

**TABLE 4:** Thermodynamical Values Considering Solvation by the ICPM Model.<sup>a,b</sup>

	<b>Methods</b>	<b><math>\Delta E</math></b>	<b><math>\Delta E_0</math></b>	<b><math>\Delta E_{298}</math></b>	<b><math>\Delta H_{298}</math></b>	<b><math>\Delta G_{298}</math></b>
<b>Trans-Preference Energy</b>	B3LYP	4.98	4.80	4.61	4.61	4.86
	MPW1PW91	4.48	4.25	4.08	4.08	4.27
	MP2(full)	3.56	3.77	3.56	3.56	3.83
	QCISD(full)	4.35	4.39	4.18	4.18	4.40
<b>Heterolysis of Neutral Nitrous Acid</b>	B3LYP	287.35	271.64	275.53	278.01	241.66
	MPW1PW91	301.44	284.84	288.87	291.35	254.75
	MP2(full)	226.67	209.83	213.72	216.19	179.70
	QCISD(full)	244.11	226.98	231.00	233.48	196.95
<b>Heterolysis of Protonated Nitrous Acid</b>	B3LYP	25.59	17.52	18.33	20.81	-8.34
	MPW1PW91	23.22	15.30	18.36	20.84	-16.93
	MP2(full)	6.80	-0.35	-0.41	2.06	-28.76
	QCISD(full)	5.00	-2.08	-2.34	0.14	-28.01
<b>Proton Affinity of Nitrous Acid</b>	B3LYP			-30.67	-28.19	-49.59
	MPW1PW91			-30.44	-27.96	-56.62
	MP2(full)			15.41	17.89	-3.34
	QCISD(full)			11.45	13.93	-6.30

<sup>a</sup> All calculations employed the 6-311++G(2df,2p) basis set. <sup>b</sup> Preference energies, dissociation energies and proton affinities in kJ/mol.