

Abstract Submitted
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A Unified Perspective on the Nature of Bonding in Pairwise Interatomic Interactions ROBERT LUCCHESI LUCCHESI, CHARLES ROSALES, L. RIVERA-RIVERA, B. MCELMURRY, J. BEVAN, J. WALTON, Texas A&M University — Different classes of ground electronic state pairwise interatomic interactions are referenced to a single canonical potential using explicit transformations. These approaches have been applied to diatomic molecules N_2 , CO , H_2Ca_2 , O_2 ; argon dimer, and one-dimensional cuts through multidimensional potentials of $OC-HBr$, $OC-HF$, $OC-HCCH$, $OC-HCN$, $OC-HCl$, $OC-HI$, $OC-BrCl$, and $OC-Cl_2$ using accurate semi-empirically determined interatomic Rydberg-Klein-Rees (RKR) and morphed intermolecular potentials. These different bonding categories are represented in these systems which vary from van der Waals, halogen bonding, hydrogen bonding to strongly bound covalent molecules with binding energies covering three orders of magnitude from 84.5 cm^{-1} approaches were then utilized to give a unified perspective on the nature of bonding in the whole range of diatomic and intermolecular interactions investigated to 89600.6 cm^{-1} in ground state dissociation energies.

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