

Electronic Supporting information

**Separation of Am³⁺ and Eu³⁺ using hexa-n-octylnitrilo triacetamide (HONTA):
complexation, extraction, luminescence, EXAFS and DFT studies**

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S1. Purification of ^{241}Am

^{241}Am was purified from its daughter product, ^{237}Np , by first reducing Np to its +4 state using hydroxylamine hydrochloride at 1 M HNO_3 and subsequently extracting Np^{4+} by TTA (similar to the extraction of Pu^{4+} mentioned above). The aqueous phase was evaporated to dryness and a few drops of mixture of concentrated HNO_3 and HClO_4 (5:1 ratio) was added to destroy the organic impurities. Alpha spectrometry of the purified ^{241}Am stock was carried out to rule out the presence of the impurities.

S2. Radiometric assay of ^{241}Am and $^{152,154}\text{Eu}$:

^{241}Am and $^{152,154}\text{Eu}$ were assayed radiometrically using a well type NaI(Tl) scintillation counter which was interfaced with a multi-channel analyzer. For experiments where the extraction of Am or Eu were very large or very low, the aliquot size from the phase containing low counts was kept large enough to have more counts. Additionally, counting time was increased (some cases, >10 h counting time was used as against only one minute of counting time used for most samples). The counter was calibrated with known standards before the counting was done. Enough counts were collected (>10,000 counts) to neglect the counting statistics errors (<1%).

S3. EXAFS Studies

S3.1 Experimental set up

In the present study EXAFS measurements were performed on the Eu extract of HONTA in *n*-dodecane to probe the local structure surrounding Eu ions. The EXAFS measurements were carried out at the Energy-Scanning EXAFS beamline (BL-9) at the INDUS-2 Synchrotron Source (2.5 GeV, 200 mA) at the Raja Ramanna Centre for Advanced Technology (RRCAT), Indore, India. This beamline operates in an energy range of 4 to 25 KeV. The beamline optics consists of a Rh/Pt coated collimating meridional cylindrical mirror and the collimated beam reflected by the mirror is monochromatized by a Si(111) ($2d=6.2709$) based double crystal monochromator (DCM). The second crystal of DCM is a sagittal cylinder used for horizontal focusing, while an Rh/Pt coated bendable post mirror facing down was used for vertical focusing of the beam at the sample position. Rejection of the higher harmonics content in the X-ray beam

was performed by detuning the second crystal of DCM. In the present case, EXAFS measurements at Eu L3-edges were performed in fluorescence mode.

S3.2 Data Analysis

In order to take care of the oscillations in the absorption spectra, $\mu(E)$ was converted into the absorption function $\chi(E)$ defined as follows:

$$\chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu_0(E_0)} \quad (S1)$$

where E_0 is the absorption edge energy, $\mu_0(E_0)$ is the bare atom background and $\Delta\mu_0(E_0)$ is the step in $\mu(E)$ value at the absorption edge. The energy dependent absorption coefficient $\chi(E)$ was converted into the wavenumber dependent absorption coefficient $\chi(k)$ using the relation

$$K = \sqrt{\frac{2m(E - E_0)}{\hbar^2}} \quad (S2)$$

where m is the electron mass. $\chi(k)$ is weighted by k^2 to amplify the oscillation at high k and the $\chi(k)k^2$ functions were Fourier transformed in R space to generate the $\chi(R)$ *versus* R spectra in terms of the real distances from the center of the absorbing atom. The EXAFS data analysis programme, available within the IFEFFIT software package, was used for data analysis. This includes background reduction and Fourier transform to derive the $\chi(R)$ *versus* R spectra from the absorption spectra (using the ATHENA software), generation of the theoretical EXAFS spectra starting from an assumed crystallographic structure and finally fitting of the experimental data with the theoretical spectra using the ARTEMIS software.

S4. Computational studies

Coordinates in optimized structures of Am^{3+} and Ln^{3+} complexes of HMNTA at the B3LYP/SVP level of theory

$\text{Am}(\text{HMNTA})(\text{NO}_3)_2^+$

N	1.8054361	0.0568738	0.0097810
C	2.1586815	-0.1514362	1.4198673
H	2.2930070	-1.2319896	1.6000909
H	3.1277160	0.3261692	1.6594061
C	2.2388186	1.3521123	-0.5299663
H	2.8730091	1.8760632	0.2092994
H	2.8806109	1.2005640	-1.4149584
C	2.1669510	-1.0883089	-0.8360627
H	2.0619034	-0.7915545	-1.8917050
H	3.2182153	-1.4020885	-0.6740616
C	1.2061967	-2.2702294	-0.6142342
C	1.0636055	0.3162599	2.3957828
C	1.0846964	2.3017121	-0.9173467
O	-0.0933048	1.9896108	-0.6566275
O	-0.0879347	0.5069495	1.9624189
O	0.1590016	-2.0803097	0.0434195
N	1.3888415	3.4554052	-1.5272774
N	1.5060326	-3.4643384	-1.1342855
N	1.3633833	0.4704296	3.6931264
C	0.3220666	4.3547878	-1.9803952
H	0.4087885	5.3284255	-1.4665912
H	0.4134509	4.5154458	-3.0692621
H	-0.6556951	3.9101237	-1.7572889
C	2.7488521	3.8684850	-1.8736200
H	3.0166051	3.5501129	-2.8988140
H	2.8033889	4.9682322	-1.8302161
H	3.4922642	3.4735180	-1.1665664
C	0.6044052	-4.6025997	-0.9279676
H	0.1219961	-4.8790251	-1.8828090
H	1.1863429	-5.4655028	-0.5596537
H	-0.1671093	-4.3347524	-0.1949691
C	2.6870901	-3.7397366	-1.9506565
H	3.4633444	-4.2646624	-1.3627263
H	2.3914209	-4.3907010	-2.7902113
H	3.1125282	-2.8223728	-2.3789707
C	0.3347750	0.9334121	4.6312994
H	0.0694957	0.1227871	5.3334399
H	0.7262267	1.7898371	5.2079133
H	-0.5608306	1.2397186	4.0754772
C	2.6767548	0.2068592	4.2793113
H	2.5328519	-0.2334998	5.2798853
H	3.2560044	-0.5129586	3.6846922
H	3.2610718	1.1393290	4.3951345
O	-0.2590393	-0.4522478	-2.4029115
O	-3.1413758	0.4993341	1.1582148

O	-2.3542424	0.0457198	-2.2499243
O	-2.8276340	-1.6046858	0.7715357
N	-3.5645532	-0.7070390	1.3271554
N	-1.3671702	-0.2149925	-3.0207319
O	-4.5435798	-0.9672488	1.9564743
O	-1.4529858	-0.2363032	-4.2130076
Am	-1.1771142	-0.0701746	-0.1159107

Eu(HMNTA)(NO₃)₂⁺

N	-0.2098764	0.1305704	-0.1819270
C	1.1950162	-0.2902343	-0.0849279
H	1.8287217	0.6030708	0.0490355
H	1.3571060	-0.9246354	0.8064458
C	-1.1670782	-0.8774161	0.2954831
H	-0.6258064	-1.7234009	0.7575021
H	-1.7968598	-0.4564384	1.0984812
C	-0.4325829	1.4701385	0.3804580
H	-1.5177569	1.6465430	0.4467085
H	-0.0058037	1.5631874	1.3995849
C	0.1323545	2.5546225	-0.5542965
C	1.6988019	-0.9919498	-1.3589402
C	-2.0888295	-1.4461792	-0.8039407
O	-1.9241052	-1.1068233	-1.9908430
O	1.0425466	-0.8661765	-2.4089214
O	0.4819505	2.2258032	-1.7088675
N	-3.0522474	-2.3048376	-0.4431487
N	0.2287038	3.8139495	-0.1165730
N	2.8441624	-1.6869094	-1.3234919
C	-3.9957166	-2.8158903	-1.4432405
H	-3.9294345	-3.9170950	-1.4914322
H	-5.0249101	-2.5319554	-1.1600044
H	-3.7564060	-2.3913196	-2.4260240
C	-3.3144280	-2.7143244	0.9362342
H	-4.0720583	-2.0625859	1.4113851
H	-3.7044083	-3.7448209	0.9289891
H	-2.4012042	-2.7108057	1.5477598
C	0.7715997	4.8554726	-0.9942897
H	-0.0331263	5.5470557	-1.3023673
H	1.5416529	5.4264188	-0.4469327
H	1.2145914	4.3927678	-1.8854351
C	-0.2179448	4.2722181	1.1980663
H	0.6427499	4.4474357	1.8703213
H	-0.7601807	5.2249845	1.0757541
H	-0.9070984	3.5585076	1.6689489
C	3.3222227	-2.3669821	-2.5323616
H	4.2367389	-1.8742962	-2.9085393
H	3.5581197	-3.4177772	-2.2894109
H	2.5458995	-2.3310366	-3.3072433
C	3.7049293	-1.8227763	-0.1499772
H	4.7561078	-1.7203447	-0.4685197
H	3.5092810	-1.0423629	0.5975929
H	3.5839064	-2.8166417	0.3207336
Eu	-0.7103819	0.6226794	-3.0218517

O	-2.4175789	1.8317102	-1.7436332
O	-0.2681738	-0.2806878	-5.1742042
O	-2.7746967	1.5431734	-3.8515237
O	0.5670669	1.6633505	-4.7355269
N	0.4380475	0.7103237	-5.5912378
N	-3.2150142	2.0021826	-2.7436916
O	0.9397821	0.7391802	-6.6735271
O	-4.2758312	2.5420890	-2.6299565

Am(HMNTA)(NO₃)₃

N	1.8836375	0.0101515	-0.2275347
C	2.1036206	0.5976254	1.0648716
H	2.2109749	-0.2129228	1.8031927
H	3.0529904	1.1777466	1.0995786
C	1.9394767	0.8352941	-1.4021011
H	2.1121071	1.8786610	-1.0908871
H	2.7935081	0.5629677	-2.0615918
C	1.8844788	-1.4200455	-0.3690222
H	1.8849773	-1.6640374	-1.4435416
H	2.8072601	-1.8777865	0.0530378
C	0.6611442	-2.1007532	0.2916459
C	0.9516307	1.5268947	1.5174716
C	0.6407074	0.7860651	-2.2405375
O	-0.3093797	0.0977190	-1.8449343
O	-0.0068570	1.7138464	0.7540987
O	-0.1586900	-1.3994264	0.9013028
N	0.5925481	1.4552912	-3.4103584
N	0.5465920	-3.4422481	0.2324755
N	1.0432839	2.1505973	2.7085950
C	-0.6034033	1.3710134	-4.2504669
H	-1.1749754	2.3157219	-4.2105077
H	-0.3017826	1.1713220	-5.2945449
H	-1.2470302	0.5575368	-3.8902623
C	1.6538365	2.3101175	-3.9213554
H	2.1877676	1.8262352	-4.7627771
H	1.2122263	3.2517124	-4.2929310
H	2.3840356	2.5695301	-3.1432078
C	-0.6061507	-4.0991530	0.8506342
H	-1.3797831	-4.3258261	0.0953173
H	-0.2713026	-5.0370467	1.3274753
H	-1.0396258	-3.4354089	1.6109676
C	1.4040398	-4.3176166	-0.5525071
H	1.7984133	-5.1311872	0.0843044
H	0.8265510	-4.7764698	-1.3772455
H	2.2570287	-3.7796074	-0.9857887
C	-0.0347409	3.0366078	3.1492903
H	-0.6986270	2.5181010	3.8644786
H	0.4054620	3.9250000	3.6354242
H	-0.6282597	3.3498982	2.2799807
C	2.0916121	1.9235425	3.6921317
H	1.6472693	1.5491945	4.6330675
H	2.8293041	1.1879876	3.3469518
H	2.6214253	2.8691941	3.9149639

O	-2.1974600	2.3857969	-1.0763775
O	-2.2461228	-2.0276363	-1.0524548
O	-3.4256972	0.7872405	-1.8407593
O	-3.4378664	1.3907464	1.6465223
O	-3.6813528	-1.4701694	0.4583726
O	-1.8223722	0.3103374	2.5796235
N	-3.0375422	1.9924193	-1.9584039
O	-3.4106314	2.7141074	-2.8539885
N	-3.2689697	-2.3539927	-0.3656144
O	-3.7966989	-3.4372204	-0.4694029
N	-2.8307767	1.0852463	2.7225090
O	-3.1622578	1.5136567	3.8025052
Am	-1.9126452	0.2189315	0.0845503

Eu(HMNTA)(NO₃)₃

N	1.9095117	-0.0321104	-0.2523665
C	2.1175856	0.5649115	1.0371718
H	2.2212998	-0.2390886	1.7833427
H	3.0663283	1.1456533	1.0734771
C	1.9723296	0.7861847	-1.4311539
H	2.1795160	1.8242811	-1.1251733
H	2.8111653	0.4858333	-2.0980363
C	1.8889336	-1.4631676	-0.3781102
H	1.8725042	-1.7205524	-1.4495767
H	2.8095377	-1.9282015	0.0403113
C	0.6607619	-2.1166670	0.3000224
C	0.9619594	1.4972930	1.4747943
C	0.6640587	0.7689085	-2.2574650
O	-0.2766009	0.0582575	-1.8775300
O	0.0091738	1.6780093	0.7033470
O	-0.1663402	-1.3905757	0.8689630
N	0.5966072	1.4881571	-3.3955112
N	0.5481817	-3.4595577	0.2972025
N	1.0467059	2.1282420	2.6631925
C	-0.6384864	1.4874329	-4.1816470
H	-1.2366965	2.3926628	-3.9739663
H	-0.3820470	1.4556122	-5.2551325
H	-1.2371315	0.6048713	-3.9201872
C	1.6154456	2.4214314	-3.8519777
H	1.9005272	2.1902513	-4.8952271
H	1.2232814	3.4558702	-3.8257018
H	2.5210822	2.3793499	-3.2331870
C	-0.6141009	-4.0904102	0.9247429
H	-1.3721048	-4.3577442	0.1668371
H	-0.2861218	-5.0019665	1.4547362
H	-1.0657682	-3.3913525	1.6413922
C	1.4065903	-4.3632938	-0.4540913
H	1.7638422	-5.1764881	0.2042254
H	0.8424853	-4.8205348	-1.2891704
H	2.2839290	-3.8499643	-0.8686322
C	-0.0447235	2.9998692	3.1006676
H	-0.7210360	2.4652037	3.7915532
H	0.3816414	3.8808726	3.6114270

H	-0.6228630	3.3266421	2.2260430
C	2.0727317	1.8769263	3.6647933
H	1.6369623	1.3556724	4.5384701
H	2.8941714	1.2654580	3.2694200
H	2.4977173	2.8354444	4.0150758
O	-2.0802880	2.2854865	-1.2644275
O	-2.2169700	-1.9983758	-1.0873733
O	-3.5300831	0.7531114	-1.7054303
O	-3.3574480	1.5059417	1.4274274
O	-3.5466489	-1.4779587	0.5278540
O	-1.8689651	0.3494099	2.4699615
N	-3.0800284	1.9117363	-1.9679372
O	-3.5431029	2.6092700	-2.8415431
N	-3.1786132	-2.3472489	-0.3274432
O	-3.6895416	-3.4425831	-0.3975045
N	-2.8317004	1.1864784	2.5399883
O	-3.1951872	1.6592895	3.5917693
Eu	-1.8570634	0.2033181	0.0135317

Am(HMNTA)₂³⁺

N	2.7526237	-0.0159773	-0.1226061
C	3.2512248	-0.7399223	1.0610743
H	3.2005363	-1.8256593	0.8617913
H	4.3129709	-0.5020052	1.2546832
C	3.1963811	1.3898827	-0.1220983
H	3.2144030	1.7570892	0.9200242
H	4.2276883	1.4838099	-0.5090668
C	3.1297143	-0.7011479	-1.3721124
H	3.0398855	0.0132570	-2.2110514
H	4.1848451	-1.0287744	-1.3450478
C	2.1679674	-1.8618383	-1.6663181
C	2.3625327	-0.4634641	2.2838629
C	2.2062811	2.2768635	-0.8907823
O	1.0212191	1.8687539	-1.0017236
O	1.1823503	-0.0842954	2.0701258
O	1.0190360	-1.8065091	-1.1568931
N	2.6123347	3.4456610	-1.3801493
N	2.5524003	-2.8592725	-2.4591754
N	2.8405677	-0.6553118	3.5111136
C	1.6874506	4.2985864	-2.1387784
H	1.4841575	5.2262439	-1.5752723
H	2.1516516	4.5665809	-3.1033815
H	0.7486898	3.7595523	-2.3169480
C	3.9794805	3.9677614	-1.2272552
H	4.6398568	3.6082083	-2.0374355
H	3.9377240	5.0663257	-1.2819136
H	4.4095530	3.7036114	-0.2500789
C	1.6508606	-3.9883528	-2.7252714
H	1.3283155	-3.9714412	-3.7813750
H	2.1911370	-4.9320221	-2.5373256
H	0.7743256	-3.9259547	-2.0686659
C	3.8654204	-2.9383725	-3.1169381

H	4.5791181	-3.5253980	-2.5105353
H	3.7375660	-3.4473863	-4.0851363
H	4.2816852	-1.9422715	-3.3216005
C	2.0087666	-0.3663193	4.6866999
H	1.7323241	-1.3078823	5.1937566
H	2.5871593	0.2558106	5.3908399
H	1.1017030	0.1681039	4.3780683
C	4.1895334	-1.1540667	3.8140549
H	4.1256423	-1.8194272	4.6900511
H	4.6073427	-1.7402899	2.9845094
H	4.8717341	-0.3209532	4.0625800
Am	-0.0918471	-0.0128549	0.0163154
N	-2.9434953	-0.0213260	0.1157752
C	-3.3400406	-0.8489562	1.2692240
H	-3.2729895	-0.2369933	2.1871991
H	-4.3923564	-1.1766560	1.1853972
C	-3.4279355	-0.5939319	-1.1529380
H	-3.3836371	-1.6964249	-1.0860540
H	-4.4862664	-0.3304161	-1.3327178
C	-3.3787358	1.3777878	0.2793969
H	-3.3713585	1.8712519	-0.7094376
H	-4.4176102	1.4334087	0.6535605
C	-2.5213793	-0.1798602	-2.3212786
C	-2.3996265	2.1519334	1.1739499
C	-2.3773818	-2.0301009	1.4537486
O	-1.3347901	0.1401547	-2.0541258
O	-1.2116456	-1.9113222	0.9959865
O	-1.2221262	1.7183542	1.2611209
N	-2.8079815	3.2564194	1.7935173
N	-2.9987914	-0.2024329	-3.5633996
N	-2.7857553	-3.1092125	2.1170265
C	-1.8851785	-4.2542503	2.3080664
H	-1.7093042	-4.4142495	3.3860593
H	-2.3527912	-5.1614201	1.8876811
H	-0.9317309	-4.0617656	1.8009013
C	-4.1388007	-3.2487089	2.6817162
H	-4.4583657	-2.3316573	3.2002955
H	-4.8764695	-3.5160751	1.9040755
H	-4.1201073	-4.0587432	3.4257495
C	-2.1574340	0.2109435	-4.6941663
H	-2.6933086	0.9746871	-5.2836223
H	-1.2140637	0.6274301	-4.3200789
H	-1.9503969	-0.6563234	-5.3457574
C	-4.3691373	-0.6158579	-3.9056489
H	-4.7135821	-1.4476355	-3.2735160
H	-5.0755018	0.2306413	-3.8291573
H	-4.3723910	-0.9713756	-4.9470191
C	-1.8942766	4.0014786	2.6703125
H	-2.3739798	4.1468108	3.6534673
H	-0.9603512	3.4392513	2.7943084
H	-1.6783267	4.9920079	2.2326656
C	-4.1678059	3.8057464	1.6709407
H	-4.5591195	3.6991581	0.6481686

H	-4.8606055	3.3304054	2.3889206
H	-4.1268117	4.8820287	1.8967691

Eu(HMNTA)₂³⁺

N	2.7883781	-0.0165199	-0.1249756
C	3.2761349	-0.7097721	1.0765828
H	3.2651829	-1.7989765	0.8905967
H	4.3242672	-0.4391855	1.3001836
C	3.2041986	1.3936073	-0.1582547
H	3.2390916	1.7802597	0.8763212
H	4.2235804	1.5035303	-0.5718757
C	3.1471939	-0.7297501	-1.3598558
H	3.0758916	-0.0289925	-2.2119785
H	4.1930277	-1.0867450	-1.3323522
C	2.1537717	-1.8682402	-1.6327612
C	2.3454749	-0.4477963	2.2712159
C	2.1763428	2.2440346	-0.9197281
O	1.0027717	1.7985057	-1.0051198
O	1.1663433	-0.0905970	2.0213123
O	1.0099205	-1.7762536	-1.1181707
N	2.5342032	3.4174713	-1.4348142
N	2.5094414	-2.8852394	-2.4138009
N	2.7909089	-0.6303083	3.5121434
C	1.5687155	4.2232814	-2.1938131
H	1.3323457	5.1484410	-1.6390628
H	2.0145157	4.4999838	-3.1646313
H	0.6518264	3.6438909	-2.3581315
C	3.8797010	3.9994920	-1.3181524
H	4.4952968	3.7561605	-2.2031653
H	3.7795466	5.0947611	-1.2593353
H	4.3928884	3.6662845	-0.4053723
C	1.5810352	-3.9967165	-2.6600111
H	1.2890505	-4.0134211	-3.7247464
H	2.0840234	-4.9488850	-2.4180710
H	0.6894726	-3.8788217	-2.0320163
C	3.8244550	-3.0018174	-3.0637241
H	4.5492708	-3.5216166	-2.4109135
H	3.7043950	-3.5953303	-3.9830669
H	4.2232352	-2.0198206	-3.3562790
C	1.9219659	-0.3546432	4.6633810
H	1.6806590	-1.2966251	5.1870869
H	2.4533817	0.3110578	5.3651419
H	0.9976860	0.1273536	4.3218810
C	4.1446746	-1.0932432	3.8502110
H	4.0805883	-1.7277750	4.7484234
H	4.5829835	-1.7018036	3.0473821
H	4.8099705	-0.2403646	4.0771745
Eu	-0.1004731	-0.0233199	0.0168524
N	-2.9837903	-0.0005925	0.1335914
C	-3.3584855	-0.8345369	1.2855617
H	-3.2864546	-0.2270296	2.2061169
H	-4.4079602	-1.1753103	1.2170214

C	-3.4727872	-0.5602113	-1.1352832
H	-3.4625178	-1.6631855	-1.0681006
H	-4.5217873	-0.2686674	-1.3208902
C	-3.3879945	1.4024393	0.3113596
H	-3.4078964	1.8966269	-0.6769822
H	-4.4110596	1.4795775	0.7238293
C	-2.5368351	-0.1821320	-2.2939517
C	-2.3618282	2.1548943	1.1710959
C	-2.3792983	-2.0043193	1.4506256
O	-1.3485838	0.1035560	-1.9971905
O	-1.2227435	-1.8691672	0.9747439
O	-1.1976228	1.6828861	1.2327120
N	-2.7148426	3.2772426	1.7922738
N	-2.9681126	-0.2087466	-3.5544150
N	-2.7641873	-3.0916840	2.1136764
C	-1.8441926	-4.2232440	2.2917758
H	-2.3163243	-5.1424651	1.9045797
H	-0.9124819	-4.0285610	1.7464712
H	-1.6264359	-4.3626812	3.3651427
C	-4.1061637	-3.2445455	2.7019954
H	-4.4044788	-2.3483999	3.2684596
H	-4.8635729	-3.4690228	1.9300725
H	-4.0797768	-4.0881727	3.4071864
C	-2.0449369	0.0874282	-4.6582123
H	-2.4244911	0.9512788	-5.2314655
H	-1.0498771	0.3157878	-4.2585878
H	-1.9882623	-0.7836012	-5.3344856
C	-4.3139465	-0.5992114	-3.9926255
H	-4.2770523	-1.5864537	-4.4872051
H	-5.0262656	-0.6489236	-3.1598775
H	-4.6831961	0.1399168	-4.7231348
C	-1.7556352	3.9913805	2.6452286
H	-2.2134277	4.1691118	3.6335009
H	-0.8457106	3.3896839	2.7612362
H	-1.5036048	4.9668816	2.1932718
C	-4.0545683	3.8789624	1.7042628
H	-4.5158625	3.7065897	0.7210308
H	-4.7179708	3.4966544	2.5014081
H	-3.9537431	4.9675662	1.8341637

La(HMNTA)₂³⁺

N	2.9345151	-0.0242186	-0.1322542
C	3.4288180	-0.7272409	1.0617505
H	3.3996976	-1.8158989	0.8723612
H	4.4845592	-0.4726557	1.2684391
C	3.3618771	1.3831755	-0.1520936
H	3.3835839	1.7637711	0.8854456
H	4.3900048	1.4843004	-0.5462769
C	3.3076846	-0.7249535	-1.3705175
H	3.2317991	-0.0181418	-2.2175884
H	4.3590569	-1.0652073	-1.3387451
C	2.3398661	-1.8813515	-1.6700221

C	2.5274387	-0.4628404	2.2796997
C	2.3632864	2.2606358	-0.9257238
O	1.1778372	1.8512219	-1.0258577
O	1.3366011	-0.1199124	2.0632933
O	1.1809692	-1.8158603	-1.1851816
N	2.7633997	3.4250419	-1.4315111
N	2.7361310	-2.8858050	-2.4485025
N	3.0105511	-0.6324616	3.5083232
C	1.8314454	4.2630095	-2.1975709
H	1.5939430	5.1795414	-1.6287920
H	2.3078587	4.5529215	-3.1496618
H	0.9095457	3.7037152	-2.3998678
C	4.1213127	3.9706044	-1.2866337
H	4.7564006	3.6923670	-2.1473847
H	4.0508626	5.0691247	-1.2526952
H	4.5971811	3.6430678	-0.3517919
C	1.8363213	-4.0134460	-2.7252557
H	1.5356603	-4.0034607	-3.7879252
H	2.3682693	-4.9578693	-2.5182903
H	0.9462490	-3.9425805	-2.0880441
C	4.0626154	-2.9680508	-3.0796096
H	4.7851934	-3.4903750	-2.4262908
H	3.9658714	-3.5440074	-4.0127764
H	4.4508648	-1.9747046	-3.3459087
C	2.1717539	-0.3571720	4.6820147
H	1.9238518	-1.3015936	5.1985203
H	2.7312971	0.2892487	5.3795420
H	1.2486325	0.1463773	4.3692425
C	4.3735753	-1.0929001	3.8114123
H	4.3368618	-1.7052368	4.7262888
H	4.7819068	-1.7236754	3.0098635
H	5.0497360	-0.2382400	3.9956393
La	-0.0983847	-0.0313377	0.0163012
N	-3.1173978	-0.0054010	0.1438462
C	-3.5059457	-0.8157667	1.3088836
H	-3.4164846	-0.1965215	2.2203335
H	-4.5640639	-1.1299539	1.2459356
C	-3.6184373	-0.5877638	-1.1111901
H	-3.5883193	-1.6897316	-1.0304116
H	-4.6754711	-0.3147070	-1.2785491
C	-3.5335654	1.3979517	0.2944716
H	-3.5334971	1.8783884	-0.7011449
H	-4.5675894	1.4707699	0.6795791
C	-2.7171300	-0.2122092	-2.2996408
C	-2.5403160	2.1811970	1.1687989
C	-2.5610478	-2.0133002	1.4946090
O	-1.5167252	0.0656441	-2.0437890
O	-1.3911108	-1.9129530	1.0431258
O	-1.3609901	1.7502626	1.2452742

N	-2.9406507	3.2903030	1.7861653
N	-3.1914378	-0.2305983	-3.5447392
N	-2.9918779	-3.0895800	2.1484822
C	-2.1153957	-4.2549708	2.3273445
H	-2.6354398	-5.1583932	1.9651835
H	-1.1877644	-4.1103656	1.7599080
H	-1.8801651	-4.3873417	3.3981073
C	-4.3411226	-3.2045516	2.7271259
H	-4.6507611	-2.2725029	3.2235994
H	-5.0864460	-3.4875709	1.9622849
H	-4.3215030	-3.9942878	3.4929543
C	-2.3110342	0.0888270	-4.6764482
H	-2.7457781	0.9257024	-5.2504254
H	-1.3169338	0.3684685	-4.3080755
H	-2.2311208	-0.7884604	-5.3424335
C	-4.5508234	-0.6151146	-3.9437652
H	-4.5056211	-1.5191681	-4.5762700
H	-5.1959862	-0.8278748	-3.0830643
H	-5.0042413	0.1985323	-4.5356629
C	-2.0187475	4.0327430	2.6560165
H	-2.5126741	4.2223455	3.6243415
H	-1.1053817	3.4460561	2.8150850
H	-1.7625580	5.0028497	2.1945065
C	-4.2922434	3.8587514	1.6687462
H	-4.7309335	3.6695695	0.6784919
H	-4.9614941	3.4665180	2.4561812
H	-4.2197030	4.9504182	1.7925609

Pr(HMNTA)₂³⁺

N	2.8934542	-0.0233642	-0.1243089
C	3.3670274	-0.7124185	1.0828231
H	3.3565899	-1.8022660	0.8995321
H	4.4138096	-0.4448741	1.3177750
C	3.3036968	1.3859248	-0.1596572
H	3.3358915	1.7744334	0.8744872
H	4.3237692	1.5016944	-0.5709466
C	3.2537189	-0.7408990	-1.3534782
H	3.1990088	-0.0397871	-2.2066977
H	4.2951733	-1.1106945	-1.3186587
C	2.2542043	-1.8715186	-1.6433565
C	2.4298276	-0.4510920	2.2734270
C	2.2787372	2.2395249	-0.9235201
O	1.1035180	1.7987899	-1.0153995
O	1.2492573	-0.0983884	2.0229996
O	1.1051002	-1.7792317	-1.1387666
N	2.6427558	3.4143045	-1.4316167

N	2.6104083	-2.8829950	-2.4312756
N	2.8738944	-0.6332070	3.5154112
C	1.6843421	4.2266743	-2.1925102
H	1.4467704	5.1496303	-1.6345519
H	2.1365886	4.5068952	-3.1593051
H	0.7667022	3.6509578	-2.3652963
C	3.9894937	3.9910601	-1.3009876
H	4.6228730	3.7233728	-2.1662322
H	3.8945696	5.0877729	-1.2704966
H	4.4806625	3.6772414	-0.3692119
C	1.6779456	-3.9866909	-2.6962404
H	1.3817499	-3.9813583	-3.7600202
H	2.1798040	-4.9444927	-2.4754734
H	0.7888731	-3.8796133	-2.0628648
C	3.9275602	-3.0016854	-3.0761786
H	4.6383111	-3.5533117	-2.4341261
H	3.8038401	-3.5649696	-4.0139957
H	4.3453720	-2.0186537	-3.3357521
C	2.0032976	-0.3595227	4.6657835
H	1.7634920	-1.3019179	5.1894994
H	2.5319331	0.3078966	5.3680282
H	1.0780635	0.1200564	4.3235137
C	4.2288549	-1.0940062	3.8528121
H	4.1706960	-1.6978748	4.7720503
H	4.6526588	-1.7329503	3.0656684
H	4.9036065	-0.2396626	4.0437866
Pr	-0.1013005	-0.0278665	0.0076165
N	-3.0924480	-0.0031854	0.1354640
C	-3.4604070	-0.8386735	1.2855794
H	-3.3972885	-0.2291180	2.2055461
H	-4.5062926	-1.1911677	1.2157087
C	-3.5769660	-0.5607601	-1.1341742
H	-3.5745580	-1.6636394	-1.0647086
H	-4.6226997	-0.2617625	-1.3282538
C	-3.4908135	1.3988819	0.3152185
H	-3.5205431	1.8913048	-0.6738850
H	-4.5095937	1.4808850	0.7377441
C	-2.6384896	-0.1902683	-2.2953446
C	-2.4584145	2.1602035	1.1618405
C	-2.4748350	-2.0042183	1.4590425
O	-1.4490091	0.0972571	-2.0049308
O	-1.3204983	-1.8728322	0.9750844
O	-1.2892037	1.6980868	1.2130034
N	-2.8112532	3.2835431	1.7818494
N	-3.0735634	-0.2195828	-3.5545716
N	-2.8508855	-3.0870842	2.1344958

C	-1.9335430	-4.2230346	2.2961065
H	-2.4328309	-5.1445381	1.9505673
H	-1.0253679	-4.0507377	1.7055113
H	-1.6689149	-4.3430479	3.3613471
C	-4.1805966	-3.2457287	2.7462375
H	-4.5353123	-2.3069657	3.1968918
H	-4.9206256	-3.6117420	2.0118322
H	-4.1024483	-3.9896385	3.5534453
C	-2.1657573	0.1139215	-4.6598923
H	-2.6172784	0.9147837	-5.2709240
H	-1.2018795	0.4504395	-4.2600884
H	-2.0171186	-0.7731278	-5.3009121
C	-4.4188017	-0.6159190	-3.9886594
H	-4.3379237	-1.4685854	-4.6851856
H	-5.0564318	-0.9195238	-3.1497133
H	-4.9008410	0.2218743	-4.5220732
C	-1.8474652	4.0061359	2.6222670
H	-2.3037354	4.2012417	3.6078800
H	-0.9401139	3.4023419	2.7469319
H	-1.5909901	4.9734557	2.1552599
C	-4.1515588	3.8847933	1.7017327
H	-4.6334153	3.6832447	0.7343787
H	-4.7986500	3.5278662	2.5236540
H	-4.0466678	4.9768406	1.7961054

Pm(HMNTA)₂³⁺

N	2.8534145	-0.0131271	-0.1273280
C	3.3350356	-0.6971769	1.0797308
H	3.3343882	-1.7872060	0.8972744
H	4.3793937	-0.4196432	1.3134764
C	3.2558212	1.3984336	-0.1683165
H	3.2830452	1.7922410	0.8639198
H	4.2759741	1.5173233	-0.5782197
C	3.2144344	-0.7310183	-1.3570169
H	3.1581079	-0.0308913	-2.2108034
H	4.2561485	-1.0996312	-1.3222487
C	2.2142141	-1.8609883	-1.6421734
C	2.3954575	-0.4419795	2.2698135
C	2.2255537	2.2387705	-0.9398204
O	1.0550297	1.7868107	-1.0332491
O	1.2149287	-0.0896063	2.0185079
O	1.0666211	-1.7626049	-1.1358341
N	2.5811602	3.4141832	-1.4528171
N	2.5663732	-2.8771837	-2.4253924
N	2.8373809	-0.6290952	3.5115262
C	1.6177267	4.2147019	-2.2196461

H	1.3683751	5.1365656	-1.6649885
H	2.0711637	4.4974088	-3.1851576
H	0.7069287	3.6288663	-2.3947330
C	3.9222656	4.0037662	-1.3227215
H	4.5538146	3.7503650	-2.1935840
H	3.8166012	5.0992274	-1.2815598
H	4.4216369	3.6863713	-0.3966446
C	1.6308216	-3.9800116	-2.6834338
H	1.3416686	-3.9857129	-3.7490924
H	2.1267710	-4.9375030	-2.4482523
H	0.7381756	-3.8617241	-2.0571114
C	3.8836777	-3.0024523	-3.0689165
H	4.5955867	-3.5445492	-2.4200902
H	3.7606035	-3.5781595	-3.9992083
H	4.2995608	-2.0220137	-3.3415233
C	1.9644451	-0.3618315	4.6616202
H	1.7266546	-1.3068167	5.1815315
H	2.4904983	0.3043741	5.3669452
H	1.0383778	0.1162628	4.3195145
C	4.1921009	-1.0899729	3.8494966
H	4.1313521	-1.7080795	4.7591406
H	4.6230176	-1.7148880	3.0550682
H	4.8621680	-0.2358624	4.0570612
Pm	-0.0998095	-0.0332268	0.0126553
N	-3.0530440	-0.0070059	0.1282269
C	-3.4319033	-0.8397698	1.2777191
H	-3.3845460	-0.2262591	2.1959136
H	-4.4749320	-1.1972159	1.1955364
C	-3.5363623	-0.5593072	-1.1439921
H	-3.5419574	-1.6623451	-1.0763546
H	-4.5792378	-0.2533195	-1.3415886
C	-3.4412064	1.3983739	0.3087784
H	-3.4500187	1.8967936	-0.6777522
H	-4.4653097	1.4884087	0.7164368
C	-2.5878365	-0.1944693	-2.2984367
C	-2.4114393	2.1384895	1.1760356
C	-2.4417849	-1.9977781	1.4705054
O	-1.3971704	0.0794286	-1.9984133
O	-1.2803708	-1.8587747	1.0078235
O	-1.2493047	1.6598790	1.2350821
N	-2.7562511	3.2580906	1.8065863
N	-3.0132930	-0.2159311	-3.5609350
N	-2.8247030	-3.0805430	2.1425910
C	-1.9031288	-4.2089289	2.3303079
H	-2.3820292	-5.1340414	1.9660704
H	-0.9781701	-4.0260532	1.7696894

H	-1.6716092	-4.3296785	3.4031130
C	-4.1671369	-3.2400405	2.7266289
H	-4.5099509	-2.3147168	3.2140060
H	-4.9034162	-3.5578163	1.9667362
H	-4.1162605	-4.0207207	3.5002484
C	-2.0876324	0.0914880	-4.6593399
H	-2.4896132	0.9331223	-5.2500125
H	-1.1051545	0.3589065	-4.2528797
H	-1.9941849	-0.7872185	-5.3216199
C	-4.3604960	-0.5909428	-4.0078135
H	-4.3043815	-1.5116633	-4.6150317
H	-5.0447942	-0.7696849	-3.1697717
H	-4.7748526	0.2144410	-4.6382856
C	-1.7923863	3.9562898	2.6675284
H	-2.2546545	4.1383274	3.6528907
H	-0.8919746	3.3414278	2.7884892
H	-1.5230042	4.9291488	2.2198531
C	-4.0884671	3.8764398	1.7209378
H	-4.5607357	3.6968658	0.7445107
H	-4.7493606	3.5133463	2.5290345
H	-3.9720272	4.9653768	1.8352448

Ho(HMNTA)₂³⁺

N	2.8936658	-0.0252262	-0.1304811
C	3.3367253	-0.6669698	1.1077319
H	3.3763300	-1.7605802	0.9533089
H	4.3597440	-0.3555174	1.3882965
C	3.2678757	1.3868026	-0.2191213
H	3.3440144	1.8037040	0.8015966
H	4.2617761	1.5203013	-0.6856654
C	3.2206862	-0.7914814	-1.3335688
H	3.2215068	-0.1118087	-2.2054270
H	4.2351575	-1.2282836	-1.2803267
C	2.1557476	-1.8662075	-1.6069405
C	2.3350917	-0.4114612	2.2459116
C	2.1850092	2.1957542	-0.9516906
O	1.0232486	1.7141818	-0.9970213
O	1.1604352	-0.0886108	1.9312236
O	1.0151612	-1.7064075	-1.1004166
N	2.4893514	3.3742390	-1.4886222
N	2.4535141	-2.9066423	-2.3807970
N	2.7170770	-0.5598753	3.5115732
C	1.4806520	4.1416559	-2.2301577
H	1.2189493	5.0586361	-1.6730491
H	1.8979540	4.4329000	-3.2092433
H	0.5831995	3.5280700	-2.3770382

C	3.8191325	3.9986413	-1.4079903
H	4.4339549	3.7412685	-2.2895064
H	3.6870980	5.0917050	-1.3874924
H	4.3500951	3.7139203	-0.4887083
C	1.4658165	-3.9655555	-2.6254935
H	1.1639626	-3.9606068	-3.6876754
H	1.9206344	-4.9441185	-2.3941469
H	0.5867190	-3.8061739	-1.9889623
C	3.7611997	-3.1015875	-3.0267244
H	4.4483227	-3.6709956	-2.3745732
H	3.6076333	-3.6793066	-3.9512793
H	4.2235061	-2.1452018	-3.3097588
C	1.7847079	-0.2832741	4.6117920
H	1.5206604	-1.2233102	5.1280994
H	2.2734717	0.3899398	5.3369027
H	0.8773248	0.1908375	4.2180075
C	4.0616950	-0.9873690	3.9264933
H	3.9658766	-1.5960573	4.8394815
H	4.5476431	-1.6109272	3.1636316
H	4.7006735	-0.1157266	4.1579130
Ho	-0.1017432	-0.0263444	0.0075854
N	-3.1010049	0.0001253	0.1404713
C	-3.4395970	-0.8826705	1.2575155
H	-3.4316625	-0.2977987	2.1953735
H	-4.4598749	-1.2983965	1.1606477
C	-3.5519946	-0.5051325	-1.1570067
H	-3.6075610	-1.6079753	-1.1157379
H	-4.5708905	-0.1519141	-1.3978163
C	-3.4549740	1.4003992	0.3750023
H	-3.5261574	1.9214684	-0.5973023
H	-4.4464424	1.4998129	0.8549311
C	-2.5429592	-0.1538984	-2.2640618
C	-2.3608765	2.1147027	1.1853851
C	-2.3891019	-1.9931181	1.4182093
O	-1.3633189	0.1035479	-1.9090899
O	-1.2432310	-1.7920517	0.9387417
O	-1.2048490	1.6173404	1.1809546
N	-2.6518562	3.2351605	1.8408544
N	-2.9087975	-0.1607318	-3.5442911
N	-2.7053731	-3.1062641	2.0740517
C	-1.7295357	-4.1941641	2.2191017
H	-2.1796570	-5.1356785	1.8602993
H	-0.8317511	-3.9659179	1.6313883
H	-1.4585859	-4.3161461	3.2825324
C	-4.0261814	-3.3474944	2.6780284
H	-4.4370632	-2.4353777	3.1353793

H	-4.7403452	-3.7485257	1.9363015
H	-3.9084811	-4.0935377	3.4784166
C	-1.9367567	0.1603394	-4.5975658
H	-2.3371852	0.9769307	-5.2230984
H	-0.9871703	0.4700568	-4.1450922
H	-1.7763739	-0.7242404	-5.2390734
C	-4.2382331	-0.5233543	-4.0513572
H	-4.1440481	-1.3887733	-4.7303889
H	-4.9330239	-0.7922991	-3.2468760
H	-4.6608953	0.3209805	-4.6231485
C	-1.6354878	3.9104461	2.6576193
H	-2.0529481	4.1092967	3.6594730
H	-0.7478698	3.2718749	2.7458546
H	-1.3575992	4.8739983	2.1950312
C	-3.9757273	3.8777375	1.8238564
H	-4.4959154	3.7170801	0.8689457
H	-4.6050711	3.5173304	2.6579156
H	-3.8342558	4.9630384	1.9436511

Tm(HMNTA)₂³⁺

N	2.8119410	-0.0184914	-0.1324843
C	3.2702914	-0.6861208	1.0889659
H	3.2903341	-1.7776039	0.9175419
H	4.3026463	-0.3924719	1.3535077
C	3.2034898	1.3919482	-0.1980904
H	3.2781841	1.7927028	0.8290183
H	4.2010197	1.5192139	-0.6580868
C	3.1401527	-0.7633652	-1.3510192
H	3.0999704	-0.0754787	-2.2154964
H	4.1683591	-1.1687330	-1.3208569
C	2.0979533	-1.8631332	-1.6039698
C	2.2901534	-0.4300002	2.2444235
C	2.1298534	2.2170237	-0.9251611
O	0.9667576	1.7410410	-0.9819722
O	1.1166977	-0.0858851	1.9481527
O	0.9643044	-1.7243114	-1.0764085
N	2.4442806	3.4003349	-1.4455386
N	2.4044641	-2.9011791	-2.3772357
N	2.6879530	-0.5977406	3.5024683
C	1.4435384	4.1843691	-2.1803512
H	1.1898937	5.0979366	-1.6140173
H	1.8644052	4.4819283	-3.1560383
H	0.5407711	3.5803898	-2.3343990
C	3.7787162	4.0128818	-1.3545887
H	4.3912648	3.7656575	-2.2405943
H	3.6556723	5.1065213	-1.3154492

H	4.3076543	3.7083514	-0.4405156
C	1.4362204	-3.9836719	-2.5957601
H	1.1121549	-3.9919516	-3.6513382
H	1.9183405	-4.9501193	-2.3688426
H	0.5672729	-3.8404815	-1.9415950
C	3.7036086	-3.0701637	-3.0472553
H	4.4146840	-3.6236256	-2.4071749
H	3.5450133	-3.6531024	-3.9677267
H	4.1399675	-2.1047163	-3.3406220
C	1.7765805	-0.3180485	4.6194237
H	1.5101679	-1.2585720	5.1335201
H	2.2847928	0.3444961	5.3409830
H	0.8685786	0.1692081	4.2434601
C	4.0317942	-1.0509742	3.8917482
H	3.9404007	-1.6670247	4.8002421
H	4.4948313	-1.6750403	3.1150860
H	4.6888762	-0.1924664	4.1212852
Tm	-0.0996226	-0.0225454	0.0165355
N	-3.0130535	-0.0077971	0.1384568
C	-3.3629048	-0.8673614	1.2729298
H	-3.3343821	-0.2681523	2.2012026
H	-4.3921037	-1.2624901	1.1879807
C	-3.4697316	-0.5431545	-1.1474429
H	-3.4919636	-1.6465061	-1.0913797
H	-4.5012849	-0.2208868	-1.3756962
C	-3.3906240	1.3937752	0.3416166
H	-3.4520279	1.8962251	-0.6409396
H	-4.3908034	1.4863162	0.8039890
C	-2.4804481	-0.1768929	-2.2658364
C	-2.3151745	2.1293782	1.1559148
C	-2.3296137	-1.9920867	1.4363478
O	-1.3000402	0.0905323	-1.9206062
O	-1.1823135	-1.8059129	0.9557498
O	-1.1571913	1.6374093	1.1732956
N	-2.6218228	3.2575646	1.7900949
N	-2.8596900	-0.1818474	-3.5420309
N	-2.6623278	-3.1000797	2.0929966
C	-1.7029180	-4.2027256	2.2363624
H	-2.1673958	-5.1367374	1.8762311
H	-0.8022178	-3.9868578	1.6483601
H	-1.4330856	-4.3305858	3.2993752
C	-3.9862483	-3.3182092	2.6992024
H	-4.3717061	-2.4031685	3.1730520
H	-4.7140198	-3.6896578	1.9554045
H	-3.8836664	-4.0793789	3.4872497
C	-1.9010093	0.1505021	-4.6042401

H	-2.2974319	0.9901198	-5.2014867
H	-0.9381651	0.4317178	-4.1613886
H	-1.7687718	-0.7200040	-5.2706410
C	-4.1930785	-0.5468942	-4.0370264
H	-4.1050026	-1.4146373	-4.7138795
H	-4.8814739	-0.8122900	-3.2258786
H	-4.6198954	0.2957534	-4.6081816
C	-1.6205556	3.9526133	2.6091676
H	-2.0487221	4.1556630	3.6057015
H	-0.7259632	3.3258426	2.7107660
H	-1.3511508	4.9151752	2.1396602
C	-3.9503175	3.8890222	1.7487214
H	-4.4630802	3.7004507	0.7948379
H	-4.5820320	3.5442375	2.5875590
H	-3.8184020	4.9781657	1.8423517

Lu(HMNTA)₂³⁺

N	2.9296937	-0.0214083	-0.1337603
C	3.3474947	-0.6416539	1.1197484
H	3.4247801	-1.7345992	0.9753532
H	4.3511484	-0.3008628	1.4344957
C	3.2773856	1.3913456	-0.2503998
H	3.3985631	1.8191752	0.7614770
H	4.2451412	1.5378543	-0.7657803
C	3.2272530	-0.8132601	-1.3236292
H	3.2502656	-0.1473190	-2.2055955
H	4.2258562	-1.2854897	-1.2675840
C	2.1277919	-1.8579026	-1.5802370
C	2.3064219	-0.4081203	2.2278711
C	2.1526045	2.1833848	-0.9384005
O	0.9962826	1.6858691	-0.9445466
O	1.1351280	-0.1016286	1.8841205
O	0.9959670	-1.6625678	-1.0658585
N	2.4201915	3.3660689	-1.4851076
N	2.3890376	-2.9159546	-2.3428870
N	2.6567987	-0.5517035	3.5029794
C	1.3764013	4.1213206	-2.1892058
H	1.1187910	5.0315102	-1.6191607
H	1.7571565	4.4236414	-3.1796934
H	0.4840213	3.4947786	-2.3106217
C	3.7463414	4.0037347	-1.4524815
H	4.3446815	3.7254213	-2.3390091
H	3.6048782	5.0955340	-1.4615191
H	4.2992000	3.7509349	-0.5366242
C	1.3727461	-3.9531165	-2.5614081
H	1.0445398	-3.9441305	-3.6157874

H	1.8126025	-4.9405252	-2.3392654
H	0.5130297	-3.7743019	-1.9036160
C	3.6825690	-3.1521659	-3.0031927
H	4.3579838	-3.7434876	-2.3583950
H	3.5003970	-3.7242707	-3.9262071
H	4.1723134	-2.2110769	-3.2907766
C	1.6945753	-0.2868819	4.5800919
H	1.4185399	-1.2314733	5.0815958
H	2.1626352	0.3812922	5.3231805
H	0.7969117	0.1892139	4.1666197
C	3.9971936	-0.9627406	3.9485198
H	3.8895031	-1.5514273	4.8730526
H	4.4974094	-1.6012457	3.2073420
H	4.6292166	-0.0835177	4.1703591
Lu	-0.1046977	-0.0241390	0.0118528
N	-3.1151206	0.0002950	0.1404309
C	-3.4325064	-0.9030804	1.2435821
H	-3.4452928	-0.3299668	2.1885423
H	-4.4399532	-1.3476153	1.1386685
C	-3.5437334	-0.4846511	-1.1692436
H	-3.6241685	-1.5862765	-1.1397171
H	-4.5481202	-0.1078876	-1.4342652
C	-3.4541093	1.3973454	0.3980051
H	-3.5564552	1.9285580	-0.5660621
H	-4.4281811	1.4993445	0.9121757
C	-2.5027354	-0.1431164	-2.2504634
C	-2.3320511	2.1006482	1.1792926
C	-2.3537333	-1.9879388	1.3952856
O	-1.3286245	0.1033334	-1.8692206
O	-1.2143278	-1.7605942	0.9109825
O	-1.1826016	1.5883543	1.1532244
N	-2.5952954	3.2275241	1.8349238
N	-2.8402225	-0.1419378	-3.5381288
N	-2.6418552	-3.1118655	2.0452590
C	-1.6456939	-4.1831894	2.1725972
H	-2.0913287	-5.1333005	1.8315748
H	-0.7667409	-3.9459267	1.5602719
H	-1.3452255	-4.2947261	3.2292953
C	-3.9512144	-3.3816018	2.6618769
H	-4.3825508	-2.4762095	3.1133242
H	-4.6600820	-3.8084238	1.9294352
H	-3.8078757	-4.1163003	3.4686454
C	-1.8474733	0.1844199	-4.5700157
H	-2.2405558	0.9969426	-5.2054169
H	-0.9102456	0.5023654	-4.0975624
H	-1.6661752	-0.6996132	-5.2066546

C	-4.1644098	-0.4865360	-4.0716167
H	-4.0540972	-1.3017530	-4.8073769
H	-4.8542135	-0.8249585	-3.2893540
H	-4.6011780	0.3873899	-4.5859985
C	-1.5545579	3.8988676	2.6236295
H	-1.9440053	4.1018071	3.6358804
H	-0.6679382	3.2561529	2.6898221
H	-1.2843474	4.8601272	2.1518088
C	-3.9156286	3.8783028	1.8441171
H	-4.4427536	3.7451922	0.8885867
H	-4.5420508	3.5004645	2.6726215
H	-3.7667426	4.9590609	1.9910246

Vibrational frequencies of optimized structures of Am³⁺ and Ln³⁺ complexes of HMNTAcalculated at the def-SV(P)/B3LYP level of theory
Am(NTA)(NO₃)₂⁺

# mode	symmetry	wave number	IR intensity
#		cm ⁻¹	km/mol
1	a	-3.64	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7		0	0
8	a	14.87	0.49894
9	a	21.56	1.1151
10	a	28.86	0.24225
11	a	29.74	1.1019
12	a	34.01	2.53068
13	a	36.85	1.51095
14	a	52.05	0.1175
15	a	53.06	0.80393
16	a	57.76	1.70316
17	a	61.09	1.97464
18	a	70.6	0.31311
19	a	80.35	0.62935
20	a	83.75	0.39991
21	a	87.46	0.97606
22	a	96.01	1.88548
23	a	102.21	0.56745
24	a	111.42	0.6979
25	a	116.84	0.6553
26	a	120.43	1.95653
27	a	124.68	0.721
28	a	129.25	3.17444
29	a	148.37	13.7684
30	a	151.62	1.28981
31	a	162.99	8.59436
32	a	175.52	12.44501
33	a	195.68	3.51046
34	a	204.05	1.33191
35	a	207.44	3.18453

36	a	215.28	0.73714
37	a	223.99	11.01267
38	a	236.66	41.25837
39	a	248.69	80.4877
40	a	254.63	8.71882
41	a	272.76	0.90455
42	a	277.91	0.93155
43	a	285.46	9.43788
44	a	293.57	11.27988
45	a	314.5	6.50074
46	a	379.67	1.56533
47	a	399.24	20.09933
48	a	410.32	43.56402
49	a	436.68	14.44751
50	a	443.3	3.05108
51	a	462.34	19.82146
52	a	472.22	2.9447
53	a	515.32	8.81573
54	a	531.22	14.71733
55	a	574.66	0.87429
56	a	604.72	2.67647
57	a	620.5	1.11167
58	a	642.39	47.60869
59	a	653.6	45.53717
60	a	655.61	13.22974
61	a	718.53	0.26103
62	a	724.14	0.95921
63	a	754.95	60.92996
64	a	763.57	37.2577
65	a	819.13	19.31391
66	a	824.21	18.11444
67	a	825.92	15.98702
68	a	831.73	16.57011
69	a	835.74	15.29363
70	a	914.03	66.56779
71	a	960.53	11.67194
72	a	962.06	7.70007
73	a	982.81	3.60485
74	a	995.51	22.63966
75	a	1005.78	22.72187
76	a	1017.06	27.29591

77	a	1057.08	89.42143
78	a	1069.29	72.22027
79	a	1072.76	7.32701
80	a	1076.15	6.45996
81	a	1076.99	14.90879
82	a	1112.55	4.72779
83	a	1114.06	3.68464
84	a	1115.04	3.8004
85	a	1155.68	105.52196
86	a	1159.06	96.03121
87	a	1166.74	3.96942
88	a	1167.77	10.40783
89	a	1169.02	7.89497
90	a	1184.61	24.60379
91	a	1187.33	26.92728
92	a	1194.96	18.39153
93	a	1269.09	252.13152
94	a	1278.02	119.63326
95	a	1279.39	49.65174
96	a	1280.87	25.78463
97	a	1292.44	304.68161
98	a	1298.11	19.7558
99	a	1333.23	16.40615
100	a	1361.16	26.33731
101	a	1376.78	21.39002
102	a	1389.38	31.03576
103	a	1395.34	14.05517
104	a	1429.72	16.5033
105	a	1432.25	12.03573
106	a	1432.71	20.56056
107	a	1438.32	17.85211
108	a	1443.84	12.98073
109	a	1446.68	26.47184
110	a	1461.11	21.4398
111	a	1464.54	26.48456
112	a	1466.33	34.46806
113	a	1468.3	1.41657
114	a	1470.02	0.57487
115	a	1472.84	9.34417
116	a	1475.11	9.25713
117	a	1476.6	7.58118

118	a	1484.06	2.41258
119	a	1487.09	6.54312
120	a	1487.34	2.56036
121	a	1488.07	28.1824
122	a	1488.52	10.1354
123	a	1490.23	18.2346
124	a	1497.5	12.46639
125	a	1546.83	45.8861
126	a	1549.08	26.54063
127	a	1556.02	57.44112
128	a	1687.43	439.07106
129	a	1690	617.29153
130	a	1700.8	1278.04976
131	a	1709.19	1314.93183
132	a	1737.48	49.44847
133	a	2992.17	30.47809
134	a	3012.49	16.99449
135	a	3019.52	15.26158
136	a	3022.66	19.10157
137	a	3023.81	16.33899
138	a	3025.13	16.23272
139	a	3031.44	24.11487
140	a	3031.75	20.0408
141	a	3032.87	17.38467
142	a	3077.74	3.22976
143	a	3082.49	3.48062
144	a	3104.41	3.61529
145	a	3104.68	8.65889
146	a	3105.53	6.57573
147	a	3106.56	7.0463
148	a	3107.8	0.78294
149	a	3108.22	0.66061
150	a	3112.6	2.49409
151	a	3152.79	5.98276
152	a	3157.91	5.96998
153	a	3165.92	4.91398
154	a	3183.14	0.98845
155	a	3185.19	1.06383
156	a	3189.26	0.84631
Şend			

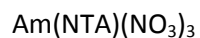
Eu(NTA)(NO₃)₂⁺

# mode	symmetry	wave number	IR intensity
#		cm ⁻¹	km/mol
1		0	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7	a	7.1	0.24207
8	a	18.53	0.74157
9	a	20.97	0.28059
10	a	22.7	0.81238
11	a	31.21	2.0104
12	a	32.98	0.17408
13	a	36.97	0.20365
14	a	39.11	0.34966
15	a	46.25	1.623
16	a	53.7	4.1526
17	a	61.46	1.04896
18	a	75.37	0.57562
19	a	82.86	0.74878
20	a	85.29	0.10411
21	a	91.54	2.00799
22	a	99.54	2.13978
23	a	103.04	0.6162
24	a	109.65	0.54285
25	a	115.08	0.55576
26	a	122.27	0.79835
27	a	130.24	0.39672
28	a	135	1.52693
29	a	148.26	6.19756
30	a	156.57	6.64755
31	a	163.4	11.35825
32	a	175.41	14.0095
33	a	194.25	7.23286
34	a	198.95	2.92317
35	a	211.08	1.00245

36	a	215.73	2.36567
37	a	233.23	7.37613
38	a	241.92	33.87418
39	a	249.58	16.33266
40	a	265.79	92.20953
41	a	279.28	0.83027
42	a	281	8.59855
43	a	287.3	12.5163
44	a	296.87	9.8409
45	a	309.7	10.32144
46	a	380.43	1.33123
47	a	396.12	11.81241
48	a	415.96	50.39587
49	a	431.4	16.32736
50	a	439.85	3.66885
51	a	459.54	19.18644
52	a	476.53	7.93557
53	a	500.23	5.60037
54	a	534.22	14.23216
55	a	571.25	6.90868
56	a	596.35	3.43068
57	a	622.37	1.68089
58	a	643.48	44.73651
59	a	652.69	44.80487
60	a	660.57	22.63581
61	a	720.12	0.05344
62	a	724.31	1.51654
63	a	758.29	65.9318
64	a	766.21	31.87743
65	a	817.16	18.5208
66	a	826.42	19.02291
67	a	828.95	18.5814
68	a	833.86	15.97597
69	a	835.81	12.09643
70	a	914.39	75.91108
71	a	953.37	8.91517
72	a	960.17	16.00672
73	a	972.42	5.36617
74	a	984.96	21.77574
75	a	996.3	15.71071
76	a	1013.42	20.91273

77	a	1059.59	63.57319
78	a	1066.76	4.17817
79	a	1067.16	9.09647
80	a	1068.77	11.35256
81	a	1070.4	63.7554
82	a	1105.38	3.35072
83	a	1105.77	2.42762
84	a	1106.49	1.238
85	a	1146.62	112.36348
86	a	1151.39	92.75748
87	a	1159.05	2.47099
88	a	1160.28	22.70695
89	a	1161.99	10.39692
90	a	1177.1	25.63181
91	a	1178.9	34.09512
92	a	1185.92	15.55968
93	a	1266.75	14.81349
94	a	1274.08	42.40689
95	a	1275.15	24.03398
96	a	1278.57	262.53794
97	a	1278.85	100.89035
98	a	1301.66	333.6559
99	a	1316.47	16.8111
100	a	1346.32	14.78322
101	a	1350.73	12.0972
102	a	1369.33	26.50362
103	a	1382.44	9.8168
104	a	1419.79	3.11595
105	a	1424.83	18.23768
106	a	1425.34	11.02032
107	a	1425.95	17.51248
108	a	1432.77	23.19148
109	a	1438.79	10.74587
110	a	1448.18	28.89747
111	a	1450.41	11.90776
112	a	1455.72	16.47825
113	a	1458.59	20.71845
114	a	1458.73	15.96693
115	a	1460.56	9.15379
116	a	1463.23	7.73972
117	a	1466.26	8.89482

118	a	1470.52	9.75452
119	a	1476.41	11.01841
120	a	1476.98	7.78221
121	a	1477.64	14.43487
122	a	1478.76	9.30566
123	a	1479.26	15.93859
124	a	1479.68	10.27322
125	a	1546.58	52.83082
126	a	1549.17	25.98842
127	a	1556.07	65.29727
128	a	1689.21	220.31524
129	a	1692.71	784.84678
130	a	1702.38	1206.38667
131	a	1708.37	1243.53426
132	a	1738.84	121.2819
133	a	3013.08	31.48788
134	a	3023.89	15.88714
135	a	3027.26	17.95549
136	a	3035.81	11.13695
137	a	3035.94	20.93961
138	a	3038.47	13.88272
139	a	3042.42	25.05836
140	a	3043.02	23.74559
141	a	3043.65	21.51776
142	a	3085.62	4.23324
143	a	3097.18	2.58716
144	a	3111.96	4.73132
145	a	3113.45	5.9604
146	a	3115.93	2.05648
147	a	3118.58	8.77044
148	a	3119.41	4.19099
149	a	3120.91	4.96939
150	a	3121.03	0.78449
151	a	3174.48	5.84572
152	a	3178.17	5.675
153	a	3187.52	4.59984
154	a	3195.64	1.03056
155	a	3197.46	1.35452
156	a	3201.61	1.12719
Şend			



# mode	symmetry	wave number	IR intensity
#		cm ⁻¹	km/mol
1		0	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7	a	31.21	0.46425
8	a	35.42	0.31886
9	a	37.43	0.12932
10	a	42.13	0.29474
11	a	47.79	0.22828
12	a	50.68	0.67617
13	a	55.12	1.04865
14	a	58.86	0.85488
15	a	68.45	8.01023
16	a	69.92	3.75741
17	a	77.23	3.02931
18	a	79.24	5.01287
19	a	86.58	1.56537
20	a	95.82	1.96327
21	a	99.28	1.68943
22	a	109.32	0.5644
23	a	114.89	0.10374
24	a	117.82	0.29734
25	a	138.75	2.74369
26	a	141.64	3.62078
27	a	145.81	4.10714
28	a	149.06	1.16431
29	a	152.55	0.42578
30	a	157.63	0.58071
31	a	163.41	0.31601
32	a	179.27	8.31356
33	a	186.45	2.18763
34	a	190.19	2.75895
35	a	194.35	10.88228

36	a	200.49	11.80054
37	a	203.62	1.49107
38	a	206.88	12.68512
39	a	211.37	16.12835
40	a	215.99	8.71485
41	a	217.03	46.26275
42	a	221.92	49.57157
43	a	223.87	46.7701
44	a	235.39	2.92005
45	a	239.72	3.89703
46	a	246.18	11.93159
47	a	281.29	2.69362
48	a	284.61	6.04477
49	a	289.45	5.16028
50	a	295.17	3.72664
51	a	296.6	3.03145
52	a	352.59	3.66041
53	a	387.49	19.46088
54	a	388.59	19.40549
55	a	423.54	1.69612
56	a	430.43	3.98843
57	a	432.16	3.8783
58	a	461.73	14.18847
59	a	515.76	13.73065
60	a	518.89	13.60441
61	a	562.6	8.44138
62	a	585.71	0.35589
63	a	587.06	0.82059
64	a	621.08	0.33437
65	a	640.94	20.00923
66	a	642.42	21.05918
67	a	725.23	0.14725
68	a	726.88	0.09268
69	a	727.22	0.38303
70	a	762.03	33.38085
71	a	763.38	33.45382
72	a	769.31	14.24422
73	a	805.59	21.5904
74	a	823.53	15.39752
75	a	824.79	11.93829
76	a	834.19	15.68476

77	a	835.06	18.55317
78	a	836.06	19.58734
79	a	917.34	15.80891
80	a	963.66	3.5267
81	a	965.58	2.16516
82	a	970.36	0.74026
83	a	992.89	2.65255
84	a	1002.35	33.07008
85	a	1002.54	30.94778
86	a	1077.23	7.25916
87	a	1080.45	9.48847
88	a	1081.16	13.83644
89	a	1084.59	42.19627
90	a	1085.23	40.35977
91	a	1087.02	38.05731
92	a	1116.41	1.4684
93	a	1117.64	3.05419
94	a	1118.58	5.19762
95	a	1159.64	181.21541
96	a	1160.99	179.75223
97	a	1166.72	5.46046
98	a	1168.31	5.98325
99	a	1168.68	9.92783
100	a	1173.28	0.8229
101	a	1217.81	17.35675
102	a	1218.21	17.51841
103	a	1277.62	1.17139
104	a	1285.17	48.76524
105	a	1285.71	47.08865
106	a	1288.42	16.72745
107	a	1335.86	235.04397
108	a	1340.89	276.05247
109	a	1341.81	22.54131
110	a	1343.83	137.25433
111	a	1346.8	336.88944
112	a	1364.97	11.74342
113	a	1406.31	30.18724
114	a	1406.57	23.87254
115	a	1429.86	10.18751
116	a	1430.73	14.7192
117	a	1431.52	12.64738

118	a	1434.71	23.24558
119	a	1436.1	10.89907
120	a	1437.41	44.0762
121	a	1452.84	13.8448
122	a	1454.25	8.60673
123	a	1459.36	3.08471
124	a	1460.64	8.32346
125	a	1461.58	23.74256
126	a	1464.56	5.61964
127	a	1466.41	9.43063
128	a	1466.59	23.15687
129	a	1472.25	6.90142
130	a	1475.29	1.97641
131	a	1478.67	5.18597
132	a	1481.16	11.78893
133	a	1486	17.58628
134	a	1489.09	17.86495
135	a	1490.54	25.4835
136	a	1544.82	87.38213
137	a	1545.39	78.57846
138	a	1547.8	65.38326
139	a	1639.78	618.90161
140	a	1642.79	607.24
141	a	1652.89	532.96453
142	a	1702.9	970.90747
143	a	1705.66	908.90383
144	a	1733.66	274.25566
145	a	2931.06	61.48392
146	a	2932.68	60.04716
147	a	2937.97	72.72196
148	a	2995.24	37.68439
149	a	3000	34.87415
150	a	3000.98	32.55201
151	a	3010.19	39.21115
152	a	3013.38	39.11721
153	a	3014.83	35.04265
154	a	3063.23	12.63956
155	a	3063.92	14.483
156	a	3070.31	11.93464
157	a	3080.49	2.76616
158	a	3085.74	4.32431

159	a	3086.88	7.75474
160	a	3088.12	4.90037
161	a	3090.93	8.87286
162	a	3093.53	8.10863
163	a	3149.56	7.62752
164	a	3154.6	6.03518
165	a	3156	2.26294
166	a	3157.57	1.61847
167	a	3158.79	6.20231
168	a	3161.37	0.46578
Şend			

Eu(NTA)(NO₃)₃

# mode	symmetry	wave number	IR intensity
#		cm**(-1)	km/mol
1		0	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7	a	3.98	0.6015
8	a	24.24	0.76582
9	a	33.73	0.32329
10	a	36.5	0.14454
11	a	38.68	0.11627
12	a	45.89	0.41212
13	a	49.05	0.86688
14	a	53.95	0.99509
15	a	56.02	0.53445
16	a	57.49	0.39336
17	a	64.45	0.99755
18	a	69.72	7.00619
19	a	73.52	2.61664
20	a	77.94	2.19734
21	a	85.65	4.76017
22	a	93.02	1.39029
23	a	96.86	2.03642
24	a	101.32	2.50259

25	a	115.32	0.20979
26	a	117.3	0.02452
27	a	119.13	0.23277
28	a	153.82	3.10027
29	a	155.03	2.44767
30	a	156.57	0.77459
31	a	158.13	3.83851
32	a	185.66	9.14185
33	a	189.21	1.75072
34	a	191.95	0.41786
35	a	198.23	1.07688
36	a	200.15	3.01795
37	a	203.12	2.76858
38	a	206.81	1.81753
39	a	208.44	8.43588
40	a	211.55	14.31443
41	a	214.32	9.09613
42	a	216.46	4.86296
43	a	226.43	50.40311
44	a	236.84	71.471
45	a	240.87	57.24422
46	a	245.68	31.04292
47	a	280.04	6.36705
48	a	281.08	4.07655
49	a	287.52	2.78675
50	a	288.4	3.10414
51	a	289.49	7.62422
52	a	353.11	2.98545
53	a	385.77	20.82586
54	a	387.28	20.91135
55	a	423.61	2.40541
56	a	428.36	4.67423
57	a	429.8	4.24917
58	a	459.55	14.52319
59	a	514.09	14.08402
60	a	514.63	15.10257
61	a	561.06	10.73185
62	a	585.89	0.1469
63	a	586.68	0.30263
64	a	621.51	0.48649
65	a	641.73	23.06027

66	a	642.63	22.59503
67	a	727.33	0.15517
68	a	728.25	0.35735
69	a	728.49	0.06076
70	a	765.23	31.763
71	a	766.8	25.20214
72	a	771.77	13.34135
73	a	807.29	20.19991
74	a	824.94	13.3113
75	a	826.36	12.97542
76	a	837.71	15.44572
77	a	837.93	14.9362
78	a	838.15	27.4243
79	a	917.47	15.46856
80	a	963.35	2.95331
81	a	963.68	2.57647
82	a	968.64	1.05655
83	a	990.92	1.12201
84	a	1000.07	34.58107
85	a	1001.86	32.64258
86	a	1070.88	5.56686
87	a	1072.05	6.10153
88	a	1072.76	11.09871
89	a	1088.34	36.81121
90	a	1089.35	40.62751
91	a	1090.75	38.54925
92	a	1108.77	0.91963
93	a	1109.59	1.82967
94	a	1109.69	1.11564
95	a	1156.12	180.60829
96	a	1156.28	174.77501
97	a	1162.17	1.24816
98	a	1164.27	15.20985
99	a	1164.44	14.23074
100	a	1170.67	0.13188
101	a	1216.44	14.8394
102	a	1218.15	16.59742
103	a	1275.37	0.93184
104	a	1284.47	50.47471
105	a	1284.89	46.64319
106	a	1287.83	14.38982

107	a	1339.67	29.46587
108	a	1340.29	27.78161
109	a	1353.94	455.45166
110	a	1356.43	250.25922
111	a	1360.31	310.87086
112	a	1361.83	5.78752
113	a	1406.35	27.52456
114	a	1406.86	28.68616
115	a	1425.95	11.75102
116	a	1426.75	13.74902
117	a	1428.06	12.66492
118	a	1434.08	11.45586
119	a	1435.71	35.77351
120	a	1436.86	21.39081
121	a	1449.91	16.86633
122	a	1450.03	10.36969
123	a	1455.24	10.86102
124	a	1458.16	4.92325
125	a	1459.79	3.19982
126	a	1462.06	4.93693
127	a	1464.01	22.79114
128	a	1465.27	19.31075
129	a	1471.01	9.75658
130	a	1473.19	3.06386
131	a	1473.63	3.51118
132	a	1475.02	2.17662
133	a	1486.69	25.47742
134	a	1487.36	20.86128
135	a	1488.94	35.3521
136	a	1545.97	79.36789
137	a	1546.88	81.67104
138	a	1549.16	73.19063
139	a	1637.17	556.61073
140	a	1638.85	563.46808
141	a	1650.39	485.91266
142	a	1705.08	934.09787
143	a	1705.69	926.22207
144	a	1733.85	236.61118
145	a	2950.19	64.8094
146	a	2951.93	62.07574
147	a	2956.74	70.30075

148	a	3024.5	33.6048
149	a	3025.26	33.30536
150	a	3025.41	29.05958
151	a	3039.27	42.99656
152	a	3039.55	34.48031
153	a	3039.97	23.97314
154	a	3087.72	14.26153
155	a	3089.74	14.65665
156	a	3089.92	14.94659
157	a	3099.81	0.51191
158	a	3101.67	4.88954
159	a	3102.53	4.89667
160	a	3118.61	9.38311
161	a	3119.51	8.36806
162	a	3120.28	9.01574
163	a	3177.83	6.86369
164	a	3179.13	6.83119
165	a	3179.71	6.94967
166	a	3180.86	0.9957
167	a	3181.77	0.96252
168	a	3184.5	0.53495
Şend			

Am(NTA)₂³⁺

# mode	symmetry	wave number	IR intensity
#		cm**(-1)	km/mol
1		0	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7	a	21.3	0.02528
8	a	25.87	3.04021
9	a	27.53	3.21333
10	a	34.64	1.24587
11	a	35.22	1.25294
12	a	36.7	0.56563
13	a	37.21	0.82584

14	a	60.2	2.37831
15	a	70.69	0.03126
16	a	76.78	1.68387
17	a	77.36	4.02589
18	a	77.95	3.17026
19	a	79.53	0.42829
20	a	87.03	0.2381
21	a	87.89	0.32704
22	a	94.75	0.04045
23	a	110.97	4.51143
24	a	112.53	0.73249
25	a	113.47	0.23972
26	a	126.92	1.69634
27	a	128.85	32.37831
28	a	137.71	5.39106
29	a	139.99	10.64866
30	a	142.61	9.18411
31	a	144.82	4.87741
32	a	150.95	2.0417
33	a	152.95	7.92179
34	a	155.13	15.32756
35	a	157.7	7.66635
36	a	158.34	9.2467
37	a	167.04	2.60616
38	a	170.15	2.50381
39	a	176.03	1.65379
40	a	188.11	0.2651
41	a	193.96	0.00454
42	a	198.59	0.14675
43	a	199.68	0.1652
44	a	199.95	0.19648
45	a	201.11	0.09945
46	a	204.66	0.16798
47	a	208.79	0.21981
48	a	212.9	0.12092
49	a	213.51	0.18721
50	a	214.86	1.37939
51	a	215.71	1.41879
52	a	258.51	35.56359
53	a	264.9	0.40062
54	a	286.05	1.65025

55	a	287.9	3.30157
56	a	288.14	1.23565
57	a	289.72	3.76347
58	a	302.15	3.9783
59	a	303.6	2.55875
60	a	304.39	3.66393
61	a	306.18	6.87926
62	a	306.59	1.54376
63	a	308.44	3.85616
64	a	382.38	0.05233
65	a	385.88	0.01926
66	a	403.06	26.47786
67	a	404.01	47.98404
68	a	404.34	6.32131
69	a	404.97	43.21157
70	a	439.65	22.73134
71	a	440.55	21.67852
72	a	441.56	16.74673
73	a	441.75	20.86524
74	a	464.17	78.37795
75	a	469.25	1.08377
76	a	481.66	0.00821
77	a	489.02	0.07531
78	a	517.19	13.50361
79	a	517.91	24.79662
80	a	518.89	6.30212
81	a	519.62	15.72984
82	a	592.26	3.65383
83	a	594.81	1.44094
84	a	621.85	5.90416
85	a	622.47	11.64838
86	a	622.95	0.22201
87	a	623.59	6.27938
88	a	649.64	70.4482
89	a	656.9	14.15888
90	a	658.29	23.65327
91	a	658.68	9.80575
92	a	659.34	76.67454
93	a	659.45	105.88352
94	a	813.96	48.87029
95	a	815.57	0.01741

96	a	835.06	4.52306
97	a	835.45	1.25782
98	a	835.54	13.55175
99	a	835.74	17.46646
100	a	910.81	125.92986
101	a	913.56	2.7592
102	a	959.07	11.52574
103	a	959.93	9.17968
104	a	960.37	15.9763
105	a	961.51	12.71508
106	a	982.47	11.91264
107	a	983.08	1.7342
108	a	1000.82	10.37553
109	a	1001.38	10.33197
110	a	1001.47	21.14641
111	a	1002.92	17.68838
112	a	1024.17	73.33761
113	a	1026.34	17.93822
114	a	1067.58	4.38809
115	a	1068.47	11.06569
116	a	1070.86	19.37177
117	a	1071.41	5.1412
118	a	1072.98	11.10781
119	a	1074.45	22.35057
120	a	1105.02	4.53792
121	a	1105.84	3.61539
122	a	1106.1	4.35895
123	a	1106.82	6.92829
124	a	1106.88	1.11076
125	a	1107.15	3.19759
126	a	1139.58	41.37879
127	a	1140.92	37.74877
128	a	1141.26	48.75815
129	a	1142.87	43.8737
130	a	1158.88	1.29837
131	a	1159.26	0.56034
132	a	1159.34	1.55598
133	a	1159.7	0.88292
134	a	1160.39	1.34849
135	a	1161.29	1.93208
136	a	1183.48	15.0648

137	a	1184.01	31.47426
138	a	1184.24	50.51586
139	a	1185.27	44.98763
140	a	1185.64	4.96148
141	a	1187.07	6.30941
142	a	1265.14	49.74058
143	a	1265.87	18.17241
144	a	1266.66	89.77052
145	a	1266.83	107.56128
146	a	1266.96	54.25156
147	a	1269.32	1.77891
148	a	1282.69	9.6914
149	a	1282.97	1.09618
150	a	1311.6	2.6858
151	a	1311.72	25.25255
152	a	1312.83	11.58256
153	a	1313.28	17.95268
154	a	1375.03	11.44472
155	a	1375.36	12.8582
156	a	1377.36	11.2533
157	a	1378.43	12.6547
158	a	1384.29	3.74836
159	a	1385.17	3.1632
160	a	1426.05	21.34706
161	a	1427.76	21.95339
162	a	1428.06	15.59754
163	a	1428.28	29.47106
164	a	1428.89	9.25046
165	a	1429.17	16.86008
166	a	1438.61	15.05083
167	a	1439.42	3.97334
168	a	1442.05	11.48383
169	a	1443.04	6.16168
170	a	1443.41	16.91349
171	a	1444.11	5.80148
172	a	1452.67	32.33781
173	a	1453.12	32.61793
174	a	1453.52	52.63274
175	a	1455.48	37.45233
176	a	1455.98	115.95324
177	a	1457.26	5.73883

178	a	1462.51	11.24254
179	a	1462.71	9.08617
180	a	1463.18	8.78054
181	a	1464.49	12.99218
182	a	1464.88	5.70178
183	a	1465.54	3.93527
184	a	1466.49	8.06886
185	a	1467.64	20.33501
186	a	1467.78	4.69796
187	a	1469.21	13.02773
188	a	1471.7	13.11597
189	a	1472.54	1.32426
190	a	1477.47	7.56381
191	a	1478.2	7.36432
192	a	1478.79	7.36538
193	a	1479.2	14.3246
194	a	1479.71	7.81852
195	a	1479.82	3.93327
196	a	1482.15	13.25044
197	a	1483.16	12.54874
198	a	1484.4	8.96348
199	a	1485.95	25.91346
200	a	1486.14	7.56586
201	a	1488.7	16.13006
202	a	1529.79	10.03221
203	a	1530.58	9.18441
204	a	1532.31	19.94761
205	a	1533.13	13.90761
206	a	1538.52	399.60236
207	a	1545.52	3.8574
208	a	1676.94	33.50882
209	a	1677.8	28.17238
210	a	1680.13	2170.02935
211	a	1685.21	1470.91376
212	a	1685.76	1448.76003
213	a	1724.77	0.40888
214	a	3015.98	7.80525
215	a	3016.42	7.93375
216	a	3016.53	7.66868
217	a	3017.58	8.56915
218	a	3019.44	4.89601

219	a	3020.24	2.68501
220	a	3022.15	7.50276
221	a	3022.61	4.15874
222	a	3022.84	9.41554
223	a	3023.39	5.43601
224	a	3023.63	10.96089
225	a	3023.78	6.24838
226	a	3026.06	4.83352
227	a	3026.18	5.0635
228	a	3026.41	9.59899
229	a	3026.45	3.37579
230	a	3026.97	6.93071
231	a	3027.12	4.91915
232	a	3065.62	10.79282
233	a	3066.71	9.25768
234	a	3070.89	0.40835
235	a	3071.91	0.36882
236	a	3072.01	0.42143
237	a	3073.35	0.55378
238	a	3104.42	1.54622
239	a	3104.66	1.33243
240	a	3104.73	1.57621
241	a	3104.98	1.46507
242	a	3105.46	1.30032
243	a	3105.52	1.47504
244	a	3113.3	0.31529
245	a	3116.47	0.5341
246	a	3118.06	2.05635
247	a	3118.42	1.14434
248	a	3118.69	1.55054
249	a	3119.81	1.49739
250	a	3143.92	1.3674
251	a	3144.12	0.62968
252	a	3145.47	1.64433
253	a	3145.53	1.50038
254	a	3152.18	2.44511
255	a	3156.11	2.8
256	a	3174.58	0.93147
257	a	3175.09	1.62877
258	a	3175.29	1.10964
259	a	3175.57	1.22153

260	a	3175.84	1.5606
261	a	3176.65	1.51396
\$end			

Eu(NTA)₂³⁺

# mode	symmetry	wave number	IR intensity
#		cm**(-1)	km/mol
1	a	-23.96	0
2	a	-19.12	0
3		0	0
4		0	0
5		0	0
6		0	0
7		0	0
8		0	0
9	a	17.7	0.04843
10	a	20.77	1.51898
11	a	21.34	1.33938
12	a	29.31	1.25141
13	a	30.72	1.01064
14	a	32.29	1.57066
15	a	32.88	1.86791
16	a	34.7	0.06614
17	a	35.3	0.11346
18	a	41.93	0.07106
19	a	54.23	1.44309
20	a	64.32	1.01527
21	a	66.58	1.33724
22	a	71.41	1.70335
23	a	73.81	1.45256
24	a	74.36	3.17792
25	a	77.46	0.52404
26	a	79.55	0.91373
27	a	83.87	0.17583
28	a	87.52	0.98174
29	a	103.57	6.39186
30	a	110.23	1.27809
31	a	116.69	0.46238
32	a	127.55	1.23539

33	a	130.38	2.06954
34	a	133.12	3.32661
35	a	136.9	1.72656
36	a	137.82	2.2589
37	a	139.54	0.98133
38	a	142.36	1.98891
39	a	151.21	5.98391
40	a	152.19	50.3925
41	a	159.32	7.33704
42	a	161.53	12.26854
43	a	167.32	9.60668
44	a	174.81	19.97
45	a	177.47	23.80868
46	a	183.08	1.03809
47	a	190.84	0.11459
48	a	207.54	0.88191
49	a	210.17	1.85139
50	a	211.86	5.01087
51	a	212.85	4.19142
52	a	256.07	50.5044
53	a	260.27	3.93177
54	a	281.42	2.09169
55	a	284.19	5.06568
56	a	284.73	3.94672
57	a	286.96	1.97731
58	a	294.5	2.30562
59	a	296.43	4.11786
60	a	296.96	2.25205
61	a	299.44	4.54627
62	a	300.65	4.41501
63	a	310.35	3.35814
64	a	378.05	0.08499
65	a	380.86	0.07893
66	a	403.36	51.60718
67	a	403.91	22.11038
68	a	405.49	35.30103
69	a	408.11	6.70458
70	a	437.37	12.92003
71	a	438.04	33.64274
72	a	438.53	40.63092
73	a	446.43	1.89563

74	a	461.87	70.87054
75	a	465.56	0.09961
76	a	480.88	0.24844
77	a	487.07	0.02004
78	a	512.62	23.4716
79	a	515.83	23.75964
80	a	516.3	8.47279
81	a	517.97	7.88069
82	a	585.29	4.15193
83	a	589.57	1.61028
84	a	619.07	6.98895
85	a	620.46	8.54065
86	a	621.33	3.92909
87	a	622.95	1.12319
88	a	647.67	68.37307
89	a	654.85	4.51844
90	a	656.31	83.72149
91	a	656.84	45.33242
92	a	657.31	85.43953
93	a	659.05	29.71373
94	a	816	56.56575
95	a	817.89	0.30659
96	a	835.48	2.38498
97	a	835.92	20.36056
98	a	836.15	17.95165
99	a	839.11	1.0266
100	a	910.61	107.35318
101	a	913.6	8.25785
102	a	958.18	12.77797
103	a	959.25	9.44086
104	a	960.42	15.19653
105	a	961.43	12.59798
106	a	980.32	15.00428
107	a	981.47	4.48536
108	a	996.09	15.8475
109	a	998.17	10.88208
110	a	999.4	15.92993
111	a	1000.6	17.54531
112	a	1015.28	46.43219
113	a	1018.32	23.7142
114	a	1057.84	10.33835

115	a	1061.39	1.48765
116	a	1061.75	12.43437
117	a	1063.11	17.26446
118	a	1063.89	8.30505
119	a	1068.19	17.1935
120	a	1098.26	4.66705
121	a	1098.75	2.829
122	a	1099.23	4.8277
123	a	1099.37	2.10054
124	a	1099.62	0.87407
125	a	1100.59	3.8995
126	a	1144.83	55.55965
127	a	1145.04	48.73278
128	a	1145.36	27.16117
129	a	1145.71	72.8599
130	a	1153.24	0.84757
131	a	1153.86	4.27742
132	a	1154.56	1.24888
133	a	1155.39	4.53803
134	a	1155.86	4.48725
135	a	1159.9	6.9629
136	a	1179.47	20.38713
137	a	1181.12	36.81719
138	a	1181.51	44.98506
139	a	1181.87	6.13582
140	a	1182.52	8.50991
141	a	1182.88	17.48674
142	a	1261.42	64.41078
143	a	1265.47	66.2371
144	a	1265.88	53.84611
145	a	1266.01	42.84637
146	a	1266.96	85.21397
147	a	1268.42	11.04295
148	a	1277.08	6.14419
149	a	1278.39	2.1054
150	a	1312.55	8.43206
151	a	1313.23	17.13884
152	a	1313.85	29.48887
153	a	1314.92	7.80843
154	a	1372.26	10.09357
155	a	1374.03	13.7247

156	a	1374.51	12.97509
157	a	1375.71	13.33057
158	a	1379.74	8.59358
159	a	1380.42	3.17984
160	a	1420.22	23.62237
161	a	1422.46	12.50524
162	a	1422.63	25.11725
163	a	1424.18	20.08247
164	a	1424.48	22.02058
165	a	1424.71	6.74152
166	a	1435.77	11.00311
167	a	1436.9	0.7119
168	a	1439.72	18.20391
169	a	1440.19	2.80149
170	a	1440.43	16.53391
171	a	1441.46	6.05949
172	a	1449.06	11.22248
173	a	1449.78	23.00528
174	a	1452.54	92.34698
175	a	1452.95	36.83462
176	a	1453.86	22.91474
177	a	1454.53	46.12576
178	a	1458.82	4.9124
179	a	1459.9	10.27867
180	a	1460.14	6.15913
181	a	1460.44	27.3065
182	a	1461.81	6.36845
183	a	1463.2	4.64542
184	a	1463.82	9.75814
185	a	1463.99	4.36028
186	a	1464.33	5.10253
187	a	1466.91	10.35046
188	a	1468.42	8.53899
189	a	1470.69	3.15984
190	a	1474.27	14.91074
191	a	1475.1	16.5143
192	a	1475.55	14.73339
193	a	1476.25	11.48927
194	a	1476.45	11.79624
195	a	1476.99	3.12667
196	a	1477.06	0.08883

197	a	1479.13	15.75887
198	a	1480.62	3.65633
199	a	1481.14	20.23229
200	a	1482.96	21.30011
201	a	1484.31	12.1203
202	a	1532.63	16.71579
203	a	1535.4	14.77106
204	a	1536.24	8.91537
205	a	1541.4	462.49496
206	a	1549.3	0.934
207	a	1553.64	4.73964
208	a	1676.77	164.69572
209	a	1681.32	1848.10083
210	a	1686.88	1358.20194
211	a	1688.74	1441.12996
212	a	1701.29	134.0644
213	a	1726.42	1.38056
214	a	3031.72	8.84128
215	a	3033.67	8.5948
216	a	3034.02	8.90419
217	a	3034.55	9.10606
218	a	3037.62	7.56076
219	a	3039.51	6.86588
220	a	3046.38	5.73073
221	a	3046.6	5.60904
222	a	3047.34	7.9631
223	a	3047.49	4.24262
224	a	3047.83	6.11742
225	a	3048.26	4.64286
226	a	3050.36	6.27642
227	a	3050.46	4.91652
228	a	3050.59	6.16684
229	a	3051	7.52563
230	a	3051.11	3.59641
231	a	3052.67	9.6117
232	a	3082.69	9.65406
233	a	3083.15	7.49037
234	a	3087.52	0.34271
235	a	3088.63	0.76873
236	a	3090.06	0.54508
237	a	3090.98	1.67078

238	a	3126.62	1.81028
239	a	3128.25	0.16762
240	a	3128.68	1.51132
241	a	3129.22	1.48414
242	a	3129.4	1.6864
243	a	3129.55	1.36961
244	a	3130.59	1.41632
245	a	3137.76	0.3464
246	a	3139.39	0.39926
247	a	3141.33	0.71159
248	a	3141.42	0.6892
249	a	3142.38	1.93479
250	a	3167.95	0.65351
251	a	3171.49	1.99967
252	a	3173.52	2.04615
253	a	3178.33	2.32368
254	a	3180.6	2.47697
255	a	3198.32	2.67206
256	a	3200.85	1.23562
257	a	3201.16	1.40302
258	a	3201.53	0.88539
259	a	3201.6	1.65464
260	a	3201.79	1.9953
261	a	3206.36	1.76336
\$end			

La(NTA)₂³⁺

# mode	symmetry	wave number	IR intensity
#		cm**(-1)	km/mol
1	a	-43.17	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7		0	0
8	a	13.99	0.03515
9	a	18.88	1.50277
10	a	20.23	1.26495

11	a	24.62	1.00516
12	a	29.51	0.87012
13	a	31.47	0.78666
14	a	31.76	0.54461
15	a	36.77	0.15779
16	a	42.92	0.39799
17	a	47.85	0.43675
18	a	51.66	0.2617
19	a	56.68	0.77983
20	a	62.54	0.39946
21	a	67.69	1.94959
22	a	71.03	3.49615
23	a	72.38	4.59564
24	a	75.38	1.39778
25	a	76.21	0.51461
26	a	77.48	0.87994
27	a	84.2	0.26646
28	a	96.67	1.23207
29	a	103.27	0.29516
30	a	107.47	6.98536
31	a	116.89	0.52187
32	a	117.82	1.17909
33	a	123.56	2.34484
34	a	126.02	0.15259
35	a	128.6	1.09276
36	a	129.99	1.39729
37	a	134.78	1.13163
38	a	142.27	0.27387
39	a	149.86	12.30008
40	a	150.48	15.7981
41	a	155.36	9.65407
42	a	156.17	7.55324
43	a	161.64	66.92733
44	a	172.22	24.26403
45	a	174.83	23.99093
46	a	188.22	1.93741
47	a	192.24	0.1323
48	a	207.35	1.81976
49	a	209.62	1.16225
50	a	212.77	3.56641
51	a	213.16	4.37453

52	a	261.34	30.97182
53	a	262.52	35.63445
54	a	282.36	2.46412
55	a	283.95	0.48336
56	a	285.8	7.03079
57	a	286.56	3.24904
58	a	295.62	3.42869
59	a	296.46	2.17758
60	a	298.02	5.75629
61	a	298.84	5.88802
62	a	299.07	1.89749
63	a	315.05	3.47566
64	a	380.19	0.9848
65	a	382.61	0.16503
66	a	400.91	23.53956
67	a	402.02	44.02501
68	a	402.24	30.32563
69	a	404.52	32.86577
70	a	438.36	22.69998
71	a	439.04	27.26294
72	a	439.18	8.49552
73	a	440.05	14.59762
74	a	465.35	75.03462
75	a	468.27	2.99944
76	a	478.62	1.38126
77	a	483.68	0.02612
78	a	511.03	15.01581
79	a	514.64	7.25304
80	a	514.93	25.00806
81	a	515.89	11.42343
82	a	590.63	6.43691
83	a	593.05	2.48693
84	a	622.05	10.93983
85	a	623.07	9.74935
86	a	623.56	5.1952
87	a	624.34	6.4309
88	a	649.59	72.37112
89	a	654.68	0.75723
90	a	657.69	27.6601
91	a	657.96	8.8522
92	a	658.97	117.67602

93	a	659.94	80.04406
94	a	817.87	64.08956
95	a	819.78	0.7279
96	a	836.5	16.72739
97	a	836.82	13.10336
98	a	837.3	3.86366
99	a	837.71	3.78091
100	a	914.82	110.21311
101	a	917.21	8.31858
102	a	962.25	6.98317
103	a	962.4	4.74317
104	a	962.82	16.34185
105	a	963.6	12.51702
106	a	983.42	7.73649
107	a	984.19	4.9485
108	a	1004.35	18.65867
109	a	1006.14	16.98915
110	a	1006.61	21.56225
111	a	1007.78	22.13152
112	a	1029.09	74.66841
113	a	1030.12	7.19985
114	a	1062.63	9.83789
115	a	1068	9.14703
116	a	1068.33	0.62564
117	a	1068.78	6.70765
118	a	1069.72	23.14257
119	a	1071.38	14.73854
120	a	1107.32	4.84498
121	a	1108.66	4.8343
122	a	1108.77	3.2481
123	a	1108.78	4.97261
124	a	1109.08	4.27882
125	a	1110.28	0.3484
126	a	1148.72	51.04392
127	a	1149.71	59.7981
128	a	1149.86	37.64096
129	a	1150.43	64.11776
130	a	1162.73	2.45194
131	a	1163.18	1.76737
132	a	1163.5	0.97042
133	a	1164.18	3.01271

134	a	1164.6	3.1304
135	a	1170.84	5.84965
136	a	1185.8	21.16885
137	a	1188.5	10.59013
138	a	1188.95	10.60357
139	a	1189.32	28.37935
140	a	1189.68	19.29205
141	a	1190.04	36.20687
142	a	1263.46	66.44273
143	a	1268.77	41.70969
144	a	1269.25	55.99955
145	a	1269.48	102.67429
146	a	1269.97	58.15821
147	a	1271.81	5.90859
148	a	1294.38	4.95545
149	a	1294.55	2.69036
150	a	1324.17	14.37913
151	a	1324.79	14.18376
152	a	1325.46	15.85367
153	a	1325.92	15.98056
154	a	1386.99	10.42672
155	a	1387.12	25.48013
156	a	1388.97	17.63917
157	a	1390	19.17634
158	a	1395.94	4.66688
159	a	1396.77	1.93609
160	a	1428.82	23.70625
161	a	1429.39	37.88264
162	a	1429.59	8.2757
163	a	1431.1	34.9662
164	a	1431.38	6.54335
165	a	1432.2	19.08076
166	a	1444.65	10.38328
167	a	1445.3	2.62601
168	a	1448.29	11.44254
169	a	1448.73	7.16576
170	a	1449.23	16.30768
171	a	1451.85	8.93865
172	a	1460.33	13.57206
173	a	1460.95	32.56465
174	a	1461.95	32.45123

175	a	1462.09	40.44602
176	a	1462.31	99.46614
177	a	1463.52	23.02899
178	a	1467.93	23.14275
179	a	1471.36	7.20377
180	a	1471.7	17.02144
181	a	1471.89	10.83736
182	a	1472.42	13.12004
183	a	1472.66	7.13634
184	a	1472.76	1.41694
185	a	1473.49	7.65824
186	a	1473.8	8.84998
187	a	1475.41	15.73875
188	a	1479.7	5.20808
189	a	1480.79	6.33877
190	a	1483.93	5.97067
191	a	1484.84	29.43186
192	a	1485.58	5.08766
193	a	1485.91	7.90662
194	a	1486.47	4.35893
195	a	1486.9	11.00214
196	a	1486.96	8.89093
197	a	1491.31	12.75366
198	a	1492.19	22.37844
199	a	1492.44	1.38534
200	a	1496.64	25.5118
201	a	1497.05	14.69589
202	a	1536.87	17.46963
203	a	1537.91	5.64961
204	a	1538.3	23.25362
205	a	1538.66	14.83874
206	a	1543.71	404.87582
207	a	1550.41	0.29163
208	a	1681.55	551.95799
209	a	1684.01	4.84888
210	a	1685.2	1696.87884
211	a	1687.64	1338.09596
212	a	1688.39	1377.55243
213	a	1725.29	1.41353
214	a	3019.99	7.68336
215	a	3020.08	10.01836

216	a	3020.93	9.21476
217	a	3022.59	9.46344
218	a	3024.09	9.16641
219	a	3028.33	7.11062
220	a	3034.92	6.56484
221	a	3035.38	5.95672
222	a	3035.86	4.93417
223	a	3035.98	8.74978
224	a	3036.21	6.9789
225	a	3036.62	4.94198
226	a	3039.24	2.14597
227	a	3039.25	9.06295
228	a	3039.31	5.67627
229	a	3039.4	6.38503
230	a	3039.87	4.44911
231	a	3041.9	10.47549
232	a	3069.31	13.8627
233	a	3070.49	12.25198
234	a	3074.89	1.11528
235	a	3075.16	0.64957
236	a	3076.17	0.88941
237	a	3079.07	2.85429
238	a	3112.75	1.85526
239	a	3114.6	0.38598
240	a	3115.9	1.57561
241	a	3116.01	1.54319
242	a	3116.09	1.79321
243	a	3116.49	1.50381
244	a	3116.83	1.5146
245	a	3126.61	0.54496
246	a	3127.82	0.65014
247	a	3128.56	0.92025
248	a	3129.5	0.96207
249	a	3130.35	2.07693
250	a	3155.42	1.02239
251	a	3158.6	2.32455
252	a	3160.11	2.35773
253	a	3162.73	2.67219
254	a	3164.71	2.87483
255	a	3187.4	0.88914
256	a	3187.85	1.11269

257	a	3187.97	1.30029
258	a	3188.79	3.19011
259	a	3188.98	0.77506
260	a	3189.21	1.52095
261	a	3194.1	1.68549
\$end			

Pr(NTA)₂³⁺

# mode	symmetry	wave number	IR intensity
#		cm**(-1)	km/mol
1		0	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7	a	8.67	0.06602
8	a	14.95	0.06297
9	a	19.62	0.89583
10	a	21.32	1.26017
11	a	27.55	1.00782
12	a	28.66	1.29084
13	a	31.48	1.25961
14	a	32.03	1.0107
15	a	35.33	0.4305
16	a	44.57	0.52374
17	a	46.84	0.17461
18	a	48.86	0.07201
19	a	50.9	0.1423
20	a	57.17	0.41701
21	a	61.45	0.01092
22	a	65.71	2.70143
23	a	72.46	3.42344
24	a	73.71	0.98977
25	a	75.57	4.01997
26	a	77.37	0.18175
27	a	79.14	0.3335
28	a	82.24	0.04281
29	a	103.23	5.93699

30	a	111.13	0.97271
31	a	115.54	0.45214
32	a	117.33	0.79226
33	a	130.41	1.26873
34	a	132.89	0.07296
35	a	134.69	0.63283
36	a	135.89	0.89134
37	a	138.93	2.24326
38	a	143.22	0.54586
39	a	150.37	4.73929
40	a	151.78	7.20049
41	a	155.46	12.1736
42	a	156.28	10.51986
43	a	158.17	61.76313
44	a	173.74	29.41478
45	a	176.36	31.07988
46	a	183.21	0.88377
47	a	190.62	0.05026
48	a	208.87	1.91212
49	a	210.42	1.31592
50	a	213.05	4.4941
51	a	213.87	5.31787
52	a	257.43	63.70513
53	a	261.37	7.06452
54	a	280.56	3.69535
55	a	282.99	1.49662
56	a	284.91	7.6259
57	a	286.81	3.90442
58	a	295.21	2.52846
59	a	295.48	4.47106
60	a	296.13	1.02314
61	a	297.46	4.92737
62	a	298.48	4.81785
63	a	311.77	3.38
64	a	378.32	0.77923
65	a	381.11	0.10465
66	a	401.84	15.84827
67	a	402.49	28.71426
68	a	403	55.21207
69	a	405.13	35.90956
70	a	437.76	21.73344

71	a	438.32	21.2328
72	a	438.84	19.92325
73	a	439.4	14.95341
74	a	464.62	76.2889
75	a	468.56	0.57303
76	a	477.44	1.93298
77	a	482.39	0.01273
78	a	511.79	16.58263
79	a	514.9	16.24826
80	a	516.06	18.11923
81	a	517.13	13.08374
82	a	588.14	5.23739
83	a	591.72	2.52719
84	a	620.14	10.08649
85	a	621.43	11.4587
86	a	621.58	2.55298
87	a	622.46	5.07458
88	a	646.58	73.55242
89	a	653.35	1.76769
90	a	655.15	21.65791
91	a	655.72	25.2128
92	a	656.4	99.28197
93	a	656.62	103.33538
94	a	817.58	70.38151
95	a	819.7	0.01571
96	a	835.07	21.52038
97	a	835.33	13.94501
98	a	835.65	8.4561
99	a	835.76	3.62888
100	a	913.97	105.94133
101	a	916.8	13.51903
102	a	962.14	10.63626
103	a	963.07	6.61716
104	a	963.85	15.44671
105	a	964.31	11.78054
106	a	983.18	12.60886
107	a	984.21	5.0536
108	a	1002.92	19.4504
109	a	1004.01	15.0426
110	a	1005.83	19.90853
111	a	1007.15	21.23523

112	a	1022.52	46.59235
113	a	1025.17	23.32727
114	a	1063.23	9.09727
115	a	1068.19	2.51498
116	a	1068.43	1.02628
117	a	1069.18	30.16199
118	a	1069.67	6.24394
119	a	1072.42	15.41624
120	a	1106.91	3.80235
121	a	1107.79	5.02598
122	a	1108.35	3.67438
123	a	1108.69	3.96173
124	a	1109.49	4.66171
125	a	1110.03	0.01507
126	a	1153.27	52.90502
127	a	1154.39	39.19349
128	a	1154.78	60.24114
129	a	1155.39	64.50952
130	a	1162.92	1.5459
131	a	1163.88	5.4996
132	a	1164.15	0.72224
133	a	1164.97	5.23402
134	a	1165.32	5.43641
135	a	1170.56	6.8366
136	a	1186.85	16.27135
137	a	1188.86	1.64921
138	a	1189.67	7.35251
139	a	1190.09	25.03639
140	a	1190.26	27.00173
141	a	1190.74	37.79432
142	a	1264.51	65.64871
143	a	1268.43	27.51842
144	a	1268.99	97.90741
145	a	1269.23	90.95073
146	a	1269.73	60.97279
147	a	1272	7.44324
148	a	1291.56	3.3271
149	a	1294.06	2.86952
150	a	1326.59	15.35489
151	a	1327.67	15.14806
152	a	1328.45	17.57793

153	a	1328.61	18.36947
154	a	1386.15	17.74863
155	a	1388.29	18.95946
156	a	1388.49	18.44887
157	a	1390.09	20.21574
158	a	1394.64	6.03828
159	a	1395.36	3.79154
160	a	1428.31	26.14985
161	a	1429.85	18.99932
162	a	1430.44	26.48912
163	a	1431.95	21.27184
164	a	1432.23	33.53782
165	a	1432.46	6.27764
166	a	1443.73	14.68701
167	a	1444.52	0.59953
168	a	1447.4	12.51741
169	a	1447.89	2.35291
170	a	1448.34	13.21502
171	a	1449.91	9.57706
172	a	1458.62	37.23018
173	a	1459.97	56.37573
174	a	1461.07	33.67817
175	a	1461.41	39.94884
176	a	1463.02	75.04278
177	a	1463.79	8.50594
178	a	1467.54	26.98281
179	a	1469.47	22.28882
180	a	1470.24	4.49899
181	a	1470.91	11.21778
182	a	1472.16	11.28805
183	a	1472.82	12.20495
184	a	1473.53	5.09704
185	a	1473.74	1.99331
186	a	1474.02	13.04096
187	a	1474.86	13.41139
188	a	1478.42	4.27163
189	a	1480.59	6.21518
190	a	1483.69	13.01067
191	a	1484.98	7.34927
192	a	1485.18	21.65469
193	a	1485.61	7.47377

194	a	1486.02	9.30491
195	a	1486.38	4.9777
196	a	1486.49	4.0492
197	a	1490.51	16.22189
198	a	1491.21	17.4367
199	a	1491.74	7.37862
200	a	1495.6	26.76641
201	a	1496.17	17.61786
202	a	1535.46	7.84261
203	a	1536.6	10.05612
204	a	1537.3	11.74774
205	a	1538.02	19.60791
206	a	1543.45	435.46723
207	a	1551.12	0.75235
208	a	1677.52	186.80149
209	a	1677.79	21.87985
210	a	1681	1922.74592
211	a	1684.91	1437.58385
212	a	1685.1	1497.83003
213	a	1725.51	1.1741
214	a	3019.03	9.39188
215	a	3019.75	9.75335
216	a	3020.58	10.08593
217	a	3021.05	10.67703
218	a	3023.77	9.83568
219	a	3027.55	8.38918
220	a	3035.63	5.67232
221	a	3035.68	5.95311
222	a	3035.89	7.0713
223	a	3036.22	3.05615
224	a	3036.26	8.77988
225	a	3036.46	6.62477
226	a	3038.99	6.63527
227	a	3039.71	5.80485
228	a	3039.82	5.30233
229	a	3039.98	7.0736
230	a	3040.27	4.86249
231	a	3041.69	10.52907
232	a	3069.39	12.84189
233	a	3069.83	8.77389
234	a	3074.89	0.81578

235	a	3075.14	1.19537
236	a	3076.56	0.86865
237	a	3079.38	2.58826
238	a	3112.29	1.90707
239	a	3114.33	0.27854
240	a	3114.78	1.65298
241	a	3116.23	1.29259
242	a	3116.26	1.77065
243	a	3116.55	1.40689
244	a	3117.11	1.41055
245	a	3127.1	0.63321
246	a	3128.67	0.63792
247	a	3128.81	0.76761
248	a	3129.5	0.81925
249	a	3130.94	1.51912
250	a	3156.26	1.3749
251	a	3159.91	2.21741
252	a	3160.72	2.22027
253	a	3162.19	2.38815
254	a	3163.39	2.67773
255	a	3188.16	2.94965
256	a	3188.68	0.72895
257	a	3188.89	1.96964
258	a	3188.91	1.11617
259	a	3189.87	0.52428
260	a	3190.02	2.08803
261	a	3193.63	1.7828
Şend			

Ho(NTA)₂³⁺

# mode	symmetry	wave number	IR intensity
#		cm ⁻¹	km/mol
1		0	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7	a	13.94	0.65543

8	a	17	0.18717
9	a	17.71	0.62412
10	a	26.89	0.32371
11	a	28.65	0.96145
12	a	31.19	2.44736
13	a	32.05	1.92056
14	a	36.13	2.04682
15	a	38.64	1.39961
16	a	42.06	2.57042
17	a	45.33	0.82299
18	a	46.12	0.01181
19	a	48.18	0.05347
20	a	50.44	0.08659
21	a	54.96	0.51124
22	a	64.86	5.1
23	a	77.56	2.37988
24	a	79.54	0.88464
25	a	80.47	1.26048
26	a	81.9	1.24041
27	a	85.27	2.06587
28	a	85.68	0.87152
29	a	92.56	8.88333
30	a	113.52	0.3144
31	a	121.75	0.77484
32	a	123.44	0.69395
33	a	132.04	2.44544
34	a	132.92	0.25329
35	a	135.92	1.09022
36	a	137.46	1.25434
37	a	138.93	4.06172
38	a	140.57	1.06424
39	a	150.22	28.6875
40	a	153.89	4.06043
41	a	154.48	4.05087
42	a	164.19	14.50466
43	a	164.92	17.01771
44	a	173.02	10.36421
45	a	176.15	24.79883
46	a	176.51	21.50966
47	a	183.54	0.49335
48	a	214.86	0.88875

49	a	215.83	0.87389
50	a	218.39	2.64911
51	a	218.99	2.81813
52	a	258.15	52.8586
53	a	262.79	1.60558
54	a	281.65	3.69799
55	a	284.39	1.70984
56	a	286.65	7.57703
57	a	287.67	5.08746
58	a	294.41	1.3817
59	a	294.51	2.52714
60	a	295.24	0.61147
61	a	296.37	3.11624
62	a	297.97	2.72252
63	a	312	2.50851
64	a	374.45	0.22963
65	a	376.84	0.1002
66	a	403.9	14.55201
67	a	404.13	48.75966
68	a	405.06	27.75623
69	a	407.35	29.78079
70	a	438.76	23.20659
71	a	439.7	25.228
72	a	440.27	10.138
73	a	441.09	11.71125
74	a	467.92	61.92372
75	a	472.06	0.24522
76	a	478.82	6.59114
77	a	483.11	0.02296
78	a	513.28	17.4009
79	a	515.36	20.92898
80	a	516.78	12.31469
81	a	517.31	12.6277
82	a	584.36	3.39062
83	a	586.53	1.00411
84	a	618.89	6.03775
85	a	619.81	6.66201
86	a	620.33	2.25488
87	a	620.8	3.85947
88	a	645.91	51.60318
89	a	652.98	5.84089

90	a	653.95	5.76926
91	a	654.44	38.19158
92	a	655.01	117.0965
93	a	655.26	85.41679
94	a	818.53	84.90282
95	a	821.91	0.06141
96	a	833.52	21.71446
97	a	833.84	8.61081
98	a	834.15	17.33747
99	a	834.38	7.03972
100	a	915.31	97.28179
101	a	918.05	11.29821
102	a	962.34	11.8854
103	a	964.18	6.9907
104	a	964.63	13.62495
105	a	964.9	17.00795
106	a	981.78	21.61136
107	a	983.28	4.93856
108	a	1002.02	20.11667
109	a	1003.55	13.48284
110	a	1004.99	21.13804
111	a	1005.27	19.83437
112	a	1013.55	28.06587
113	a	1015.6	15.38435
114	a	1065.5	9.81274
115	a	1068.93	6.64941
116	a	1069.94	11.81206
117	a	1071.99	16.82917
118	a	1074.11	3.63489
119	a	1074.67	22.64343
120	a	1106.82	3.72496
121	a	1107.99	5.05231
122	a	1108.08	2.71781
123	a	1108.73	3.71978
124	a	1109.61	0.00149
125	a	1110	4.34807
126	a	1160.65	35.78461
127	a	1161.14	17.67811
128	a	1161.32	45.48498
129	a	1161.61	42.15817
130	a	1163.51	13.74658

131	a	1164.03	1.96477
132	a	1165.26	36.22644
133	a	1167.16	37.77071
134	a	1167.72	35.23074
135	a	1171.11	15.82525
136	a	1188.71	6.05232
137	a	1189.49	1.27719
138	a	1191.96	7.25888
139	a	1192.12	10.00171
140	a	1192.71	28.87399
141	a	1193.44	24.78054
142	a	1265.51	61.4338
143	a	1269.69	27.74133
144	a	1269.92	53.63651
145	a	1270.5	64.78625
146	a	1270.88	121.02517
147	a	1273.04	7.62085
148	a	1287.76	2.13578
149	a	1292.28	1.48779
150	a	1332.99	18.67803
151	a	1333.77	17.67309
152	a	1334.71	23.04453
153	a	1335.19	22.5551
154	a	1386.82	19.48327
155	a	1386.91	19.77472
156	a	1389.7	21.4461
157	a	1391.15	22.75187
158	a	1393.28	8.86604
159	a	1394.43	8.14945
160	a	1428.99	23.40945
161	a	1431.44	18.1127
162	a	1432.89	20.95496
163	a	1433.31	30.19808
164	a	1433.54	9.49568
165	a	1434.56	15.16898
166	a	1442.71	33.2947
167	a	1443.55	2.13135
168	a	1446.07	10.79295
169	a	1446.71	5.19941
170	a	1447.13	8.10179
171	a	1449.03	7.36689

172	a	1456.41	25.36762
173	a	1458.84	20.74395
174	a	1459.6	35.9019
175	a	1460.63	37.46727
176	a	1463.06	86.96601
177	a	1464.28	8.39905
178	a	1467.29	26.97972
179	a	1468.61	26.59928
180	a	1469.2	11.15395
181	a	1469.81	7.77584
182	a	1470.14	10.53979
183	a	1473.31	7.62019
184	a	1473.76	10.04481
185	a	1473.96	5.68823
186	a	1474.31	12.55173
187	a	1475.53	13.86018
188	a	1477.81	5.83218
189	a	1480.19	4.30083
190	a	1483.39	18.18144
191	a	1484.83	11.53948
192	a	1485.62	22.14526
193	a	1486.05	3.21233
194	a	1486.32	1.40518
195	a	1486.46	11.38046
196	a	1486.83	1.33117
197	a	1490.73	18.14023
198	a	1491.21	12.14998
199	a	1494.07	14.47209
200	a	1495.89	32.07302
201	a	1496.93	13.57739
202	a	1537.96	5.44606
203	a	1538.82	11.52137
204	a	1539.17	11.89861
205	a	1540.1	15.42112
206	a	1544.97	456.86688
207	a	1553.72	0.8218
208	a	1680.16	216.29428
209	a	1681.36	10.2956
210	a	1683.31	1657.61439
211	a	1689.04	1496.35928
212	a	1689.61	1504.55675

213	a	1732.38	0.93972
214	a	3018.02	11.08506
215	a	3018.98	11.55297
216	a	3020.3	10.51473
217	a	3020.45	11.4123
218	a	3023.85	8.46075
219	a	3026.96	8.54968
220	a	3035.88	5.5743
221	a	3036.16	5.63901
222	a	3036.2	7.13564
223	a	3036.42	6.54759
224	a	3036.71	5.09935
225	a	3036.81	6.45349
226	a	3039.37	5.97768
227	a	3039.73	8.9507
228	a	3039.75	1.61022
229	a	3040.09	7.01162
230	a	3040.28	4.49999
231	a	3042.33	9.37767
232	a	3068.66	10.56058
233	a	3069.25	8.23754
234	a	3074.14	1.22953
235	a	3075.21	1.08571
236	a	3076.85	1.21854
237	a	3079.12	2.53571
238	a	3112.8	1.81529
239	a	3115.1	1.57354
240	a	3115.2	0.27957
241	a	3115.98	1.51896
242	a	3116.26	1.70133
243	a	3116.46	1.36278
244	a	3116.84	1.42465
245	a	3127.11	0.48651
246	a	3129.21	0.59871
247	a	3129.63	0.79919
248	a	3129.86	0.69677
249	a	3131.33	1.38054
250	a	3157.08	1.35097
251	a	3160.02	2.04275
252	a	3161.61	2.02757
253	a	3161.9	2.25446

254	a	3166.22	2.48028
255	a	3187.85	1.3302
256	a	3187.97	1.17407
257	a	3188.57	1.44517
258	a	3188.69	1.13458
259	a	3188.84	1.10652
260	a	3190.65	1.97904
261	a	3193.15	2.13792
Şend			

Tm(NTA)₂³⁺

# mode	symmetry	wave number	IR intensity
#		cm ^{**} (-1)	km/mol
1		0	0
2		0	0
3		0	0
4		0	0
5		0	0
6		0	0
7	a	14.49	0.82694
8	a	18.71	0.38364
9	a	19.16	0.69804
10	a	28.67	0.51598
11	a	30.13	1.39403
12	a	32.46	2.46033
13	a	33.99	1.96656
14	a	36.1	0.39593
15	a	38.53	1.10836
16	a	43.62	0.08344
17	a	50.29	1.71948
18	a	50.88	1.79825
19	a	51.12	0.26621
20	a	54.66	0.18262
21	a	57.08	0.63445
22	a	66.75	5.82942
23	a	79.55	2.26001
24	a	81.57	0.09814
25	a	82.11	1.90349
26	a	83.2	0.94942

27	a	85.9	2.18469
28	a	87.56	0.47096
29	a	94.74	10.48045
30	a	114.67	0.33325
31	a	123.2	0.72303
32	a	124.68	0.94949
33	a	132.22	3.08754
34	a	133.85	0.10743
35	a	137.71	2.87644
36	a	139.66	4.45479
37	a	140.85	2.37858
38	a	142.08	1.11296
39	a	148.41	26.02991
40	a	154.02	4.63742
41	a	154.97	3.46757
42	a	167.92	21.26218
43	a	169.07	17.08184
44	a	175.56	16.304
45	a	178.14	23.47995
46	a	179.27	5.75828
47	a	189.54	0.32284
48	a	216.21	1.02214
49	a	216.64	1.26906
50	a	220.44	1.72712
51	a	220.81	1.89109
52	a	257.87	46.10134
53	a	263.8	1.63789
54	a	282.7	3.08425
55	a	283.74	2.47964
56	a	286.94	5.05501
57	a	288.22	3.89479
58	a	294.99	2.15353
59	a	295.28	2.4462
60	a	296.13	0.55016
61	a	298.14	4.02755
62	a	298.69	3.14318
63	a	313.1	2.72251
64	a	375.82	0.05864
65	a	378.49	0.11967
66	a	405.23	23.24352
67	a	405.53	33.60754

68	a	406.68	30.09684
69	a	408.61	26.8955
70	a	440.19	27.22123
71	a	441.48	37.13574
72	a	441.6	2.07527
73	a	442.4	7.376
74	a	467.63	64.08252
75	a	471.41	0.117
76	a	482.87	1.96868
77	a	488.4	0.01331
78	a	512.99	17.0615
79	a	516.47	18.68299
80	a	518.1	16.18667
81	a	519.21	11.80614
82	a	585.93	3.07781
83	a	589.48	1.34927
84	a	620.14	5.27805
85	a	621.1	3.95802
86	a	621.22	4.42868
87	a	622.68	4.16652
88	a	647.62	51.05735
89	a	655.12	0.64877
90	a	655.7	8.25382
91	a	656.13	74.3792
92	a	657.43	88.20438
93	a	657.67	82.34084
94	a	817.88	75.41825
95	a	821.14	0.02083
96	a	834.99	4.89713
97	a	835.39	2.33816
98	a	835.43	22.00438
99	a	836.12	17.37732
100	a	914.84	92.17271
101	a	918.01	15.5184
102	a	962.91	11.9724
103	a	964.64	7.96663
104	a	965.6	14.96997
105	a	966.42	11.72047
106	a	982.88	17.61234
107	a	984.62	3.99516
108	a	1002.15	19.64473

109	a	1003.69	14.03635
110	a	1005.39	19.88436
111	a	1007.12	20.71119
112	a	1017.09	34.83578
113	a	1020.25	20.44266
114	a	1064.48	9.90914
115	a	1068.23	6.00287
116	a	1069.13	12.67544
117	a	1071.78	15.94069
118	a	1072.94	7.98557
119	a	1074.7	18.00489
120	a	1107.16	3.59955
121	a	1107.94	4.41241
122	a	1108.12	3.40554
123	a	1108.9	3.72288
124	a	1109.31	0.05812
125	a	1110.14	4.38952
126	a	1158.21	51.17206
127	a	1158.96	32.63454
128	a	1159.79	50.76479
129	a	1160.05	54.59165
130	a	1163.01	4.41489
131	a	1164.09	0.98775
132	a	1164.47	13.45574
133	a	1165.87	18.35321
134	a	1166.69	19.2096
135	a	1170.65	10.54791
136	a	1188.09	12.10114
137	a	1189.67	1.96907
138	a	1191.22	18.30959
139	a	1191.42	0.70538
140	a	1191.95	35.36288
141	a	1192.37	27.53773
142	a	1264.98	61.9825
143	a	1269.53	20.663
144	a	1269.97	53.00976
145	a	1270.42	94.028
146	a	1271.03	91.14399
147	a	1273.14	9.60866
148	a	1287.36	2.38616
149	a	1292.22	1.92616

150	a	1329.24	17.84317
151	a	1330.17	15.24509
152	a	1330.76	21.89127
153	a	1331.68	20.36095
154	a	1385.68	18.48617
155	a	1386.5	18.38197
156	a	1388.9	20.84665
157	a	1390.62	20.54524
158	a	1393.05	6.61045
159	a	1394.61	7.35802
160	a	1428.38	23.30418
161	a	1430.97	18.66574
162	a	1432.65	21.74053
163	a	1433.2	26.96915
164	a	1433.38	9.36071
165	a	1434.79	14.75852
166	a	1443.51	28.01417
167	a	1444.4	0.51121
168	a	1447.04	13.62321
169	a	1447.66	1.59945
170	a	1448.58	9.77688
171	a	1450.01	7.04885
172	a	1457.09	27.48402
173	a	1458.96	22.22297
174	a	1460.75	34.59578
175	a	1461.38	36.47866
176	a	1463.01	89.99488
177	a	1463.81	10.60282
178	a	1467.29	22.41308
179	a	1468.89	29.02271
180	a	1469.7	10.71597
181	a	1470.14	6.22502
182	a	1471.54	10.3547
183	a	1473.2	8.07307
184	a	1473.84	5.18386
185	a	1473.88	11.06917
186	a	1474.17	10.34252
187	a	1475.57	13.73316
188	a	1477.63	5.52586
189	a	1480.53	4.76476
190	a	1482.96	18.91304

191	a	1484.79	10.8653
192	a	1485.37	23.21861
193	a	1485.7	10.30963
194	a	1486.07	1.24667
195	a	1486.43	2.7514
196	a	1486.73	1.70296
197	a	1490.24	17.78876
198	a	1491.25	12.87981
199	a	1493.13	13.18306
200	a	1495.69	37.31789
201	a	1496.01	7.53268
202	a	1538.05	4.25747
203	a	1539.02	9.26817
204	a	1539.58	20.39032
205	a	1540.43	14.07637
206	a	1544.74	447.52573
207	a	1553.6	0.78619
208	a	1681.33	318.99213
209	a	1683.44	62.13909
210	a	1684.78	1485.79981
211	a	1691.71	1460.41756
212	a	1693.09	1482.58133
213	a	1733.9	0.98075
214	a	3020.58	9.78241
215	a	3021.11	10.50329
216	a	3022.46	10.69039
217	a	3022.8	9.28779
218	a	3025.79	7.38064
219	a	3029.74	7.0163
220	a	3035.92	5.60504
221	a	3036.27	3.37977
222	a	3036.34	13.4023
223	a	3036.39	2.6347
224	a	3036.72	6.45395
225	a	3036.94	5.00767
226	a	3039.58	5.8102
227	a	3039.82	6.42442
228	a	3039.87	3.16814
229	a	3040.02	8.01798
230	a	3040.23	4.52344
231	a	3042.53	9.53577

232	a	3070.76	15.84391
233	a	3070.88	3.35666
234	a	3076.03	0.92937
235	a	3076.76	1.07604
236	a	3078.5	1.03974
237	a	3081.15	2.8175
238	a	3112.87	1.70279
239	a	3115.44	0.22239
240	a	3115.46	1.6157
241	a	3116.12	1.53733
242	a	3116.2	1.62531
243	a	3116.54	1.40813
244	a	3116.87	1.43687
245	a	3127.31	0.48759
246	a	3128.93	0.60252
247	a	3129.47	0.77607
248	a	3129.51	0.69631
249	a	3130.96	1.57195
250	a	3156.19	1.19707
251	a	3159.85	2.05412
252	a	3161.06	2.1112
253	a	3161.92	2.30195
254	a	3165.56	2.51503
255	a	3187.86	1.26137
256	a	3188.2	1.28218
257	a	3188.33	1.64591
258	a	3188.5	0.79453
259	a	3188.71	1.16908
260	a	3190.44	2.25667
261	a	3193.73	2.0121
Şend			

Lu(NTA)₂³⁺

# mode	symmetry	wave number	IR intensity
#		cm ⁻¹	km/mol
1		0	0
2		0	0
3		0	0
4		0	0

5		0	0
6		0	0
7	a	14.99	0.6419
8	a	15.94	1.12247
9	a	17.88	0.08693
10	a	26.48	7.02108
11	a	28.41	0.67306
12	a	29.3	1.57338
13	a	32.2	2.92773
14	a	32.91	2.47602
15	a	36.38	0.67757
16	a	46.15	0.13847
17	a	49.1	0.02928
18	a	49.61	0.30284
19	a	51.5	0.40043
20	a	53.1	0.00567
21	a	56.99	0.22415
22	a	67.04	5.02785
23	a	78.83	0.2752
24	a	80.69	1.65631
25	a	84.32	1.78756
26	a	86.03	1.55656
27	a	88.24	7.84288
28	a	89.4	2.05936
29	a	91.78	0.77534
30	a	112.3	0.48639
31	a	124.44	0.83341
32	a	125.39	0.71766
33	a	132.31	2.18516
34	a	133.78	0.59357
35	a	136.6	2.10668
36	a	138.42	0.38465
37	a	140.06	3.08966
38	a	140.56	0.43763
39	a	148.71	20.68988
40	a	156.13	2.94656
41	a	156.49	2.01735
42	a	168.93	11.51268
43	a	170.58	17.62621
44	a	171.36	16.33577
45	a	175.72	27.71566

46	a	177.97	24.90273
47	a	180.8	0.47897
48	a	217.97	0.38257
49	a	218.73	0.4568
50	a	221.41	1.49806
51	a	222.04	1.42378
52	a	259.03	47.96367
53	a	264.31	0.77061
54	a	284.45	2.67744
55	a	286.81	1.3486
56	a	288.26	6.91163
57	a	289.14	7.67666
58	a	293.87	1.52612
59	a	294.66	1.43135
60	a	295.13	0.41056
61	a	296.02	2.33318
62	a	297.31	2.17105
63	a	311.69	2.34277
64	a	372.23	0.09122
65	a	374.69	0.11471
66	a	403.72	23.23916
67	a	403.95	42.17032
68	a	404.42	26.84835
69	a	407.2	28.43942
70	a	439.71	24.71782
71	a	440.12	22.0412
72	a	440.81	4.95599
73	a	441.72	9.60978
74	a	469.99	50.62395
75	a	474.67	0.07734
76	a	476.9	15.90607
77	a	481.04	0.50033
78	a	514.74	20.56519
79	a	516.79	6.11374
80	a	516.99	27.74682
81	a	518.23	7.61051
82	a	582.9	2.98411
83	a	583.94	0.07931
84	a	617.76	3.65564
85	a	618.57	6.07877
86	a	618.96	1.72316

87	a	619.72	2.88093
88	a	644.87	40.74747
89	a	651.72	3.61083
90	a	652.61	9.23172
91	a	653.08	44.55483
92	a	653.68	121.17956
93	a	654.48	68.04244
94	a	818.78	95.83703
95	a	823.03	0.10313
96	a	832.27	14.06985
97	a	832.3	21.78998
98	a	832.99	9.61259
99	a	833.33	14.89571
100	a	916.63	102.62493
101	a	919.03	3.18176
102	a	963.56	8.29948
103	a	964.38	16.36041
104	a	965.12	3.36125
105	a	965.45	22.92535
106	a	980.87	29.17601
107	a	982.07	0.24061
108	a	1003.43	18.95978
109	a	1004.67	22.08803
110	a	1004.69	11.22703
111	a	1005.32	24.24715
112	a	1010.05	20.50981
113	a	1011.2	9.43696
114	a	1067.42	9.79648
115	a	1071.67	6.88261
116	a	1072.52	9.38776
117	a	1073.39	24.18227
118	a	1074.17	7.05593
119	a	1075.06	18.38721
120	a	1106.99	3.81348
121	a	1107.98	4.18462
122	a	1108.24	3.59102
123	a	1108.77	3.75189
124	a	1109.27	3.9897
125	a	1109.62	0.12122
126	a	1161.79	12.75968
127	a	1162.48	7.28584

128	a	1162.75	12.32153
129	a	1162.92	8.59917
130	a	1163.78	0.71363
131	a	1165.1	34.42024
132	a	1168.41	62.10659
133	a	1170.83	67.33872
134	a	1171.27	85.60527
135	a	1171.57	13.0075
136	a	1189.89	2.24918
137	a	1190.41	0.41305
138	a	1193.68	11.50944
139	a	1194.49	1.76633
140	a	1194.99	23.8998
141	a	1195.61	15.23518
142	a	1266.57	57.41919
143	a	1270.4	17.79995
144	a	1270.81	37.0321
145	a	1271.18	64.04602
146	a	1271.72	142.96703
147	a	1273.7	6.44336
148	a	1287.43	1.63916
149	a	1290.83	0.78073
150	a	1337.46	21.4252
151	a	1338.79	18.60831
152	a	1339.91	27.14522
153	a	1340.58	25.83543
154	a	1387.12	20.55354
155	a	1388.5	21.05406
156	a	1390.54	24.41751
157	a	1391.41	24.3656
158	a	1392.56	11.22169
159	a	1393.76	10.99094
160	a	1429.7	21.5911
161	a	1432.75	17.0845
162	a	1433.31	22.11653
163	a	1433.79	17.52326
164	a	1434.43	22.22485
165	a	1434.88	10.14437
166	a	1442.37	46.74303
167	a	1443.03	2.9998
168	a	1444.93	11.45148

169	a	1445.33	7.23539
170	a	1445.94	4.91716
171	a	1448.67	6.75032
172	a	1456.42	23.30803
173	a	1458.63	21.41245
174	a	1459.17	39.73097
175	a	1459.4	29.89398
176	a	1463.27	72.41211
177	a	1465.77	9.5984
178	a	1466.98	34.69863
179	a	1469.01	19.22178
180	a	1469.23	13.82852
181	a	1469.29	13.55908
182	a	1470.13	8.49043
183	a	1473.45	4.36768
184	a	1473.58	10.41269
185	a	1474.28	13.58219
186	a	1474.87	14.03388
187	a	1475.35	11.27186
188	a	1478.5	6.31557
189	a	1480.11	4.0094
190	a	1483.72	16.30885
191	a	1485.01	13.00439
192	a	1485.67	16.66641
193	a	1486.16	0.81187
194	a	1486.57	2.86188
195	a	1486.96	2.35545
196	a	1489.21	18.29718
197	a	1492.04	11.50482
198	a	1492.88	18.55068
199	a	1494.77	13.70518
200	a	1497.19	36.3268
201	a	1497.84	9.12995
202	a	1538.45	7.35251
203	a	1539.3	5.10864
204	a	1539.67	15.62344
205	a	1540.5	17.13107
206	a	1545.14	464.14168
207	a	1554.41	0.42446
208	a	1680.98	136.39002
209	a	1681.89	2.68124

210	a	1683.83	1633.5743
211	a	1689.96	1528.60414
212	a	1690.82	1521.2653
213	a	1735.27	0.42136
214	a	3016.72	11.53872
215	a	3017.15	13.40797
216	a	3018.66	12.58705
217	a	3019.07	10.98759
218	a	3022.31	8.78126
219	a	3026.39	9.01154
220	a	3036.08	2.23407
221	a	3036.11	3.99791
222	a	3036.12	12.63124
223	a	3036.34	6.17713
224	a	3036.61	6.59604
225	a	3036.7	5.04641
226	a	3039.35	5.30946
227	a	3039.64	7.81266
228	a	3039.66	2.05962
229	a	3039.93	6.75836
230	a	3040.11	4.46768
231	a	3042.46	8.7228
232	a	3067.72	8.98304
233	a	3068.2	7.17034
234	a	3073.56	1.54174
235	a	3074.16	1.12055
236	a	3075.86	1.32686
237	a	3079.01	2.45708
238	a	3112.88	1.80297
239	a	3115.54	1.58494
240	a	3115.74	0.24559
241	a	3115.92	1.53951
242	a	3116.28	1.79598
243	a	3116.42	1.25375
244	a	3116.91	1.42609
245	a	3128.09	0.50871
246	a	3129.37	0.66545
247	a	3130.46	0.68869
248	a	3130.85	0.81646
249	a	3131.45	1.19692
250	a	3157.81	1.45524

251	a	3160.67	1.83701
252	a	3161.12	2.0305
253	a	3161.35	1.96085
254	a	3165.09	2.2893
255	a	3187.03	1.21769
256	a	3187.08	1.10347
257	a	3187.17	1.19974
258	a	3187.34	1.14788
259	a	3187.68	1.13273
260	a	3190.2	1.38813
261	a	3191.85	2.46397
Şend			