Supporting Information

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

Fernanda Duarte, Esteban Vöhringer-Martinez, and Alejandro Toro-Labbé

Laboratorio de Química Teórica Computacional (QTC), Facultad de Química, Pontificia Universidad Católica de Chile, Santiago, Chile.

Table of Contents

Figure S1. Isodensity surface at 0.004 e/A³ for the neutral(left) and zwitterion(right) structure for alanine and phenylalanine, calculated from optimized structures at the B3LYP/6-31G(d,p) level of theory.

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 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](image.png)
2. Structural Rearrangement

Figure 2 shows the evolution along $\xi$ of the distances between the donor and acceptor atoms.