

Correction to “Interaction of Metal Ions with Biomolecular Ligands: How Accurate Are Calculated Free Energies Associated with Metal Ion Complexation?”

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Scrutinizing the values published in Table 4, we realized a mistake in our script that was converting stability constants obtained

Table 4. Free Energies Associated with the Complexation of Metal Ions (Mn^{2+} , Fe^{2+} , Cu^{2+} , Zn^{2+} , Cd^{2+}) in Solution, Calculated as $\Delta G = \Delta E_{\text{int}} + \Delta G_{\text{solv}} + \Delta E_{\text{ZPE}} - \Delta(RT \ln(q_{\text{trans}}q_{\text{rot}}q_{\text{vib}}))$, Using Various Methods and $[\text{M}(\text{H}_2\text{O})_6]^{2+}$ as Reference^a

complex	exp ^b	MP2/aTZ ^c	M06/TZ ^d	B3LYP/TZ ^e	B3LYP-D/TZ ^e	MPWB1K/TZ	M052X/cTZ(SMD)
$[\text{ZnX}_6]^{2+ f}$	−6.7	−4.8	−3.2	−2.1	−4.2	−1.3	−11.8
$[\text{CdX}_6]^{2+}$	−6.7	−6.2	−5.4	−5.6	−7.1	−4.8	−14.7
$[\text{CuX}_6]^{2+}$	−10.6	−22.6	−24.9	−20.4	−22.4 (−10.0)	−22.7	−23.1 (−18.2)
$[\text{FeX}_6]^{2+}$	−3.4	−0.3	0.4	1.4	−0.9	1.4	−5.7
$[\text{MnX}_6]^{2+}$	−2.0	−0.7	0.5	1.0	−1.1	0.8	−8.2
$[\text{ZnY}_6]^{2+ g}$	−3.6	−5.7	−1.6	−0.3	−4.1	−0.6	−3.0
$[\text{CdY}_6]^{2+}$	−3.7	−8.9	−4.8	−4.2	−7.1	−4.3	−5.0
$[\text{CuY}_6]^{2+}$	−5.7	−25.1	−24.5	−16.3	−20.6 (−3.2)	−23.3	−11.8 (−11.5)
$[\text{FeY}_6]^{2+}$			1.4	1.0	−2.7	0.5	−0.8
$[\text{MnY}_6]^{2+}$	−1.8	−5.5	−2.0	−0.5	−4.0	−1.2	−1.7
$[\text{ZnZ}_6]^+ h$	−2.2	12.0	13.2	14.6	12.0	12.7	−11.3
$[\text{CdZ}_6]^+$	−2.6	13.0	13.8	14.8	11.7	13.6	−10.1
$[\text{CuZ}_6]^+$	−3.0	1.4	−1.2	2.8	1.2 (7.2)	0.1	−19.1 (−19.5)
$[\text{FeZ}_6]^+$	−1.9	13.3	14.2	15.1	12.6	12.9	−10.2
$[\text{MnZ}_6]^+$	−1.9	13.3	14.7	15.0	11.4	13.1	−11.1

^aThe equilibrium geometries were obtained using the RI-DFT(PBE)/def-SV(P) method along with empirical dispersion correction. No constraints were imposed during the optimizations, and stability checks were performed. COSMO-RS was used for the calculation of the solvation energies. The values in parentheses are for tetracoordinated systems; see the text for details. All of the values are in kcal mol^{−1}. ^bExperimental values for ionic strength equal to 2 M ($[\text{MX}_6]$ systems), 0.5 M ($[\text{MY}_6]$ systems), and 0 M ($[\text{MZ}_6]$ systems). ^cRI-MP2 method, aug-cc-pVTZ basis set. ^dM06 functional, def2-TZVP basis set. ^eB3LYP functional, def2-TZVP basis set. ^f $[\text{MX}_6]^{2+}$ stands for the $[\text{M}^{\text{II}}(\text{NH}_3)_2(\text{H}_2\text{O})_4]^{2+}$ complex. ^g $[\text{MY}_6]^{2+}$ stands for the $[\text{M}^{\text{II}}(\text{Im})(\text{H}_2\text{O})_5]^{2+}$ complex. ^h $[\text{MZ}_6]^+$ stands for the $[\text{M}^{\text{II}}(\text{CH}_3\text{COO})(\text{H}_2\text{O})_5]^+$ complex.

from the literature into free energy changes associated with corresponding complexation reactions. We remedy our mistake and the correct values (column 2) listed in the new Table 4 presented below. In most cases, the values are ~ 1 kcal mol^{−1} more negative, with few exceptions that amount to 2–6 kcal mol^{−1} (more negative). The correct values are generally in slightly better agreement with the calculated values. The corrections leave our observations and conclusions mostly unchanged.

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