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Semiempirical equations of state for NaCl¹ MICHEL SANTOS, University of Sao Paulo, RENATA WENTZCOVITCH, University of Minnesota — Despite diamond anvil cell experiments having reached pressures of hundreds of GPa, measuring high pressures is still a challenge. One of the strategies adopted in high pressure measurements is to measure the lattice spacing, via x-ray diffraction, of a calibrant whose equation of state is well known. Several calibrants have been widely used, but pressure scales based on them still have great uncertainties at high pressures and temperatures (PT). NaCl has been widely used as a pressure standard, but the lack of good high P and high T equations of state limits the use of this material. We have developed strategies to produce predictive high PT equations of state by combining ab initio results with available data at low T and high P or high T and low P. The high PT equations of state obtained in this way for NaCl show excellent agreement with high PT data by Bohler and Kennedy ². Semi-empirical equations will play an important role in the development of predictive databases of thermodynamics properties of materials.

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²R. Bohler and G. Kennedy, J. Phys. Chem. Solids, 41, pp 517 (1980)

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