Supplementary Material (ESI) for PCCP

Supporting Information

Insights on the Mechanism of Proton Transfer Reactions in Amino Acids.

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Figure S2. Bond distances (in angstroms) between donor and acceptor atoms for the water–assisted proton transfer **R4**.

1. Isodensity surface

Figure 1 shows the isodensity surface at 0.004 e/A^3 for the for the neutral(left) and zwitterion(right) form for alanine and phenylalanine, calculated from optimized structures at the B3LYP/6-31G(d,p) level of theory.

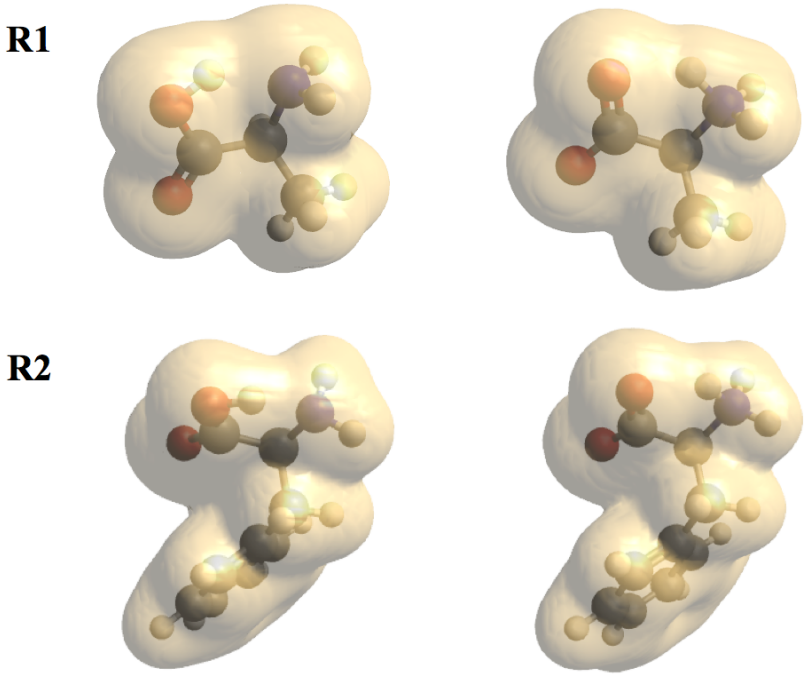

Figure 1:

2. Structural Rearrangement

Figure 2 shows the evolution along ξ of the distances between the donor and acceptor atoms.

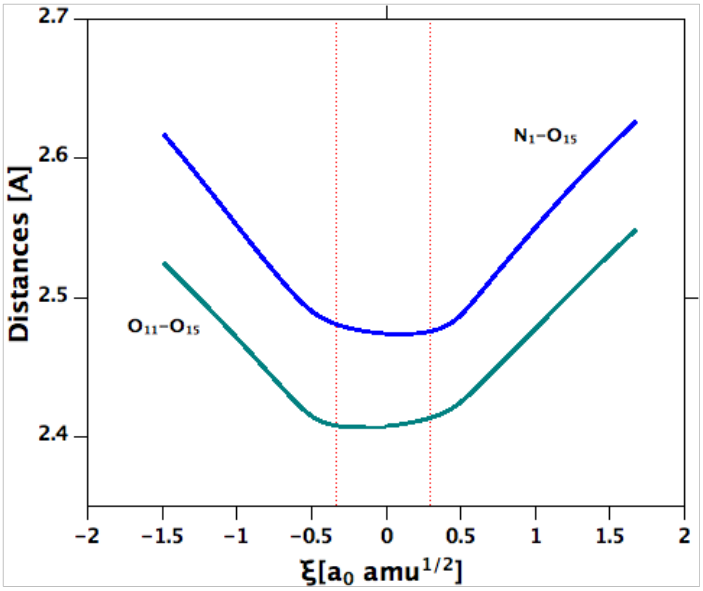

Figure 2: