Supporting Information

Cation-assisted interactions between N-heterocycles and CO_2

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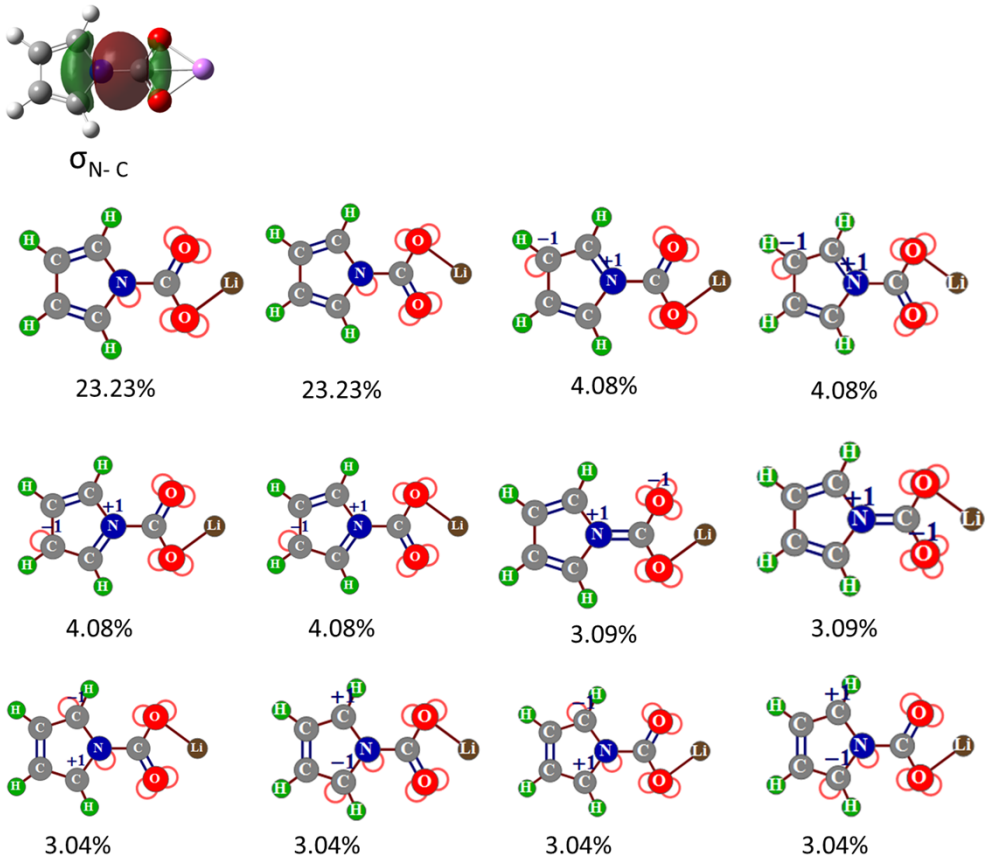
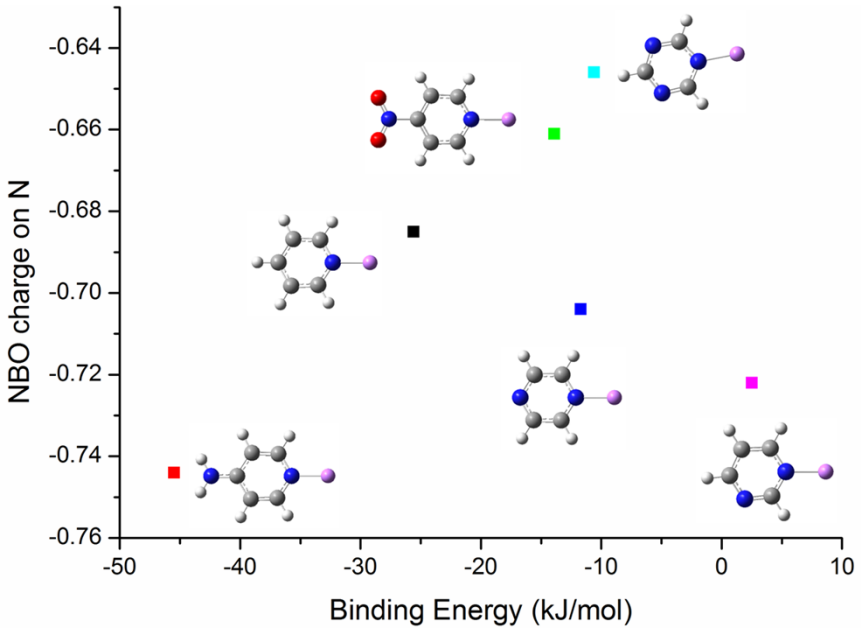
STable 1. The binding energies (kJ/mol) calculated with the B3LYP, MP2, and M06-2X methods.

Complex	B3LYP			MP2			M06-2X		
	Without Li^+	With Li^+	ΔE	Without Li^+	With Li^+	ΔE	Without Li^+	With Li^+	ΔE
1	-11.8	-25.7	-13.8	-13.3	-33.9	-20.6	-40.8	-82.2	-41.4
10	-106.8	-129.4	-22.6	-122.2	-161.4	-39.2	-160.7	-189.9	-29.2
12	-32.9	-122.1	-89.2	-11.1	-118.9	-107.8	-82.9	-177.4	-94.5

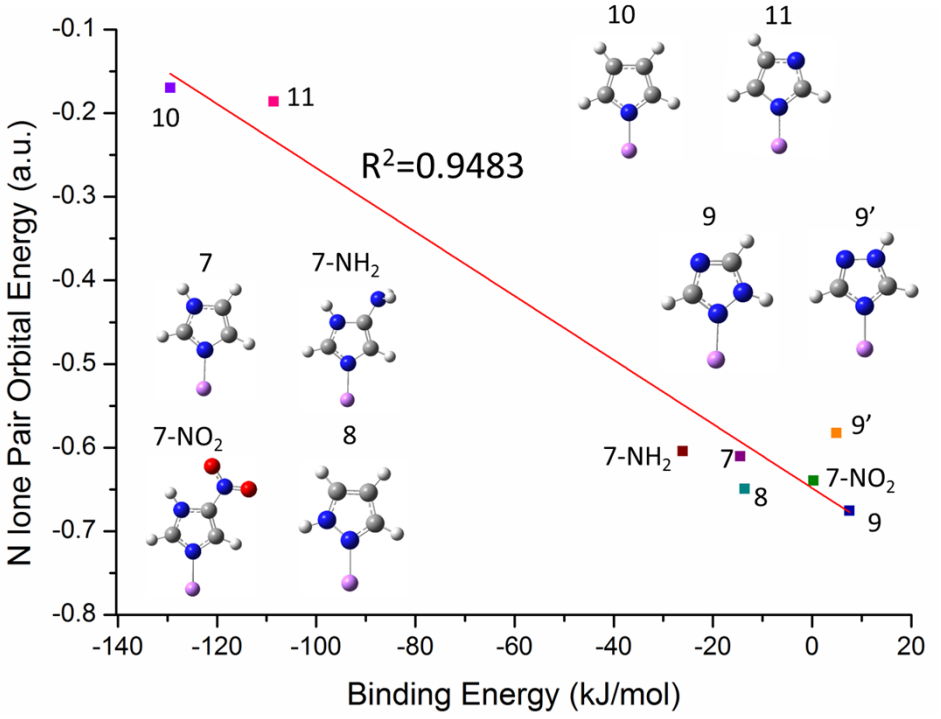
Calculations were carried out using the functionals of B3LYP,[1] MP2[2] and M06-2X [3]with the 6-31++(d,p) basis set, respectively.



SFigure 1. NBO and NRT analyses of pyrr-CO_2-Li^+complexes (**10**).



SFigure 2. Binding energy of neutral six-membered NHCs and CO_2 with Li^+ versus the NBO charge of the reacting N atom.



SFigure 3. Binding energy of five-membered NHCs and CO_2 with Li^+ versus the NBO lone pair energy of the reacting N atom.

Reference

[1] a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789.
[2] Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.
[3] Y. Zhao, D. G. Truhlar, *Acc. Chem. Res.* 2008, **41,** 157-167.