

# Experimental Study and Modeling of the Uv-Vis and Infrared Spectra of the [VO(O<sub>2</sub>)Hheida]<sup>-</sup> Complex Dissolved in Water

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## SUPPORTING INFORMATION

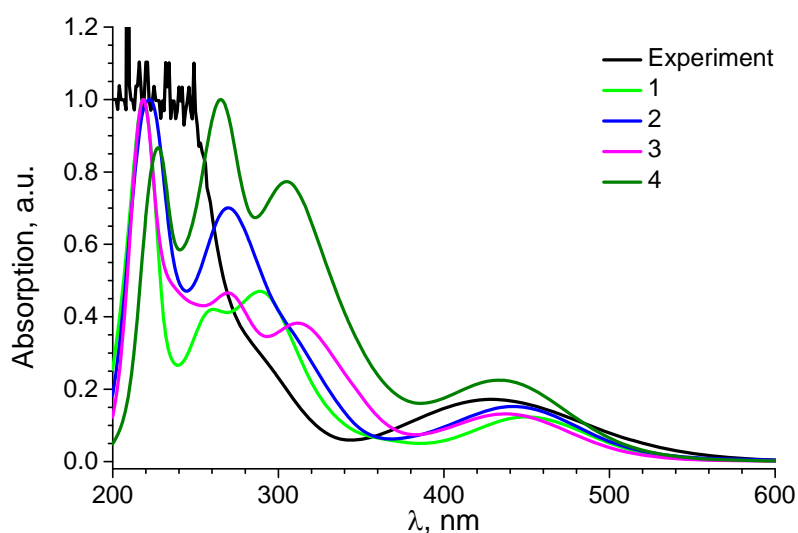
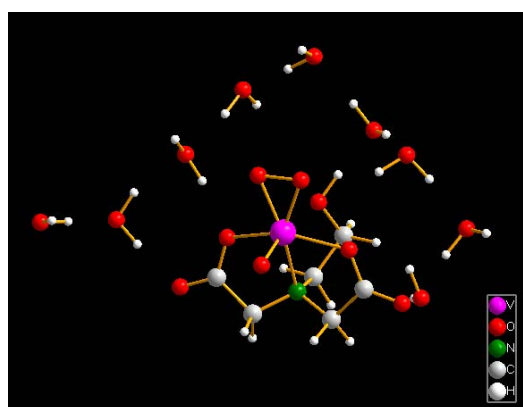
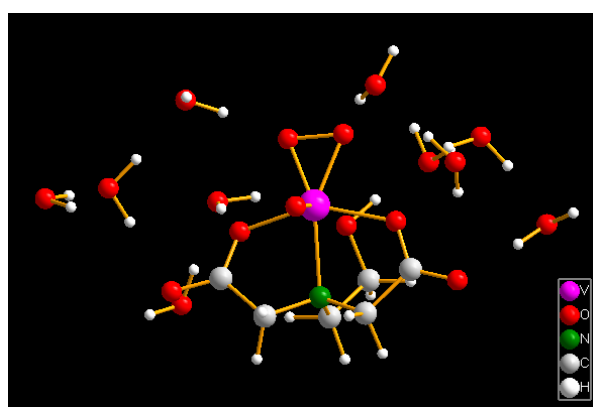


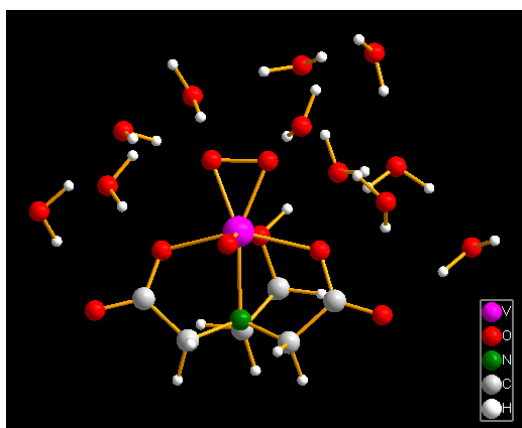
Figure S1. Apparent absorption spectra of the [VO(O<sub>2</sub>)(Hheida)]<sup>-</sup> complex dissolved in water: black line – experimental data; colored lines - spectra of [VO(O<sub>2</sub>)(Hheida)]<sup>-</sup> anion calculated with inclusion of a different number of additional water molecules in the model: light green line - [VO(O<sub>2</sub>)(Hheida)]<sup>-</sup>·9H<sub>2</sub>O (**1**), blue line - [VO(O<sub>2</sub>)(Hheida)]<sup>-</sup>·10H<sub>2</sub>O (**2**), pink line - [VO(O<sub>2</sub>)(Hheida)]<sup>-</sup>·11H<sub>2</sub>O (**3**), dark green line - [VO(O<sub>2</sub>)(Hheida)]<sup>-</sup>·12H<sub>2</sub>O (**4**).



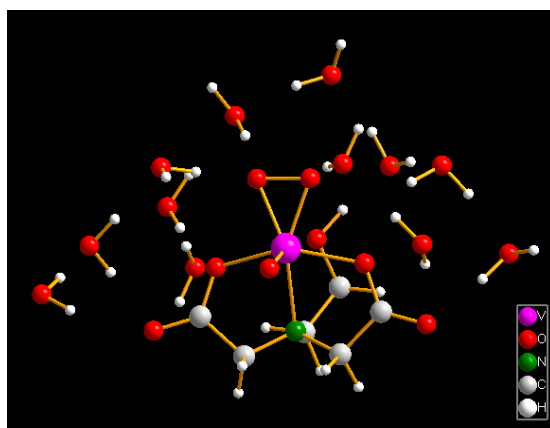
a)



b)



c)



d)

Figure S2. Optimized structure of the  $[\text{VO}(\text{O}_2)(\text{Hheida})]^-$  anion dissolved in water. In the figures the additional water molecules included in the model are shown.

(a)-  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 9\text{H}_2\text{O}$  (**1**), (b) -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 10\text{H}_2\text{O}$  (**2**), (c)-  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 11\text{H}_2\text{O}$  (**3**), (d)-  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 12\text{H}_2\text{O}$  (**4**).

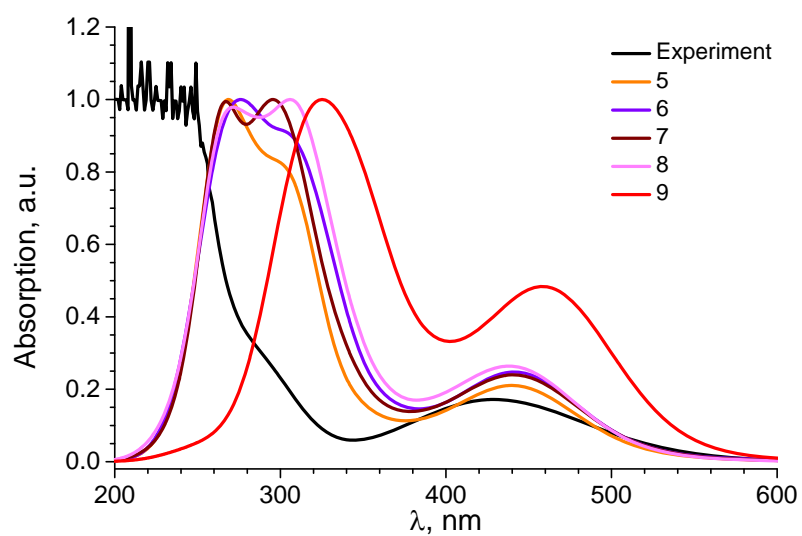


Figure S3. Apparent absorption spectra of the  $[\text{VO}(\text{O}_2)(\text{Hheida})]^-$  complex dissolved in water:

black line – experimental data; colored lines - spectra of  $[\text{VO}(\text{O}_2)(\text{Hheida})]^-$  anion calculated with inclusion of a different number of additional water molecules in the model: orange line -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 14\text{H}_2\text{O}$  (**5**), violet line -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 16\text{H}_2\text{O}$  (**6**), brown line -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 18\text{H}_2\text{O}$  (**7**), light magenta line -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 20\text{H}_2\text{O}$  (**8**), red -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 22\text{H}_2\text{O}$  (**9**).

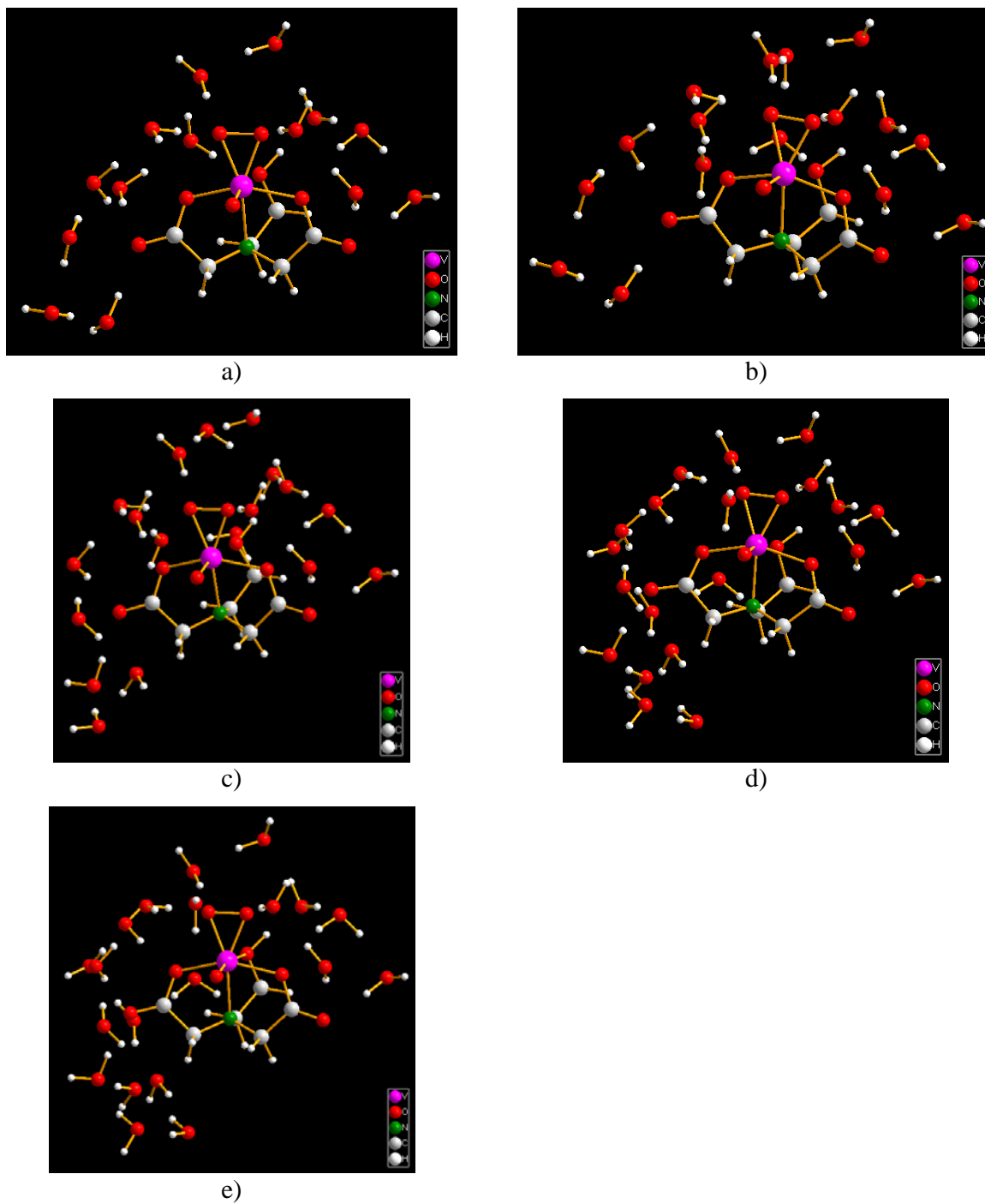


Figure S4. Optimized structure of the  $[\text{VO}(\text{O}_2)(\text{Hheida})]^-$  anion dissolved in water. In the figures the additional water molecules included in the model are shown. (a)-  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 14\text{H}_2\text{O}$  (5), (b) -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 16\text{H}_2\text{O}$  (6), (c)-  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 18\text{H}_2\text{O}$  (7), (d)-  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 20\text{H}_2\text{O}$  (8), (e) -  $[\text{VO}(\text{O}_2)(\text{Hheida})]^- \cdot 22\text{H}_2\text{O}$  (9).

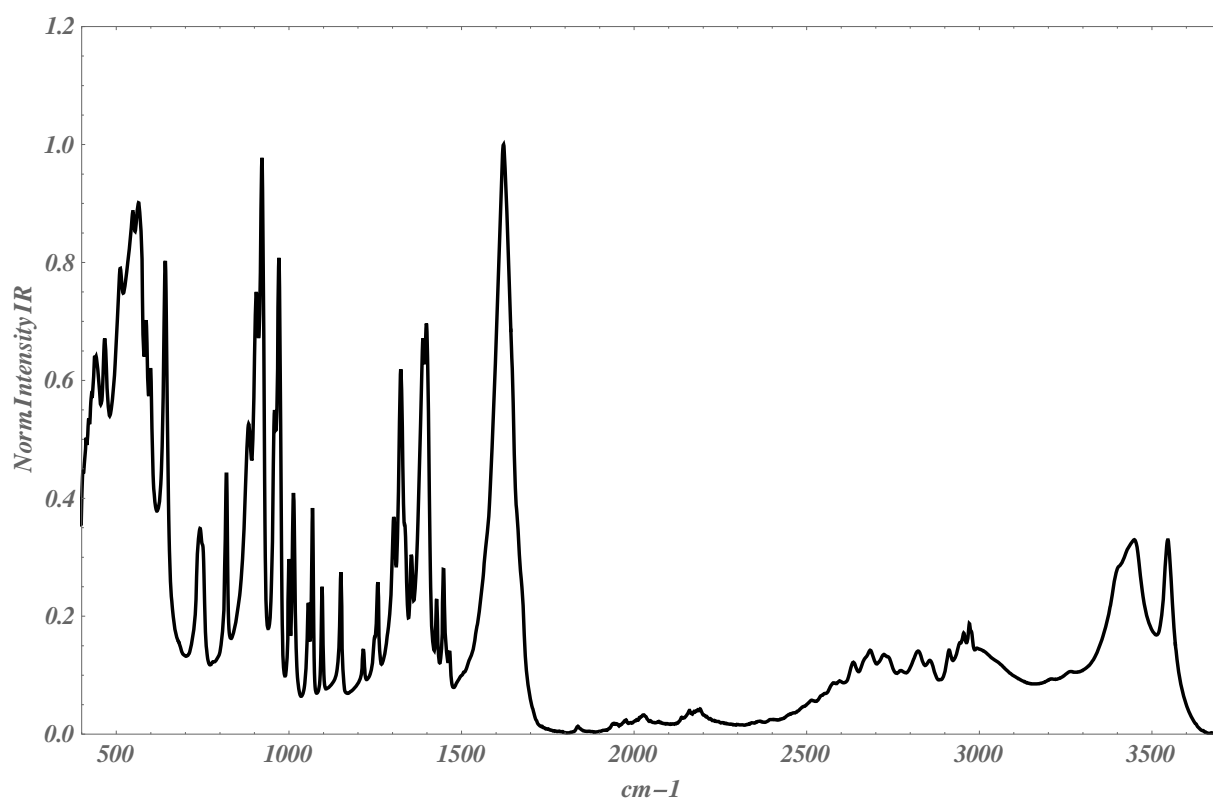


Figure S5. Infrared spectra of the K[VO(O<sub>2</sub>)(Hheida)] compound in the range 400 -3700 nm obtained by ATR method.