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Accuracy of equation-of-state formulations

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ABSTRACT

The accuracy of equation-of-state formulations is compared for theoretical total energies or experimental pressure-volume measurements for H_2, Ne, Pt, and Ta. This spans the entire range of compression found for minerals and volatiles in the Earth. The Vinet equation is found to be most accurate. The origin of the behavior of different equation-of-state formulations is discussed. It is shown that subtle phase transitions can be detected by examining the residuals from an equation-of-state fit. A change in the electronic structure of Ta is found at high pressures using this procedure, and a possible new transition in H_2.