

DFT Studies toward the Design and Discovery of a Versatile Cage-Functionalized Proton Sponge

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In the original article,^[1] Table 1 on page 421 is erroneous; the correct Table 1 is given below.

Table 1. B3LYP/6-311+G**//B3LYP/6-31G* calculated proton affinities in gas phase, water, and acetonitrile at 298 K in kJ/mol.

	Gas phase	Proton affinity (PA) ^[a]	
		Aqueous phase	Acetonitrile
1	1110.1	1297.3	1290.1
2	1091.2	1233.1	1235.2
3	1182.8	1300.7	1317.8
4	1112.9	1294.0	1291.3
5	1128.6	1289.8	1281.4
6	1156.7	1297.2	1307.7
7	1025.0 ^[b]	1205.3	1197.6
8	1099.6	1249.2	1252.5
9	1146.9	1249.2	1252.5
10	1192.0	1223.4	1267.7

[a] Zero-point energy corrected. [b] Experimental value: 1030.1 kJ/mol.^[7]

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