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New high-pressure phases in MOOH (M = Al, Ga, In)

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Abstract

A unique phase, belonging to an orthorhombic crystal system (*Pbca*, $Z = 8$), is proposed in AlOOH using crystal structure searches based on an evolutionary genetic algorithm method, combined with density functional theory. This phase features a nonlinear asymmetric doubly covalent hydrogen-bond and metal cations that are sixfold oxygen coordinated. Unlike the earlier proposed monoclinic phase, the stability region of *Pbca* (166–189 GPa) lies well below the pressure of decomposition to Al_2O_3+ice X (287 GPa). In GaOOH the *Pbca*-type phase is not energetically favorable at any pressure. In the course of evaluating the breakdown of GaOOH to its constituent oxides, we have found a new phase of Ga_2O_3 (U_2S_3-type). In InOOH, *Pbca* is energetically favorable over a narrow pressure interval (12–17 GPa). Also in InOOH, we find a new tetragonal structure ($P\bar{4}2_1m$, $Z = 4$) stable above 51 GPa. This phase has nonlinear asymmetric hydrogen-bonds and metal cations that are sevenfold oxygen coordinated. Phonon calculations confirm the vibrational stability of the new phases and show that the high-pressure polymorphs of AlOOH are likely to be important carriers of water into the deep lower mantles of Earth and rocky super-Earths.

Keywords: High pressure, first-principles, phase transitions, AlOOH; Water in Nominally Hydrous and Anhydrous Minerals