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Raman spectroscopy and X-ray diffraction *in situ* characterization of phase transitions in cristobalite under high pressure

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We have studied *in situ* the structure and optical properties of cristobalite at pressures up to 61 GPa by means of micro-Raman spectroscopy and X-ray powder diffraction. The α -cristobalite phase of SiO₂ was formed after annealing of silica sol-gel glass at 1500⁰C for 15 minutes. For generation of high-pressure a Mao-Bell and membrane type diamond anvil cells were used. On pressure increase four polymorphs were found: C-I has initial structure of α -cristobalite up to 6 GPa, C-II in the pressure range 0.2 – 14GPa, C-III from 14 to 35, C-IV above 35 GPa, and no new phase was observed up to 61 GPa. The high-pressure phase C-IV is crystalline and quenchable. The monoclinically distorted α -PbO₂-type structure provides the best fit of X-ray pattern of recovered C-IV phase.

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Experimental and Theoretical Identification of New High-Pressure TiO₂ Polymorph

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Our combined theoretical and experimental investigations have led to the discovery of a new polymorph of titanium dioxide, where titanium is seven-coordinated to oxygen in the orthorhombic OI (*Pbca*) structure. The zero-pressure bulk modulus of the new phase measured in the pressure range 19 to 36 GPa is 318(3) GPa. We demonstrate that the group IVa dioxides (TiO₂, ZrO₂, HfO₂) on compression at ambient temperature all follow the common path: Rutile → α-PbO₂-type → baddeleyite-type (MI) → orthorhombic OI (*Pbca*) structure → cotunnite-type (OII).

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Structure of Metallic and Magnetic High-Pressure Fe₃O₄ Polymorph: Experimental and Theoretical Study

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Studies of the nature of the high-pressure polymorph of magnetite, the oldest known magnetic material, have a long and controversial history. Using electrically- and laser-heated diamond anvil cells at pressures above 40 GPa we synthesized pure high-pressure Fe₃O₄ phase (h-Fe₃O₄) and performed an *in situ* structural refinement. In good agreement with our *ab initio* calculations we found that h-Fe₃O₄ adopts the CaTi₂O₄-type structure (space group *Bbmm*). Electrical resistivity and Mössbauer spectroscopy measurements show that h-Fe₃O₄ is metallic and magnetic up to at least 70 GPa. The magnetic properties are associated with one of the structural positions presumably occupied by mostly Fe²⁺ ions.