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Structure and Stability of Low-Z Ionic Solids at High Pressure. A. Lazicki^{1,2}, C.S. Yoo¹, W. Pickett², R. Scalettar², ¹Lawrence Livermore National Laboratory, Livermore, CA 94551, ²Univ. of California, Davis, CA 95616.

We explore pressure-induced phase transitions in a class of highly ionic low-Z compounds with simple structures using synchrotron x-ray diffraction and spectroscopy in diamond anvil cells and with electronic structure calculations. Results for Li_3N and Li_2O reveal some original and unexpected properties and provide a better general understanding of this class of closed-shell materials, and of their hydrogen-containing analogs NH_3 and H_2O . Li_3N has a hexagonal to cubic structural transition at 40 GPa, accompanied by a volume collapse and electronic band-gap widening. The new phase is stable to over 200 GPa, and the N^{3-} ions (isovalent to neon) retain their ionic character. Like neon, the compressibility and metallization pressure are very high. Li_2O , which is structurally and electronically similar to high pressure ice, undergoes a cubic-orthorhombic transition at 50 GPa, with a 100% increase in bulk modulus. Considered with the known behavior of alkali sulfides, the present results for Li_2O indicate a systematic high-pressure behavior of all alkali chalcogenides, including non-molecular ice at ultra-high pressure.

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