Poster

Molecular aggregations in crystals of butene isomers determined at high-pressure

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For the first time, we have determined the crystal structures of all four butene isomers: 1-butene (**B**), cis-2-butene (**CB**), trans-2-butene (**TB**), and isobutene (**IB**) at high-pressure by single-crystal X-ray diffraction techniques. These compounds, gases under ambient conditions, at high pressure and room temperature froze in their phases α at: 3.65, 1.55, 0.50 and 1.40 GPa, respectively. **B**, **CB**, **TB** and **IB** crystallise in the centrosymmetric space groups: *Pnma*, *C*2/*c*, $P2_1$/c and $P6_3/m$, respectively. Stability of these structures was maintained across the range of studied pressure. Additionally, we have correlated the physical properties of butene isomers with their crystalline packing and interatomic distances, enhancing our understanding of molecular interactions under extreme conditions.