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

Insights into the Interactions of CO_2 with Amines: a DFT Benchmark Study

Ednilsom Orestes, Célia Machado Ronconi, and José Walkimar de Mesquita Carneiro*

Instituto de Química, Universidade Federal Fluminense, Campus do Valonguinho, CEP 24020-141, Niterói, Rio de Janeiro, Brazil.

*E-mail: jose_walkimar@id.uff.br

Supporting Information

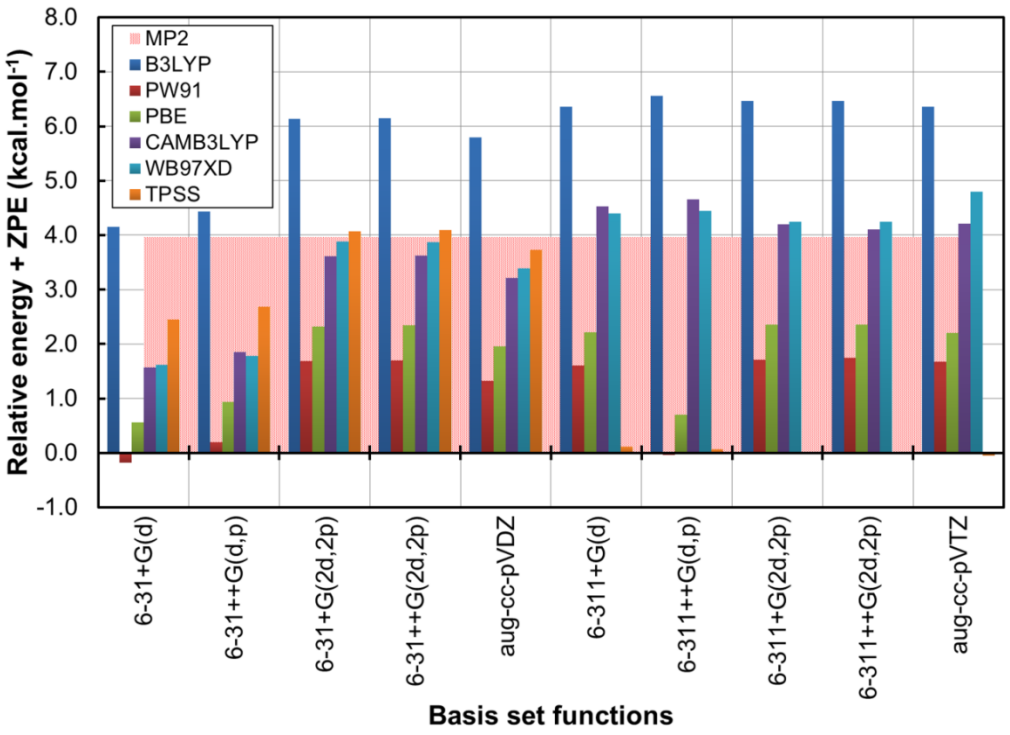


Figure S1. Zero-point corrected interaction energy between the 1,2-diaminoethane and CO_2 in kcal mol^{-1} as function of the basis set for various DFT functionals. All calculations are compared with the MP2/aug-cc-pVTZ calculation equals to 3.9 kcal mol^{-1}, represented by the bottom continuous bar.

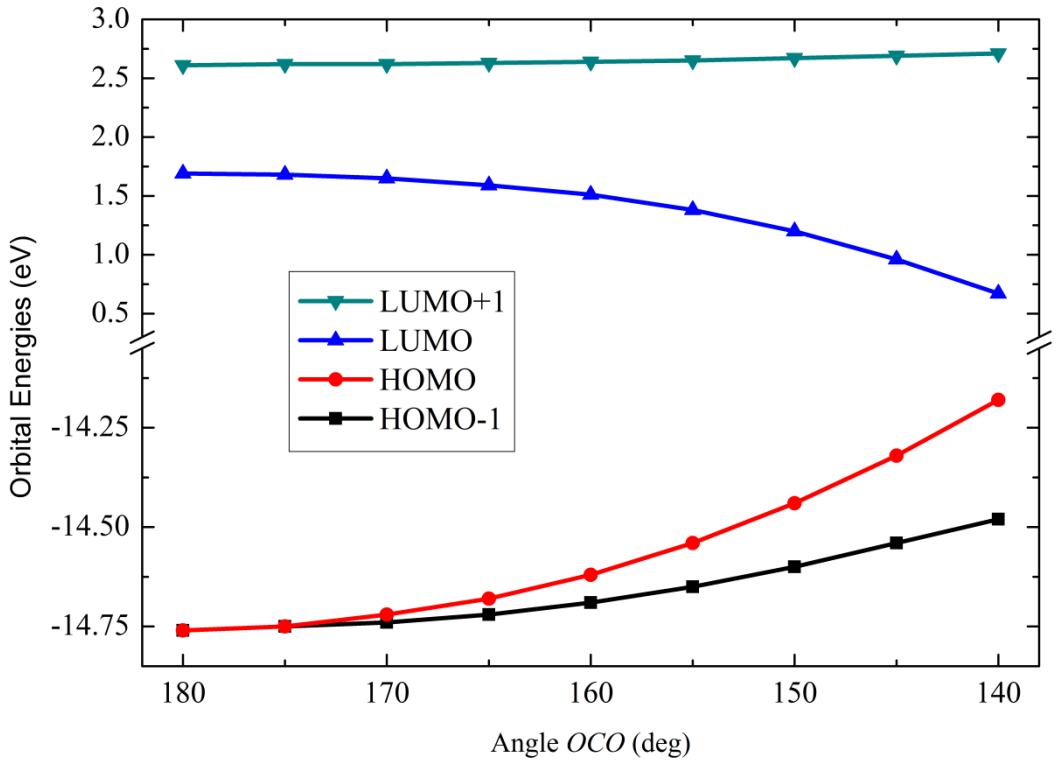
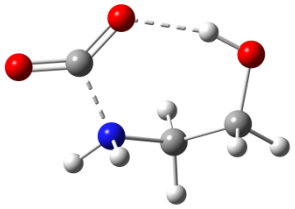
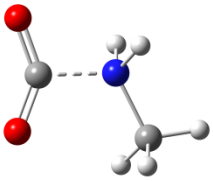
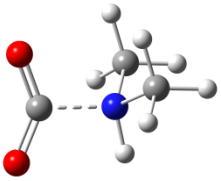
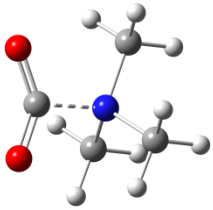
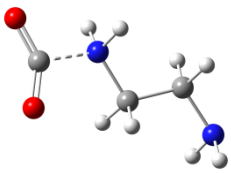
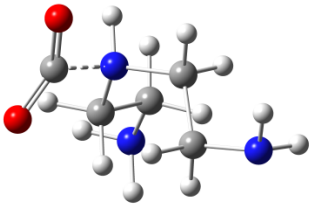
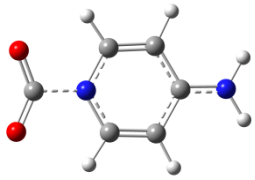
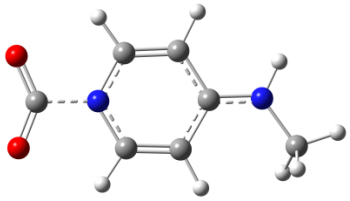
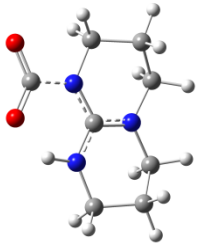
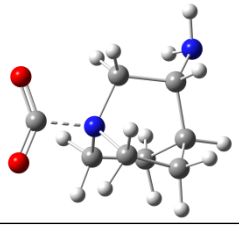


Figure S2. MP2(full)/6-311++G(2d,2p) orbital energies for CO_2 as a function of the COC angle.

Table S1. CAM-B3LYP/6-311++G(2d,2p) optimized geometries, selected geometrical parameters, and interaction energy for the zwitterion formed by a set of different amines and CO_2. Only the interaction between CO_2 and the most basic nitrogen of each amine is provided.

	OH---OCO distance	1.760 Å
	N-C distance	1.605 Å
	OCO angle	136.28º
	Int. Energy + BSSE	-2.50 kcal mol^{-1}
	N-C distance	1.625 Å
	OCO angle	138.06 º
	Int. Energy + BSSE	-0.01 kcal mol^{-1}
	N-C distance	1.606 Å
	OCO angle	137.07 º
	Int. Energy + BSSE	-2.03 kcal mol^{-1}
	N-C distance	1.655 Å
	OCO angle	136.80 º
	Int. Energy + BSSE	-0.53 kcal mol^{-1}
	N-C distance	1.636 Å
	OCO angle	135.23 º
	Int. Energy + BSSE	1.54 kcal mol^{-1}
	N-C distance	1.637 Å
	OCO angle	137.65 º
	Int. Energy + BSSE	0.64 kcal mol^{-1}

	N-C distance	1.544 Å
	OCO angle	134.19 º
	Int. Energy + BSSE	-4.67 kcal mol^{-1}
	N-C distance	1.540 Å
	OCO angle	133.95 º
	Int. Energy + BSSE	-5.54 kcal mol^{-1}
	N-C distance	1.470 Å
	OCO angle	127.94 º
	Int. Energy + BSSE	1.26 kcal mol^{-1}
	N-C distance	1.629 Å
	OCO angle	136.45 º
	Int. Energy + BSSE	-2.40 kcal mol^{-1}

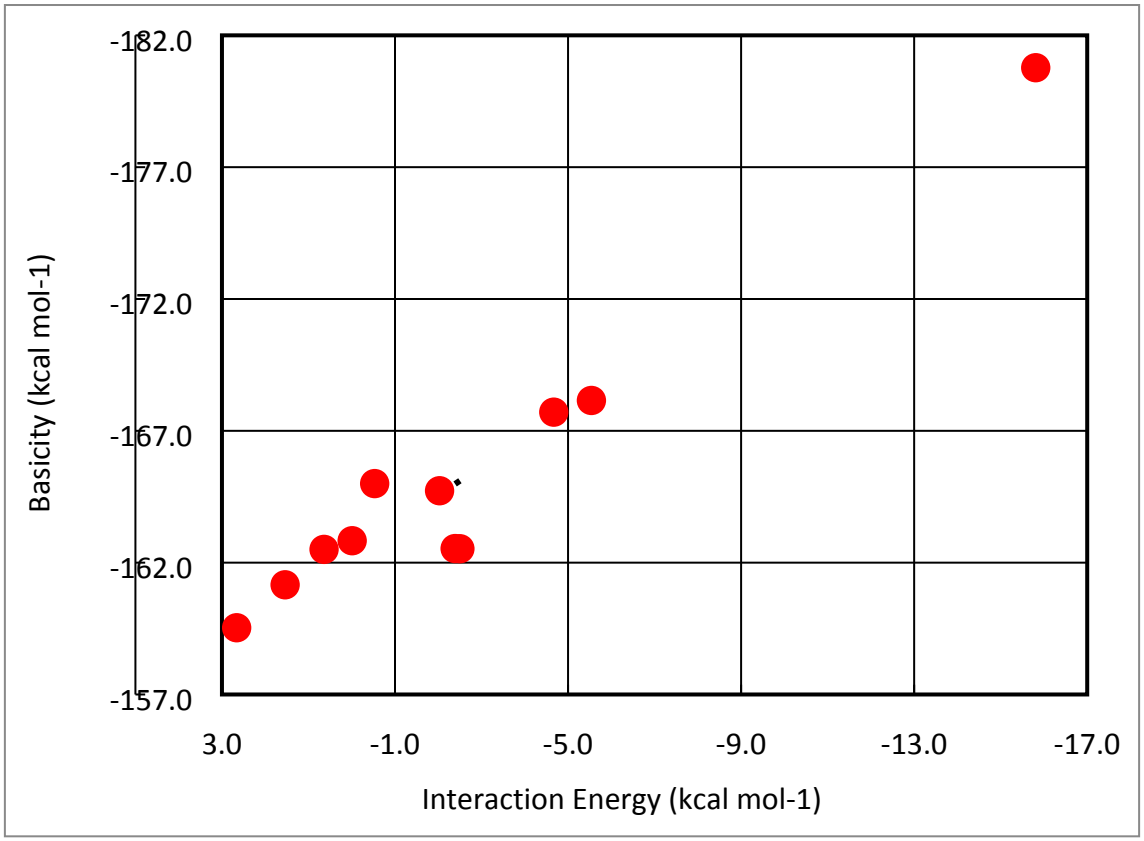


Figure S3. Correlation between the interaction energy of CO_2-amines and basicity of the amines.