Supplementary Information, "Vibrational spectroscopy of anionic nitrate complexes of UO_2^{2+} and Eu^{3+} isolated in the gas phase," G. S. Groenewold. et al.

Frequencies, intensities, and assignments for $[UO_2(NO_3)_2O]^-$, using different functionals with the StuttRSC/TZVP basis set (intensities in KM/mol).

LDA		B3LYP		PW91		
Freq	Int.	Freq.	Int.	Freq.	Int.	Assignment
840	189	942	372	820	166	Uranyl ν_3
1060	34	1051	53	1004	30	Asymmetric combination of NO_3 ν_1
1061	31	1053	24	1006	34	Symmetric combination of NO_3 ν_1
1289	69	1289	130	1221	64	Asymmetric combination of NO_3 ν_3
1299	376	1302	449	1234	370	Symmetric combination of NO_3 ν_3
1573	1122	1544	1249	1492	1120	Asymmetric combination of NO_3 ν_3
1582	266	1557	305	1506	231	Symmetric combination of NO_3 ν_3

Frequencies, intensities, and assignments for $[UO_2(NO_3)(NO_2)(O_2)]^-$, using different functionals with the StuttRSC/TZVP basis set (intensities in KM/mol).

LDA		B3LYP		PW91		
Freq	Int.	Freq.	Int.	Freq.	Int.	Assignment
925	357	953	400	902	337	Uranyl ν_3
1059	26	1048	25	1010	27	NO_3 ν_1
1228	211	1238	265	1160	204	Asymmetric stretch NO_2
1244	71	1223	48	1180	84	O_2 stretch
1298	261	1294	340	1235	250	NO_3 ν_3
1320	17	1346	30	1273	24	Symmetric stretch NO_2 (breathing)
1575	731	1545	788	1499	685	NO_3 ν_3

Coordinates for the structures of the complexes, generated by the different computational packages used, in x,y,z format.

$[UO_2(NO_3)_3]^-$, LDA/DSPP/DNP (DMol^3)

U -0.351 0.164 0.031
O -0.559 1.926 0.265
O -0.145 -1.598 -0.201
O 1.049 0.583 -1.932
O 2.080 0.463 -0.054
N 2.160 0.640 -1.312
O 3.211 0.846 -1.876
O 0.669 -0.008 2.255
N -0.413 -0.204 2.896
O -1.464 -0.235 2.178
O -0.441 -0.352 4.097
O -2.772 -0.114 -0.235
N -2.800 0.045 -1.498
O -1.668 0.277 -2.034
O -3.824 -0.019 -2.141

$[UO_2(NO_3)_2(O)]^-$, LDA/DSPP/DNP (DMol^3)

U -0.370 0.274 0.025
O -0.233 2.057 0.392
O -0.263 -1.534 -0.199
O 1.148 0.585 -1.901
O 2.132 0.274 -0.013
N 2.24 0.488 -1.258
O 3.321 0.593 -1.803
O 0.519 -0.118 2.331
N -0.615 -0.194 2.893
O -1.622 -0.058 2.129
O -0.733 -0.387 4.087
O -1.979 0.427 -1.006

$[UO_2(NO_3)_2(O)]^-$ structure with LDA/StuttRSC/TZVP (NWChem)

U	0.12336125	-0.46037980	-0.00000250
O	0.08147164	-0.30402888	1.81157322
O	0.08142874	-0.30390503	-1.81156334
O	0.90202442	1.90041005	-0.00008236
O	-2.24983898	-0.90520560	-0.00003170
O	2.40103098	0.34098681	-0.00002278
O	-1.73138837	1.19479955	-0.00007929
N	2.13959358	1.60127829	-0.00001023
N	-2.65358537	0.31694863	-0.00001195
O	3.02274828	2.44023445	0.00006998
O	-3.83790003	0.60192167	0.00007087
O	0.61624219	-2.29985575	0.00009008

$[UO_2(NO_3)_2(O)]^-$ structure with B3LYP/StuttRSC/TZVP (NWChem)

U	0.09736083	-0.36336968	-0.00009623
O	0.10471265	-0.39079323	1.78875538
O	0.10473940	-0.39089406	-1.78861784
O	0.97513944	2.02599923	-0.00003852
O	-2.36284119	-0.84504614	-0.00001120
O	2.46880158	0.44958592	-0.00000927
O	-1.85749768	1.26699683	-0.00003537
N	2.21785329	1.71350824	0.00001629
N	-2.77744832	0.37499778	0.00001627
O	3.10616257	2.55200798	0.00003448
O	-3.96604470	0.65702461	0.00003379
O	0.64686777	-2.41415049	-0.00003513

$[UO_2(NO_3)_2(O)]^-$ structure with PW91/StuttRSC/TZVP (NWChem)

U	0.10501468	-0.39200687	-0.00005504
O	0.07148837	-0.26678943	1.82588714
O	0.07150067	-0.26682364	-1.82572256
O	0.98708531	2.01431355	-0.00001048
O	-2.32180752	-0.89364354	0.00001189
O	2.45755396	0.38713708	0.00000907
O	-1.86200301	1.25086898	-0.00001508
N	2.22926808	1.67015714	0.00001810
N	-2.76580087	0.33202619	0.00001798
O	3.14823310	2.49118853	-0.00002847
O	-3.97199928	0.58324047	-0.00002743
O	0.60927214	-2.27380149	-0.00007245

$[UO_2(NO_3)(NO_2)(O_2)]^-$, LDA/DSPP/DNP ($DMol^3$)

U	-0.249	0.244	0.136
O	-0.257	2.039	0.233
O	-0.219	-1.553	0.077
O	1.035	0.341	-1.969
O	2.200	0.328	-0.162
N	2.189	0.365	-1.434
O	3.209	0.422	-2.09
O	0.706	0.132	2.415
N	-0.378	0.083	3.052
O	-1.403	0.118	2.325
O	-2.509	0.253	-0.449
O	-1.837	0.308	-1.568

$[UO_2(NO_3)(NO_2)(O_2)]^-$ structure with LDA/StuttRSC/TZVP (NWChem)

U	0.19378788	-0.13379714	-0.01102737
O	0.29492608	-0.14472665	1.77793446
O	0.10736189	-0.12144465	-1.80070809
O	0.02517898	-2.46015270	-0.01790609
N	2.43154425	1.68426473	-0.11605434
O	2.55156464	0.41937944	-0.13118885
O	1.21785226	2.05948063	-0.04983619
N	-2.59091744	0.58486805	0.13999619
O	-2.20052788	-0.63350721	0.11239386
O	-1.65288166	1.45568635	0.09552766
O	-3.76712322	0.89477307	0.20379822
O	1.30008693	-2.18392267	-0.08283844

$[UO_2(NO_3)(NO_2)(O_2)]^-$ structure with B3LYP/StuttRSC/TZVP (NWChem)

U	0.20349048	-0.04488616	-0.00133302
O	0.18110960	-0.12880980	1.77786425
O	0.21147594	0.10308047	-1.77652364
O	1.08876327	2.28636926	0.15854748
O	-2.17390476	-0.86762297	-0.07530871
O	-1.92665473	1.28484442	0.06716148
N	2.33185796	2.01814646	0.15153077
N	-2.73413542	0.28652218	-0.00475401
O	0.87851406	-2.14156130	-0.13243313
O	2.56485389	0.76998638	0.07185009
O	-3.94674970	0.42669691	-0.00582232
O	1.25109152	-3.38570962	-0.20688726

$[UO_2(NO_3)(NO_2)(O_2)]^-$ structure with PW91/StuttRSC/TZVP (NWChem)

U	0.20600187	-0.13653539	-0.01175188
O	0.30547000	-0.14321003	1.79039236
O	0.11626343	-0.11954543	-1.81435375
O	0.02925275	-2.51280606	-0.01835059
N	2.49170587	1.74417788	-0.11895874
O	2.62801518	0.46672551	-0.13484450
O	1.25917853	2.10914974	-0.05185642
N	-2.64556073	0.60771482	0.14292345
O	-2.25940793	-0.62806763	0.11503333
O	-1.69326266	1.48650396	0.09811150
O	-3.83331011	0.92793558	0.20745886
O	1.32508785	-2.23681253	-0.08441960

$[UO_2(NO_3)(NO_2)(O_2)]^-$ with linear O_2 structure with LDA/StuttRSC/TZVP (NWChem)

U	0.19035855	-0.04789028	-0.01074713
O	0.28470125	-0.01679424	1.77837825
O	0.09457164	0.00609890	-1.79932006
O	0.63963664	-2.15446662	-0.04851321
N	2.45696937	1.72565830	-0.11428246
O	2.55407057	0.45793974	-0.13144188
O	1.25157756	2.12513575	-0.04816509
N	-2.62030108	0.54388357	0.14190504
O	-2.17408424	-0.65580665	0.11511365
O	-1.72248590	1.45660094	0.09633185
O	-3.80850029	0.79959818	0.20577794
O	0.89434149	-3.40808885	-0.06870467

$[Eu(NO_3)_4]^-$ structure with LDA/StuttRSC/TZVP (NWChem)

Eu	-0.00179325	-0.00181302	-0.00000495
O	-0.79328462	1.22246274	1.93280626
N	-1.67234573	1.89426301	1.29590670
O	-2.39822876	2.70440039	1.84076123
O	0.79131406	-1.22561496	1.93270709
O	1.73904660	1.65997551	-0.03502450
O	-1.75021717	-1.65553092	-0.03960608
O	1.75069651	-1.65114018	0.03881382
O	-1.74283396	1.65979229	0.03665059
O	-0.79107281	-1.22784930	-1.93313233
O	0.79494554	1.21850988	-1.93292213
N	1.67922131	-1.88750283	1.29768288
N	1.67388110	1.88992423	-1.29536800
N	-1.67670669	-1.89281836	-1.29820496
O	2.41214175	-2.69037820	1.84386763
O	2.40432825	2.69562186	-1.84070087
O	-2.40579196	-2.69933216	-1.84415081

$[Eu(NO_3)_4]^-$ structure with B3LYP/StuttRSC/TZVP (NWChem)

Eu	-0.00021305	-0.00200005	-0.00004092
O	-0.99190049	1.17543053	1.91039389
N	-1.81871875	1.87596359	1.21768998
O	-2.59465655	2.66474195	1.72325778
O	0.98874547	-1.17913477	1.91246966
O	1.76620468	1.68321803	0.05715879
O	-1.77432226	-1.67923969	0.05510717
O	1.77692864	-1.67616906	-0.05365705
O	-1.76691057	1.68307225	-0.05826821
O	-0.99002533	-1.17985314	-1.91197685
O	0.99229741	1.17299452	-1.91125954
N	1.82386817	-1.87202460	1.22205644
N	1.81849085	1.87471888	-1.21897203
N	-1.82318386	-1.87420130	-1.22068896
O	2.60288231	-2.65663815	1.72935261
O	2.59422745	2.66335099	-1.72508104
O	-2.60216356	-2.65932874	-1.72722303

$[Eu(NO_3)_4]^-$ structure with PW91/StuttRSC/TZVP (NWChem)

Eu	0.00010604	0.00080304	0.00000976
O	-0.85089153	1.27759232	1.96616053
N	-1.75130082	1.93278124	1.31009023
O	-2.50483089	2.74123088	1.85131764
O	0.85043628	-1.27453352	1.96741052
O	1.81237438	1.68557011	-0.03837400
O	-1.81260724	-1.68355126	-0.03751157
O	1.81356278	-1.68271557	0.03904124
O	-1.81298448	1.68476342	0.03702546
O	-0.85005779	-1.27623269	-1.96635191
O	0.85093886	1.27594187	-1.96727123
N	1.75131284	-1.92990819	1.31221382
N	1.75089957	1.93218018	-1.31169284
N	-1.75055089	-1.93152578	-1.31054428
O	2.50474882	-2.73778504	1.85433472
O	2.50421248	2.74031798	-1.85356938
O	-2.50381783	-2.74002773	-1.85197000

$[Eu(NO_3)_4]^-$ structure with LDA/DSPP/DNP ($DMol^3$)

Eu	0.000	0.000	0.000
O	2.206	1.078	0.000
N	2.876	0.000	0.000
O	2.206	-1.078	0.000
O	4.091	0.000	0.000
O	0.000	1.078	-2.206
N	0.000	0.000	-2.876
O	0.000	-1.078	-2.206
O	0.000	0.000	-4.091
O	-2.206	1.078	0.000
N	-2.876	0.000	0.000
O	-2.206	-1.078	0.000
O	-4.091	0.000	0.000
O	0.000	1.078	2.206
N	0.000	0.000	2.876
O	0.000	-1.078	2.206
O	0.000	0.000	4.091