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CORRECTION

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

Katarina Ćeranić,[ab] Branislav Milovanović[b] and Milena Petković*[b]

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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 Ćeranić *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 32656–32665, https://doi.org/10.1039/D3CP03991A.

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.

[a] *Innovative Centre of the Faculty of Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia*
[b] *University of Belgrade – Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia. E-mail: milena@ffh.bg.ac.rs*

Table 1 Binding energies E_{bind} and binding energies per oxygen atom E_{bind}/n_O in Mg-crown complexes $[CMg]^{2+}$ and their hydrated counterparts $[CMg(H_2O)_2]^{2+}$ are presented in kcal mol^{-1}. $E_{bind}/(n_O + n_S)$ are binding energies per oxygen atom if solvent's oxygen atoms are also included. Geometric parameters in $[CMg(H_2O)_2]^{2+}$: relative average Mg–O and Mg–S distances with respect to r(Mg–O) in $[Mg(H_2O)_6]^{2+}$, $\bar{r}_r$(Mg–O) and $\bar{r}_r$(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, $\bar{r}_r$(Mg–O/S); difference in the two Mg–S bond lengths, Δr(Mg–S); Mg distances from the plane defined by crown's oxygen atoms/crown's and solvent's oxygen atoms, $r^{O}_{plane}/r^{O/S}_{plane}$. All distances are presented in Å

	$[CMg]^{2+}$	$[CMg(H_2O)_2]^{2+}$					
C	$E_{bind}\left(\frac{E_{bind}}{n_O}\right)$	$E_{bind}\left(\frac{E_{bind}}{n_O}\Big/\frac{E_{bind}}{n_O+n_S}\right)$	$\bar{r}_r$(Mg–O)	$\bar{r}_r$(Mg–S)	Δr(Mg–S)	$\bar{r}_r$(Mg–O/S)	$r^{O}_{plane}/r^{O/S}_{plane}$
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