

Which density functional should be used to study actinyl complexes ?

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Table S1.

Coordinates (Å) of aqua complexes $[\text{AnO}_2(\text{H}_2\text{O})_5]\text{X}^+ \cdot 10\text{H}_2\text{O}$ (An=Np, Pu or U, X = 1 or 2)

[NpO₂(H₂O)₅]⁺ · 10H₂O

93	-0.314734	-0.078548	0.236787
8	-0.261371	-0.350402	2.063525
8	2.141017	0.124384	-0.159103
8	-0.369149	0.233200	-1.617342
8	0.469201	2.283840	0.769189
8	0.735910	-2.321566	0.083791
8	-2.381383	1.331129	0.445267
8	-2.150170	-1.696926	-0.109308
1	2.626892	-0.330256	0.585956
1	2.355146	-0.390860	-1.008517
1	1.344919	2.200063	1.302915
1	0.647812	2.717045	-0.113190
1	0.738328	-2.851761	0.918143
1	0.674516	-2.902475	-0.729608
1	-2.241117	1.993212	1.219865
1	-2.522717	1.920021	-0.385072
1	-3.071571	-1.375197	0.209666
1	-2.240474	-1.898771	-1.078386
8	3.143079	-0.726906	2.248532
1	2.497639	-1.430085	2.575950
1	4.040128	-1.062776	2.447662
8	2.625698	-1.177179	-2.464013
1	1.996160	-1.944483	-2.549849

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1	3.517967	-1.570003	-2.543470
8	2.532059	2.000300	2.379653
1	2.738329	1.027532	2.469500
1	3.363285	2.397067	2.048473
8	0.187774	2.876956	-1.880922
1	0.116136	1.882447	-2.006066
1	0.777493	3.205568	-2.590244
8	1.158031	-2.490221	2.780156
1	0.484658	-1.743142	2.736362
1	0.989165	-2.971429	3.616009
8	0.691689	-3.207436	-2.434432
1	-0.177446	-2.797248	-2.749469
1	0.734896	-4.107941	-2.814714
8	-1.666283	3.091013	2.249906
1	-1.566565	2.710719	3.147176
1	-0.755702	3.016628	1.843468
8	-2.563317	2.906575	-1.675160
1	-1.601941	3.092870	-1.869474
1	-2.954301	3.772854	-1.439681
8	-4.361873	-0.527476	0.649883
1	-4.605737	-0.695703	1.583101
1	-3.830630	0.321118	0.661895
8	-1.559488	-1.828015	-2.829776
1	-1.158985	-0.934118	-2.586205
1	-2.094363	-1.693638	-3.638859

[NpO2 (H2O5)] 2+ . 10H2O

93	-0.030510	0.004021	-0.000056
8	-0.029606	0.006961	1.773632
8	2.372044	0.136603	-0.003544
8	-0.028968	0.006694	-1.773730
8	0.574674	2.329094	0.002901
8	0.849572	-2.238564	0.003422
8	-2.060401	1.295164	-0.000744
8	-1.886544	-1.529590	-0.001823

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1	2.706966	-0.302687	0.837696
1	2.703470	-0.303218	-0.846766
1	1.098314	2.504023	0.846222
1	1.097738	2.507279	-0.839282
1	0.540934	-2.693913	0.845343
1	0.542440	-2.697112	-0.836740
1	-2.069414	1.846968	0.841029
1	-2.068372	1.846922	-0.842906
1	-2.415896	-1.375880	0.839274
1	-2.414469	-1.375206	-0.843871
8	2.508857	-0.506155	2.608103
1	1.805057	-1.191371	2.767960
1	3.286785	-0.792032	3.132812
8	2.507894	-0.514683	-2.608794
1	1.804789	-1.201626	-2.765994
1	3.287090	-0.802727	-3.130380
8	1.255499	2.257538	2.600010
1	1.689923	1.376344	2.756889
1	1.774442	2.909707	3.117253
8	1.245826	2.261933	-2.600764
1	1.679081	1.381142	-2.760549
1	1.761676	2.913963	-3.121334
8	0.286199	-2.558348	2.619648
1	-0.585316	-2.104206	2.774827
1	0.258160	-3.382565	3.150806
8	0.292915	-2.559947	-2.616876
1	-0.577728	-2.105269	-2.774322
1	0.266115	-3.383356	-3.149379
8	-1.784964	1.904640	2.607588
1	-0.813611	2.046313	2.764052
1	-2.245114	2.594117	3.132134
8	-1.781938	1.908690	-2.605956
1	-0.810224	2.051840	-2.760969
1	-2.242367	2.598932	-3.129221
8	-2.369520	-1.091991	2.614007
1	-2.208284	-0.123633	2.771973

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1	-3.161374	-1.322356	3.145275
8	-2.367716	-1.090451	-2.616813
1	-2.205674	-0.122197	-2.773996
1	-3.159840	-1.319824	-3.148080

[PuO2 (H2O) 5] 1+ .10H2O

94	-0.020974	-0.004914	0.030348
8	-0.030677	-0.012229	1.843175
8	2.479817	0.256179	-0.002582
8	-0.028499	-0.005361	-1.779712
8	0.472725	2.463133	0.014976
8	0.974908	-2.303813	0.012030
8	-2.206322	1.224865	0.005064
8	-1.884595	-1.671416	0.001721
1	2.750033	-0.254477	0.807567
1	2.725286	-0.237843	-0.831994
1	1.042488	2.547046	0.827738
1	1.022960	2.545078	-0.810276
1	0.582207	-2.721106	0.825639
1	0.592391	-2.706794	-0.812714
1	-2.113763	1.798205	0.813686
1	-2.111187	1.771644	-0.821845
1	-2.404989	-1.420411	0.811946
1	-2.380604	-1.422285	-0.824013
8	2.479645	-0.498705	2.663246
1	1.747157	-1.170510	2.728965
1	3.204694	-0.841104	3.225710
8	2.447789	-0.486694	-2.671145
1	1.722065	-1.169631	-2.728950
1	3.176888	-0.823605	-3.231642
8	1.230190	2.209164	2.661380
1	1.642221	1.303427	2.725493
1	1.789583	2.795898	3.211044
8	1.177913	2.203183	-2.662769
1	1.598232	1.300349	-2.723352

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1	1.721436	2.789983	-3.228191
8	0.271727	-2.542745	2.671510
1	-0.545783	-1.977245	2.720268
1	0.092514	-3.318752	3.240634
8	0.297783	-2.508381	-2.671242
1	-0.532758	-1.959526	-2.722257
1	0.144640	-3.279327	-3.254770
8	-1.744606	1.875317	2.657200
1	-0.756036	1.975089	2.724885
1	-2.124539	2.589976	3.208379
8	-1.742662	1.838554	-2.660448
1	-0.753529	1.955630	-2.722188
1	-2.133414	2.542791	-3.217514
8	-2.347971	-1.062042	2.660152
1	-2.070530	-0.107840	2.711321
1	-3.143567	-1.137183	3.225466
8	-2.300472	-1.068014	-2.674603
1	-2.047145	-0.105488	-2.724592
1	-3.084061	-1.168094	-3.252773

[PuO2 (H2O) 5] 2+ . 10H2O

94	-0.024935	-0.000823	0.040202
8	-0.026882	-0.007848	1.800532
8	2.377250	0.154309	-0.011256
8	-0.024871	-0.002682	-1.719333
8	0.562365	2.329826	0.007953
8	0.872658	-2.232525	0.005003
8	-2.058843	1.281749	-0.004275
8	-1.870779	-1.536147	-0.005482
1	2.711276	-0.312016	0.813973
1	2.690905	-0.289955	-0.859545
1	1.108869	2.494472	0.837368
1	1.079579	2.503614	-0.837036
1	0.533943	-2.692293	0.833460
1	0.554608	-2.678061	-0.838798

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1	-2.047111	1.856076	0.821375
1	-2.053983	1.827541	-0.850441
1	-2.413726	-1.351695	0.821028
1	-2.388278	-1.365371	-0.851796
8	2.510599	-0.491975	2.611004
1	1.825014	-1.190321	2.783879
1	3.300070	-0.755104	3.130493
8	2.492783	-0.496672	-2.611940
1	1.806061	-1.201064	-2.762652
1	3.278025	-0.767534	-3.133692
8	1.261093	2.240524	2.610701
1	1.704488	1.362897	2.763964
1	1.773954	2.900624	3.123184
8	1.212625	2.250688	-2.607665
1	1.657665	1.373409	-2.753070
1	1.713064	2.903916	-3.141000
8	0.265728	-2.582274	2.615408
1	-0.611509	-2.142012	2.771821
1	0.239055	-3.419418	3.125998
8	0.294609	-2.557786	-2.610261
1	-0.585154	-2.118538	-2.759225
1	0.275912	-3.383321	-3.139821
8	-1.762720	1.908742	2.608550
1	-0.791906	2.048261	2.769623
1	-2.228058	2.599726	3.125728
8	-1.767215	1.884606	-2.609219
1	-0.793994	2.035464	-2.752034
1	-2.231711	2.568392	-3.136681
8	-2.396071	-1.065047	2.605575
1	-2.225410	-0.101124	2.777455
1	-3.201534	-1.293742	3.115820
8	-2.362335	-1.075044	-2.613729
1	-2.200901	-0.106256	-2.770373
1	-3.155660	-1.308209	-3.140802

[UO2 (H2O) 5] 1+ .10H2O

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92	0.012216	-0.303613	0.038875
8	0.158260	-0.369177	1.931851
8	2.441124	0.143283	-0.158886
8	-0.047543	-0.340784	-1.841052
8	0.431431	2.191998	0.013760
8	1.029908	-2.529546	0.042255
8	-2.084234	1.103943	0.140046
8	-1.981949	-1.707073	0.050217
1	2.942635	-0.082773	0.664883
1	2.852544	-0.265306	-0.990628
1	0.940963	2.436958	0.844654
1	0.967087	2.369443	-0.803258
1	0.546466	-3.044619	0.779855
1	0.979254	-2.988863	-0.837317
1	-1.969324	1.659714	0.962309
1	-2.013468	1.686506	-0.670942
1	-2.468329	-1.392816	0.881606
1	-2.494681	-1.376378	-0.771059
8	2.685630	0.160093	2.577735
1	1.769069	-0.258733	2.513500
1	3.140134	-0.253095	3.340208
8	2.992409	-0.656738	-2.607395
1	2.439483	-1.476980	-2.774102
1	3.883905	-0.864206	-2.953566
8	1.260403	2.452036	2.557975
1	1.927679	1.710477	2.702550
1	1.665354	3.263676	2.925692
8	0.977246	2.038764	-2.673398
1	1.181589	1.068681	-2.678128
1	1.560504	2.445016	-3.346832
8	-0.213084	-3.208348	2.250633
1	-0.151411	-2.237919	2.454015
1	-1.173691	-3.332243	2.094204
8	1.104820	-2.615106	-2.686641
1	0.474364	-1.839473	-2.557663

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1	0.744558	-3.149842	-3.423588
8	-1.621460	1.746050	2.722909
1	-0.629050	1.727736	2.767261
1	-1.889408	2.512092	3.270523
8	-1.851636	1.882516	-2.442245
1	-0.873015	1.896615	-2.644533
1	-2.227973	2.661061	-2.900635
8	-2.788862	-0.943805	2.504608
1	-2.323299	-0.086423	2.689409
1	-3.734943	-0.755701	2.669297
8	-3.090977	-0.737120	-2.190694
1	-2.590248	0.098181	-2.391882
1	-4.011840	-0.438178	-2.046417

[UO2 (H2O) 5] 2+ .10H2O

92	-0.025654	-0.004084	-0.002179
8	-0.027731	-0.010607	1.791440
8	2.392588	0.139831	-0.012969
8	-0.024380	-0.006565	-1.796155
8	0.582381	2.338809	0.009344
8	0.857734	-2.255634	0.008627
8	-2.060979	1.305232	-0.001213
8	-1.897205	-1.532113	-0.005523
1	2.739392	-0.290771	0.826610
1	2.728733	-0.297086	-0.856401
1	1.102587	2.519247	0.853422
1	1.102539	2.529715	-0.830490
1	0.548547	-2.709682	0.853309
1	0.552399	-2.717657	-0.831498
1	-2.073374	1.856949	0.840732
1	-2.073781	1.858058	-0.843003
1	-2.426446	-1.375783	0.837275
1	-2.425274	-1.373903	-0.848975
8	2.536320	-0.483135	2.608572
1	1.833381	-1.165632	2.772698

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1	3.311287	-0.763668	3.140665
8	2.534153	-0.518949	-2.611339
1	1.830404	-1.203523	-2.767921
1	3.312521	-0.810362	-3.132311
8	1.258007	2.264039	2.605780
1	1.693491	1.383254	2.761954
1	1.775562	2.916123	3.124447
8	1.237933	2.280106	-2.602400
1	1.666728	1.399123	-2.766722
1	1.751586	2.930491	-3.127195
8	0.281450	-2.594171	2.610442
1	-0.584965	-2.133961	2.767697
1	0.241565	-3.425690	3.129266
8	0.297301	-2.595959	-2.603972
1	-0.566470	-2.133697	-2.767983
1	0.261164	-3.425031	-3.127067
8	-1.789430	1.910550	2.606734
1	-0.817437	2.040084	2.768151
1	-2.243525	2.604825	3.130110
8	-1.788718	1.920757	-2.603121
1	-0.816406	2.054865	-2.762037
1	-2.244420	2.617006	-3.122444
8	-2.402119	-1.091533	2.597633
1	-2.228307	-0.126721	2.761379
1	-3.206888	-1.310764	3.113845
8	-2.398968	-1.086131	-2.605975
1	-2.225970	-0.120969	-2.767479
1	-3.202696	-1.305300	-3.123793
