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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

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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.

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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, $\Delta r$(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) | $\Delta r$(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 |