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## **Accessory Publication**

## Ligand exchange processes on the solvated zinc cation II. $[Zn(H_2O)_4L]^{2+} \cdot 2H_2O \ with \ L = NH_3, \ NH_2(CH_3), \ NH(CH_3)_2 \ and \ N(CH_3)_3$

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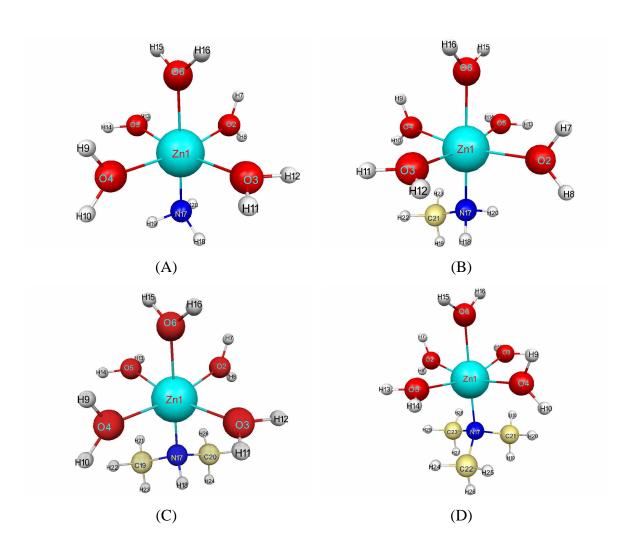


Figure S1. Calculated structures (RB3LYP/6-311+ $G^{**}$ ) of  $[Zn(H_2O)_5L]^{2+}$  (L = NH<sub>3</sub> (A),

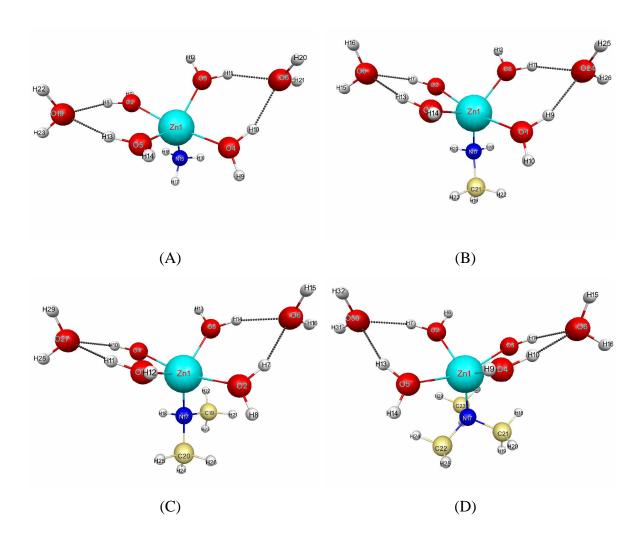


Figure S2. Calculated structures (RB3LYP/6-311+G\*\*) of  $[Zn(H_2O)_4L]^{2+}\cdot 2H_2O$  (L = NH<sub>3</sub> (A), NH<sub>2</sub>CH<sub>3</sub> (B), NH(CH<sub>3</sub>)<sub>2</sub> (C) and N(CH<sub>3</sub>)<sub>3</sub> (D)).

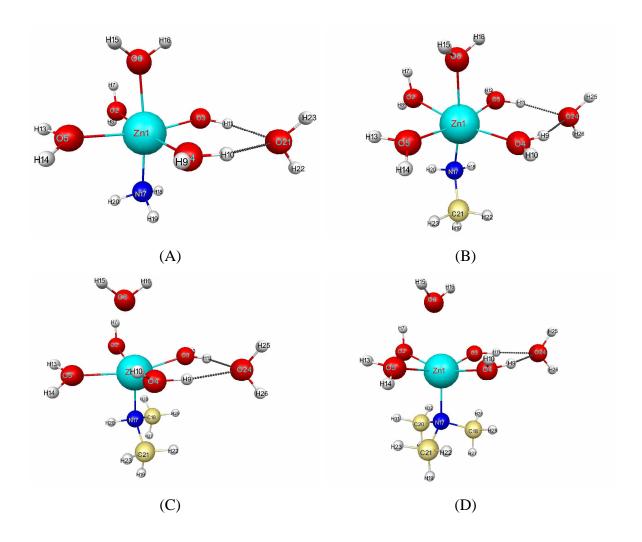


Figure S3. Calculated structures (RB3LYP/6-311+G\*\*) of  $\{[Zn(H_2O)_5L]^{2+}\cdot H_2O\}^{\ddagger}$  (L = NH<sub>3</sub> (A), NH<sub>2</sub>CH<sub>3</sub> (B), NH(CH<sub>3</sub>)<sub>2</sub> (C) and N(CH<sub>3</sub>)<sub>3</sub> (D)).

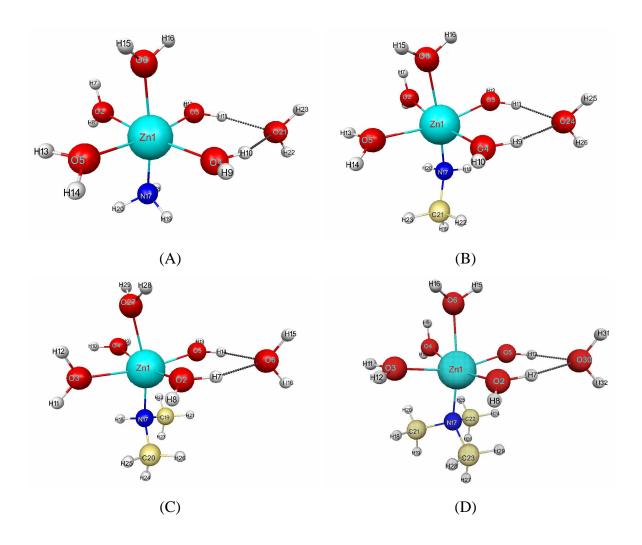


Figure S4. Calculated structures (RB3LYP/6-311+G\*\*) of  $[Zn(H_2O)_5L]^{2+} \cdot H_2O$  (L = NH<sub>3</sub> (A), NH<sub>2</sub>CH<sub>3</sub> (B), NH(CH<sub>3</sub>)<sub>2</sub> (C) and N(CH<sub>3</sub>)<sub>3</sub> (D)).