Supporting information

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SI Text

Details of Crystal Structure Predictions. Detailed structure searches through crystal structure analysis by particle-swarm optimization (CALYPSO) code were performed at 0.02, 0.1, 0.5, 1, 1.5, and 2 TPa with system sizes at 4, 8, 12, 16, 20, and 24 atoms per simulation cell, respectively. We choose the population size for each generation as 40 structures, and structures for the first generation were produced randomly with symmetry constraints. All structures were locally optimized using the Vienna Ab Initio Simulation Package code. The 60% structures of each generation with lower enthalpies were used to generate the structures for the next generation by PSO operation, and the remaining 40% structures were randomly generated to increase the structural diversity. The inertia weight is dynamically varied and decrease linearly from 0.9 to 0.4. We keep the self-confidence factor and the swarm confidence factor as constant 2. The magnitudes of the velocities are confined within the range of [−0.2,0.2]. By the use of these parameters, we were able to find the experimentally observed ϵ- and ζ-O_8 structures in the 5th and 3rd generations at CALYPSO runs with 8 atoms per simulation cell at 0.02 and 0.1 TPa, respectively.

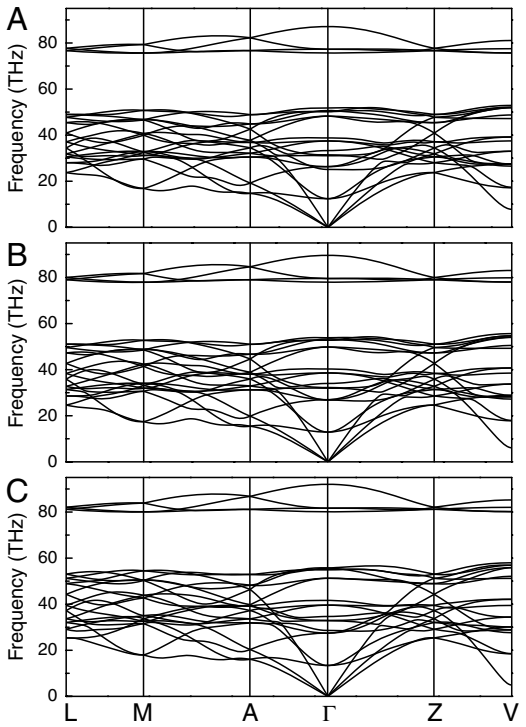

Fig. S1. Phonon dispersions of ζ-O_8 at (*A*) 1.6, (*B*) 1.8, and (*C*) 2 TPa.

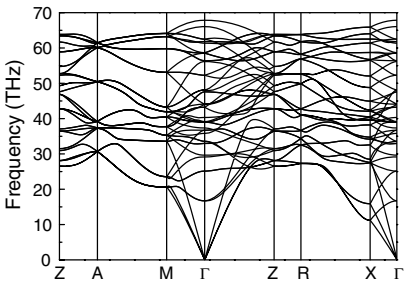

Fig. S2. Phonon dispersions of θ-O_4 at 2 TPa. The absence of imaginary frequency within the entire Brillouin zone suggested that θ-O_4 is dynamically stable.