

A diglycolamide-functionalized TREN-based dendrimer with a ‘crab-like’ grip for the complexation of actinides and lanthanides

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1. Solvent extraction studies

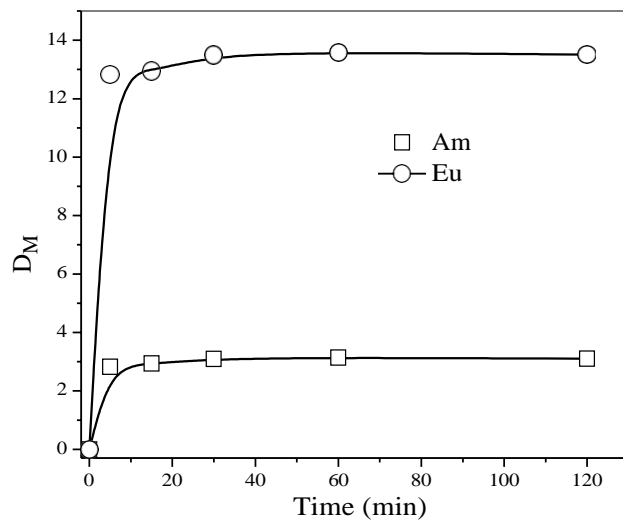


Fig.S1 Effect of equilibration time on the extraction of Am^{3+} and Eu^{3+} ; Org. phase: 1.0 mM TREN-G1-DGA in 5% iso-decanol/n-dodecane; Aq. phase: 3 M HNO_3 .

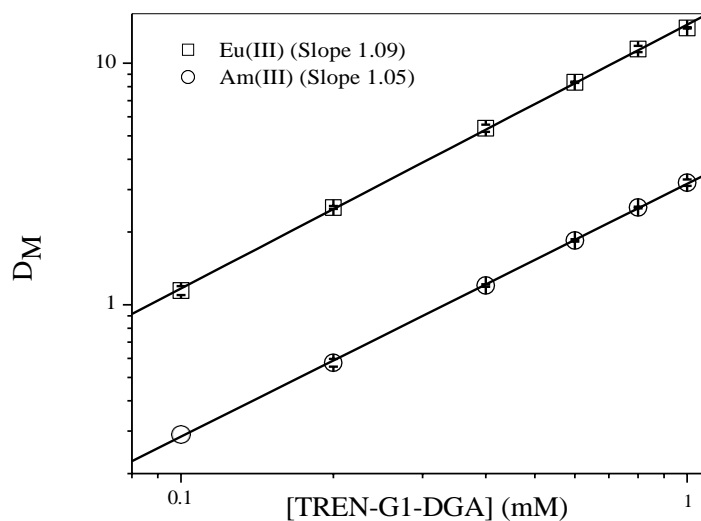


Fig. S2 Effect of the TREN-G1-DGA concentration on the extraction of Am^{3+} and Eu^{3+} ; Org. phase: TREN-G1-DGA in 5% iso-decanol/n-dodecane; Aq. phase: 3 M HNO_3 .

Table S1. Separation behavior of Am³⁺ and Eu³⁺ from nitrate media

[NaNO ₃] ^a , M	SF (D _{Eu} /D _{Am})	[HNO ₃], M	SF (D _{Eu} /D _{Am})
0.1	2	0.5	1.91
0.5	2.35	1	2.21
1	2.29	3	4.38
3	2.17	6	6.11
6	2.06		

^aAlso contained 0.01 M HNO₃ to prevent the hydrolysis of the metal ion

2. Luminescence studies

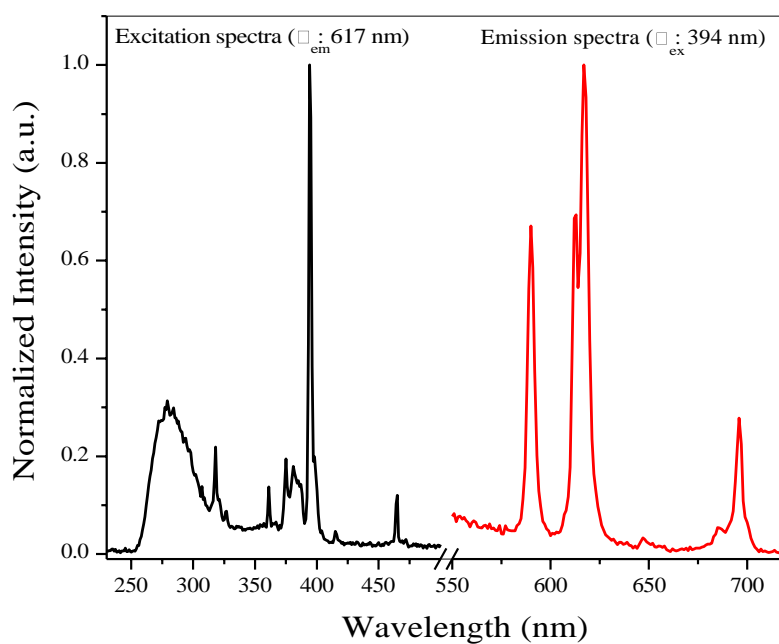


Fig. S3 Luminescence (excitation and emission) spectra of the Eu³⁺ extract using 10 mM TEHDGA in 5% iso-decanol/n-dodecane (λ_{em} : 617 nm in the excitation scan and λ_{ex} : 394 nm in the emission scan).

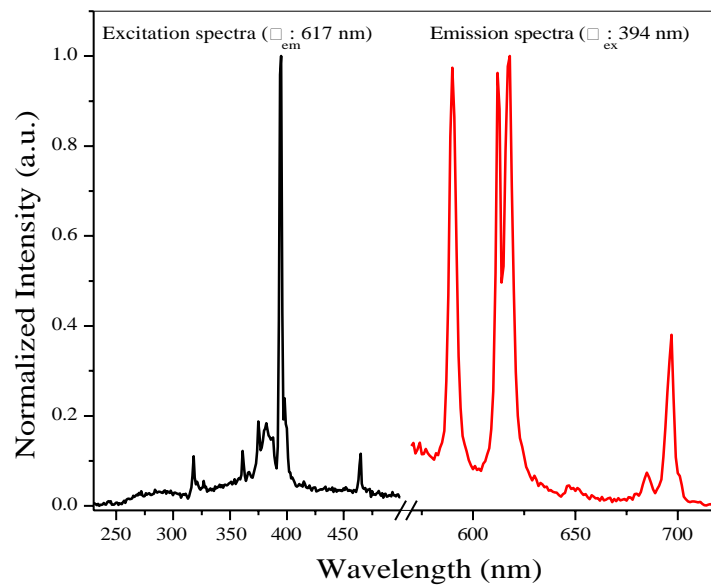


Fig. S4 Luminescence (excitation and emission) spectra of the Eu³⁺ extract using 10 mM TODGA in 5% iso-decanol/n-dodecane (λ_{em}: 617 nm in the excitation scan and λ_{ex}: 394 nm in the emission scan).

3. DFT Studies

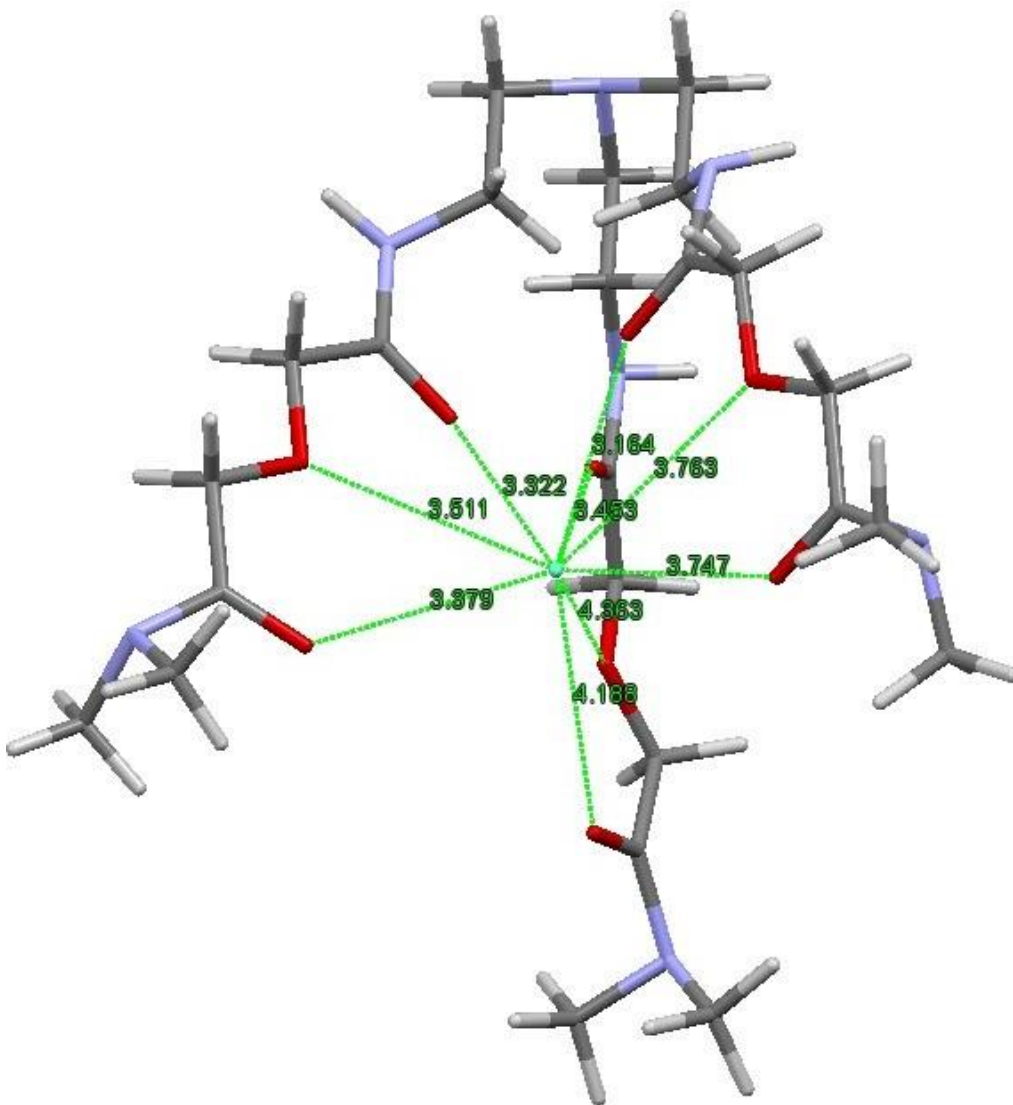


Fig.S5 Schematic 3D structure of the EuL³⁺ type of complex of DGA-TREN with closest proximity of all the three DGA arms required for the similar nine-coordination environment as observed in case of the corresponding TODGA complex.

Table S2: Coordinates of the optimized geometries of free TREN-G1-DGA and its complexes with Am³⁺ and Eu³⁺

Free TREN-G1-MDGA

N	1.9551722	0.3987592	-0.1668552
C	1.7444939	0.8372542	-1.5562784
H	1.1906709	1.7985858	-1.5530860
H	2.7231943	1.0478182	-2.0650476
C	2.1258689	1.5491030	0.7372999
H	2.5829970	1.1935806	1.6857549
H	2.8380407	2.2908656	0.2903506
C	3.0822772	-0.5477306	-0.0556343
H	3.0895747	-1.2155988	-0.9429691
H	4.0555698	0.0147569	-0.0767635
C	0.7764737	2.1982334	1.0888671
H	0.2496812	2.5032302	0.1430642
H	0.1392235	1.4102790	1.5494140
C	0.9024487	-0.1584191	-2.3741489
H	1.4069817	-1.1531531	-2.4118712
H	-0.0454988	-0.3159713	-1.8165079
C	3.0736445	-1.4486180	1.1939169
H	4.1147968	-1.8068553	1.3387508
H	2.8226739	-0.8233368	2.0948200
N	2.2544208	-2.6504760	1.0801020
N	0.5656286	0.3520418	-3.7066953
N	0.8642492	3.3097125	2.0452708
C	1.6016440	0.1864478	-4.7244114
H	1.5122848	1.0031099	-5.4804462
H	2.5882146	0.3324873	-4.2357538
C	-0.8084806	0.0895717	-4.1280553
H	-1.0035872	-0.9846086	-4.3911612
H	-1.4738474	0.3190299	-3.2669641
C	1.8615605	4.3340863	1.7365028
H	1.8628508	5.0916309	2.5510849
H	2.8692841	3.8679471	1.7589015
C	-0.4523798	3.8034201	2.4300689
H	-0.9334677	4.4502154	1.6380853
H	-1.1212669	2.9221879	2.5426529
C	2.6298632	-3.7370952	1.9684315
H	2.0666079	-4.6529343	1.6735325
H	3.7050913	-3.9683139	1.8018339
C	0.8513750	-2.5290312	0.7300946
H	0.1588109	-2.7492238	1.5903649
H	0.6588690	-1.4784762	0.4192332
C	0.5347461	-3.4712225	-0.4521612

H	0.7080403	-4.5337460	-0.1571639
H	1.2412680	-3.2560164	-1.2761054
C	-1.2707742	0.9754210	-5.2979818
H	-0.6784355	0.7594785	-6.2184225
H	-1.1314757	2.0487655	-5.0544649
C	-0.4675342	4.5602357	3.7736883
H	0.1814107	5.4656551	3.7357699
H	-0.0867762	3.9027521	4.5813967
C	1.7183521	5.0662557	0.3722838
H	1.6970754	4.3204919	-0.4514877
H	0.7768152	5.6540784	0.3223964
C	1.6453715	-1.1478827	-5.5145042
H	2.4697988	-1.0719644	-6.2560187
H	0.6947052	-1.3049866	-6.0696158
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H	-2.3470741	5.5480016	3.5171057
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N	1.9002952	-2.3345776	-4.7108708
H	1.1090023	-2.7871275	-4.2245916
C	-3.5708455	1.8052246	-5.6213574
O	-3.2826186	2.9940548	-5.4580675
C	-5.0236062	1.4065005	-5.9491685
H	-5.6146832	2.3505086	-5.8880760
H	-5.0899071	1.0220576	-7.0015357
O	-5.5287781	0.4339978	-5.0379951
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H	-10.6851487	-0.5521078	-4.8971104
H	-10.0762137	0.9899494	-4.1936911
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O	4.2479694	4.3563535	-0.7380193
C	5.0723238	6.6168866	-0.5865871
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H	5.9609573	6.3273458	0.0307804
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H	5.9665860	9.1394765	-1.0577066
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H	-4.6229154	-2.1489682	-8.2430244
H	-5.6471775	-3.6170371	-8.5417016
C	-6.4846841	-3.7941208	-5.9352726
H	-6.4378630	-3.7933343	-4.8311133
H	-7.4557652	-3.3264811	-6.2185781
H	-6.4965632	-4.8491025	-6.3021499
C	4.0791877	-4.6800751	4.8494873
O	4.9139790	-3.7754645	4.8399050
C	4.3959575	-6.0178484	5.5376462
H	4.6545038	-5.8021321	6.6058992
H	5.3170429	-6.4357240	5.0571816
O	3.3051050	-6.9093173	5.4334548
C	3.5186868	-8.1592427	6.0222802
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H	3.7228579	-8.0592925	7.1216081
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N	2.2707155	-10.2949291	6.3215157
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H	3.5680083	-11.8982196	6.7705998
H	4.2862800	-10.2753377	7.0003761
C	1.0792977	-11.1202136	6.1904305
H	1.3225337	-12.0867977	5.6907403
H	0.6362676	-11.3450456	7.1898641
H	0.3425495	-10.5617623	5.5803471
C	3.1659146	-2.8082956	-4.5220838
O	4.1758536	-2.2895424	-5.0204186
C	3.2710030	-4.0382689	-3.6028473
H	2.2682994	-4.3960454	-3.2880912
H	3.7866040	-4.8538225	-4.1728133
O	3.9746362	-3.7438938	-2.4048052
C	5.3645763	-3.5828064	-2.5723533
H	5.7920269	-4.4605411	-3.1287312
H	5.5903840	-2.6828124	-3.1904213

C	6.0209481	-3.4914216	-1.1817335
O	5.3646867	-3.6159150	-0.1496690
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C	8.0663521	-3.1635898	0.1170405
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H	8.8970351	-3.9049254	0.1873669
H	8.4972131	-2.1436494	0.2582150
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H	7.6675633	-3.2415054	-3.2754374
H	8.6167954	-2.0138246	-2.3686802
H	9.1003327	-3.7486488	-2.3194917

Am(TREN-G1-MDGA)³⁺

N	3.0819049	-0.6171911	-0.0670933
C	3.9677007	-0.3593858	-1.2135426
H	4.3740791	0.6692060	-1.1249153
H	4.8633089	-1.0321524	-1.1776114
C	3.3402626	0.2537365	1.0845167
H	2.6812247	-0.0729391	1.9167634
H	4.3964656	0.1520830	1.4537664
C	3.0057073	-2.0372523	0.2639309
H	2.9318634	-2.6088822	-0.6859944
H	3.9391665	-2.4006332	0.7752270
C	2.9881540	1.7276824	0.7665431
H	3.9071411	2.3326169	0.5519944
H	2.3915486	1.7039249	-0.1699568
C	3.2950487	-0.5285665	-2.5903443
H	4.0829599	-0.8103109	-3.3403219
H	2.6084566	-1.4011763	-2.5303226
C	1.7561017	-2.4150699	1.0991900
H	1.8948000	-2.1331463	2.1751972
H	0.9186106	-1.7928498	0.7111584
N	1.3928435	-3.8201567	0.9695834
N	2.5164703	0.6278359	-3.0785491
N	2.1754300	2.3801428	1.8055188
C	3.3953697	1.7224256	-3.5211034
H	4.2289982	1.7866022	-2.7918482
H	3.8754991	1.5087037	-4.5136129
C	1.5636730	0.2016929	-4.1166587
H	1.4407435	1.0195718	-4.8580843
H	1.9627009	-0.6669730	-4.7017088
C	2.9687114	2.8023363	2.9768785
H	3.7517128	2.0317991	3.1397348
H	3.5111268	3.7609249	2.7738572
C	1.3454781	3.4576767	1.2494977

H	0.9818454	4.0965154	2.0889935
H	1.9123633	4.1221372	0.5491235
C	2.0961219	-4.7793450	1.8244127
H	3.0608115	-4.3203801	2.1276519
H	1.5297808	-4.9732536	2.7719890
C	-0.0131101	-4.1032380	0.7398929
H	-0.1988705	-5.1847453	0.9413947
H	-0.6826115	-3.5071815	1.4187006
C	-0.3883142	-3.8052150	-0.7268836
H	0.2515854	-4.4172986	-1.3948928
H	-0.2198283	-2.7353848	-0.9723523
C	0.1779102	-0.1838865	-3.5696020
H	0.2811235	-0.7547596	-2.6197314
H	-0.3450369	-0.8468095	-4.2969891
C	0.1310460	2.8625396	0.5113465
H	0.4078293	2.3953670	-0.4624975
H	-0.6204076	3.6535034	0.3023845
C	2.1171975	2.9634393	4.2750644
H	1.0438397	2.8241494	4.0167477
H	2.3901797	2.1687313	5.0020787
C	2.7378686	3.1225851	-3.5624486
H	3.5171467	3.8737199	-3.3028562
H	1.9426178	3.1810681	-2.7889394
C	2.3534148	-6.1492903	1.1141395
H	1.8081122	-6.1451221	0.1445837
H	3.4331839	-6.2593323	0.8823041
N	-1.7830192	-4.1039872	-1.0681858
H	-1.9916690	-5.0409514	-1.4294762
N	1.9477164	-7.3110644	1.8767172
H	2.6636694	-7.9295594	2.3306724
N	2.2385136	4.2407482	4.9425690
H	3.0130539	4.4244625	5.6246969
N	-0.4497175	1.8498628	1.3935398
H	0.2270133	1.5669052	2.1340317
N	-0.6463800	1.0054855	-3.3381588
H	-0.2791660	1.9515062	-3.6594720
N	2.1684036	3.5366425	-4.8381120
H	2.8164431	3.8060037	-5.6261342
C	-1.8880366	0.9745950	-2.8667213
O	-2.4762449	-0.0754399	-2.4720462
C	-2.6257532	2.3176913	-2.8339934
H	-1.9836869	3.0983212	-2.3666156
H	-2.8478771	2.6531919	-3.8749923
O	-3.8261814	2.1300551	-2.0882162
C	-4.4820897	3.3329730	-1.7326785
H	-5.0139570	3.7633881	-2.6148449

H	-3.7396327	4.0908828	-1.3804969
C	-5.4607254	3.0085531	-0.5928395
O	-5.4477791	1.8536837	-0.0929542
N	-6.2932656	3.9746506	-0.1552492
C	-7.2441047	3.6950976	0.9242326
H	-7.0019378	4.3147571	1.8162618
H	-8.2739317	3.9475407	0.5888104
H	-7.1893467	2.6232052	1.1890786
C	-6.3247787	5.3442283	-0.6734373
H	-7.3029966	5.5494189	-1.1631651
H	-6.2000579	6.0622978	0.1668310
H	-5.5165328	5.5316271	-1.4045660
C	1.4310101	5.2859716	4.6337431
O	0.5482270	5.2614415	3.7603338
C	1.7041695	6.5629429	5.4495515
H	0.7624504	7.1586793	5.4389282
H	2.4864253	7.1557572	4.9146414
O	2.0864675	6.2585881	6.7792531
C	3.2078714	6.9158407	7.3140328
H	3.3003451	7.9588802	6.9231736
H	3.0360456	6.9916502	8.4111631
C	4.5138785	6.1174139	7.0526278
O	4.4749193	5.0706274	6.3823407
N	5.6728561	6.5936044	7.5920359
C	6.9103472	5.8361761	7.4197093
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H	7.3144462	5.5247470	8.4098819
H	6.6917193	4.9386595	6.8106846
C	5.7811844	7.7931572	8.4159633
H	6.6118331	8.4329701	8.0419165
H	4.8544176	8.3961657	8.3926771
H	6.0030815	7.5298711	9.4766914
C	-1.5882540	1.1993456	1.1676599
O	-2.2978567	1.3834506	0.1447512
C	-2.0548791	0.1999548	2.2344377
H	-1.3547534	-0.6693674	2.2963973
H	-2.0870381	0.6954090	3.2336142
O	-3.3552307	-0.2269914	1.8458949
C	-4.0518724	-0.9682574	2.8328566
H	-4.1797219	-0.3525233	3.7549336
H	-3.4834045	-1.8910045	3.1127747
C	-5.4114676	-1.3471504	2.2255635
O	-5.6012360	-1.1429636	0.9993402
N	-6.3477209	-1.8870050	3.0314324
C	-6.1483932	-2.1560441	4.4586959
H	-6.6369051	-1.3748488	5.0843852

H	-6.6065635	-3.1367305	4.7083637
H	-5.0750535	-2.2147295	4.7213746
C	-7.6818081	-2.1956370	2.5088736
H	-7.8578034	-3.2942367	2.5253268
H	-8.4514900	-1.7060627	3.1447002
H	-7.7632939	-1.8185517	1.4726347
C	-2.7897340	-3.2312696	-0.9179648
C	-4.1678921	-3.6522551	-1.4424892
H	-4.0727203	-4.3066298	-2.3412146
H	-4.7235664	-4.2217050	-0.6560467
O	-4.8442903	-2.4465215	-1.7705933
C	-6.0636380	-2.6298734	-2.4717067
H	-6.7827380	-3.2306701	-1.8616630
H	-5.8791224	-3.1796803	-3.4260090
C	-6.6280022	-1.2275030	-2.7479055
O	-2.6491089	-2.0966592	-0.4030208
O	-6.0358778	-0.2356018	-2.2546574
N	-7.7363843	-1.1186208	-3.5077364
C	-8.2836744	0.2023803	-3.8281915
H	-9.3167192	0.2934271	-3.4257178
H	-7.6390093	0.9800368	-3.3794679
H	-8.3198978	0.3364684	-4.9317713
C	-8.4370531	-2.2539206	-4.1131456
H	-8.1557528	-3.2144912	-3.6410939
H	-9.5316800	-2.1205659	-3.9771452
H	-8.2272405	-2.3118094	-5.2054291
C	0.6722843	-7.7658806	1.8517537
O	-0.2648251	-7.2171622	1.2444276
C	0.4484307	-9.0835791	2.6173350
H	0.5898779	-9.9267142	1.8974686
H	-0.6186262	-9.0933896	2.9395125
O	1.3053414	-9.1950078	3.7395732
C	2.0306737	-10.3884922	3.9074214
H	2.1481536	-10.5376999	5.0044361
H	1.4686586	-11.2698828	3.5131762
C	3.4356757	-10.2970279	3.2501339
O	3.7658130	-9.2636488	2.6427512
N	4.2756815	-11.3638052	3.3815144
C	3.9621045	-12.5956902	4.0971119
H	4.0857870	-13.4737375	3.4227887
H	4.6505010	-12.7302880	4.9631507
H	2.9239933	-12.6011163	4.4781488
C	5.6172775	-11.2980832	2.8047673
H	6.3872080	-11.3978601	3.6033536
H	5.7626934	-12.1230589	2.0710794
H	5.7352438	-10.3226739	2.2962603

C	0.8658057	3.7653833	-5.0701265
O	-0.0767957	3.4487129	-4.3009681
C	0.5713508	4.4555672	-6.4127555
H	0.5615433	3.6762590	-7.2148803
H	-0.4570706	4.8800788	-6.3383149
O	1.5185349	5.4731852	-6.6682666
C	2.0735883	5.5528424	-7.9602462
H	1.3141732	5.3354511	-8.7504395
H	2.3914828	6.6105530	-8.0932693
C	3.3015023	4.6145633	-8.1040204
O	3.6186366	3.8707144	-7.1557282
N	4.0025722	4.6454967	-9.2703978
C	5.1914165	3.8075072	-9.4217361
H	5.3342210	3.2240414	-8.4929482
H	5.0674399	3.1152547	-10.2847193
H	6.0881708	4.4415547	-9.6049826
C	3.6969023	5.5092807	-10.4073889
H	2.7493810	6.0619119	-10.2654349
H	4.5134654	6.2505165	-10.5669521
H	3.6024169	4.8989565	-11.3338308
Am	-4.1062055	-0.0933691	-0.6960982

Eu(TREN-G1-MDGA)³⁺

N	4.0206785	-0.0384972	0.2723740
C	4.4589272	0.2392507	-1.1041272
H	4.1083363	1.2520578	-1.3776898
H	5.5813264	0.2671774	-1.1806881
C	4.2997135	1.0845408	1.1785150
H	3.9705910	0.7818926	2.1957167
H	5.4039479	1.2824502	1.2502807
C	4.6094343	-1.2824288	0.7931492
H	4.5811301	-2.0431909	-0.0153518
H	5.6913517	-1.1302666	1.0490961
C	3.5477098	2.3983316	0.8044792
H	4.2420994	3.0955308	0.2744265
H	2.7461569	2.1402214	0.0799002
C	3.8642195	-0.7598441	-2.1479593
H	4.6543859	-1.4707494	-2.4904749
H	3.0889751	-1.3642864	-1.6262172
C	3.8420415	-1.8726149	2.0183319
H	4.5669811	-2.0842678	2.8432848
H	3.1488008	-1.0953060	2.4036545
N	3.0539849	-3.0572195	1.7210273

N	3.2314114	-0.1363954	-3.2973370
N	2.9119413	3.0776208	1.9188041
C	4.0419064	0.4043569	-4.3748994
H	5.1053174	0.2687805	-4.0834226
H	3.8995577	-0.1755851	-5.3218413
C	1.7939300	-0.2033939	-3.4348790
H	1.5309971	0.1469572	-4.4537157
H	1.4214182	-1.2568690	-3.3511558
C	3.7117045	3.7163006	2.9493295
H	4.7770530	3.6010784	2.6534581
H	3.5113396	4.8156505	2.9838971
C	1.4736355	3.2134517	1.9315804
H	1.1941495	3.8136056	2.8209239
H	1.1052785	3.7769462	1.0362293
C	3.7412643	-4.3345417	1.5894275
H	4.8200130	-4.1141061	1.4476340
H	3.6676208	-4.9428668	2.5279972
C	1.6390517	-3.0577142	2.0184927
H	1.3024439	-4.1122245	2.0665974
H	1.4176433	-2.6102716	3.0206866
C	0.8173859	-2.3256687	0.9200634
H	1.4626426	-2.2553987	0.0180266
H	0.5256401	-1.3008596	1.2257513
C	1.0465453	0.6845562	-2.3940622
H	1.7196337	1.5233959	-2.1214747
H	0.7953418	0.1126889	-1.4776757
C	0.7449589	1.8403503	2.0044625
H	1.3944007	1.1370099	2.5638797
H	0.5469478	1.4298233	0.9942315
C	3.5421061	3.1559999	4.4029264
H	3.2863071	2.0756575	4.3599181
H	4.5203854	3.2540836	4.9232508
C	3.8232404	1.9173240	-4.7024755
H	4.7906381	2.3275235	-5.0672798
H	3.5456597	2.4678158	-3.7784084
C	3.2740716	-5.2262598	0.3996053
H	2.9335541	-4.5827727	-0.4395481
H	4.1487410	-5.8156613	0.0479205
N	-0.3850381	-3.0474860	0.5241668
H	-0.1711051	-3.9727307	0.0799741
N	2.2239805	-6.1844345	0.7136095
H	2.5140457	-7.1319828	1.0767781
N	2.5630329	3.8439616	5.2305159
H	2.8865946	4.6775210	5.7918615
N	-0.5173796	1.8978635	2.7258438
H	-0.3825648	1.9611035	3.7582538

N	-0.1751600	1.2901486	-2.9068903
H	0.0178400	2.0753255	-3.5686350
N	2.8369961	2.1963835	-5.7342682
H	3.1648902	2.2112180	-6.7366356
C	-1.4120258	0.9577648	-2.5215766
O	-1.6782592	0.0663470	-1.6793048
C	-2.5636462	1.7637929	-3.1301896
H	-2.2274076	2.7768468	-3.4523149
H	-2.9803997	1.2301589	-4.0219858
O	-3.5412920	1.8583874	-2.0965022
C	-4.6549309	2.6670604	-2.4097787
H	-5.2164423	2.2506175	-3.2838214
H	-4.3221210	3.6987193	-2.6803997
C	-5.5514892	2.6945671	-1.1604731
O	-5.2401672	1.9835970	-0.1772337
N	-6.6440362	3.4921459	-1.1746913
C	-7.5043476	3.5772481	0.0055501
H	-7.5429830	4.6271761	0.3730906
H	-8.5385509	3.2545644	-0.2491068
H	-7.0937865	2.9226018	0.7964918
C	-7.0334765	4.3498914	-2.2947053
H	-8.1075722	4.1852229	-2.5320608
H	-6.8960802	5.4244749	-2.0339026
H	-6.4475537	4.1316342	-3.2072726
C	1.3340514	3.3813756	5.5434961
O	0.8210502	2.3332641	5.0970772
C	0.5898520	4.2389912	6.5858155
H	0.8828448	3.8666444	7.5983673
H	-0.4993868	4.0393068	6.4590382
O	0.8670699	5.6179363	6.4239935
C	1.2069875	6.3624079	7.5731364
H	0.8731048	7.4079405	7.3773606
H	0.6545439	6.0027535	8.4743482
C	2.7408318	6.3455376	7.8171866
O	3.4754569	5.6909112	7.0555379
N	3.2351485	7.0714970	8.8579287
C	4.6742583	7.0737355	9.1170449
H	5.0779202	8.1101703	9.0521501
H	4.8836872	6.6726364	10.1355373
H	5.1704003	6.4353237	8.3632493
C	2.4251882	7.8404971	9.7972474
H	2.8424865	8.8646601	9.9052999
H	1.3762747	7.9422715	9.4573816
H	2.4278436	7.3624084	10.8044072
C	-1.7172578	1.7925371	2.1505122
O	-1.8968180	1.6301629	0.9203654

C	-2.9412166	1.8222182	3.0702944
H	-2.6880999	1.4906366	4.1043139
H	-3.3535238	2.8610669	3.1263651
O	-3.8874220	0.9427530	2.4683351
C	-5.0861121	0.7498097	3.1857079
H	-5.6935827	1.6904949	3.2016775
H	-4.8671172	0.4719837	4.2439209
C	-5.8545048	-0.3757452	2.4716952
O	-5.4050815	-0.8306308	1.3951223
N	-6.9940332	-0.8302545	3.0447091
C	-7.5174161	-0.3496984	4.3248777
H	-8.6238712	-0.3321489	4.2769865
H	-7.2176148	-1.0171804	5.1625589
H	-7.1815059	0.6831364	4.5450175
C	-7.7277957	-1.9389470	2.4338961
H	-7.7969562	-2.7899667	3.1492623
H	-8.7582562	-1.6171501	2.1631318
H	-7.1895092	-2.2661952	1.5263163
C	-1.6197018	-2.5399569	0.5520309
C	-2.7393658	-3.4190337	-0.0178088
H	-2.3455342	-4.1463927	-0.7681561
H	-3.2305612	-3.9929455	0.8044836
O	-3.6599789	-2.5137129	-0.6211656
C	-4.7591067	-3.1172738	-1.2708880
H	-5.4052368	-3.6569702	-0.5341249
H	-4.4071681	-3.8648703	-2.0219899
C	-5.5488261	-1.9858845	-1.9559376
O	-1.9140778	-1.3983384	0.9768744
O	-5.1885156	-0.8003487	-1.7746161
N	-6.6052658	-2.3275640	-2.7333566
C	-7.3604243	-1.2923128	-3.4374890
H	-8.4241035	-1.3024785	-3.1080674
H	-6.9130501	-0.3084525	-3.2052615
H	-7.3291653	-1.4696265	-4.5352626
C	-7.0412998	-3.7003223	-2.9850910
H	-8.1426613	-3.7684803	-2.8532956
H	-6.7985550	-4.0084975	-4.0269514
H	-6.5744936	-4.4174449	-2.2857160
C	0.9361488	-6.0799829	0.3312073
O	0.4281177	-5.0879169	-0.2410438
C	0.0915427	-7.3407280	0.6097044
H	0.1651907	-7.9953049	-0.2933123
H	-0.9717370	-7.0119832	0.6936529
O	0.4989455	-8.0067229	1.7882831
C	0.7247360	-9.3984715	1.7308167
H	0.4556554	-9.8012290	2.7332927

H	0.0522236	-9.8900645	0.9853017
C	2.2143556	-9.7154311	1.4268664
O	3.0124773	-8.7809214	1.2323054
N	2.6061467	-11.0202242	1.4074815
C	1.7354345	-12.1554012	1.6933403
H	0.6682021	-11.8676727	1.7241151
H	1.8589289	-12.9272866	0.9013435
H	2.0041977	-12.6272232	2.6710531
C	4.0113899	-11.3448738	1.1748718
H	4.4410812	-11.8616375	2.0640980
H	4.1104237	-12.0172069	0.2922368
H	4.5659732	-10.4049810	0.9909047
C	1.6002069	2.6862080	-5.5192196
O	1.0760470	2.8585176	-4.3964179
C	0.8560935	3.0967774	-6.8055262
H	-0.2370255	3.0235849	-6.5909399
H	1.0854089	4.1742212	-6.9958002
O	1.2015288	2.2765485	-7.9045781
C	1.5367353	2.9012016	-9.1258689
H	1.2092282	2.2096024	-9.9340748
H	0.9772835	3.8574202	-9.2658188
C	3.0665168	3.1408172	-9.2348614
O	3.8034262	2.8439301	-8.2769299
N	3.5556915	3.6565163	-10.3955733
C	4.9993521	3.8398965	-10.5478048
H	5.4950421	3.5370382	-9.6068994
H	5.3812920	3.2155846	-11.3869855
H	5.2311566	4.9056686	-10.7672887
C	2.7518270	3.9798431	-11.5705651
H	1.6697846	3.9982962	-11.3392772
H	3.0328428	4.9872096	-11.9491612
H	2.9261187	3.2444489	-12.3903470
Eu	-3.5590529	0.1028086	-0.0644949