

SUPPORTING INFORMATION

Identification and Characterization of Molecular Bonding Structures by *ab initio* Quasi-atomic Orbital Analyses

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Supporting Information Description:

The Supporting Information contains orbital plots from the present study but created with different isosurface values (as indicated in each Figure caption).

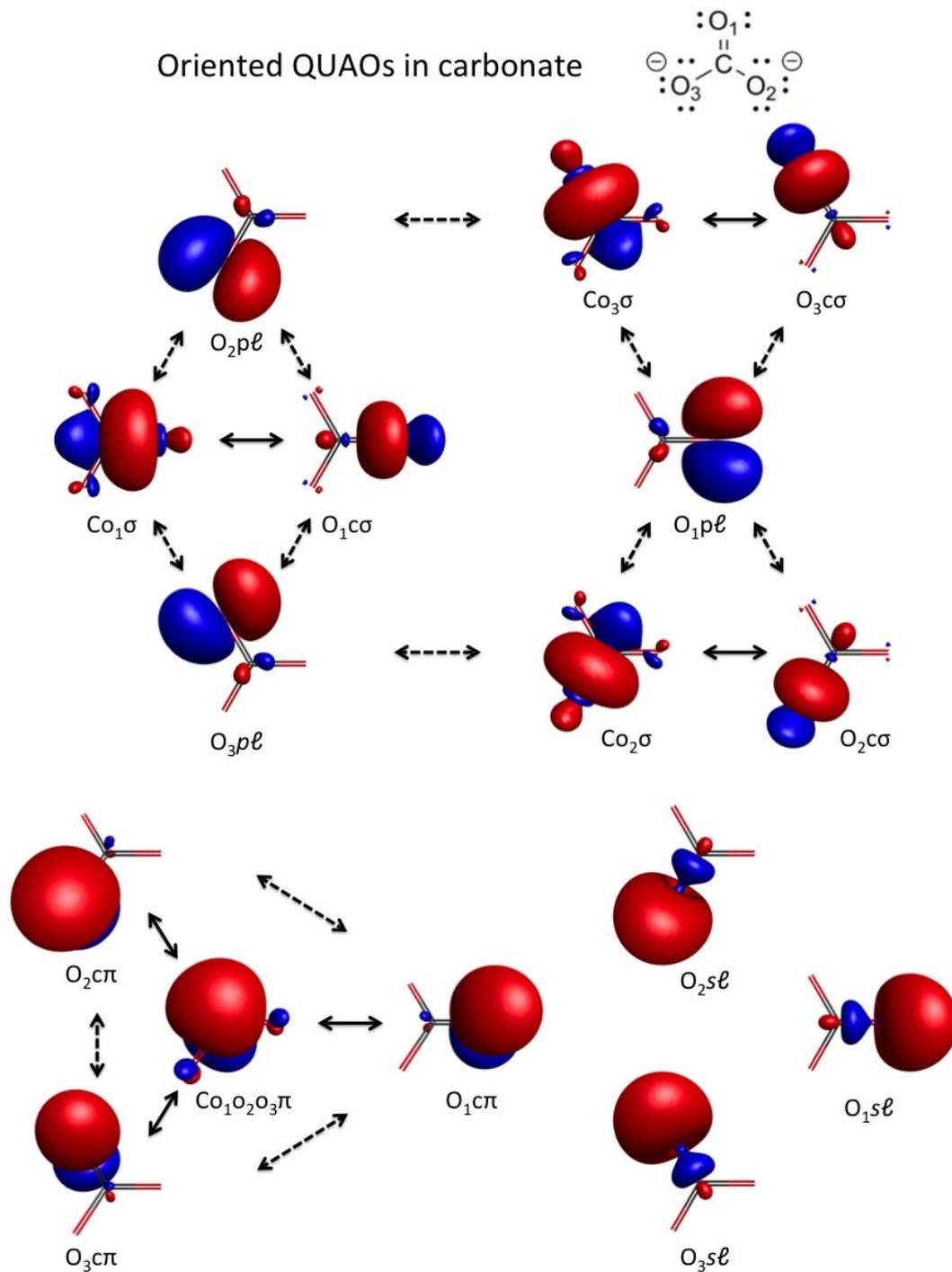


Figure S1. Oriented QUAOs in carbonate shown with absolute orbital values of 0.05 (e/bohr^3)^{1/2}. The orbital label is given beneath each orbital. A solid arrow between two orbitals indicates a firm bond between the orbitals. A dashed arrow between two orbitals indicates a weak bond between the orbitals. (The two dashed arrows for the weakly bonded pairs $\{\text{O}_2 p\ell, \text{O}_3 c\sigma\}$ and $\{\text{O}_3 p\ell, \text{O}_2 c\sigma\}$ are not shown.)

Oriented QUAOs in diborane

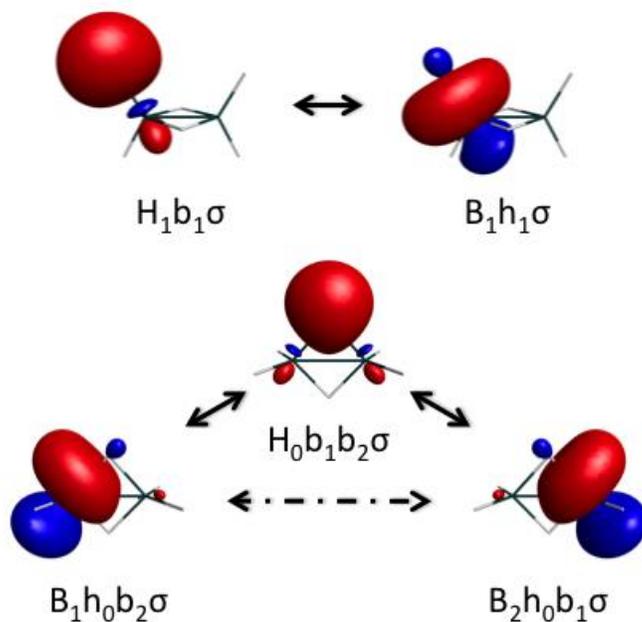


Figure S2. Oriented QUAOs in diborane shown with absolute orbital values of $0.05 \text{ (e/bohr}^3)^{1/2}$. The orbital label is given beneath each orbital. A solid arrow between two orbitals indicates a firm bond between the orbitals. A dot-dashed arrow between two orbitals indicates a weak bond between the orbitals in terms of the kinetic bond order (see text). Only one of the four equivalent terminal bonds and one of the two three-center bridge bonds are shown.

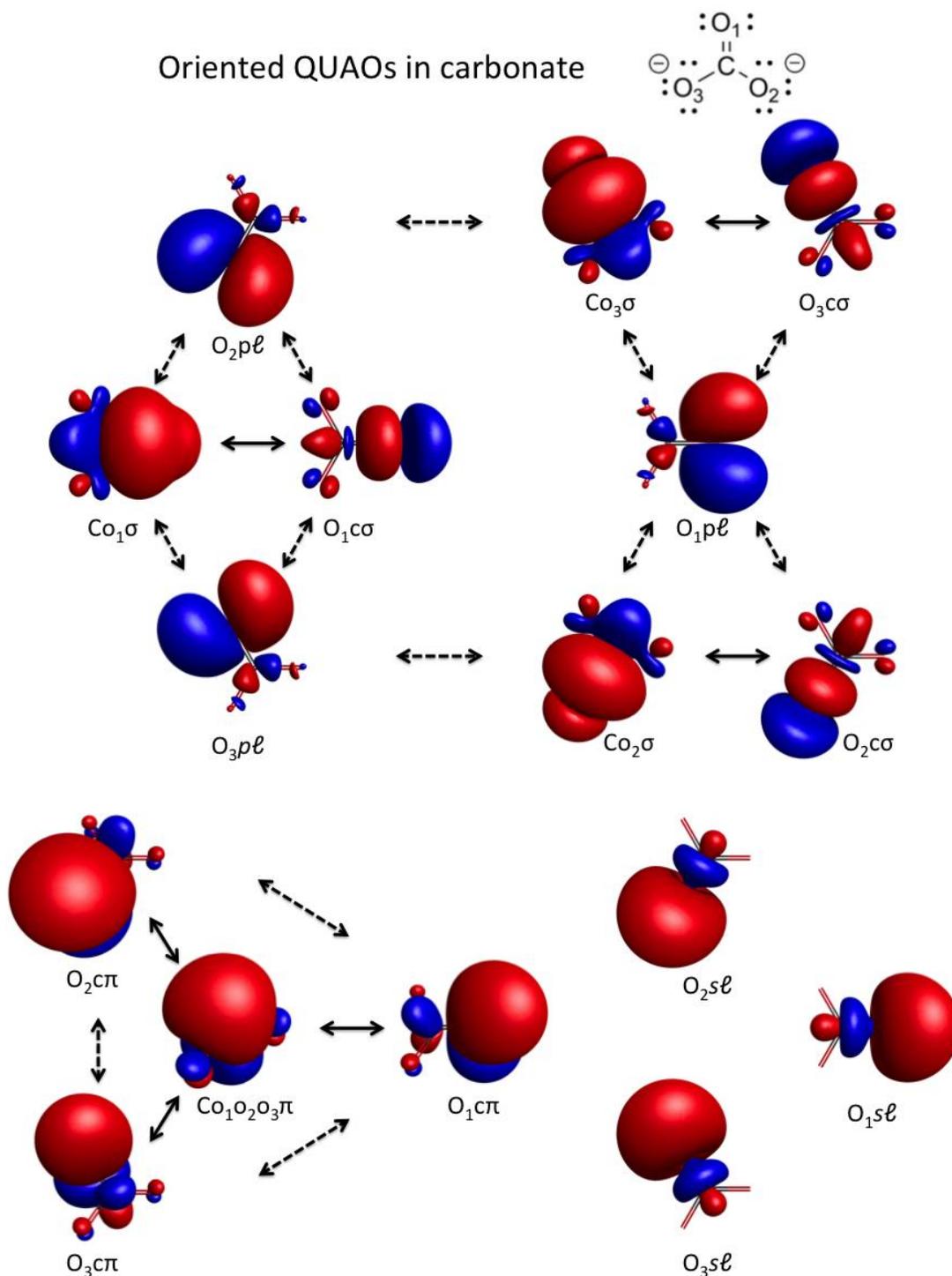


Figure S3. Oriented QUAOs in carbonate shown with absolute orbital values of $0.02 \text{ (e/bohr}^3)^{1/2}$. The orbital label is given beneath each orbital. A solid arrow between two orbitals indicates a firm bond between the orbitals. A dashed arrow between two orbitals indicates a weak bond between the orbitals. (The two dashed arrows for the weakly bonded pairs $\{\text{O}_2p\ell, \text{O}_3\sigma\}$ and $\{\text{O}_3p\ell, \text{O}_2\sigma\}$ are not shown.)

Oriented QUAOs in diborane

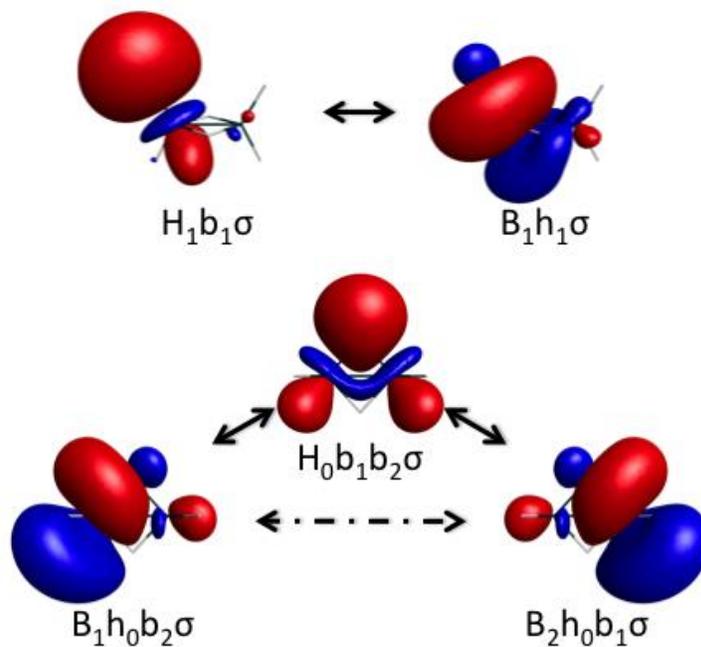


Figure S4. Oriented QUAOs in diborane shown with absolute orbital values of $0.02 \text{ (e/bohr}^3)^{1/2}$. The orbital label is given beneath each orbital. A solid arrow between two orbitals indicates a firm bond between the orbitals. A dot-dashed arrow between two orbitals indicates a weak bond between the orbitals in terms of the kinetic bond order (see text). Only one of the four equivalent terminal bonds and one of the two three-center bridge bonds are shown.