On the route from atom to equation of state

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The new results reflect the capabilities of the shell model in developing thermal equations of state (EOSs). The most general characteristic, called "rigidity," has been identified and introduced for three model objects. Simple formulas link control parameters of the two levels to form a hierarchy. For a polyatomic shell molecule, "rigidity" reflects the fact of an electron-nuclear device, forms a model potential, and makes it possible to predict critical parameters based on their relationship with the coordinates of singular points. For an atom, "rigidity" reflects its shell structure (in terms of principal quantum numbers). It makes it possible to calculate the degree of overlapping of atoms in a molecule, which is necessary to calculate the rigidity of a molecule. The third object is a model of a molecule in the form of a point center (PC), for which, by analogy, it is possible to introduce a new characteristic—"effective" rigidity, determined by its practical dimensions, manifested as a result of the action of the forces of attraction and repulsion. The ratio of their diameters turned out to be the control parameter of the EOS of interacting PCs, which forms all the above parameters, including the critical compressibility factor (CCF). As a result, the revealed hierarchy makes it possible, by specifying one number (characteristic of the outer atom), to calculate the critical parameters and CCF of a substance from polyatomic molecules. Tested for several substances—F_2, CO_2, CF_4, CCl_4, $SnCl_4$, SF_6. The maximum discrepancy with the experimental value of the CCF is 3%.