# Ionic moduli: A new semi-empirical model describing the compression of crystalline ionic compounds

DANIEL R. HUMMER[1]

[1]Department of Earth, Planetary and Space Sciences, University of California Los Angeles, Los Angeles, CA 90095

The compressibility of a material (or its reciprocal, the bulk modulus) is a fundamental parameter governing the behavior of materials at non-ambient conditions, but there currently exists no quantitative model explaining the bulk modulus of a material in terms of simpler parameters. A novel, semi-empirical model is presented which quantitatively predicts the bulk modulus of a crystalline ionic compound in terms of the compression of its constituent ions. The model assumes that ions are elastic spheres which compress reproducibly and independently of their environment, according to a simple first order equation of state. This framework introduces a new physical parameter unique to each ion called the ionic modulus, which is defined analogously to the bulk modulus of a material. Testing this model against P-V compression data for the alkali halides reveals that the model correctly predicts the bulk moduli of strongly ionic compounds within 10% error, significantly better than expected by statistics alone given the number of model parameters. In addition, it is demonstrated that the compressibility of most alkali metal and halide ions are a simple linear function of the zero pressure ionic radius. The results indicate that to a large extent, electron clouds compress reproducibly according to a simple physical law relating to the radial distribution of electrons.