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Correction: Density functional theory study of crown ether–magnesium complexes: from a solvated ion to an ion trap

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Correction for 'Density functional theory study of crown ether–magnesium complexes: from a solvated ion to an ion trap' by Katarina Čeranić *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 32656–32665, <https://doi.org/10.1039/D3CP03991A>.

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Some of the data presented in Table 1 of the original article was incorrect, the Mg–O distance in the reference structure was 2.113 Å, the correct value is 2.067 Å. The correct data relating to this difference of 0.046 Å is shown in Table 1.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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Table 1 Binding energies E_{bind} and binding energies per oxygen atom $E_{\text{bind}}/n_{\text{O}}$ in Mg-crown complexes $[\text{CMg}]^{2+}$ and their hydrated counterparts $[\text{CMg}(\text{H}_2\text{O})_2]^{2+}$ are presented in kcal mol^{-1} . $E_{\text{bind}}/(n_{\text{O}} + n_{\text{S}})$ are binding energies per oxygen atom if solvent's oxygen atoms are also included. Geometric parameters in $[\text{CMg}(\text{H}_2\text{O})_2]^{2+}$: relative average Mg–O and Mg–S distances with respect to $r(\text{Mg–O})$ in $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$, $\bar{r}_{\text{r}}(\text{Mg–O})$ and $\bar{r}_{\text{r}}(\text{Mg–S})$, with O and S being the crown's and the solvent's oxygen atoms, respectively; relative average magnesium-oxygen distances that take into account both crown's and solvent's oxygen atoms, $\bar{r}_{\text{r}}(\text{Mg–O/S})$; difference in the two Mg–S bond lengths, $\Delta r(\text{Mg–S})$; Mg distances from the plane defined by crown's oxygen atoms/crown's and solvent's oxygen atoms, $r_{\text{plane}}^{\text{O}}/r_{\text{plane}}^{\text{O/S}}$. All distances are presented in Å

C	$[\text{CMg}]^{2+}$	$[\text{CMg}(\text{H}_2\text{O})_2]^{2+}$	$\bar{r}_{\text{r}}(\text{Mg–O})$	$\bar{r}_{\text{r}}(\text{Mg–S})$	$\Delta r(\text{Mg–S})$	$\bar{r}_{\text{r}}(\text{Mg–O/S})$	$r_{\text{plane}}^{\text{O}}/r_{\text{plane}}^{\text{O/S}}$
	$E_{\text{bind}} \left(\frac{E_{\text{bind}}}{n_{\text{O}}} \right)$	$E_{\text{bind}} \left(\frac{E_{\text{bind}}}{n_{\text{O}}} / \frac{E_{\text{bind}}}{n_{\text{O}} + n_{\text{S}}} \right)$					
1	–276.1 (–69.0)	–334.7 (–83.7/–55.8)	–0.028	1.243	2.633	0.396	0.865/0.021
2	–292.9 (–73.2)	–353.0 (–88.2/–58.8)	–0.086	0.074	0.159	–0.033	0.158/0.130
3	–306.3 (–76.6)	–362.4 (–90.6/–60.4)	–0.060	0.045	0.000	–0.025	0.000/0.000
4	–288.9 (–72.2)	–351.8 (–87.9/–58.6)	–0.056	0.040	0.107	–0.024	0.158/0.000
5	–285.6 (–71.4)	–348.7 (–87.2/–58.1)	–0.056	0.046	0.133	–0.022	0.192/0.018
6	–307.2 (–76.8)	–365.3 (–91.3/–60.9)	–0.060	0.041	0.009	–0.026	0.003/0.008
7	–310.9 (–77.7)	–370.8 (–92.7/–61.8)	–0.021	0.037	0.008	–0.002	0.012/0.021
8	–308.2 (–77.0)	–373.2 (–93.3/–62.2)	0.016	0.033	0.027	0.022	0.032/0.006
9	–289.1 (–57.8)	–345.2 (–69.0/–49.3)	0.098	0.456	1.032	0.200	0.596/0.010
10	–293.9 (–58.8)	–352.8 (–70.6/–50.4)	–0.009	0.061	0.001	0.011	0.002/0.058
11	–314.3 (–62.9)	–371.9 (–74.4/–53.1)	0.046	0.021	0.011	0.039	0.002/0.008
12	–266.7 (–53.3)	–335.1 (–67.0/–47.9)	0.287	0.037	0.071	0.215	0.102/0.083
13	–305.4 (–61.1)	–365.7 (–73.1/–52.2)	0.032	0.021	0.006	0.029	0.003/0.004
14	–308.8 (–61.8)	–367.9 (–73.6/–52.6)	0.034	0.023	0.000	0.031	0.001/0.002
15	–326.9 (–65.4)	–383.6 (–76.7/–54.8)	0.106	–0.005	0.000	0.074	0.000/0.000
16	–317.6 (–63.5)	–376.0 (–75.2/–53.7)	0.107	–0.009	0.002	0.073	0.004/0.003
17	–316.0 (–63.2)	–375.9 (–75.2/–53.7)	0.108	–0.009	0.003	0.074	0.008/0.007
18	–313.1 (–62.6)	–372.4 (–74.5/–53.2)	0.096	–0.013	0.000	0.065	0.000/0.000
19	–308.2 (–61.6)	–370.0 (–74.0/–52.9)	0.098	–0.010	0.000	0.068	0.000/0.000
20	–314.5 (–62.9)	–371.6 (–74.3/–53.1)	0.100	–0.012	0.011	0.068	0.021/0.018
21	–310.4 (–62.1)	–369.8 (–74.0/–52.8)	0.097	–0.003	0.033	0.069	0.068/0.055
22	–307.4 (–61.5)	–369.9 (–74.0/–52.8)	0.096	–0.003	0.014	0.068	0.033/0.030
23	–297.4 (–59.5)	–362.4 (–72.5/–51.8)	0.098	–0.013	0.019	0.066	0.038/0.028
24	–297.4 (–59.5)	–363.6 (–72.7/–51.9)	0.088	–0.011	0.000	0.059	0.000/0.000
25	–288.4 (–57.7)	–355.8 (–71.2/–50.8)	0.085	–0.014	0.018	0.057	0.035/0.027
26	–279.2 (–55.8)	–347.6 (–69.5/–49.7)	0.081	–0.015	0.037	0.053	0.071/0.056
27	–325.5 (–54.2)	–375.2 (–62.5/–46.9)	0.307	0.012	0.048	0.233	0.340/0.000
28	–331.2 (–55.2)	–383.5 (–63.9/–47.9)	0.403	0.011	0.001	0.305	0.020/0.009
29	–350.6 (–58.4)	–387.0 (–64.5/–48.4)	0.211	0.646	1.352	0.320	0.252/0.098

