

## **A new rare earth disilicate (REE<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>; REE = Dy, Tm, Lu; type-L): Evidence for non-quenchable 10 GPa polymorph with silicon in fivefold trigonal bipyramidal coordination?**

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### **ABSTRACT**

A new structure type (L) is reported for disilicates of the middle and heavy rare earth elements (REE) quenched from 10 GPa, 1600–1700 °C. Crystal data are: triclinic, space group *PT*, *Z* = 6; Dy<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>: *a* = 6.5971(3), *b* = 6.6504(2), *c* = 18.0582(6) Å,  $\alpha$  = 83.791(2),  $\beta$  = 88.653(2),  $\gamma$  = 88.498(2)°, *V* = 787.2 Å<sup>3</sup>, and *D<sub>x</sub>* = 6.242 g/cm<sup>3</sup>; Tm<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>: *a* = 6.5499(2), *b* = 6.5876(2), *c* = 17.8916(7) Å,  $\alpha$  = 83.828(1),  $\beta$  = 88.368(1),  $\gamma$  = 88.152(2)°, *V* = 766.9 Å<sup>3</sup>, and *D<sub>x</sub>* = 6.574 g/cm<sup>3</sup>; Lu<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>: *a* = 6.5240(2), *b* = 6.5553(2), *c* = 17.7909(6) Å,  $\alpha$  = 83.977(2),  $\beta$  = 88.074(2),  $\gamma$  = 87.846(2)°, *V* = 755.8 Å<sup>3</sup>, and *D<sub>x</sub>* = 6.830 g/cm<sup>3</sup>. The type-L structure comprises linear trisilicate [Si<sub>3</sub>O<sub>10</sub>]<sup>8-</sup> and orthosilicate [SiO<sub>4</sub>]<sup>4-</sup> ions cross linked by REE<sup>3+</sup> in one sevenfold and five eightfold coordinated positions (to 3.0 Å), and is assembled from alternating (001) strips of the type-B structure of REE<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> and a sheared structure containing structural elements found in the type-B structure but with Si distributed with 50% occupancy over two face-sharing tetrahedra. The geometry of these half-occupied tetrahedra is consistent with decomposition of a SiO<sub>5</sub> trigonal bipyramid during quenching of the pressure.