

Mechanism of Isostructural Phase Transition in Isobutane under High Pressure

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Isostructural phase transitions are rare and intriguing phenomena in crystallography. In this study, we present a high-pressure single-crystal X-ray diffraction investigation of isobutane, revealing an isostructural transition between two polymorphs (α and β) within the orthorhombic *Pnma* space group. The transition occurs over a wide pressure range and is characterized by a distinct reorientation of isobutane molecules while maintaining the overall symmetry and connectivity of the crystal structure.

We introduce an orientational order parameter to quantitatively describe the molecular tilt associated with the transition and model its evolution with pressure. Hirshfeld surface analysis[1] highlights the role of subtle changes in intermolecular distances in stabilizing the high-pressure β -form. Our findings demonstrate how minor molecular adjustments can induce profound effects on packing and phase behavior, offering insights into the behavior of van der Waals solids under compression.

This work contributes to a broader understanding of polymorphism and pressure-induced transformations in aliphatic hydrocarbons, with implications for energy materials and molecular solid-state design.

[1] Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D., Spackman, M. A. (2021). *J. Appl. Crystallogr.* **54**, 1006.

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