Atomic Factorization of Molecular Interactions

The long-range dispersion interaction, or London dispersion potential, $C_6/R^6$ is numerically computed using factorized expressions relying only on the dynamic polarizabilities of the individual atoms at imaginary frequencies. The derived expressions are shown to independently agree with an alternative derivation. The dynamic dipole polarizabilities, evaluated at imaginary frequencies, are tabulated for hydrogen and lithium atoms to be used in the $C_6$ factorized expressions (which are numerically integrated by Gaussian quadrature method). This method yields $C_6$ dispersion coefficients in agreement with the latest theoretical values for the homo-nuclear atom interactions of H-H and Li-Li configurations and the hetero-nuclear interaction Li(2S)-H(1S). Higher energy hetero-nuclear dispersion coefficients appear to diverge from previous theoretical values possibly limiting the applicability of the current methodology. The dynamic dipole polarizabilities for the Li atom in the 2S, 2P, and 3S states were additionally calculated from a large basis configuration interaction calculation, encompassing frequency ranges into the positive energy continuum.

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