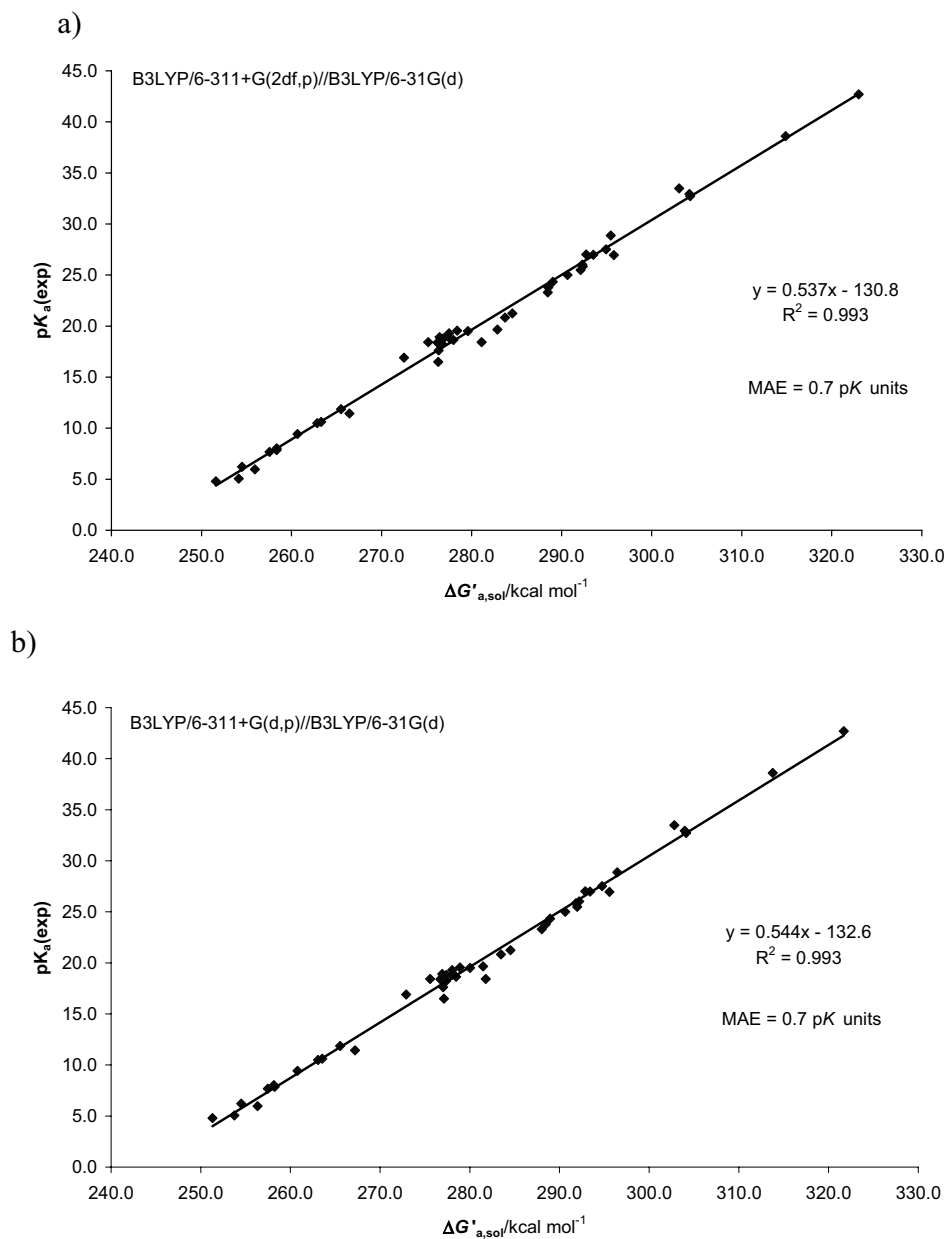


Electronic Supplemental Informations for the paper:

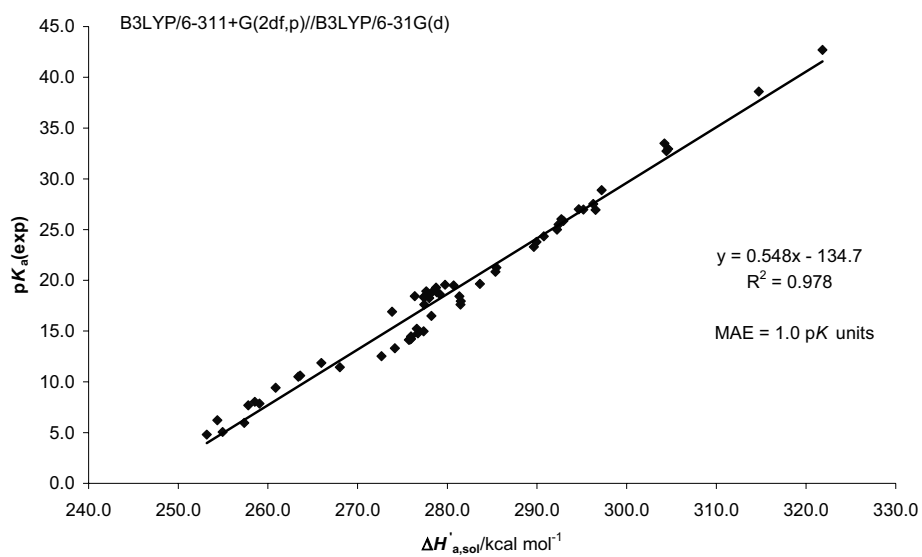
## **Basicity of Organic Bases and Superbases in Acetonitrile by the Polarized Continuum Model and DFT Calculations**

Zoran Glasovac, Mirjana Eckert-Maksić and Zvonimir B. Maksić

- 1. Figure S1.** Correlation between  $pK_a(\text{exp})$  and  $\Delta G'_{\text{a,sol}}(\text{B}_\alpha\text{H}^+)$  for a set of nitrogen bases (excluding pyridines) estimated by B3LYP(S) and B3LYP(L) methods. ....Page 2
- 2. Figure S2.** Correlation between  $pK_a(\text{exp})$  and  $\Delta H'_{\text{a,sol}}(\text{B}_\alpha\text{H}^+)$  for a set of nitrogen bases estimated by B3LYP(L) methods. ....Page 3
- 3. Table S1.** The change in Gibbs free energies of solvation for the series of bases upon protonation using different  $w(\phi)$  and  $w(\theta)$  parameters for defining grid at the isodensity surface. ....Page 4.



**Figure S1.** Correlation between  $pK_a(\text{exp})$  and  $\Delta G'_{a,\text{sol}}(\text{B}_\alpha\text{H}^+)$  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  $\text{p}K_{a}(\text{exp})$  and  $\Delta H_{a,sol}^{\circ}(\text{B}_{\alpha}\text{H}^{+})$  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  $w(\phi)$  and  $w(\theta)$  parameters for defining grid at the isodensity surface.<sup>[a]</sup>

Base	$w(\phi)$ and $w(\theta)$ parameters used for the definition of grid								$\Delta(\Delta G_{sol})$	
	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
DMA <sub>n</sub>	-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 <sub>3</sub> N	-52.21	-52.21	-52.24	-52.21	-52.21	-52.21	-52.21	-52.21	-52.22	0.01
Et <sub>3</sub> N	-45.06	-45.04	-45.17	-45.08	-45.06	-45.06	-45.03	-45.12	-45.08	0.03
NH <sub>3</sub>	-75.14	-75.14	-72.23	-68.08	-75.14	-64.30	-72.25	-72.23	-71.82	2.81
EtNH <sub>2</sub>	-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

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

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[a] all values are in in kcal mol<sup>-1</sup>.