f | 1 | · | 2 | · |
| 2e | 1 | · | 2 | · |
| 2b | · | · | · | · |

Total number of modes:

$$21A_g + 24B_g = 45$$