

# $\zeta$ -Y<sub>2</sub>[Si<sub>2</sub>O<sub>7</sub>]: Ein neuer Strukturtyp in der Yttrialit-Reihe

$\zeta$ -Y<sub>2</sub>[Si<sub>2</sub>O<sub>7</sub>]: A New Structure Type within the Yttrialite Series

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During attempts of preparing yttrium oxotellurates(IV) using Y<sub>2</sub>O<sub>3</sub> and TeO<sub>2</sub> in YCl<sub>3</sub> fluxes, the occasional reaction of these educts with the walls of the evacuated silica ampoules led to colourless, lath-shaped single crystals of Y<sub>2</sub>[Si<sub>2</sub>O<sub>7</sub>] in the new  $\zeta$ -type structure as a minor by-product which was investigated by X-ray diffraction. The title compound crystallizes monoclinically in the space group  $P2_1/m$  ( $a = 503.59(5)$ ,  $b = 806.47(8)$ ,  $c = 732.65(7)$  pm,  $\beta = 108.633(6)^\circ$ ) with two formula units per unit cell. The crystallographically unique Y<sup>3+</sup> cation is coordinated by seven oxygen atoms ( $d(\text{Y}-\text{O}) = 221 - 248$  pm) arranged in the shape of a slightly distorted monocapped octahedron. The isolated oxodisilicate units [Si<sub>2</sub>O<sub>7</sub>]<sup>6-</sup> consist of two Si<sup>4+</sup> cations and seven O<sup>2-</sup> anions of which five are crystallographically independent. These pyroanions ( $d(\text{Si}-\text{O}) = 161 - 168$  pm,  $\angle(\text{O}-\text{Si}-\text{O}) = 91 - 117^\circ$ ,  $\angle(\text{Si}-\text{O}-\text{Si}) = 156^\circ$ ) exhibit an almost perfectly eclipsed conformation built of a horseshoe-shaped backbone with the two silicon and three of the oxygen atoms situated on the mirror planes of the unit cell. The remaining four oxide anions complete this [Si<sub>2</sub>O<sub>7</sub>]<sup>6-</sup> entity of two vertex-sharing [SiO<sub>4</sub>]<sup>4-</sup> tetrahedra as terminal ligands for silicon. Assembled in planar layers parallel to  $(-1\ 0\ 1)$ , the [Si<sub>2</sub>O<sub>7</sub>]<sup>6-</sup> anions are packed with their wide basal faces of the tetrahedra pointing towards the small waist of the adjacent units and *vice versa*. The yttrium cations reside between these layers in order to interconnect them three-dimensionally.

*Key words:* Yttrium, Oxodisilicates, Yttrialite, Crystal Structures