

virial theorem

Interrelates the kinetic, T , and potential, V , energy of a system in its stationary states. The molecular electronic virial theorem is formulated (J.Slater) as follows:

$$2\langle T_{el} \rangle = - \langle V \rangle - \sum_{\alpha} \sum_{\beta > \alpha} R_{\alpha\beta} (\partial U / \partial R_{\alpha\beta})$$

where U is the potential energy function for nuclear motion and the sum runs over all internuclear distances. The true wavefunctions must satisfy the virial theorem.

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