| $SiO_2$ | *hP*15 | (180) $P6_222$ – kc |
|---|---|---|

**$SiO_2$ quartz β** [1], quartz high
Structural features: $SiO_4$ tetrahedra (split O site) share vertices to form a 3D-framework with twisted chains and narrow channels of hexagonal cross-section parallel to [001].

Wright A.F., Lehmann M.S. (1981) [1]
$O_2Si$
$a = 0.49977$, $c = 0.54601$ nm, $c/a = 1.093$, $V = 0.1181$ nm$^3$, $Z = 3$

| site | Wyck. | sym. | *x* | *y* | *z* | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 12*k* | 1 | 0.4164 | 0.1783 | 0.19143 | 0.5 | |
| Si2 | 3*c* | 222 | $^1/_2$ | 0 | 0 | | |

Experimental: single crystal, diffractometer, neutrons, R = 0.038, T = 863 K

Remarks: Phase stable at T > 846 K. Cell parameters from [2]. Short interatomic distances for partly occupied site(s). The authors state that high-symmetry β-quartz is not achieved as a stable structure and the average structure is probably of dynamic nature. Distortions within the $SiO_4$ tetrahedra may be reduced by displacing Si into a split position in Wyckoff position 6*g*; an alternative model with O in Wyckoff position 6*j* was tested and rejected (R = 0.053).

References: [1] Wright A.F., Lehmann M.S. (1981), J. Solid State Chem. 36, 371-380. [2] Ackermann R.J., Sorrell C.A. (1974), J. Appl. Crystallogr. 7, 461-467.