

Isosymmetric Reversible Phase Transition in Sodium Oxalate

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Oxalate ions are widely used in the design of supramolecular structures. Anhydrous metal oxalates (like sodium oxalate) are interesting because they have not H-bonds and their structures are determined by the interactions in the system "oxalate-anions - metal cations" only.

At 3.8 GPa an isosymmetric phase transition was observed, preserving the P21/c space group despite a jumpwise change in cell parameters and volume. The orientation of oxalate-ions and the coordination of sodium-cations by oxygen atoms change jumpwise at the transition point. The packing of the centroids of oxalate-anions remains preserved to a large extent. It distorts anisotropically with increasing pressure.

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