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Bonding Changes in Compressed Carbon Dioxide: A New Stishovite-like Phase of CO₂

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At ambient conditions, carbon dioxide (CO₂) is a prototypical molecular system, with strong covalent O=C=O molecular bonds and relatively weak quadrupolar interactions between molecules. At high pressures and temperatures, CO₂ transforms to a series of solid polymorphs with differing crystal structures, intermolecular interactions and chemical bonding. In particular, two fully covalent (extended) solid phases have been reported above 40GPa, with characteristics analogous to SiO₂ polymorphs. First, CO₂-V (above 40GPa and 1500K), consists of a network of corner sharing CO₄ tetrahedra and is structurally similar to SiO₂ tridymite¹. And, recently, an extended-solid amorphous phase (*a-carbonia*), similar to amorphous silica, has been reported at room temperature above 40GPa². Here, we present a new stishovite-like CO₂ phase VI, formed by compressing CO₂-II above 50GPa and 550K. We define the PT stability domain for the new solid, and present Raman and X-Ray diffraction results consistent with a 6-fold average coordination within a P42/mnm structure. Finally, we propose a phase/bonding diagram for carbon dioxide describing the systematic relationship between its molecular and extended phases at high pressures and temperatures. 1] V. Iota, *et al.*, Science **283**, 1510 (1999). 2] M. Santoro, *et al.* Nature **441**, 857 (2006).