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Structure and binding of Mg(II) ions and di-metal bridge complexes with biological phosphates and phosphoranes

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Both the online and the print versions of this article show an error in Table 2 and a missing line in Table 3. The correct tables appear below.

Table 2 Geometries of phosphorane complexes with hydrated Mg2+ binding (Å)

Molecule	equatorial				axial			
	bridging	non-bridging			endo-cyclic		exo-cyclic	
$P-O(H)/P^{-}_{..}O$	P-O(C)	$P-O(H)/P^{-}_{..}O$	HB	P-O:Mg	P-O	HB	P-O	HB
$[EPA]^{2-}_{aq}$	1.716	1.547	-	-	1.946	-	1.803	-
$[Mg(H_2O)_5(EPA)]$	1.665	1.572	+	1.574	1.744	-	1.874	+
$[Mg(H_2O)_4(b\text{-}EPA)]$	1.651	-	-	1.567	1.901	+	1.768	+
$[Mg(H_2O)_3(OH)(b\text{-}EPA)]^{1-}$	1.673	-	-	1.550	1.981	+	1.778	+
$[EPAH_2]$	1.653	1.630	-	-	1.727	-	1.674	-
$[EPAH]^{-}(\uparrow)$	1.706	1.661	-	-	1.893	-	1.715	-
$[EPAH]^{-}(\downarrow)$	1.714	1.665	-	-	1.779	-	1.790	-
$\left[Mg(H_2O)_5(EPAH)\right]^{1+}_{exo}$	1.641	1.693	+	1.547	1.743	-	1.740	+
$\left[Mg(H_2O)_5(EPAH)\right]^{1+}_{endo}$	1.626	1.679	+	1.540	1.938	+	1.649	-
$[Mg(H_2O)_4(OH)(EPAH)]$	1.663	1.642	-	1.542	1.827	+	1.705	-

Bridging/non-bridging distinguishes between oxygens which are bridged between a P and C atom versus an O which is bonded only to P (or in the case of neutral phosphates bound to H as well). $[EPA]^{2-}_{aq}$ optimization was preformed using the PCM solvation model (see text). (↑) or (↓) indicate the orientation of the proton on the non-bridging O relative to the ethylene ring. Columns headed by HB indicate the presence (+) or absence (-) of a hydrogen bond between a Mg^{2+}-water and the phosphorane oxygen. Deviations are shown in parentheses. Subscripts exo/endo distinguish which axial oxygen atom is hydrogen bonded

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Table 3 Ligand substitution energies (kcal/mol)

	Gas phase properties				ΔG_{aq}	
L	ΔE	ΔH	$-T\Delta S$	ΔG	PCM	COSMO
mono-dentate reactions						
CH_3COOH	–12.93	–13.49	1.33	–12.16	6.18	5.59
H_3PO_4	–22.56	–23.28	1.41	–21.86	1.93	1.67
DMPH	–28.77	–29.33	1.34	–27.99	5.47	4.60
EPH	–29.19	–29.63	1.37	–28.26	1.08	1.43
OH^-	–229.69	–230.03	–0.36	–230.39	–4.45	6.23
CH_3O^-	–218.66	–217.17	0.52	–216.65	–7.47	–0.18
CH_3COO^-	–203.76	–204.78	2.22	–202.56	–5.81	–0.88
$EPAH^-$	–205.14	–204.47	4.09	–200.38	–6.96	–2.84
DMP^-	–200.01	–200.07	3.14	–196.93	–6.40	–3.43
EP^-	–197.98	–198.15	3.86	–194.29	–5.61	–2.37
$H_2PO_4^-$	–196.06	–196.58	2.52	–194.06	–6.21	–3.48
HPO_4^{2-}	–396.14	–398.62	6.08	–392.53	–6.97	1.04
EPA^{2-}	–395.72	–394.63	5.78	–388.86	–6.12	4.79
bi-dentate reactions						
b-DMP^-	18.42	16.98	–11.23	5.75	–0.13	–0.94
b-EP^-	14.51	13.22	–11.46	1.77	–5.54	–5.95
b-EPA^{2-}	8.31	7.25	–11.07	–3.82	–8.71	–9.13

Mono-dentate reactions are of the form $[Mg(H_2O)_6]^{2+} + L^{-q} \rightarrow [Mg(H_2O)_5(L)]^{2-q} + H_2O$ and bi-dentate reactions are of the form $[Mg(H_2O)_5(L)]^{-q} \rightarrow [Mg(H_2O)_4(b\text{-}L)]^{-q} + H_2O$ where b-L indicates a ligand bound bi-dentate to Mg^{2+}. Due to the instability of $[EPA]^{2-}$ in the gas phase, the structure was first optimized using the PCM solvation model (see text). Single point energies were then calculated for the optimized structure in the gas phase. Columns headed with PCM and COSMO indicate ΔG_{aq} single point calculations performed with the PCM and COSMO solvation models