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Supplementary Information

Ab Initio, DFT and Semi-Empirical Studies on Interactions of Phosphoryl, Carbonyl, Imino and Thiocarbonyl Ligands with the Li^+ Cation: Affinity and Associated Parameters

Leonardo M. da Costa,[a] Lílian W. C. Paes[b] and José Walkimar de M. Carneiro*[,a]

[a]Instituto de Química, Universidade Federal Fluminense, Outeiro de São João Batista, s/n, 24020-141 Niterói-RJ, Brazil

[b]Departamento de Ciências Exatas, Escola de Engenharia Industrial e Metalurgia de Volta Redonda, Universidade Federal Fluminense, Av. Dos Trabalhadores,420, Vila Santa Cecília, 27255125 Volta Redonda-RJ, Brazil

Table S1. MP2/6-311+G(d,p) Merz-Kollman charges (e^-) on the Li^+ cation for the phosphoryl, carbonyl, imino and thiocarbonyl derivatives

Substituent	P=O	C=O	C=N	C=S
NH_2	0.929	0.911	0.905	0.899
OCH_3	0.931	0.912	0.906	0.901
OH	0.932	0.912	0.906	0.903
CH_3	0.934	0.913	0.908	0.905
H	0.934	0.913	0.908	0.905
Cl	0.935	0.914	0.909	0.905
CN	0.937	0.915	0.910	0.908
NO_2	0.938	0.917	0.911	0.908

Table S2. Values of electrostatic (ionic component), orbital (covalent component) interaction and the Pauli repulsion for the carbonyl compounds (kcal mol^{-1})

Carbonyl ligands	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}
$O=C(CH_3)–PhNH_2$	–49.85	–25.53	19.38
$O=C(CH_3)–PhOCH_3$	–46.68	–24.79	18.67
$O=C(CH_3)–PhCH_3$	–43.32	–23.90	18.09
$O=(CH_3)–Ph$	–41.03	–23.74	17.58
$O=C(CH_3)–PhCl$	–39.37	–23.21	17.60
$O=C(CH_3)–PhCN$	–33.49	–23.07	16.79
$O=C(CH_3)–PhNO_2$	–32.69	–22.84	16.47

Table S3. Values of electrostatic (ionic component), orbital (covalent component) interaction and the Pauli repulsion for the phosphoryl compounds (kcal mol^{-1})

Phosphoryl ligands	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}
$O=P(CH_3)_2–PhNH_2$	–59.05	–26.56	19.99
$O=P(CH_3)_2–PhOCH_3$	–57.11	–26.36	19.66
$O=P(CH_3)_2–PhCH_3$	–55.85	–26.21	19.54
$O=P(CH_3)_2–Ph$	–53.75	–26.11	19.24
$O=P(CH_3)_2–PhCl$	–52.25	–26.03	19.13
$O=P(CH_3)_2–PhCN$	–47.91	–25.77	18.68
$O=P(CH_3)_2–PhNO_2$	–45.23	–25.59	18.59

Table S4. Values of electrostatic (ionic component), orbital (covalent component) interaction and the Pauli repulsion for the imino compounds (kcal mol^{-1})

Imino ligands	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}
$HN=C(CH_3)–PhNH_2$	–45.69	–27.50	18.74
$HN=C(CH_3)–PhOCH_3$	–42.47	–26.77	17.88
$HN=C(CH_3)–PhCH_3$	–39.48	–25.99	17.31
$HN=C(CH_3)–Ph$	–37.56	–25.94	16.88
$HN=C(CH_3)–Ph$	–35.55	–25.78	16.82
$HN=C(CH_3)–PhCN$	–29.87	–25.07	16.03
$HN=C(CH_3)–PhNO_2$	–29.21	–24.53	15.74

Table S5. Values of electrostatic (ionic component), orbital (covalent component) interaction and the Pauli repulsion for the thiocarbonyl compounds (kcal mol^{-1})

Thiocarbonyl ligands	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}
$S=C(CH_3)–PhNH_2$	–38.38	–27.84	16.85
$S=C(CH_3)–PhOCH_3$	–30.99	–26.98	15.46
$S=C(CH_3)–PhCH_3$	–27.60	–26.21	14.89
$S=C(CH_3)–Ph$	–25.43	–25.17	14.37
$S=C(CH_3)–PhCl$	–23.57	–25.86	14.29
$S=C(CH_3)–PhCN$	–17.43	–25.12	13.41
$S=C(CH_3)–PhNO_2$	–16.59	–24.64	13.10

*e-mail: walk@vm.uff.br