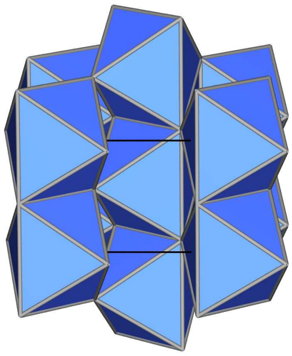
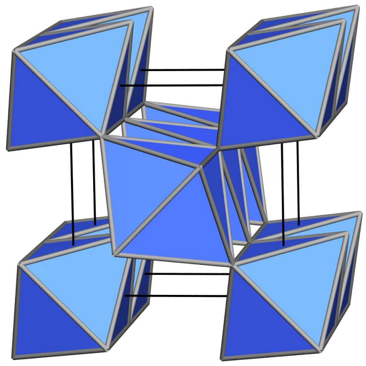
Beispiel I: Struktur von Stishovit (Rutil-Typ)

Kristallogr. Daten:
- ◇ RG $P4_2/mnm$, Z=2
- ◇ $a = 4.173$ Å
- ◇ $c = 2.657$ Å
- ◇ Si auf 2(a): 0,0,0
- ◇ O auf 4(f): 0.301,x,0





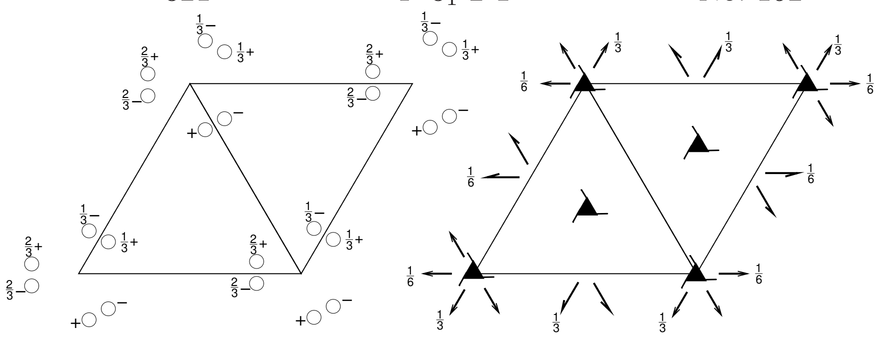
Beispiel II: Struktur von α-Quarz

Raumgruppe $P3_121$

Auszug aus den *Internationalen Tabellen*

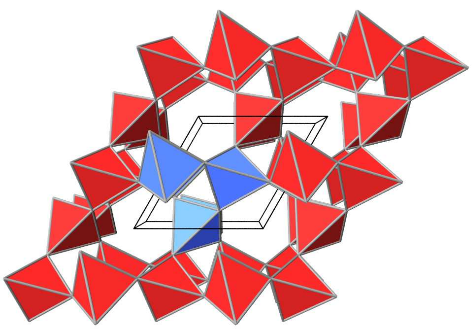
P 3_1 2 1

Trigonal	321	P 3_1 2 1	No. 152	D_3^4



Origin at centre $3_1 21$ [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
				Special: as above only
3	b	2	$x, 0, \frac{5}{6};\ 0, x, \frac{1}{6};\ \bar{x}, \bar{x}, \frac{1}{2}.$	
3	a	2	$x, 0, \frac{1}{3};\ 0, x, \frac{2}{3};\ \bar{x}, \bar{x}, 0.$	



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