

A UNIFIED PERSPECTIVE ON THE NATURE OF PAIRWISE INTERATOMIC INTERACTIONS FROM Ar₂ TO CARBON MONOXIDE.

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A method is developed that gives a unified perspective on the nature of a wide range of pairwise interatomic interactions. The approach is applied to the diatomic molecules CO, H₂⁺, H₂, HF, LiH, Li₂, O₂, and Ar₂, and one-dimensional cuts through the potentials of OC-HBr, OC-HF, OC-HCCH, OC-HCN, OC-HCl, OC-HI, OC-BrCl, and OC-Cl₂. Systems selected for investigation illustrate different bond categories varying from van der Waals, halogen bonded, hydrogen bonded to strongly bound covalently bound carbon monoxide with binding energies varying over almost three orders of magnitude, from 99.3 cm⁻¹ to 90683 cm⁻¹. Accurate semi-empirically determined Rydberg-Klein-Rees or morphed interatomic potentials are used in transformations for this wide range of species to a reduced potential demonstrating commonality in their fundamental nature.