Supporting Information

Author: Satoru Tsushima

Title: Hydration and water exchange mechanism of UO$_2$$^{2+}$ ion revisited: The validity of the "n+1" model

1. Structures of UO$_2$$^{2+}$ hydrate obtained at the B3PW91 level in the aqueous phase

<table>
<thead>
<tr>
<th>UO$_2$(H$_2$O)$_5$$^{2+}$ : &quot;5&quot;(A1 type)</th>
<th>UO$_2$(H$_2$O)$_5$$^{2+}$ : &quot;5&quot;(A1 type)</th>
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<tbody>
<tr>
<td>u -0.000729</td>
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2. Structures of UO$_2$$^{2+}$ hydrate obtained at the MP2 level in the gas phase

<table>
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<tr>
<th>UO$_2$(H$_2$O)$_5$$^{2+}$ : &quot;4+1&quot;(A2 type)</th>
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3. Structure of UO$_2$(H$_2$O)$_5^+$ and NpO$_2$(H$_2$O)$_5^{2+}$ obtained at the B3LYP level in the aqueous phase

4. Coordinates of precursors, intermediates, and transitions states in Fig. 1 and Fig. 3
Fig. 1 A2 "4+1" with one hydrogen bond

Fig. A3 "4+1" with two hydrogen bond

Fig. 1 TSA12

Fig. 2 A4 "6+1" with two hydrogen bond

Fig. 3 B1 "5+1" with one hydrogen bond

Fig. 3 B2 "5+1" with two hydrogen bond
Fig. 3 TSB23

5. Coordinates of $\text{UO}_2(\text{H}_2\text{O})_{2\text{+}}$ in Fig.2(a) and Fig.2(b)
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