

pK_a data of superbases from the article

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A New Class of Organosuperbases *N*-Alkyl- and *N*-Aryl-1,3-dialkyl-4,5-dimethylimidazol-2-ylidene Amines: Synthesis, Structure, pK_{BH⁺} Measurements, and Properties

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Table 1. Summary of basicity (pK_a) measurements in acetonitrile and calculations of the title compounds.

Base	Structure	Basicity		ΔNICS(1)	Change of dihedral angle on protonation
		pK _a (pK _{BH⁺}) MeCN	GB _{calc}		
1a		30.21	257.8	-4.23	24.6 → 84.5 (exp: 87.7) ^a
1b		29.90	256.2	-4.01	22.6 → 73.9
1c		27.98	254.7	-3.88	13.1 → 80.5
1d		26.29	253.1	-3.44	15.8 → 30.1
1e		27.2	253.4	-2.90	11.5 → 72.0

1f		29.97	259.2	-3.89	30.6 → 89.4
1g		29.47	257.6	-4.38	25.7 → 89.9 (exp: 88.5) ^a
1h		23.26	249.4	-2.98	28.3 (exp: 34.8) ^a → 57.5 (exp: 70.0) ^a
1i		25.54	250.2	-2.18	4.2 → 3.4 (exp: 7.9) ^a
1j		25.33	251.0	-2.31	2.8 → 10.5 (exp: 12.7) ^a
1k		24.46	248.0	-2.52	0.8 → 20.1

^a Value obtained from the crystal structure.