Supporting information for

The Mechanism of Water Exchange in Aqueous Uranyl(VI) Hydrate. A Density-Functional Molecular Dynamics Study. Michael Bühl*, Hendrik Kabrede

Structures of $[\text{UO}_2(\text{OH}_2)_5]^{2+} \cdot \text{H}_2\text{O}$, $[\text{UO}_2(\text{OH}_2)_6]^{2+}$, and $[\text{UO}_2(\text{OH}_2)_4]^{2+} \cdot 2\text{H}_2\text{O}$, optimized in vacuo with the CPMD program (xyz format in Å)

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21
[UO2(OH2)4](2+).2H2O
U -0.18246 0.837899 -0.0317506
O 0.689518 1.09079 -1.56822
O -1.05666 0.585429 1.50323
O 1.20991 2.56513 1.03115
O -1.81338 2.46708 -0.612787
O 1.44867 -0.795512 0.526319
O -1.5443 -0.91918 -1.08571
O -1.87117 3.86183 -2.74685
O 1.50466 -2.19635 2.65403
H 1.93213 3.06796 0.596488
H 1.12926 2.90407 1.9488
H -1.87429 3.05282 -1.47386
H -2.57079 2.69367 -0.0330736
H 2.20238 -1.01967 -0.0588974
H 1.51133 -1.38591 1.3838
H -1.48106 -1.23039 -2.01474
H -2.28943 -1.40232 -0.667663
H -2.54195 3.70318 -3.44304
H -1.7158 4.82816 -2.72875
H 1.35173 -3.163 2.63356
H 2.17264 -2.03728 3.3526
```

```
21
[UO2(OH2)5](2+).H2O (bridging)
U -0.227546 -0.264853 -0.176269
O -0.782177 1.29924 -0.831707
O 0.165262 -1.88509 0.464406
O 1.55266 2.73108 2.3015
O -0.122134 0.542195 2.14724
O -1.41486 -1.17276 -2.18439
O -2.53105 -0.626598 0.672954
O 1.5689 -0.876 -1.87821
O 1.937 0.915106 0.238077
H 1.21954 3.64587 2.17428
H 2.24054 2.80353 2.99842
H -1.56075 -2.10845 -2.44146
H -1.96161 -0.620513 -2.78342
H -2.86724 -1.41756 1.14614
H -3.25883 0.030851 0.649565
H 2.10337 -1.6894 -1.74877
H 1.60949 -0.664964 -2.8348
H -0.0485255 -0.0760427 2.90449
H 0.348886 1.38814 2.40368
H 2.60763 1.04719 -0.462924
H 1.98722 1.69358 0.859913
```

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21
[UO2(OH2)6](2+)
U 0.160023 0.0646654 0.0240776
O 0.434931 0.252894 1.78089
O 0.391697 -0.0641363 -1.74438
O 2.17523 1.51683 -0.0315919
O 2.06734 -1.5733 0.00481551
O -0.705763 2.34399 -0.56315
O -0.69645 -2.29541 0.596171
O -2.10861 0.506158 1.19239
O -2.25265 -0.629297 -1.21737
H 2.57482 1.92758 0.764237
H 2.66123 1.85228 -0.813927
H 2.63398 -1.80693 0.77064
H 2.56868 -1.80391 -0.806572
H -1.20266 2.95646 0.0185212
H -0.6221 2.77548 -1.43957
H -1.0438 -2.48089 1.49524
H -0.229557 -3.11103 0.315231
H -2.98694 0.451547 0.761168
H -2.23789 0.683273 2.14772
H -2.53714 -1.56187 -1.11286
H -2.27504 -0.465305 -2.18439
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