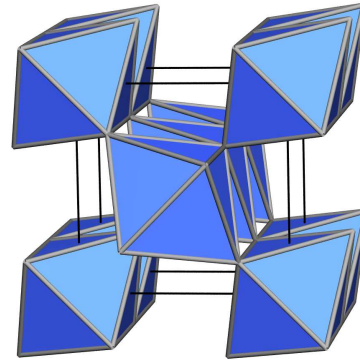
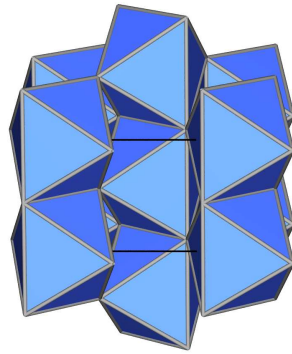


Beispiel I: Struktur von Stishovit (Rutil-Typ)

Kristallogr. Daten:

- ◇ RG $P4_2/mnm$, $Z=2$
- ◇ $a = 4.173 \text{ \AA}$
- ◇ $c = 2.657 \text{ \AA}$
- ◇ Si auf 2(a): $0,0,0$
- ◇ O auf 4(f): $0.301,x,0$



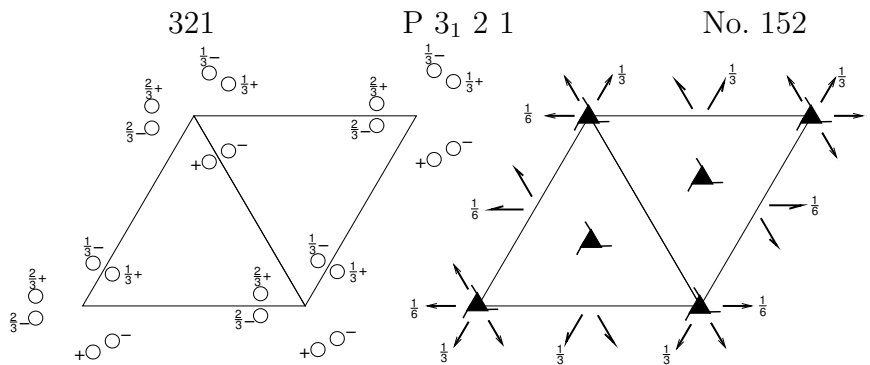
Beispiel II: Struktur von α -Quarz

Raumgruppe $P3_121$

Auszug aus den *Internationalen Tabellen*

$P 3_1 2 1$
 D_3^4

Trigonal



Origin at centre 3_121 [2-axis normal to $(11\bar{2}0)$]

Number of positions,
Wyckoff notation,
and point symmetry

Co-ordinates of equivalent positions

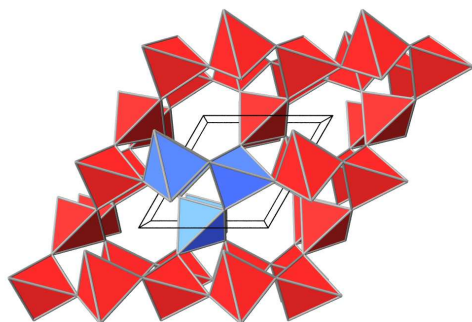
Conditions limiting
possible reflections

6	c	1	$x, y, z; \bar{y}, x - y, \frac{1}{3} + z; y - x, \bar{x}, \frac{2}{3} + z;$ $y, x, \bar{z}; \bar{x}, y - x, \frac{1}{3} - z; x - y, \bar{y}, \frac{2}{3} - z$	hkil: No conditions 000l: $l=3n$
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3	b	2	$x, 0, \frac{5}{6}; 0, x, \frac{1}{6}; \bar{x}, \bar{x}, \frac{1}{2}.$
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3	a	2	$x, 0, \frac{1}{3}; 0, x, \frac{2}{3}; \bar{x}, \bar{x}, 0.$
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Special: as above only



Kristallographische Daten:

- ◇ Raumgruppe $P3_121$, $Z=3$
- ◇ $a = 4.775 \text{ \AA}$, $c = 5.3046 \text{ \AA}$
- ◇ Si auf 3(a): $0.4570, 0, \frac{1}{3}$
- ◇ O auf 6(c): $0.408, 0.2881, 0.2300$