Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supplemental Informations for the paper:

Basicity of Organic Bases and Superbases in Acetonitrile by the Polarized Continuum Model and DFT Calculations

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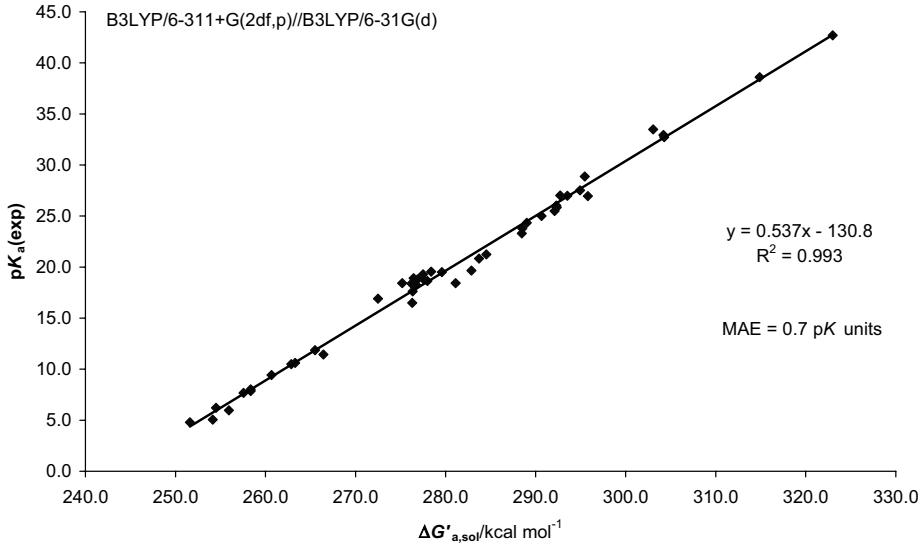
a)



b)

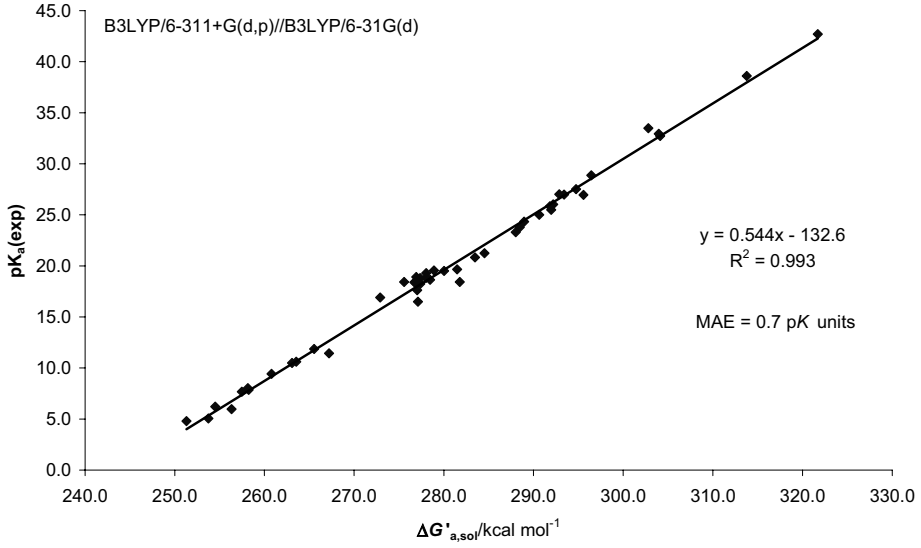


Figure S1. Correlation between pK_a(exp) and $\Delta G'_{a,sol}(B_\alpha H^+)$ for a set of nitrogen bases (excluding pyridines) estimated by B3LYP(S) and B3LYP(L) methods presented in (a) and (b), respectively.

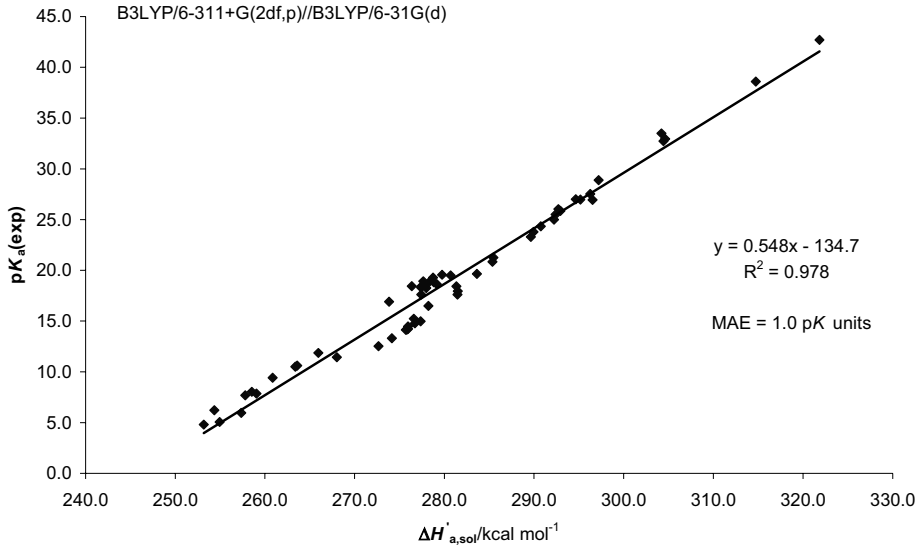


Figure S2. Correlation between pK_a(exp) and $\Delta H'_{a,sol}(B_\alpha H^+)$ for a set of nitrogen bases estimated by B3LYP(L) methods.

Table S1. The change in Gibbs free energies of solvation for the series of bases upon protonation using different w(ϕ) and w(θ) parameters for defining grid at the isodensity surface.[a]

	w(ϕ) and w(θ) parameters used for the definition of grid								$\Delta(\Delta G_{sol})$	
Base	**100 / 20**	**100 / 10**	**100 / 5**	**60 / 15**	**80 / 40**	**40 / 20**	**20 / 10**	**10 / 5**	**average**	STDEV
P4*tBu	-24.31	-24.13	-24.45	-24.22	-24.31	-24.27	-23.94	**n/c**	-24.23	0.12
P3*tBu	-25.99	-26.11	-25.71	-25.88	-25.98	-25.96	-26.05	**n/c**	-25.96	0.09
P2*tBu	-29.81	-29.96	-30.43	-29.77	-29.83	-29.83	-30.00	-30.20	-29.98	0.17
P2*Me	-29.69	-29.43	-29.50	-29.69	-29.68	-29.70	-29.23	-29.03	-29.49	0.20
P1*Ph	-32.49	-32.63	-31.03	-32.66	-32.53	-32.47	-32.54	-31.91	-32.28	0.41
P1*tBu	-34.97	-34.88	-34.81	-34.93	-34.96	-34.98	-34.82	-35.29	-34.95	0.10
P1*Et_pyr	-31.58	**n/c**	-32.15	-31.66	-31.60	-31.54	-31.58	-32.18	-31.76	0.23
P1*H_pyr	-31.49	-31.25	-30.69	-31.52	-31.51	-31.48	-31.22	-31.52	-31.34	0.21
P1*Me	-35.62	-35.71	-36.42	-35.67	-35.61	-35.61	-35.66	-36.41	-35.84	0.29
P1*H	-36.02	-35.92	-35.51	-36.00	-36.00	-36.02	-35.89	-35.30	-35.83	0.21
MTTT	-31.08	-31.00	-30.83	-31.11	-31.06	-31.09	-31.01	-30.22	-30.92	0.20
MTBD	-37.56	-37.61	-37.83	-37.57	-37.57	-37.57	-37.57	-38.41	-37.71	0.20
TBD	-39.08	-38.98	-39.19	-39.05	-39.06	-39.07	-39.06	-39.22	-39.09	0.06
DBU	-38.08	-38.08	-38.28	-38.09	-38.08	-38.08	-38.08	-38.31	-38.14	0.08
DBN	-40.12	-40.12	-40.22	-40.13	-40.12	-40.13	-40.15	-39.97	-40.12	0.04
TMG	-41.03	-41.02	-41.36	-41.05	-41.03	-41.04	-40.93	-41.34	-41.10	0.13
TMG*Me	-39.82	-39.81	-39.90	-39.81	-39.81	-39.82	-39.78	-40.12	-39.86	0.08
TMG*Ph	-36.65	-36.78	-36.45	-36.64	-36.63	-36.69	-36.72	-36.34	-36.61	0.11
BGV	-37.99	-38.00	-37.12	-38.04	-38.06	-37.88	-38.26	-38.06	-37.93	0.21
QQ	-46.11	-46.08	-46.08	-46.12	-46.11	-46.11	-46.04	-46.34	-46.12	0.05
TMP	-42.91	-43.06	-43.24	-42.93	-42.89	-42.91	-43.00	-43.62	-43.07	0.18
DMAn	-44.59	-44.57	-44.45	-44.60	-44.59	-44.57	-44.60	-45.11	-44.64	0.12
pyrr*H	-52.53	-52.55	-52.47	-52.53	-52.53	-52.53	-52.56	-52.89	-52.57	0.08
pyrr*Me	-48.30	-48.29	-47.92	-48.32	-48.31	-48.31	-48.29	-47.75	-48.19	0.18
Me_3N	-52.21	-52.21	-52.24	-52.21	-52.21	-52.21	-52.21	-52.21	-52.22	0.01
Et_3N	-45.06	-45.04	-45.17	-45.08	-45.06	-45.06	-45.03	-45.12	-45.08	0.03
NH_3	-75.14	-75.14	-72.23	-68.08	-75.14	-64.30	-72.25	-72.23	-71.82	2.81
$EtNH_2$	-59.73	-59.73	-59.85	-59.74	-59.73	-59.74	-59.71	-59.98	-59.78	0.07
1An	-54.12	-54.27	-54.53	-54.11	-54.13	-54.11	-54.11	-55.76	-54.39	0.38
2An	-51.97	-52.16	-51.90	-52.02	-51.97	-52.00	-52.38	-52.37	-52.10	0.15
3An	-52.32	-52.49	-52.62	-52.34	-52.33	-52.29	-52.81	-52.98	-52.52	0.21
4An	-50.92	-50.87	-50.31	-50.93	-50.92	-50.94	-50.95	-50.08	-50.74	0.27
5An	-55.04	-55.65	-51.98	-54.85	-54.88	-54.90	-56.14	-53.54	-54.62	0.93
6An	-51.06	-51.05	-51.35	-51.24	-51.08	-51.23	-50.13	-48.46	-50.70	0.70
7An	-57.94	-58.69	-55.13	-57.56	-57.86	-57.97	-59.08	-57.84	-57.76	0.71
8An	-51.39	-51.61	-51.05	-51.42	-51.40	-51.42	-51.40	-50.76	-51.31	0.20
9An	-60.02	-59.89	-61.13	-60.41	-60.11	-59.88	-60.06	-60.92	-60.30	0.39
10An	-59.59	-59.95	-59.10	-59.49	-59.55	-59.62	-60.00	-56.75	-59.26	0.66
1P	-49.10	-49.10	-49.12	-49.10	-49.10	-49.10	-49.08	-48.36	-49.01	0.16
2P	-46.20	-46.20	-46.14	-46.19	-46.20	-46.20	-46.21	-46.31	-46.21	0.03
3P	-43.75	-43.78	-43.64	-43.77	-43.75	-43.74	-43.64	-43.72	-43.72	0.04
4P	-41.44	-41.51	-41.28	-41.43	-41.43	-41.45	-41.53	-40.47	-41.32	0.22

5P	-44.20	-44.16	-44.35	-44.18	-44.20	-44.18	-44.13	-44.67	-44.26	0.13
6P	-47.30	-47.31	-47.64	-47.30	-47.30	-47.31	-47.30	-47.22	-47.33	0.08
7P	-45.35	-45.35	-45.87	-45.35	-45.35	-45.35	-45.39	-45.55	-45.44	0.13
9P	-39.59	-39.59	-39.97	-39.58	-39.60	-39.59	-39.52	-39.81	-39.66	0.12
8P	-44.37	-44.37	-44.94	-44.37	-44.37	-44.36	-44.46	-44.74	-44.50	0.17
10P	-45.74	-45.75	-46.57	-45.72	-45.74	-45.73	-45.96	-46.06	-45.91	0.21
11P	-45.31	-45.33	-45.53	-45.32	-45.32	-45.30	-45.34	-45.51	-45.37	0.07

[a] all values are in in kcal mol^{-1}.