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Structural Modifications of Cold and Dense Cesium, Calcium, Barium, and Selenium

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Following the development of high brilliance synchrotron x-ray sources, high density crystalline structures of elemental solids have been vastly studied at room temperature and elevated pressures. In the last decades, experimental and computational results have unveiled a vast diversity of crystalline structures adopted by many dense elements. Both complex modulated and exotic structures have been observed [1] and predicted [2]. In this communication, we report results of systematic searches for structural modifications taking place at very low temperature (T>10 K) and high pressure (P<50 GPa) in selected elementals solids. Results for cesium, calcium, barium, and selenium are presented. An extension of the known P-T phase diagram to lower temperature for cesium and selenium indicates that both elements do not adopt crystalline structures different that those already known and documented. We show that calcium at low temperature and high pressure, however, exhibits unusual and large dynamical fluctuations leading to a tetragonal distortion of the simple cubic structure known to exist at room temperature and about 30 GPa. The large amplitude fluxional behaviour leads to the appearance of a new phase, nested at T<30K between 40 and 45 GPa. Finally, barium when compressed at low temperature, transforms into a crystalline structure unobserved at high pressure and room temperature. It is found that, below 140K and in the pressure range of 13 to 35 GPa, barium does not adopt the phase IV structure, i.e., the modulated incommensurate cell, but undergoes a transition from phase II (P63/mmc) to an orthorhombic (Pmna) cell. This new structure corresponds to phase VI. On the basis of an x-ray diffraction study along quasi-isobaric and isothermal paths, we conclude that Ba-VI is most likely metastable. Our results suggest the need to scrutiny other dense elements at very low temperature. Under those conditions, unusual structural modifications are ought to be observed.

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