Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supplementary Information

Near Equivalence of Polarizability and Bond Flux for Describing Covalent Bond Rearrangements

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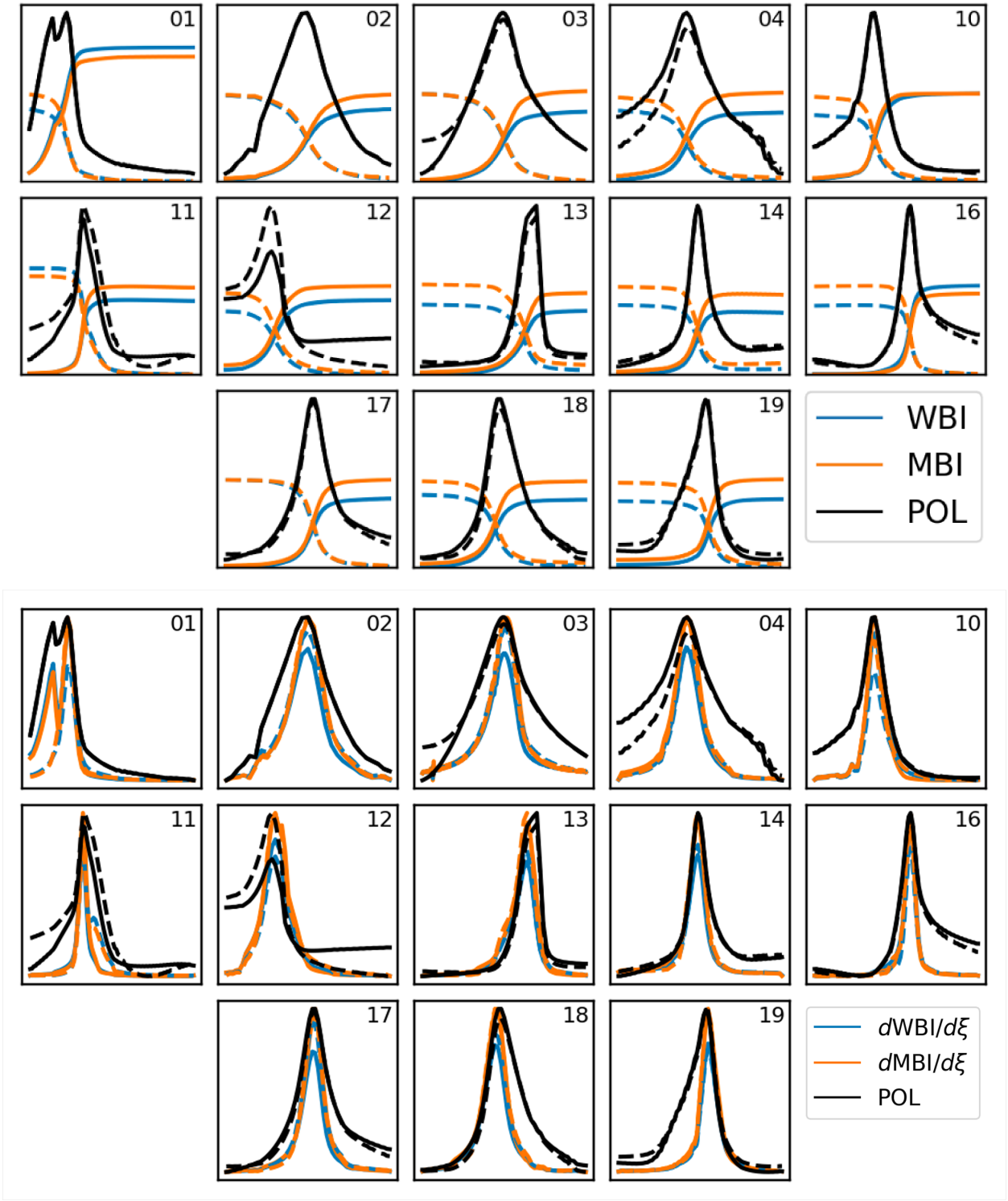

Figure 1: *Bond order and bond order flux compared to parallel polarizability for 13 hydrogen combustion reactions.* The Wiberg (blue) and Mayer (orange) bond indices plotted alongside the bond projected polarizability (black). The plots are overlaid and are plotted on separate scales. Solid and broken lines indicate forming and breaking bonds, respectively.

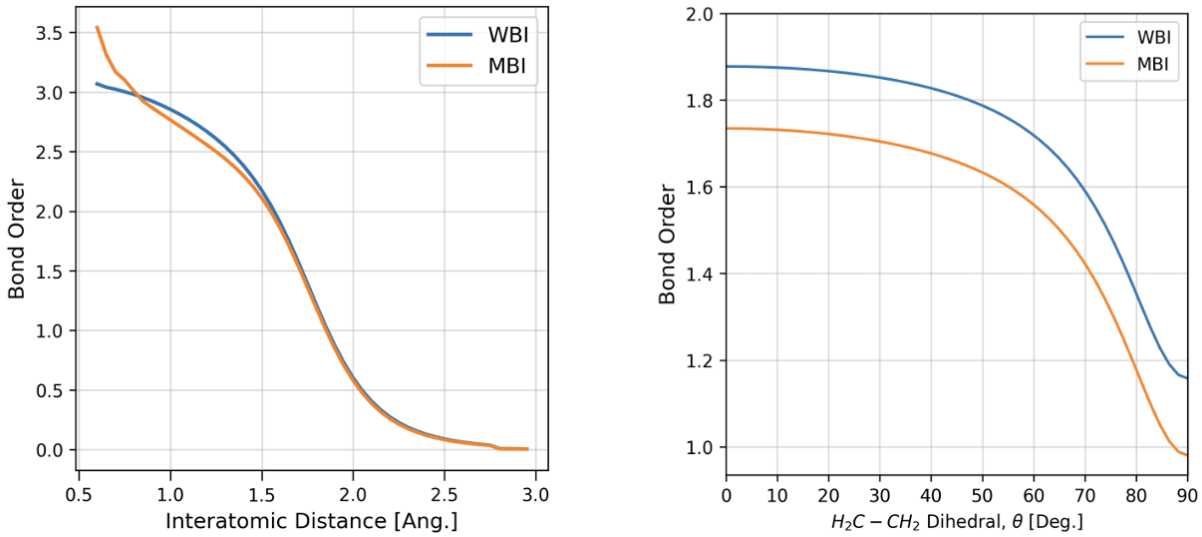

Figure 2: *Nitrogen molecule dissociation and Ethene bond rotation* Bond order, bond order flux, and polarizability profiles computed with spin-unrestricted CASSCF(6,6)/cc-pVTZ and CASSCF(2,2)/cc-pVTZ for nitrogen and ethene, respectively.

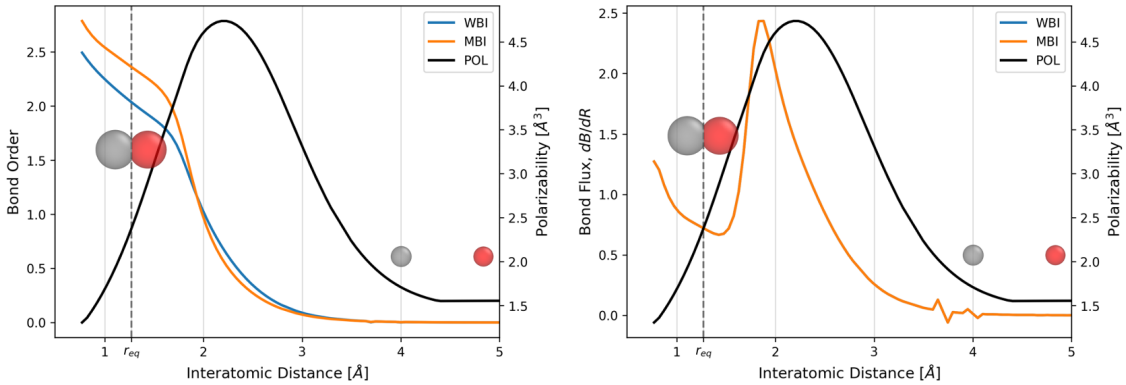

Figure 3: *Carbon monoxide bond dissociation* Bond order, bond flux, and bond-projected polarizability profiles computed with CASCI(10,8)/cc-pVTZ. Vertical dashed line indicates equilibrium bond length.

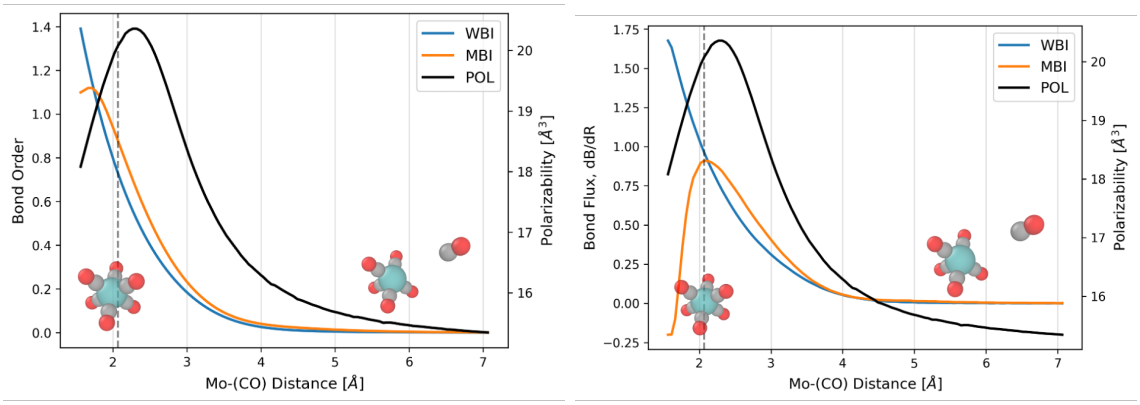

Figure 4: *Molybdenum-carbon bond dissociation in* $Mo(CO)_6$ Bond order, bond flux, and bond-projected polarizability profiles computed with ωB97x-v/def2-TZVP. Vertical dashed line indicates equilibrium bond length.

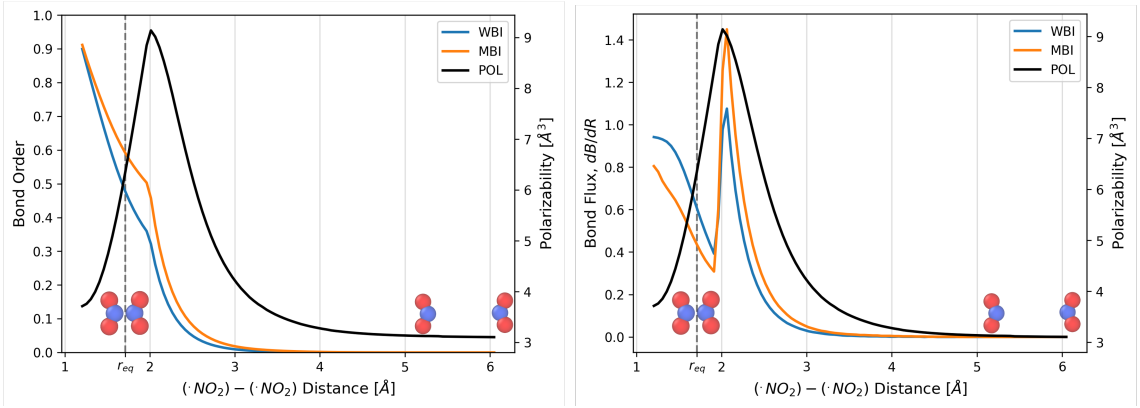

Figure 5: *Dinitrogen tetroxide dissociation* Bond order, bond flux, and bond-projected polarizability profiles computed with ωB97x-v/cc-pVTZ. Vertical dashed line indicates equilibrium bond length.