Article

Supplementary Materials: Reaction Mechanism of CO_2 with Choline-Amino Acid Ionic Liquids: A Computational Study

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Keywords: CO2 capture; Ionic Liquids; DFT; Reaction mechanisms

Supplementary Materials

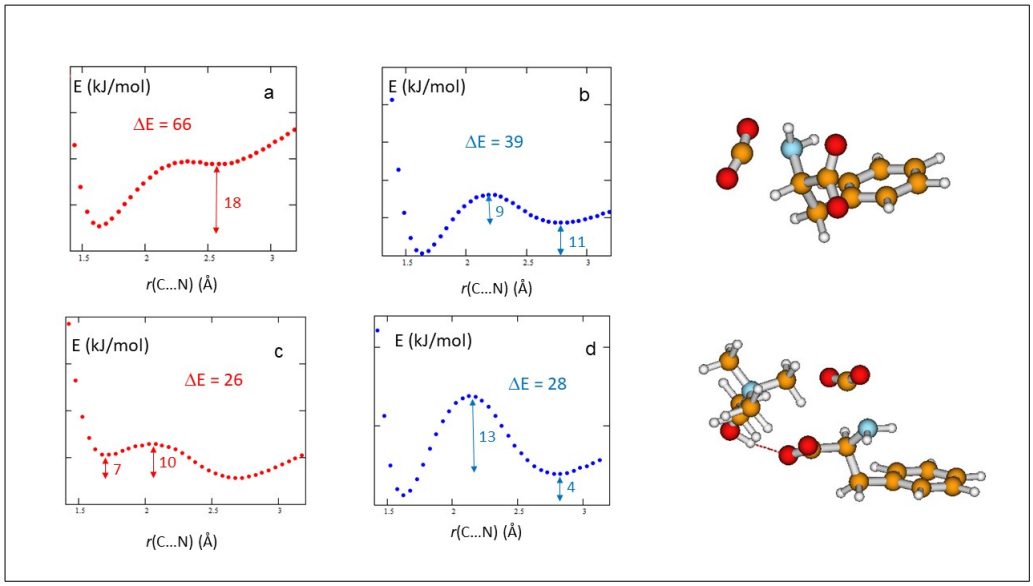

Figure S1. M062X/6-311++G** PES calculated at various C...N distances of [Phe] in vacuum (a) and PCM (b) and [Phe][Ch] in vacuum (c) and PCM (d) and M062X/6-311++G**(PCM) structure of the saddle points.
ΔE is calculated as $E_{[Phe-CO2]^-} - (E_{[Phe]^-} + E_{CO2})$
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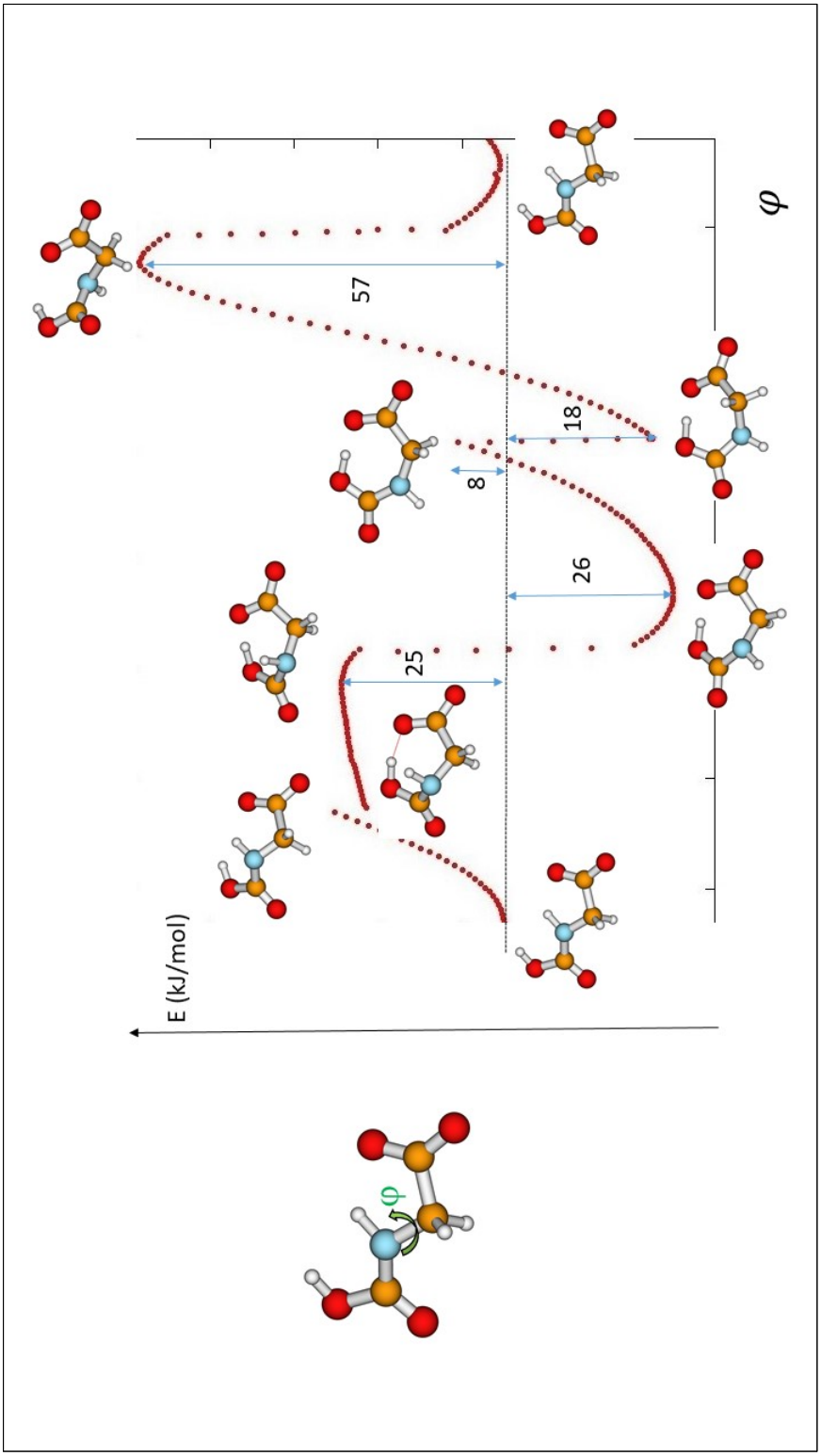

Figure S2. M062X/6-311++G** energy profile in function of the dihedral angle (ϕ) that describes the torsion about the C-N bond of the [Gly] anion calculated by PCM model. The stationary points localized in the PES scansion are reproduced in Figure.