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A new dense silica polymorph: A possible link between tetrahedrally and octahedrally coordinated silica

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Abstract

We present the discovery of a novel dense silica polymorph retrieved from shock-wave and diamond-anvil cell experiments. This polymorph is the first observed silicate composed of face-sharing polyhedra and it has a density similar to stishovite. Sterical constraints on the bond angles induce an intrinsic disorder of Si positions, such that the Si-coordination is transitional between four- and sixfold. The structure provides a mechanism for this coordination change in silica and other silicates at high temperature that is fundamentally different from mechanisms at 300 K. The new polymorph also illustrates how the face-sharing polyhedra, naturally occurring along previously proposed compression mechanisms for dense silicate melts, can be constructed without inferring unphysically small bond angles.