

Abstract Submitted
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Van der Waals forces between large molecules and nanoscale structures ALLAN PIERCE¹, Retired — Theories of forces between multi-atom structures go back to Fritz London; each structure is an assembly of electrons and nuclei, with net separation distance R . Coulomb-potential terms in the overall Hamiltonian, expanded in inverse powers of R , yield a leading relevant interaction Hamiltonian that varies asymptotically as R^{-3} . A second-order perturbation procedure yields the the correction to the lowest energy level, varying as R^{-6} . The principal difficulty is evaluating the matrix elements, products of which appear in each term of the sum giving the coefficient of R^{-6} . Each such matrix element involves tensorial products of dipole moment vector operators. An approximation, derived from experimental results used by Denbigh (1940) in regard to the polarizability of molecules, is that the dominant contribution comes from separate covalent bonds and that the contributions are additive. Matrix elements for a given covalent bond can be satisfactorily and simply calculated using an LCAO approximation. An additional approximation is that only two states are relevant for any given covalent bond. Results yield approximate insight that forces should be viewed as forces between bonds and that the forces depend tensorially on the bond directional orientations.

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