Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Photodynamic behavior of electronic coupling in N-methylformamide dimer

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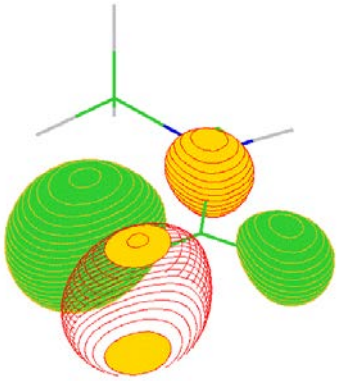
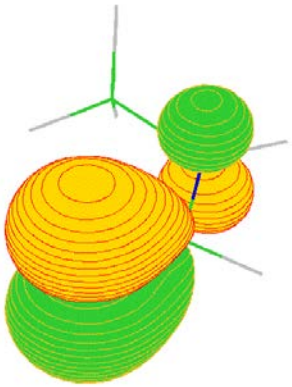
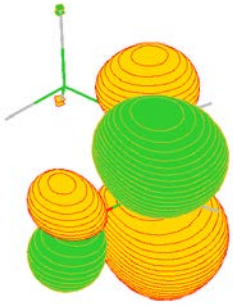
Supporting Material



The non-bonding orbital localized on O atom

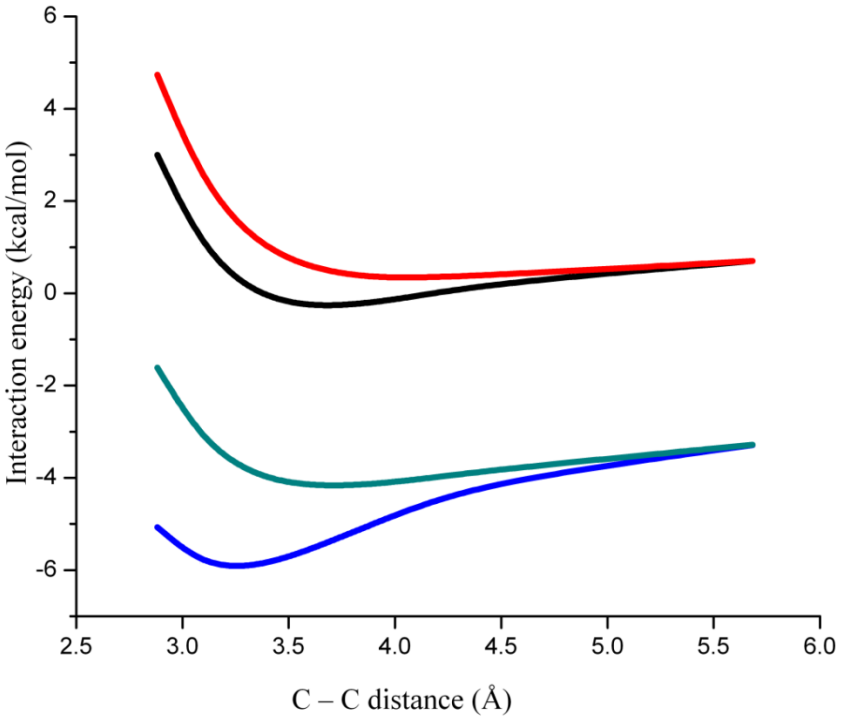


The π orbital localized on CO bond and non-bonidng orbital of N atom with π symmetry

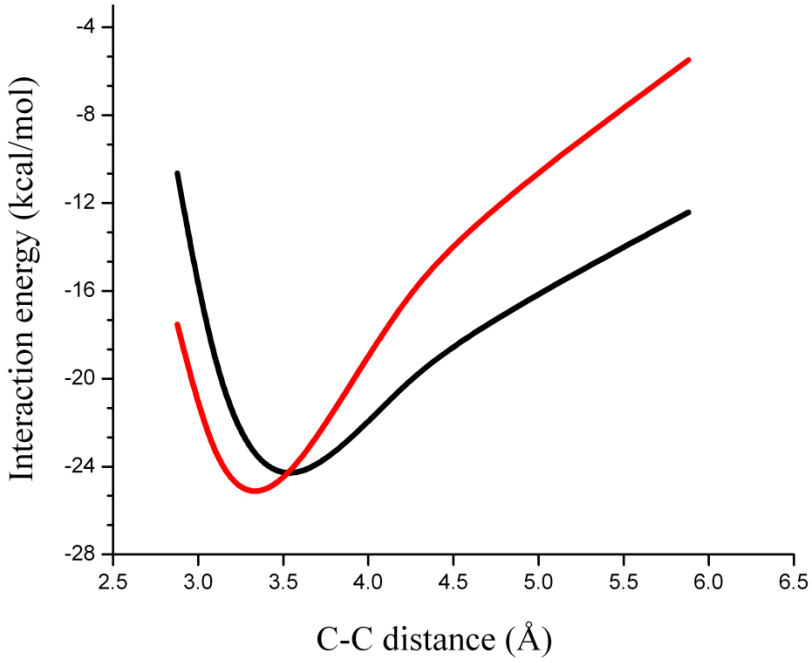


The antibonding π* orbital

S1. The molecular orbitals inolved in the electronic configurations of the excited states of formamide



S2. The scan of the interaction energies of N-methyl formamide with respect to C...C distance (C atoms of CO carbonyl group) calculated at the CASSCF level with (red line) and without (black line) BSSE included and CASPT2 level with (green line) and without (blue line) BSSE included.



S3. The scan of the interaction energies of N-methylformamide in the complex with water molecus with respect to C...C distance (C atoms of CO carbonyl group) calculated at the CASSCF (black line) and CASPT2 (red line) methods, respectively.