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Origin of Hydrogen Bonding: Natural Bond Orbital Electron Donor-Acceptor Interactions

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Abstract : We perform computational investigation using density functional theory, B3LYP with aug-cc-pVTZ basis set followed by natural bond orbital analysis (NBO), which provides best single “natural Lewis structure” (NLS) representation of chosen wavefunction (Ψ) with natural resonance theory (NRT) to provide an analysis of molecular electron density in terms of resonance structures (RS) and weights (w). We selected for the study a wide range of gas phase dimers (B…HA), with hydrogen bond dissociation energies (ΔEB…H) that span more than two orders of magnitude. We demonstrate that charge transfer from a donor Lewis-type NBO (nB:) to an acceptor non-Lewis-type NBO (σHA*) is the primary cause for H-bonding not classical electrostatic (dipole-dipole or ionic). We provide a variety of structure, and spectroscopic descriptors to support the conclusion, such as IR frequency shift (ΔνHA), H-bond penetration distance (ΔRB..H), bond order (bB..H), charge-transfer (CTB→HA) and the corresponding donor-acceptor stabilization energy (ΔE(2)).

Keywords : natural bond orbital, hydrogen bonding, electron donor, electron acceptor
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