Valence State Atoms in Molecules and Universal Scaling of RKR Potential Curves

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Based on Ruedenberg's bond analysis we describe a Valence State (VS) Atom as an Atom-in-a-Molecule devoid of wave interference. The spectroscopic behaviour of diatoms is rationalized to an unprecedented degree of universality if the VS energy is taken as the asymptotic reference level. A universal VS potential function reproduces the Rydberg-Klein-Rees (RKR) curves of fifty molecules to an accuracy of 1.4% within the Coulson-Fischer range ($0.5\ R_e < R < 1.5\ R_e$). The scaled RKR curves coalesce into virtually a single curve in this range. A combination of the VS and Morse potential functions allows to obtain the same accuracy over the whole range of distances up to $R \rightarrow \infty$. An arithmetic combination rule is established for scaled force constant increments, which are transferable from homo- to heteronuclear molecules to an accuracy of 1.6 % in the harmonic wavenumber of 42 diatoms covering the full range of bond polarity.