

Supplementary Information

Revisiting the covalent nature of halogen bonding: polarized three-center four-electron bond

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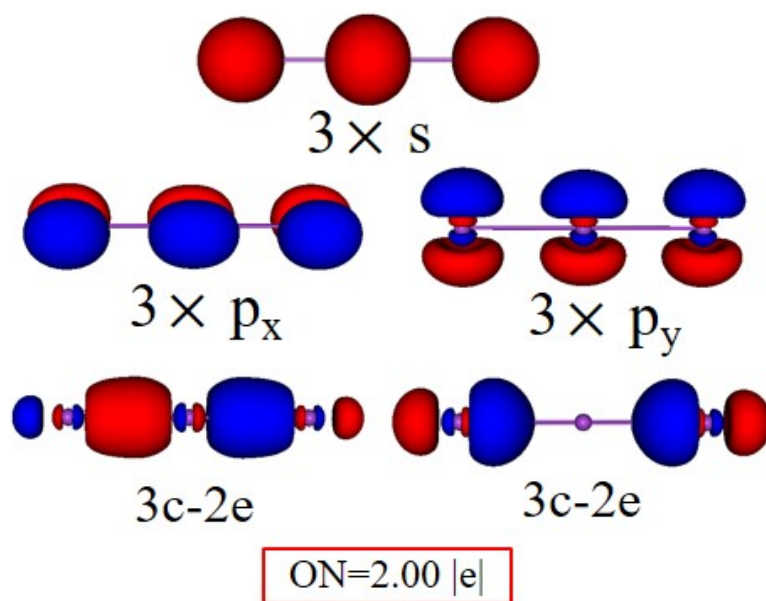


Figure S1. Full AdNDP bonding frameworks of I_3^-

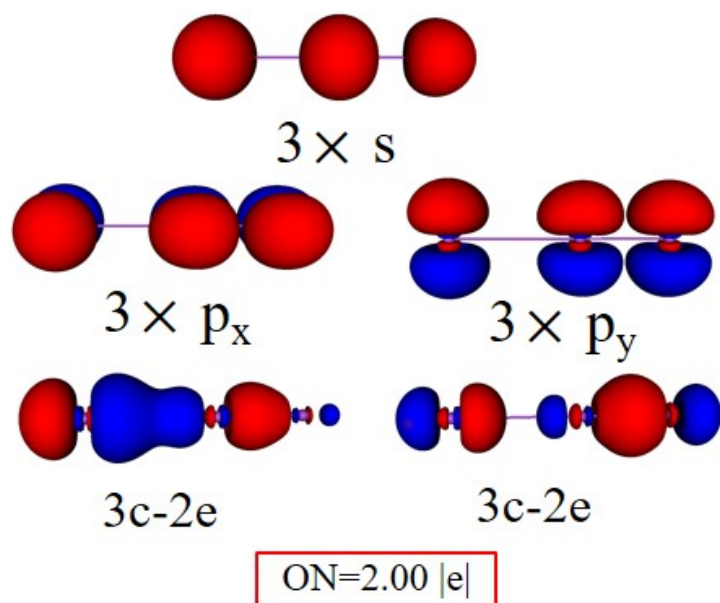


Figure S2. Full AdNDP bonding frameworks of I₂...I⁻ (I₁...I₂ distance of 4.00 Å)

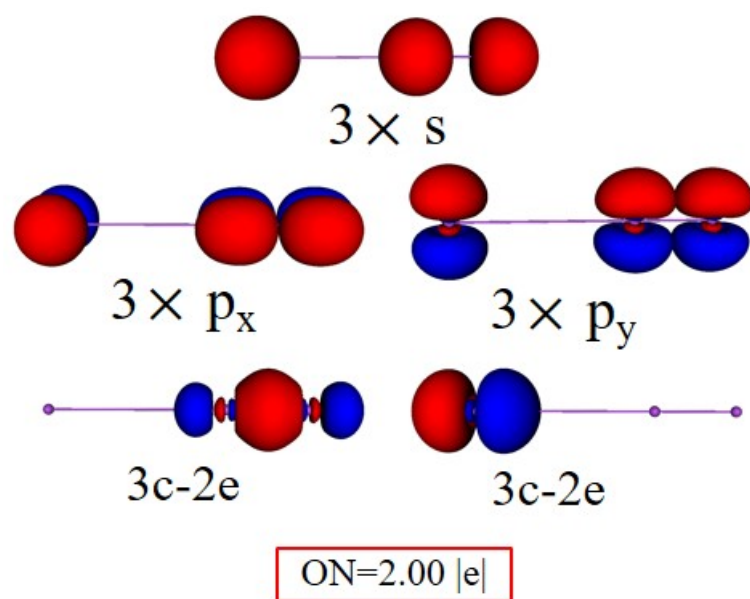


Figure S3. AdNDP bonding frameworks of I₂...I⁻ (I₁...I₂ distance of 6.00 Å)

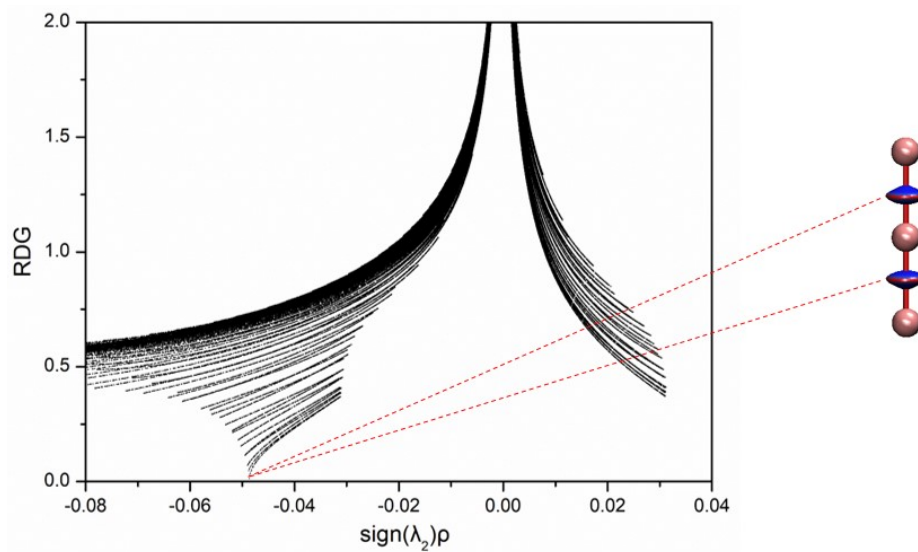


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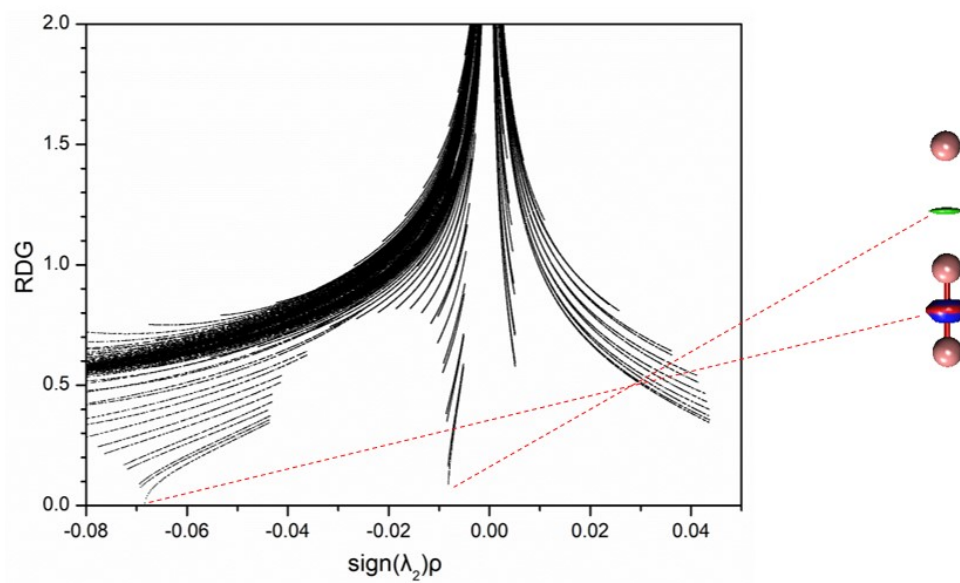


Figure S5. Plots of the reduced density gradient (RDG in a.u.) against the sign of the second Hessian eigenvalue multiplied by the electron density ($\text{sign}(\lambda_2)\rho$) in a. u.) for $\text{I}_2 \cdots \text{I}^-$ ($\text{I}_1 \cdots \text{I}_2$ distance of 4.00 Å) with NCI isosurfaces at 0.40

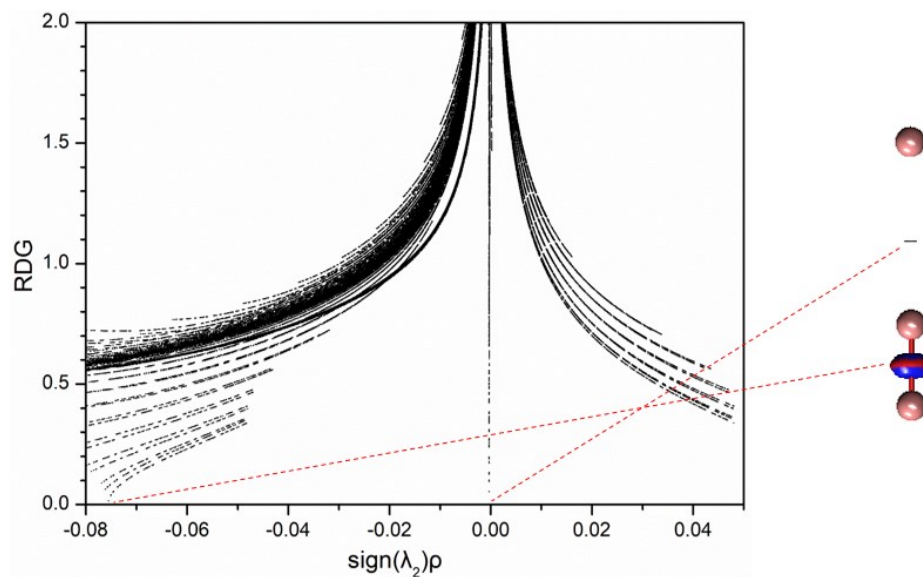


Figure S6. Plots of the reduced density gradient (RDG in a.u.) against the sign of the second Hessian eigenvalue multiplied by the electron density ($\text{sign}(\lambda_2)\rho$) in a. u.) for $\text{I}_2 \dots \text{I}^-$ ($\text{I}_1 \dots \text{I}_2$ distance of 6.00 Å) with NCI isosurfaces at 0.40