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Supporting Information

Experimental and Theoretical Studies on the Extraction Behavior of Cf(III) by NTAamide(C8) Ligand and the Seperation of Cf(III)/Cm(III)

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1. Concentration of Cf^{3+}

The Cf^{3+} concentration in the solution can be calculated from the liquid scintillation number and the following formula:

$$\lambda = \frac{\ln 2}{t_{1/2}} \quad (1)$$

$$N = \frac{A}{\lambda} \quad (2)$$

$$n = \frac{N}{N_A} \quad (3)$$

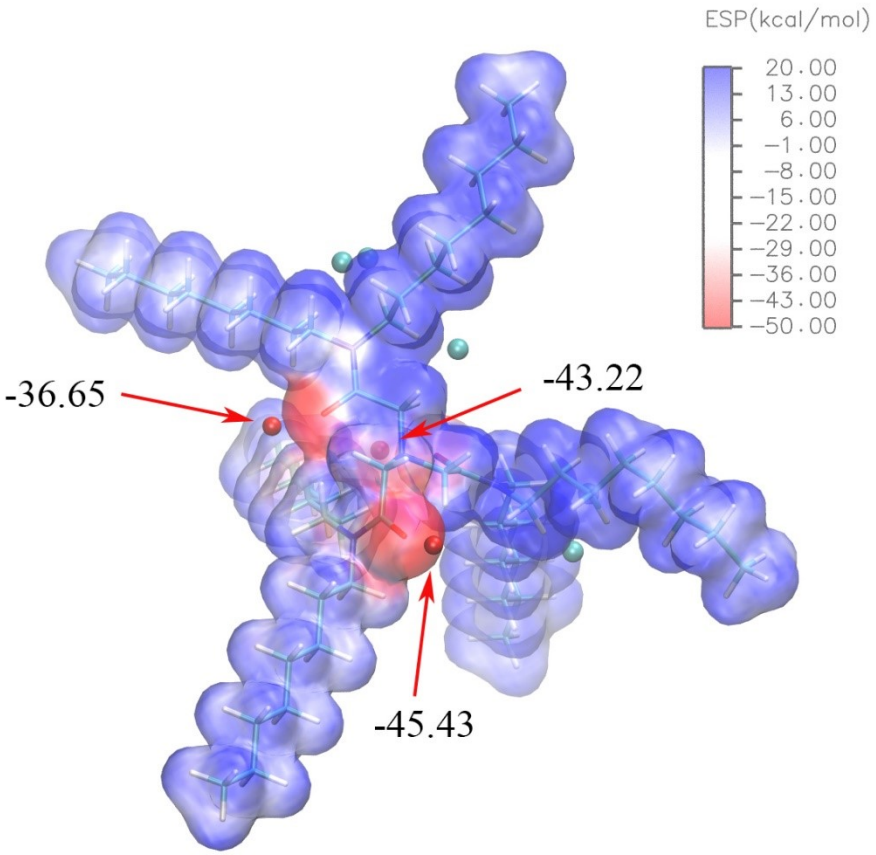
Table S1. Nuclear properties of ^{252}Cf and its decay daughter ^{248}Cm

Nuclide	Half-life (year)	Radioactivity（Ci /g）	Spontaneous fission half-life(year)	Fission fraction (%)	Spontaneous fission yield (n s-1 g-1)
^{252}Cf	2.645	5.38×10^{2}	85	3.09	2.3×10^{12}
^{248}Cm	3.4×10^{5}	4.25×10^{-3}	41	8.39	1.2×10^{7}

After liquid scintillation measurement and deducting the background, the radioactivity of the Cf(III) solution used in the experiment was about 800 cpm, and the radioactivity of the Cf(III) solution obtained after stripping was 910 cpm.

After calculation, the Cf(III) concentration in the solution is about 9.60×10^{-8}mol/L, and the concentration of Cf(III) solution obtained after stripping is 1.09×10^{-7}mol/L.

2. The electrostatic potential (ESP) of NTAamide(C8)



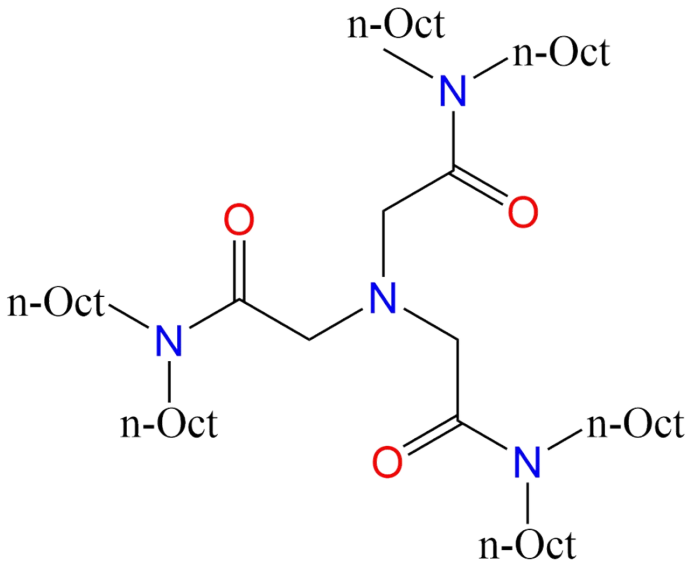


Figure S1. The maps of ESP and structure of NTAamide(C8).

3. Mulliken population analysis (MPA)

Table S2. Differences in charge transfer of metal ions with complexes and trivalent metal ions calculated from Mulliken charges

Species	ΔQ (An)	ΔQ (L)	ΔQ (NO_3)
$CfL(NO_3)_3$	1.564	0.408	1.155
$CmL(NO_3)_3$	1.559	0.415	1.146
$[CfL_2][NO_3]_3$	1.564	0.672	0.892
$[CmL_2][NO_3]_3$	1.557	0.663	0.893

4. Cartesian coordinates coordinates of optimized structures

(1) CfL(NO_3)$_3$	Standard orientation		
Center Number Atomic Number Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	0.48941	0.64907	0.30150
C	-0.77507	1.27437	-0.30262
H	-0.53089	1.95863	-1.12903
H	-1.25681	1.87290	0.47797
C	-3.09421	0.68708	-0.74295
C	-3.67432	0.65746	0.67699
H	-3.18463	1.68076	-1.20386
H	-3.69092	-0.00599	-1.34744
O	0.48776	-0.57793	0.54992
O	-3.10562	-0.04489	1.54044
C	1.61125	2.87250	0.34721
C	1.19679	3.68986	1.58054
H	0.98963	3.14002	-0.51121
H	2.64349	3.11171	0.06848
C	1.34199	5.20037	1.34757
H	0.15755	3.45158	1.84491
H	1.81090	3.38767	2.43902
C	0.92983	6.03159	2.56883
H	2.38505	5.42831	1.08454
H	0.73370	5.49733	0.48030
H	-0.11845	5.84847	2.83685
H	1.54460	5.78127	3.44243
C	2.74213	0.79284	1.19369
C	3.72268	0.21632	0.16406
H	2.39755	0.00969	1.87153
H	3.22889	1.56603	1.79646
C	4.96266	-0.39550	0.831200
H	3.20635	-0.55128	-0.42638
H	4.03150	1.00917	-0.53340

C	5.95009	-0.98760	-0.18202
H	5.47039	0.37261	1.43272
H	4.64395	-1.17859	1.53258
H	5.47803	-1.78218	-0.77360
H	6.31263	-0.22056	-0.87912
N	1.55718	1.41712	0.56460
C	-5.51273	2.17141	-0.03633
C	-5.10781	3.65273	-0.03447
H	-6.57744	2.07691	0.20220
H	-5.38656	1.73738	-1.03211
C	-5.94804	4.48557	-1.01300
H	-5.21686	4.05634	0.98125
H	-4.04265	3.74065	-0.29194
C	-5.54932	5.96627	-1.03076
H	-5.85002	4.06750	-2.02562
H	-7.0103	4.39571	-0.74470
H	-5.66900	6.42044	-0.03897
H	-4.50074	6.09134	-1.33037
C	-5.36203	1.28737	2.31321
C	-6.42129	0.18632	2.45472
H	-5.79773	2.26957	2.52833
H	-4.54358	1.11965	3.01590
C	-7.01926	0.14379	3.86844
H	-7.22517	0.35013	1.72231
H	-5.96578	-0.78241	2.21808
C	-8.08295	-0.94958	4.02675
H	-6.21241	-0.02485	4.59486
H	-7.45795	1.12357	4.11039
H	-8.91874	-0.79315	3.33187
H	-7.65818	-1.94019	3.82581
N	-4.78381	1.36063	0.95410
N	-1.70307	0.22274	-0.73107
H	-6.16804	6.53444	-1.73522
H	1.04416	7.10461	2.37460
H	6.82237	-1.42029	0.32209

H	-8.49101	-0.95866	5.04459
C	-1.31413	-0.37330	-2.01372
C	-1.85035	-1.80788	-2.11124
H	-1.64095	0.24499	-2.86158
H	-0.22104	-0.43578	-2.05648
O	-2.17533	-2.39906	-1.05688
C	-1.54529	-1.76121	-4.57700
C	-2.71101	-1.07110	-5.30035
H	-1.12910	-2.55045	-5.21175
H	-0.72950	-1.05627	-4.39519
C	-2.29278	-0.49220	-6.65945
H	-3.52590	-1.79381	-5.44247
H	-3.11279	-0.26998	-4.66370
C	-3.44588	0.20995	-7.38715
H	-1.46435	0.21681	-6.51574
H	-1.89945	-1.30097	-7.29154
H	-4.27624	-0.48300	-7.57300
H	-3.83648	1.04778	-6.79527
C	-2.41324	-3.80100	-3.38876
C	-1.27219	-4.82454	-3.32024
H	-2.96156	-3.89898	-4.33236
H	-3.11771	-3.96250	-2.57046
C	-1.78893	-6.26635	-3.42855
H	-0.55221	-4.63086	-4.12889
H	-0.73246	-4.69603	-2.37482
C	-0.66356	-7.30517	-3.34806
H	-2.51216	-6.45022	-2.62191
H	-2.33815	-6.38878	-4.37417
H	0.06200	-7.16856	-4.16092
H	-0.12319	-7.22338	-2.39757
N	-1.93893	-2.40249	-3.31021
H	-3.11941	0.60803	-8.35502
H	-1.06153	-8.32432	-3.42263
O	0.23504	-2.27759	3.14282
O	-2.95078	-2.68128	3.22447

O	-0.78333	-0.36217	3.17955
O	0.85223	-0.74880	4.58866
O	-5.01535	-3.40135	3.06107
O	-3.86696	-2.88055	1.26729
N	0.12484	-1.11980	3.67250
N	-3.97960	-3.00513	2.53599
O	-1.24611	-4.46890	1.28336
O	0.31833	-5.60775	0.25137
O	0.32279	-3.41497	0.21927
N	-0.18175	-4.53557	0.57589
Cf	-1.48329	-1.95281	1.30348

(1) $CmL(NO_3)_3$ Standard orientation

Center Number Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
C		0.48941	0.64907	0.30150
C		-0.77507	1.27437	-0.30262
H		-0.53089	1.95863	-1.12903
H		-1.25681	1.87290	0.47797
C		-3.09421	0.68708	-0.74295
C		-3.67432	0.65746	0.67699
H		-3.18463	1.68076	-1.20386
H		-3.69092	-0.00599	-1.34744
O		0.48776	-0.57793	0.54992
O		-3.10562	-0.04489	1.54044
C		1.61125	2.87250	0.34721
C		1.19679	3.68986	1.58054
H		0.98963	3.14002	-0.51121
H		2.64349	3.11171	0.06848
C		1.34199	5.20037	1.34757
H		0.15755	3.45158	1.84491
H		1.81090	3.38767	2.43902
C		0.92983	6.03159	2.56883

H	2.38505	5.42831	1.08454
H	0.73370	5.49733	0.48030
H	-0.11845	5.84847	2.83685
H	1.54460	5.78127	3.44243
C	2.74213	0.79284	1.19369
C	3.72268	0.21632	0.16406
H	2.39755	0.00969	1.87153
H	3.22889	1.56603	1.79646
C	4.96266	-0.39550	0.83120
H	3.20635	-0.55128	-0.42638
H	4.03150	1.00917	-0.53340
C	5.95009	-0.98760	-0.18202
H	5.47039	0.37261	1.43272
H	4.64395	-1.17859	1.53258
H	5.47803	-1.78218	-0.77360
H	6.31263	-0.22056	-0.87912
N	1.55718	1.41712	0.56460
C	-5.51273	2.17141	-0.03633
C	-5.10781	3.65273	-0.03447
H	-6.57744	2.07691	0.20220
H	-5.38656	1.73738	-1.03211
C	-5.94804	4.48557	-1.01300
H	-5.21686	4.05634	0.98125
H	-4.04265	3.74065	-0.29194
C	-5.54932	5.96627	-1.03076
H	-5.85002	4.06750	-2.02562
H	-7.01030	4.39571	-0.74470
H	-5.66900	6.42044	-0.03897
H	-4.50074	6.09134	-1.33037
C	-5.36203	1.28737	2.31321
C	-6.42129	0.18632	2.45472
H	-5.79773	2.26957	2.52833
H	-4.54358	1.11965	3.01590
C	-7.01926	0.14379	3.86844
H	-7.22517	0.35013	1.72231

H	-5.96578	-0.78241	2.21808
C	-8.08295	-0.94958	4.02675
H	-6.21241	-0.02485	4.59486
H	-7.45795	1.12357	4.11039
H	-8.91874	-0.79315	3.33187
H	-7.65818	-1.94019	3.82581
N	-4.78381	1.36063	0.95410
N	-1.70307	0.22274	-0.73107
H	-6.16804	6.53444	-1.73522
H	1.04416	7.10461	2.37460
H	6.82237	-1.42029	0.32209
H	-8.49101	-0.95866	5.04459
C	-1.31413	-0.37330	-2.01372
C	-1.85035	-1.80788	-2.11124
H	-1.64095	0.24499	-2.86158
H	-0.22104	-0.43578	-2.05648
O	-2.17533	-2.39906	-1.05688
C	-1.54529	-1.76121	-4.57700
C	-2.71101	-1.07110	-5.30035
H	-1.12910	-2.55045	-5.21175
H	-0.72950	-1.05627	-4.39519
C	-2.29278	-0.49220	-6.65945
H	-3.52590	-1.79381	-5.44247
H	-3.11279	-0.26998	-4.66370
C	-3.44588	0.20995	-7.38715
H	-1.46435	0.21681	-6.51574
H	-1.89945	-1.30097	-7.29154
H	-4.27624	-0.48300	-7.57300
H	-3.83648	1.04778	-6.79527
C	-2.41324	-3.80100	-3.38876
C	-1.27219	-4.82454	-3.32024
H	-2.96156	-3.89898	-4.33236
H	-3.11771	-3.96250	-2.57046
C	-1.78893	-6.26635	-3.42855
H	-0.55221	-4.63086	-4.12889

H	-0.73246	-4.69603	-2.37482
C	-0.66356	-7.30517	-3.34806
H	-2.51216	-6.45022	-2.62191
H	-2.33815	-6.38878	-4.37417
H	0.06200	-7.16856	-4.16092
H	-0.12319	-7.22338	-2.39757
N	-1.93893	-2.40249	-3.31021
H	-3.11941	0.60803	-8.35502
H	-1.06153	-8.32432	-3.42263
O	0.23504	-2.27759	3.14282
O	-2.95078	-2.68128	3.22447
O	-0.78333	-0.36217	3.17955
O	0.85223	-0.74880	4.58866
O	-5.01535	-3.40135	3.06107
O	-3.86696	-2.88055	1.26729
N	0.12484	-1.11980	3.67250
N	-3.97960	-3.00513	2.53599
O	-1.24611	-4.46890	1.28336
O	0.31833	-5.60775	0.25137
O	0.32279	-3.41497	0.21927
N	-0.18175	-4.53557	0.57589
Cm	-1.48329	-1.95281	1.30348

(1) $[CfL_2][NO_3]_3$ Standard orientation

Center Number Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
	Cf	-1.74020	-1.99121	1.34296
	C	0.21650	0.64762	0.90474
	C	-1.22507	0.87164	0.40794
	H	-1.23070	1.64923	-0.32546
	H	-1.84630	1.15337	1.23242
	C	-3.11401	-0.15048	-0.66899
	C	-4.00950	0.25313	0.51718

H	-3.11781	0.63012	-1.40148
H	-3.48849	-1.05287	-1.10627
O	0.57619	-0.49257	1.29843
O	-3.74383	-0.16648	1.67338
C	0.66153	3.00141	0.46538
C	0.11087	3.80144	1.66260
H	-0.10291	2.89996	-0.27672
H	1.49914	3.51893	0.04628
C	-0.33621	5.19730	1.18758
H	-0.72605	3.28372	2.08278
H	0.87546	3.90505	2.40343
C	-0.88643	5.99510	2.38493
H	0.50029	5.71630	0.76689
H	-1.10047	5.09358	0.44662
H	-1.72220	5.47604	2.80574
H	-0.12141	6.09959	3.12592
C	2.46658	1.45253	1.37752
C	3.35051	1.05443	0.18040
H	2.48191	0.67094	2.10805
H	2.84085	2.35531	1.81249
C	4.79668	0.82831	0.66058
H	2.97450	0.15232	-0.25583
H	3.33496	1.83663	-0.54952
C	5.67890	0.42944	-0.53691
H	5.17288	1.73013	1.09608
H	4.81230	0.04598	1.39066
H	5.30212	-0.47236	-0.97301
H	5.66413	1.21160	-1.26684
N	1.08615	1.66657	0.91628
C	-5.38882	1.53386	-1.03088
C	-4.67143	2.87459	-1.28060
H	-6.44577	1.67439	-1.11936
H	-5.06227	0.81545	-1.75375
C	-5.00245	3.37907	-2.69884
H	-4.99994	3.59448	-0.56027

H	-3.61451	2.73558	-1.18983
C	-4.28420	4.71811	-2.94839
H	-4.67382	2.65951	-3.41854
H	-6.06007	3.51834	-2.79104
H	-4.61317	5.43840	-2.22925
H	-3.22697	4.57866	-2.85599
C	-5.91399	1.42962	1.46366
C	-7.03418	0.38827	1.64601
H	-6.34626	2.39150	1.28276
H	-5.31674	1.46785	2.35098
C	-7.91325	0.78547	2.84696
H	-7.63402	0.35040	0.76073
H	-6.60094	-0.57365	1.82454
C	-9.03249	-0.25636	3.03249
H	-7.31210	0.82376	3.73163
H	-8.34710	1.74672	2.66857
H	-9.63404	-0.29540	2.14827
H	-8.59844	-1.21806	3.21145
N	-5.06961	1.04720	0.32139
N	-1.73987	-0.36979	-0.19171
H	-4.51274	5.06734	-3.93386
H	-1.19789	6.96447	2.05497
H	6.68318	0.27157	-0.20330
H	-9.64272	0.02045	3.86712
C	-0.88403	-0.75762	-1.32371
C	-1.41935	-2.05934	-1.95183
H	-0.89004	0.02209	-2.05668
H	0.11656	-0.91505	-0.97878
O	-2.01947	-2.90438	-1.23802
C	-0.54999	-1.30759	-4.09669
C	-1.57232	-0.31067	-4.67752
H	-0.04935	-1.81123	-4.89709
H	0.16630	-0.77786	-3.50437
C	-0.84181	0.72516	-5.55537
H	-2.28889	-0.83957	-5.27162

H	-2.07372	0.19195	-3.87754
C	-1.86366	1.72457	-6.13063
H	-0.12464	1.25283	-4.96284
H	-0.34163	0.22383	-6.35830
H	-2.58233	1.19922	-6.72332
H	-2.36158	2.22675	-5.32778
C	-1.75097	-3.54178	-3.85011
C	-0.66165	-4.62710	-3.76654
H	-2.00709	-3.37198	-4.87500
H	-2.61895	-3.86660	-3.31500
C	-1.18828	-5.93120	-4.39575
H	0.20823	-4.30135	-4.29741
H	-0.40920	-4.80173	-2.74121
C	-0.10069	-7.01899	-4.31499
H	-2.05830	-6.25721	-3.86489
H	-1.44028	-5.75566	-5.42053
H	0.77050	-6.69316	-4.84457
H	0.15035	-7.19661	-3.29024
N	-1.24589	-2.29436	-3.25677
H	-1.35585	2.44309	-6.73997
H	-0.46760	-7.92323	-4.75458
C	0.22396	-4.61786	1.81259
C	-1.22229	-4.85179	2.28869
H	-1.23318	-5.62860	3.02431
H	-1.82952	-5.14037	1.45691
C	-3.13277	-3.83713	3.33442
C	-4.00882	-4.24447	2.13497
H	-3.14419	-4.61786	4.06726
H	-3.51752	-2.93676	3.76601
O	0.58119	-3.47491	1.42658
O	-3.73025	-3.82296	0.98279
C	0.67876	-6.96784	2.25374
C	0.15090	-7.76751	1.04729
H	-0.09701	-6.87266	2.98500
H	1.51320	-7.48115	2.68378

C	-0.29710	-9.16379	1.51649
H	-0.68159	-7.25320	0.61390
H	0.92712	-7.86741	0.31802
C	-0.82552	-9.96692	0.31343
H	0.53498	-9.67801	1.95093
H	-1.07335	-9.06181	2.24514
H	-1.65757	-9.45308	-0.12116
H	-0.04927	-10.06920	-0.41590
C	2.48450	-5.40668	1.36753
C	3.34951	-5.00090	2.57498
H	2.50403	-4.62588	0.63626
H	2.87079	-6.30706	0.93866
C	4.80181	-4.76893	2.11597
H	2.96281	-4.09946	3.00338
H	3.32759	-5.78141	3.30632
C	5.66161	-4.36751	3.32824
H	5.18881	-5.66917	1.68626
H	4.82635	-3.98661	1.38607
H	5.27425	-3.46720	3.75779
H	5.63675	-5.15033	4.05716
N	1.10055	-5.63036	1.81071
C	-5.40461	-5.53303	3.66052
C	-4.68163	-6.86867	3.92196
H	-6.46201	-5.68110	3.73175
H	-5.09503	-4.81222	4.38771
C	-5.02942	-7.37468	5.33575
H	-4.99424	-7.59104	3.19765
H	-3.62395	-6.72236	3.84672
C	-4.30763	-8.71030	5.59489
H	-4.71408	-6.65322	6.05975
H	-6.08723	-7.51947	5.41384
H	-4.62432	-9.43240	4.87163
H	-3.24998	-8.56606	5.51544
C	-5.89158	-5.42968	1.15958
C	-7.01430	-4.39495	0.96193

H	-6.32107	-6.39431	1.33298
H	-5.28092	-5.46366	0.28116
C	-7.87295	-4.79907	-0.24982
H	-7.62671	-4.36011	1.83862
H	-6.58444	-3.43037	0.78901
C	-8.99569	-3.76503	-0.45174
H	-7.25926	-4.83467	-1.12599
H	-8.30265	-5.76302	-0.07602
H	-9.60842	-3.72807	0.42486
H	-8.56542	-2.80111	-0.62744
N	-5.06706	-5.04413	2.31417
N	-1.75285	-3.61248	2.87738
H	-4.54677	-9.06066	6.57739
H	-1.13689	-10.93660	0.64140
H	6.67132	-4.20608	3.01233
H	-9.59353	-4.04778	-1.2933
C	-0.91491	-3.21795	4.02034
C	-1.46665	-1.91862	4.63849
H	-0.92634	-3.99698	4.75479
H	0.08968	-3.05567	3.68869
O	-2.06040	-1.07872	3.91343
C	-0.62475	-2.66362	6.79682
C	-1.64994	-3.66629	7.36189
H	-0.13938	-2.15695	7.60400
H	0.10423	-3.18913	6.21506
C	-0.92640	-4.69731	8.25049
H	-2.37857	-3.14115	7.94439
H	-2.13592	-4.17160	6.55406
C	-1.95013	-5.70231	8.81207
H	-0.19814	-5.22075	7.66796
H	-0.44059	-4.19242	9.05974
H	-2.67930	-5.18102	9.39555
H	-2.43531	-6.20675	8.00259
C	-1.83528	-0.43719	6.53353
C	-0.75160	0.65490	6.46565

H	-2.10441	-0.61003	7.55467
H	-2.69823	-0.11777	5.98677
C	-1.29379	1.95544	7.08799
H	0.11278	0.33355	7.00789
H	-0.48647	0.83132	5.44381
C	-0.21089	3.04892	7.02232
H	-2.15833	2.27651	6.54518
H	-1.55897	1.77809	8.10909
H	0.65399	2.72859	7.56515
H	0.05460	3.22674	6.00133
N	-1.31423	-1.68117	5.94642
H	-1.44623	-6.41817	9.42731
H	-0.58916	3.95153	7.45508

(1) $[CmL_2][NO_3]_3$ Standard orientation

Center Number Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
C		0.20718	0.67143	0.87471
C		-1.22612	0.91022	0.37066
H		-1.22282	1.68659	-0.36565
H		-1.85206	1.20391	1.19027
C		-3.11202	-0.11932	-0.70009
C		-4.00184	0.27112	0.49478
H		-3.12393	0.66528	-1.42841
H		-3.48300	-1.01964	-1.14278
O		0.55317	-0.47337	1.26315
O		-3.72224	-0.15106	1.64594
C		0.66406	3.01354	0.45858
C		0.11134	3.80147	1.65945
H		-0.09728	2.91795	-0.28623
H		1.50346	3.53425	0.04630
0C		-0.33440	5.19700	1.18892
H		-0.72573	3.28024	2.07496

H	0.87406	3.90085	2.40321
C	-0.88512	5.99267	2.38572
H	0.50255	5.71579	0.77044
H	-1.09822	5.09460	0.44648
H	-1.72215	5.47393	2.80439
H	-0.12122	6.09461	3.12778
C	2.45897	1.45488	1.37153
C	3.34754	1.05436	0.17894
H	2.46531	0.67193	2.10049
H	2.83645	2.35451	1.81202
C	4.79209	0.82793	0.66340
H	2.97198	0.15259	-0.25779
H	3.33639	1.83624	-0.55145
C	5.67647	0.42978	-0.53336
H	5.16744	1.72943	1.09980
H	4.80593	0.04537	1.39324
H	5.30138	-0.47274	-0.96967
H	5.66142	1.21166	-1.26350
N	1.08258	1.67910	0.90065
C	-5.39329	1.53718	-1.03440
C	-4.67319	2.87383	-1.28200
H	-6.45020	1.67794	-1.11986
H	-5.07002	0.81804	-1.75820
C	-5.00505	3.37863	-2.69716
H	-4.99785	3.59347	-0.55995
H	-3.61606	2.73177	-1.19303
C	-4.28555	4.71670	-2.94594
H	-4.67851	2.65905	-3.41793
H	-6.06199	3.51957	-2.78668
H	-4.61191	5.43646	-2.22450
H	-3.22861	4.57592	-2.85607
C	-5.91194	1.43108	1.45838
C	-7.03184	0.38870	1.64207
H	-6.34593	2.39245	1.28004
H	-5.31246	1.46858	2.34408

C	-7.91179	0.78682	2.84252
H	-7.63189	0.35036	0.75701
H	-6.59811	-0.57289	1.82096
C	-9.03124	-0.25470	3.02790
H	-7.31102	0.82586	3.72758
H	-8.34546	1.74836	2.66349
H	-9.63213	-0.29380	2.14366
H	-8.59748	-1.21629	3.20742
N	-5.06861	1.05512	0.31244
N	-1.73817	-0.33310	-0.22473
H	-4.51630	5.06790	-3.92976
H	-1.19470	6.96232	2.05641
H	6.68057	0.27315	-0.19873
H	-9.64167	0.02230	3.86214
C	-0.88113	-0.72351	-1.35241
C	-1.41593	-2.03247	-1.96259
H	-0.89203	0.04946	-2.09306
H	0.12208	-0.87033	-1.00794
O	-2.01564	-2.86395	-1.23227
C	-0.54607	-1.30425	-4.10301
C	-1.56889	-0.30972	-4.67794
H	-0.04702	-1.80939	-4.90318
H	0.17381	-0.77555	-3.51259
C	-0.83995	0.72341	-5.55465
H	-2.28702	-0.83805	-5.26952
H	-2.06798	0.19263	-3.87574
C	-1.86284	1.71940	-6.13024
H	-0.12295	1.25145	-4.96215
H	-0.34004	0.22136	-6.35667
H	-2.58030	1.19125	-6.72310
H	-2.36297	2.22073	-5.32813
C	-1.74911	-3.53385	-3.85308
C	-0.66091	-4.62216	-3.77042
H	-2.00493	-3.36484	-4.87798
H	-2.61641	-3.85655	-3.31631

C	-1.18997	-5.92788	-4.39472
H	0.20795	-4.29889	-4.30511
H	-0.40549	-4.79438	-2.74586
C	-0.10149	-7.01485	-4.31252
H	-2.05892	-6.25216	-3.86059
H	-1.44502	-5.75603	-5.41951
H	0.76727	-6.69102	-4.84624
H	0.15306	-7.18756	-3.28763
N	-1.24385	-2.28344	-3.26353
H	-1.35645	2.43814	-6.73977
H	-0.46915	-7.92163	-4.74605
C	0.21528	-4.63648	1.83465
C	-1.22405	-4.88310	2.31747
H	-1.22707	-5.66147	3.05264
H	-1.83647	-5.17491	1.48937
C	-3.13072	-3.86971	3.36549
C	-4.00067	-4.26313	2.15733
H	-3.14651	-4.65419	4.09188
H	-3.51439	-2.97135	3.80789
O	0.56099	-3.48946	1.45161
O	-3.70542	-3.83654	1.01108
C	0.67929	-6.97674	2.26027
C	0.14841	-7.76961	1.05237
H	-0.09324	-6.88485	2.99399
H	1.51578	-7.49185	2.68505
C	-0.29588	-9.16818	1.51663
H	-0.68590	-7.25386	0.62483
H	0.92223	-7.86491	0.31976
C	-0.82472	-9.96603	0.31107
H	0.53785	-9.68259	1.94699
H	-1.07094	-9.07076	2.24793
H	-1.65806	-9.45116	-0.11963
H	-0.04928	-10.0633	-0.41960
C	2.47847	-5.40841	1.37271
C	3.34686	-5.00411	2.57873

H	2.49192	-4.62503	0.64411
H	2.86714	-6.30592	0.93745
C	4.79719	-4.76955	2.11575
H	2.96002	-4.10480	3.01045
H	3.32907	-5.78664	3.30850
C	5.66234	-4.36576	3.32467
H	5.18402	-5.66911	1.68519
H	4.81714	-3.98716	1.38599
H	5.27606	-3.46512	3.75512
H	5.64183	-5.14720	4.05502
N	1.09651	-5.63978	1.82288
C	-5.40617	-5.53587	3.66600
C	-4.68308	-6.86893	3.92371
H	-6.46328	-5.68182	3.73643
H	-5.09653	-4.81530	4.39443
C	-5.03277	-7.37553	5.33372
H	-4.99398	-7.59012	3.19702
H	-3.62556	-6.72172	3.84965
C	-4.30884	-8.70919	5.59304
H	-4.72110	-6.65405	6.05909
H	-6.09000	-7.52283	5.40774
H	-4.61986	-9.43081	4.86681
H	-3.25152	-8.56172	5.51892
C	-5.88966	-5.43355	1.16587
C	-7.0129	-4.39751	0.96550
H	-6.32069	-6.39740	1.33858
H	-5.27716	-5.46822	0.28887
C	-7.87400	-4.80044	-0.24756
H	-7.62583	-4.36245	1.84175
H	-6.58205	-3.43372	0.79235
C	-8.99669	-3.76509	-0.44886
H	-7.26051	-4.83617	-1.12401
H	-8.30481	-5.76451	-0.07475
H	-9.61056	-3.72980	0.42662
H	-8.56584	-2.80095	-0.62166

N	-5.06525	-5.05251	2.32361
N	-1.75126	-3.64654	2.90850
H	-4.55193	-9.06192	6.57330
H	-1.13419	-10.93750	0.63484
H	6.67021	-4.20337	3.00393
H	-9.59336	-4.04515	-1.29195
C	-0.91349	-3.25275	4.05075
C	-1.46416	-1.94623	4.65220
H	-0.93213	-4.02514	4.79262
H	0.09381	-3.09943	3.72400
O	-2.05695	-1.11772	3.91464
C	-0.62068	-2.66773	6.80498
C	-1.64588	-3.66786	7.36502
H	-0.13560	-2.16001	7.61206
H	0.11035	-3.19210	6.22448
C	-0.92385	-4.69706	8.25158
H	-2.37530	-3.14364	7.94613
H	-2.13065	-4.17268	6.55545
C	-1.94958	-5.69847	8.81187
H	-0.19542	-5.22093	7.66924
H	-0.43819	-4.19224	9.06050
H	-2.67880	-5.17392	9.39349
H	-2.43478	-6.20265	8.00237
C	-1.83311	-0.44475	6.53635
C	-0.74972	0.64957	6.46912
H	-2.10329	-0.61420	7.55739
H	-2.69373	-0.12731	5.98626
C	-1.29522	1.95198	7.08558
H	0.11301	0.33111	7.01634
H	-0.48037	0.82294	5.44818
C	-0.21209	3.04517	7.01960
H	-2.15829	2.27133	6.53885
H	-1.56423	1.77806	8.10634
H	0.65103	2.72567	7.56496
H	0.05563	3.22058	5.99854

N	-1.31226	-1.69301	5.95545
H	-1.44849	-6.41403	9.42912
H	-0.59102	3.94923	7.44903
Cm	-1.73763	-1.98777	1.34437