

Effect of branching in the alkyl chain of diglycolamides on the sequestration of tetravalent actinides: Solvent extraction and theoretical studies

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Valence adjustment and purification of actinide tracers

Neptunium(IV)

A ferrous sulfamate solution (0.3 M) was freshly prepared by dissolving a known amount of iron powder (BDH) in sulfamic acid (Aldrich). The resultant Fe(II) sulfamate solution along with a few drops of hydroxylamine nitrate (1 M) was used for as the conversion of Np into its Np(IV) state. A HTTA solution in xylene was used for the extraction of Np(IV) from 1 M HNO₃ medium. The Np(IV) loaded organic solution was back extracted with 8 M HNO₃. The back extracted aqueous phase was washed multiple times to remove any traces of organic impurities. The purity of the tracer was ascertained by α - and γ -ray spectrometry.

Plutonium(IV)

The oxidation state of Pu was adjusted to the Pu(IV) state using a 0.05 M solution of NaNO₂ (Merck). Ammonium metavanadate (Aldrich) was used as the holding oxidant for Pu(IV) stabilization. The Pu(IV) was purified using Dowex 1X8 anion exchange resin and the purity of the tracer was ascertained by α - and γ -ray spectrometry.

Thorium(IV)

Th(IV) was separated from an aged uranyl solution kept in 6 M HCl. Uranium has tendency to form an anionic tetrachloro complex and hence a liquid anion exchanger was used for its separation and purification. 0.1 M Aliquat 336 was dissolved in chloroform and used for the separation of U(VI) from Th(IV). The aqueous phase containing Th(IV) was washed with 0.1 M Aliquat 336-chloroform for better purification. The purity of the tracer was ascertained by α - and γ -ray spectrometry.

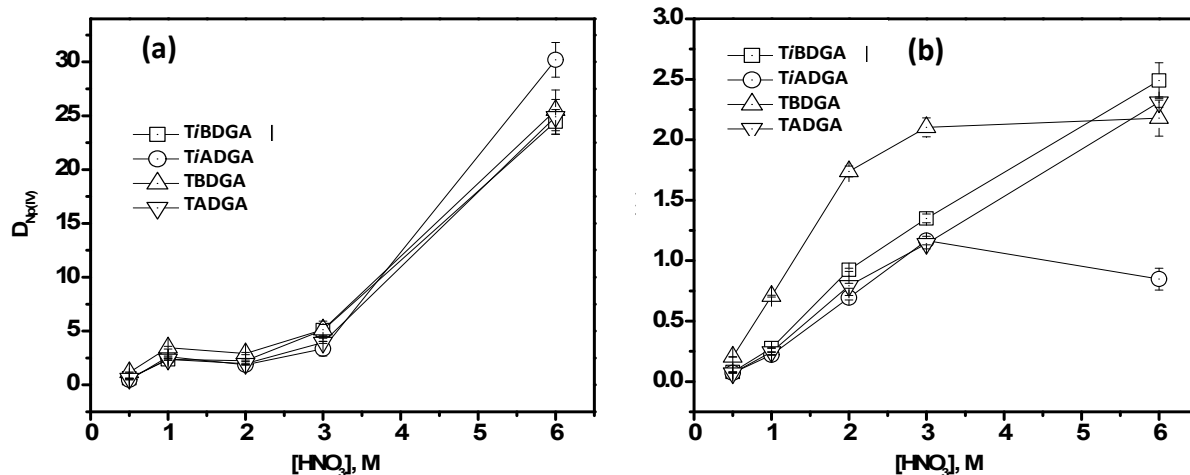


Figure S1. Effect of feed acidity in the extraction of (a) Np(IV) and (b) Th(IV) by different DGA derivatives, solvent: octanol, T: 298 K.

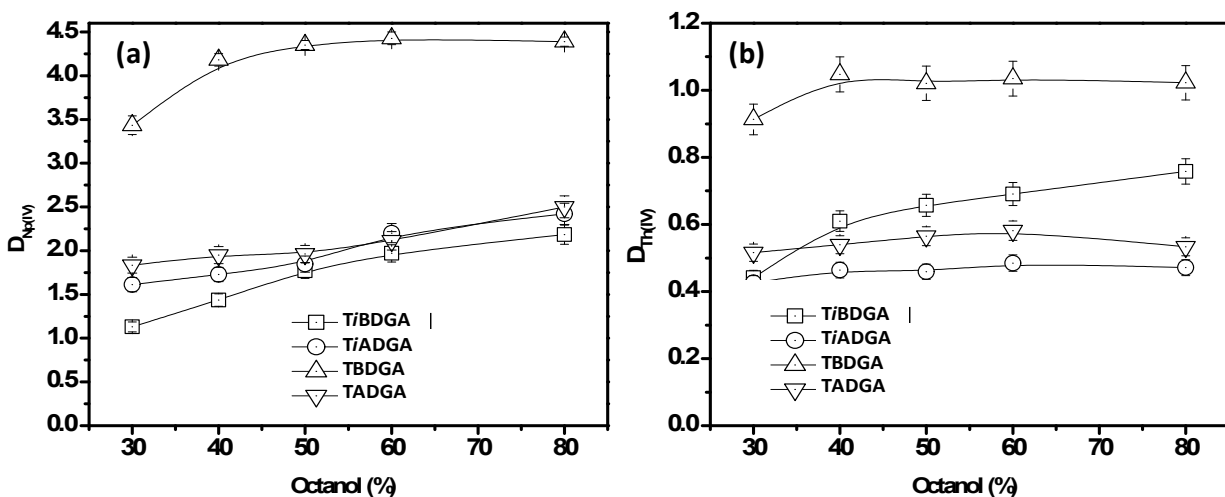


Figure S2. Effect of varying octanol content on the extraction of (a) Np(IV) and (b) Th(IV) by different DGA derivatives, T : 298 K.

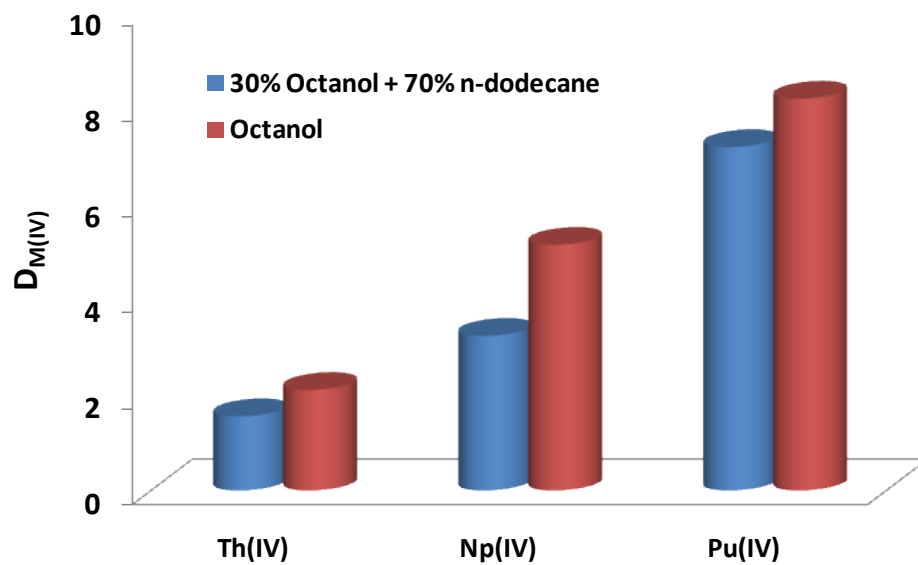


Figure S3. Comparison of the distribution ratio of different tetravalent actinides with *n*-butyl DGA derivative TMDGA in 30% octanol + 70% *n*-dodecane and pure octanol at 3 M HNO₃, T: 298 K.

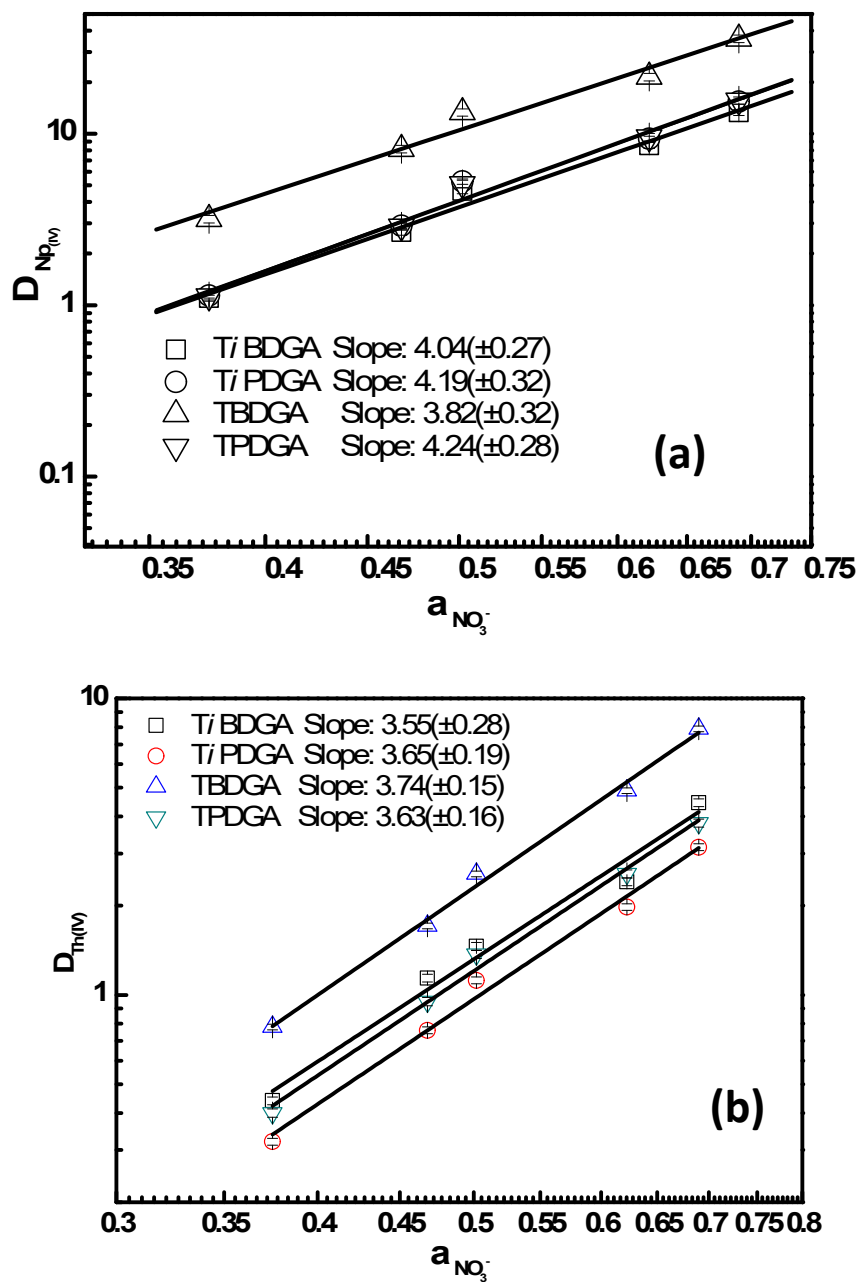


Figure S 4. Effect of nitrate activity on the extraction of (a) Np(IV), and (b) Th(IV) by different DGA derivatives, solvent: 30% octanol + 70% *n*-dodecane, [HNO₃] : 0.5 M T: 298 K.

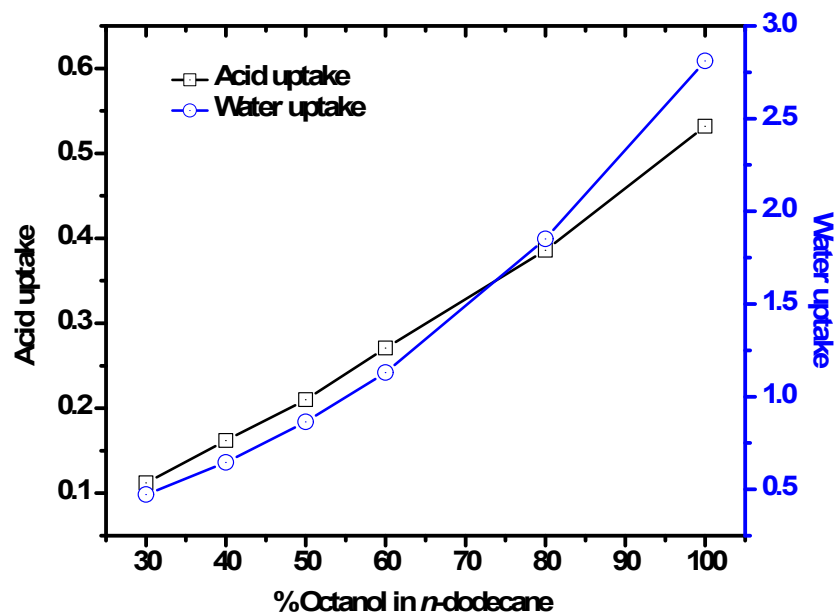


Figure S5. Water and acid uptake by octanol-*n*-dodecane mixtures, [HNO₃]: 3 M HNO₃, T : 298 K.

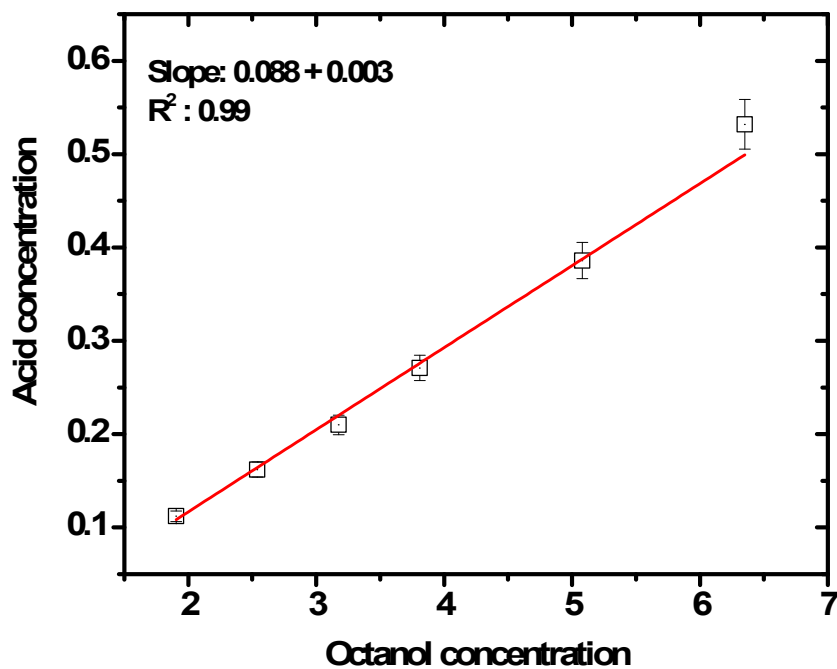


Figure S6. Acid uptake by octanol-*n*-dodecane mixtures, [HNO₃]: 3 M HNO₃, T: 298 K.

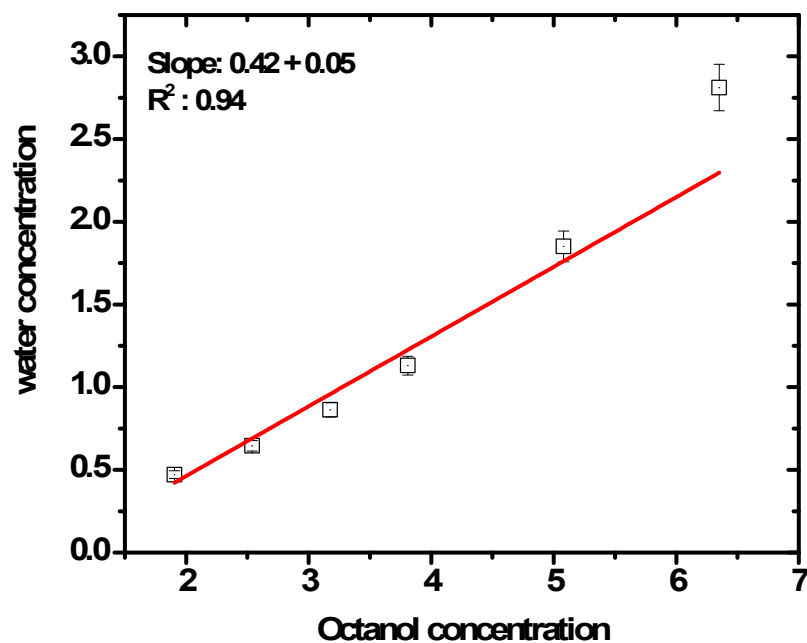


Figure S7. Water uptake by octanol-*n*-dodecane mixtures, [HNO₃]: 3 M HNO₃, T: 298 K.

Cartesian coordinates of the optimized structures of the An⁴⁺ complexes of DGA derivatives

Th(IV)-*n*-Butyl DGA

C	-6.1488891	-4.7828933	3.8359690
C	-4.7125565	-4.3192764	3.5346215
C	-4.0992353	-5.0689788	2.3389885
N	-2.6998583	-4.6877830	2.0467468
C	-2.3677067	-3.7388498	1.1653565
C	-3.4805845	-3.0401859	0.3723073
O	-2.8461429	-2.0393493	-0.4182605
C	-3.7179760	-1.2707999	-1.2486489
C	-2.8167331	-0.2901524	-2.0110388
N	-3.3569025	0.6679289	-2.7617990
C	-4.8171846	0.8600779	-2.9009373
C	-5.4010324	1.8960112	-1.9247173
C	-6.9043537	2.1313666	-2.1557118
C	-1.6432492	-5.3754802	2.8193941
C	-1.1921731	-6.6997041	2.1817119
C	-0.1598084	-7.4412547	3.0486416
O	-1.1692882	-3.3926313	0.9437220
O	0.1691806	-2.9843623	-1.5799222
C	1.2027578	-3.6842826	-1.7898815
N	1.3134262	-4.5072099	-2.8386659
C	2.5040553	-5.3477535	-3.0915835

C	2.3896643	-6.7758869	-2.5324377
C	3.5879270	-7.6569595	-2.9285966
O	-1.5609090	-0.4407924	-1.8879763
O	1.9193330	-2.7921592	0.2984952
C	2.9722535	-2.3494114	1.1496477
C	2.3701916	-1.3002721	2.0861587
N	3.0708687	-0.8317389	3.1170533
C	4.4392797	-1.2895395	3.4420243
C	4.4853744	-2.3999347	4.5047080
C	5.9264062	-2.7823576	4.8874779
C	2.3736104	-3.5595369	-0.8114299
O	1.1965884	-0.8890189	1.8221219
C	-2.4770212	1.6378877	-3.4574825
C	-2.1383406	1.2303656	-4.8996048
C	-1.2729591	2.2889439	-5.6065011
C	2.4830043	0.2209583	3.9824119
C	2.8044778	1.6454378	3.5012877
C	2.2547637	2.7150614	4.4622437
C	0.2146357	-4.5933245	-3.8254837
C	0.4219610	-3.6777855	-5.0433834
C	-0.6972656	-3.8378724	-6.0868085
H	-4.7001368	-3.2216211	3.3368551
H	2.2990764	-6.7366410	-1.4208675
H	-4.0100116	-3.7669008	-0.2901945
H	-4.2310095	-2.5806615	1.0568538
H	-4.0974364	-6.1635019	2.5320251
H	-4.7169147	-4.9284599	1.4273052
H	-6.1443559	-5.8793043	4.0387669
H	-6.7804677	-4.6434716	2.9269349
H	-2.0517752	-5.5523486	3.8372298
H	-0.7903557	-4.6745560	2.9178255
H	-0.7642374	-6.4893893	1.1741117
H	-0.6010748	-7.6425134	4.0526328
H	0.7155771	-6.7735162	3.2303440
H	-4.4674702	-0.7290758	-0.6276755
H	-4.2624890	-1.9434406	-1.9549082
H	-5.3282497	-0.1201834	-2.7923251
H	-4.9957674	1.1768162	-3.9512545
H	-4.8516507	2.8582551	-2.0374487
H	-7.0639727	2.4666019	-3.2070661
H	-7.4511667	1.1638738	-2.0580637
H	-1.5563010	1.7485947	-2.8504896
H	-3.0076503	2.6133337	-3.4420110
H	-1.6044153	0.2524275	-4.8859519
H	-0.3341203	2.4432617	-5.0247246
H	-1.8061730	3.2679869	-5.5920292
H	3.7874826	-1.8834227	0.5431256
H	3.4028418	-3.2093829	1.7131845
H	4.9942144	-0.3943781	3.7969121
H	4.9508110	-1.6108300	2.5099430
H	3.9345813	-2.0630190	5.4131217

H	6.4531296	-1.8785656	5.2729231
H	6.4832049	-3.0937900	3.9719161
H	2.8826923	0.0501010	5.0047999
H	1.3874869	0.0558058	4.0150377
H	2.3721370	1.7924099	2.4848552
H	2.6923492	2.5577239	5.4761333
H	1.1545559	2.5748458	4.5769650
H	2.7303200	-4.5579827	-0.4685086
H	3.2201722	-3.0356949	-1.3179838
H	3.4079238	-4.8373175	-2.6974519
H	2.6384020	-5.3802128	-4.1937488
H	3.6527651	-7.7031356	-4.0404318
H	4.5332142	-7.1726463	-2.5876143
H	-0.7273081	-4.3380964	-3.3000937
H	0.1483252	-5.6564394	-4.1427645
H	0.4741166	-2.6198249	-4.6978042
H	-1.6800073	-3.6086322	-5.6102291
H	-0.7543955	-4.9052050	-6.4044433
N	1.5032937	0.7394422	-1.1468847
O	1.6149919	-0.5529756	-1.3252612
O	2.2529300	1.5340800	-1.6495457
O	0.5149858	1.0650672	-0.3785351
H	3.9419565	-3.2989763	4.1279387
H	-5.2220278	1.5655402	-0.8745227
H	-3.0796070	1.0740818	-5.4775039
H	-4.0735634	-4.4739356	4.4340318
H	-2.0765047	-7.3590894	2.0184064
H	1.4471936	-7.2413309	-2.9031512
H	3.9084214	1.7677214	3.4025393
H	1.4039297	-3.9040049	-5.5209649
C	-6.7821456	-4.0429646	5.0210908
H	-7.8161042	-4.4045958	5.2069032
H	-6.1997889	-4.1988189	5.9560906
H	-6.8377257	-2.9467942	4.8366660
C	0.3149441	-8.7605514	2.4262418
H	0.7988628	-8.5961751	1.4368041
H	1.0543913	-9.2684947	3.0819505
H	-0.5319962	-9.4655327	2.2718779
C	-7.5029538	3.1624965	-1.1905876
H	-7.0041866	4.1518262	-1.2923100
H	-8.5854348	3.3113609	-1.3914371
H	-7.3988913	2.8395411	-0.1306302
C	-0.9296958	1.9156459	-7.0538616
H	-0.2988422	2.6978756	-7.5278561
H	-0.3678103	0.9558024	-7.1056431
H	-1.8467759	1.8051720	-7.6745097
C	-0.4999679	-2.9481649	-7.3207346
H	-0.4689515	-1.8693920	-7.0470731
H	0.4505777	-3.1880962	-7.8471574
H	-1.3275090	-3.0872040	-8.0489688
C	3.5021359	-9.0785530	-2.3593973

H	2.5832527	-9.6017179	-2.7067631
H	4.3737649	-9.6879881	-2.6803985
H	3.4894409	-9.0735270	-1.2462934
N	-2.2845750	0.0878717	1.8916966
O	-3.0783410	0.6245753	2.6219012
O	-1.6836796	-1.0245186	2.1868228
O	-1.9639764	0.5562940	0.7215201
Th	-0.3571043	-1.2424030	0.0381120
C	5.9904866	-3.9005522	5.9353980
H	7.0435236	-4.1445641	6.1915150
H	5.4777798	-3.6048101	6.8777590
H	5.5103701	-4.8347941	5.5666453
C	2.5455567	4.1464028	3.9929936
H	2.0813552	4.3532033	3.0028166
H	2.1427992	4.8893877	4.7142892
H	3.6390577	4.3301617	3.8990104

Th(IV)-*iso*-Butyl DGA

C	-6.2998852	-4.5712444	3.6458251
C	-4.8395331	-4.1084392	3.4901863
C	-4.1474564	-5.0183649	2.4438700
N	-2.7424735	-4.6752464	2.1205155
C	-2.4190673	-3.7559472	1.2036368
C	-3.5342570	-3.0944506	0.3846350
O	-2.9103089	-2.1010330	-0.4236176
C	-3.7998233	-1.3496474	-1.2540034
C	-2.9194740	-0.3434863	-2.0061311
N	-3.4617145	0.6171666	-2.7530312
C	-4.9206077	0.8022092	-2.9227147
C	-5.5329762	1.9745826	-2.1181039
C	-6.9906899	2.1730421	-2.5723209
C	-1.6551385	-5.3443197	2.8712701
C	-0.9940213	-6.5294805	2.1295426
C	0.1493394	-7.0772454	3.0025816
O	-1.2215733	-3.4176106	0.9622659
O	0.0969751	-3.0265260	-1.5791460
C	1.1431810	-3.7081258	-1.7897362
N	1.2604052	-4.5385314	-2.8332010
C	2.4671919	-5.3673461	-3.0611852
C	2.4884942	-6.7390451	-2.3423330
C	3.8359907	-7.4245536	-2.6343676
O	-1.6608950	-0.4734991	-1.8785066
O	1.8568052	-2.7768838	0.2820856
C	2.9055703	-2.3292745	1.1364537
C	2.2985521	-1.2864182	2.0761424
N	2.9954213	-0.8338087	3.1198479
C	4.3358097	-1.3614511	3.4671163
C	4.3562109	-2.6424443	4.3388175
C	5.8232478	-3.0586241	4.5537726

C	2.3215588	-3.5381070	-0.8285061
O	1.1363449	-0.8603519	1.7869322
C	-2.5589157	1.5970665	-3.4114404
C	-1.8918646	1.1065151	-4.7168850
C	-0.9265028	2.2010672	-5.2071303
C	2.4545024	0.2751386	3.9453349
C	3.0998359	1.6526162	3.6622273
C	2.5028888	2.6777209	4.6441086
C	0.1513497	-4.6125039	-3.8137502
C	0.1404155	-3.4779521	-4.8652540
C	-1.0875337	-3.6686516	-5.7739611
H	-4.8495284	-3.0669612	3.0880856
H	2.4314356	-6.5483356	-1.2433411
H	-4.0420795	-3.8493395	-0.2639416
H	-4.3024458	-2.6323151	1.0458692
H	-4.1410001	-6.0659819	2.8098055
H	-4.7379298	-5.0310812	1.5026212
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H	-6.8489313	-4.5626856	2.6779536
H	-2.0922988	-5.6926210	3.8288825
H	-0.8917749	-4.5745786	3.1067826
H	-0.5511685	-6.1211673	1.1914142
H	-0.2384968	-7.4961218	3.9586511
H	0.8925722	-6.2885517	3.2563904
H	-4.5610689	-0.8303451	-0.6307856
H	-4.3253180	-2.0319766	-1.9653490
H	-5.4403383	-0.1475812	-2.6723460
H	-5.0897195	0.9698160	-4.0073648
H	-4.9663570	2.8960860	-2.3882067
H	-7.0617608	2.3760251	-3.6636609
H	-7.6115421	1.2753518	-2.3494538
H	-1.7814599	1.8760153	-2.6706033
H	-3.1705770	2.5007078	-3.6147028
H	-1.2879935	0.2055168	-4.4605727
H	-0.1606545	2.4508451	-4.4402526
H	-1.4725247	3.1376366	-5.4626012
H	3.7150806	-1.8482303	0.5332911
H	3.3462587	-3.1894619	1.6888642
H	4.8633290	-0.5433725	4.0006347
H	4.9107487	-1.5281147	2.5303394
H	6.3785659	-2.2873976	5.1334810
H	6.3609407	-3.2117523	3.5914549
H	2.6185128	-0.0052064	5.0064274
H	1.3616319	0.3155216	3.7656820
H	2.6490973	2.3711330	5.7035678
H	1.4109720	2.8124498	4.4728756
H	2.7195524	-4.5185785	-0.4819955
H	3.1410688	-2.9883858	-1.3526351
H	3.3660978	-4.7767063	-2.7817420
H	2.5403294	-5.5233906	-4.1570076
H	3.9459146	-7.6495435	-3.7192199

H	4.7014668	-6.7949371	-2.3296787
H	-0.7998326	-4.6022779	-3.2423377
H	0.2337219	-5.5976854	-4.3168392
H	0.0182449	-2.5180073	-4.3120361
H	-2.0361141	-3.6967871	-5.1921487
H	-1.0184821	-4.6162829	-6.3548034
N	1.3627730	0.7252432	-1.2339754
O	1.5018773	-0.5684361	-1.3823342
O	2.0765941	1.5241119	-1.7816985
O	0.3905773	1.0474671	-0.4459266
H	3.8508998	-3.4566538	3.7643336
H	4.1905860	1.5730941	3.8844606
N	-2.3556764	0.0537415	1.8982930
O	-3.1512405	0.5847458	2.6310393
O	-1.7516119	-1.0580377	2.1870705
O	-2.0361655	0.5285035	0.7304666
Th	-0.4320264	-1.2708040	0.0269283
H	-7.4490156	3.0342983	-2.0412086
H	-0.3914032	1.8696414	-6.1232452
H	-1.1658860	-2.8372719	-6.5076274
H	3.9109817	-8.3880646	-2.0864743
H	5.8795784	-4.0087748	5.1265632
H	0.6877564	-7.8965272	2.4786869
H	-6.8464189	-3.9057155	4.3476048
H	2.9875702	3.6688797	4.5132502
C	3.6129179	-2.4874883	5.6759799
H	4.0586513	-1.6779529	6.2973469
H	2.5310136	-2.2682506	5.5393226
H	3.6843118	-3.4278378	6.2639370
C	2.9405628	2.1021314	2.2020625
H	3.4131682	1.3897858	1.4878957
H	1.8698565	2.2140717	1.9216343
H	3.4334569	3.0857552	2.0445671
C	1.3035353	-7.6431920	-2.7209167
H	0.3227107	-7.1923110	-2.4527190
H	1.2975443	-7.8694558	-3.8114013
H	1.3758182	-8.6148638	-2.1863186
C	1.4371024	-3.3997926	-5.6875569
H	1.6171197	-4.3389806	-6.2594669
H	1.3764025	-2.5736877	-6.4290804
H	2.3294767	-3.1982858	-5.0544195
C	-2.9060480	0.7185517	-5.8058714
H	-3.5518027	1.5812718	-6.0875858
H	-2.3789701	0.3914526	-6.7286991
H	-3.5654335	-0.1223904	-5.4940976
C	-5.4323553	1.7868522	-0.5961954
H	-6.0520006	0.9240135	-0.2552264
H	-4.3861825	1.6405509	-0.2451583
H	-5.8223224	2.6850376	-0.0701616
C	-4.1116762	-4.0699345	4.8441387
H	-4.0510839	-5.0830733	5.3035137

H	-3.0834947	-3.6549409	4.7595359
H	-4.6657340	-3.4205023	5.5557869
C	-1.9892148	-7.6395263	1.7513245
H	-1.4673879	-8.4684998	1.2253776
H	-2.4721287	-8.0784811	2.6537891
H	-2.7912939	-7.2767020	1.0703229

Th(IV)-*n*-Amyl DGA

C	-6.1259117	-4.8562082	3.8564140
C	-4.7010432	-4.3702244	3.5410494
C	-4.0825985	-5.1198716	2.3480437
N	-2.6870261	-4.7263137	2.0531156
C	-2.3647456	-3.7744506	1.1714929
C	-3.4841841	-3.0903032	0.3752018
O	-2.8591662	-2.0867951	-0.4194701
C	-3.7378518	-1.3308658	-1.2543739
C	-2.8459395	-0.3424771	-2.0178088
N	-3.3948546	0.6108677	-2.7679971
C	-4.8570439	0.7912596	-2.9039493
C	-5.4465893	1.8200577	-1.9236152
C	-6.9529425	2.0383376	-2.1451934
C	-1.6233036	-5.4046390	2.8246446
C	-1.1595983	-6.7223588	2.1823645
C	-0.1315821	-7.4643325	3.0525346
O	-1.1699926	-3.4143146	0.9514198
O	0.1578640	-3.0039984	-1.5777204
C	1.2012557	-3.6882871	-1.7909956
N	1.3194871	-4.5141390	-2.8364701
C	2.5250443	-5.3318972	-3.0941810
C	2.4475281	-6.7585540	-2.5250771
C	3.6569747	-7.6154176	-2.9364684
O	-1.5886113	-0.4821089	-1.8955602
O	1.9096812	-2.7881689	0.2959218
C	2.9558149	-2.3387836	1.1517359
C	2.3387621	-1.3055516	2.0959235
N	3.0263664	-0.8482567	3.1405268
C	4.3933619	-1.3058109	3.4725528
C	4.4328608	-2.4427294	4.5070887
C	5.8710562	-2.8302259	4.8914960
C	2.3748804	-3.5416908	-0.8190306
O	1.1659894	-0.8965024	1.8245098
C	-2.5231079	1.5892024	-3.4623559
C	-2.1734612	1.1831249	-4.9022355
C	-1.3069785	2.2452609	-5.6003427
C	2.4246029	0.1871388	4.0168952
C	2.7675514	1.6207652	3.5793483
C	2.1952393	2.6690980	4.5489781
C	0.2152218	-4.6287939	-3.8144013
C	0.4022841	-3.7320053	-5.0496391

C	-0.7159237	-3.9341366	-6.0857441
H	-4.7086033	-3.2745564	3.3330399
H	2.3731213	-6.7150589	-1.4126956
H	-4.0060804	-3.8251096	-0.2843016
H	-4.2393711	-2.6353599	1.0575682
H	-4.0695242	-6.2132775	2.5465706
H	-4.7025459	-4.9897878	1.4363917
H	-6.1016963	-5.9500570	4.0758383
H	-6.7685410	-4.7412005	2.9506717
H	-2.0306461	-5.5885977	3.8416449
H	-0.7777562	-4.6952547	2.9254733
H	-0.7252150	-6.5023558	1.1798102
H	-0.5830436	-7.6862017	4.0486290
H	0.7371847	-6.7927504	3.2560791
H	-4.4947870	-0.7958511	-0.6367077
H	-4.2731064	-2.0119207	-1.9597487
H	-5.3596449	-0.1935106	-2.7962510
H	-5.0404431	1.1086851	-3.9531608
H	-4.9080542	2.7879074	-2.0392949
H	-7.1252240	2.3781212	-3.1940466
H	-7.4910131	1.0647710	-2.0483262
H	-1.6060328	1.7109406	-2.8519250
H	-3.0643549	2.5587688	-3.4504334
H	-1.6360464	0.2074248	-4.8845254
H	-0.3714801	2.4028498	-5.0123545
H	-1.8424676	3.2241283	-5.5909534
H	3.7656171	-1.8566295	0.5505320
H	3.3967120	-3.1980474	1.7080837
H	4.9372279	-0.4166527	3.8575529
H	4.9197019	-1.5993382	2.5393780
H	3.8723936	-2.1303294	5.4182913
H	6.3924667	-1.9376992	5.3111799
H	6.4402093	-3.1124176	3.9727682
H	2.7981241	-0.0114409	5.0441988
H	1.3276915	0.0288287	4.0184739
H	2.3672230	1.7939494	2.5541085
H	2.5869765	2.4764131	5.5764552
H	1.0880186	2.5469267	4.6145194
H	2.7542089	-4.5334309	-0.4811744
H	3.2072098	-2.9977736	-1.3281143
H	3.4215102	-4.7989402	-2.7131503
H	2.6492846	-5.3695237	-4.1972737
H	3.7035323	-7.6705604	-4.0496531
H	4.5998245	-7.1098518	-2.6169046
H	-0.7260226	-4.3769499	-3.2863139
H	0.1603283	-5.6978020	-4.1138073
H	0.4361402	-2.6670791	-4.7243125
H	-1.7030537	-3.7029773	-5.6169216
H	-0.7615100	-5.0109563	-6.3755867
N	1.4610676	0.7351024	-1.1547462
O	1.5878213	-0.5569538	-1.3254237

O	2.2010950	1.5352659	-1.6630689
O	0.4696566	1.0538616	-0.3878005
H	3.8954674	-3.3329924	4.1024033
H	-5.2566408	1.4906638	-0.8751734
H	-3.1103011	1.0234849	-5.4861044
H	-4.0525501	-4.5058013	4.4365775
H	-2.0396690	-7.3842308	2.0074367
H	1.5089899	-7.2444202	-2.8788303
H	3.8745006	1.7382721	3.5166249
H	1.3868065	-3.9494799	-5.5256052
C	-6.7754797	-4.1145217	5.0372548
H	-6.1297238	-4.2283485	5.9389350
H	-6.7990492	-3.0215714	4.8149573
C	0.3720263	-8.7743889	2.4229947
H	0.8310570	-8.5512864	1.4301561
H	-0.4998341	-9.4367591	2.2116146
C	-7.5676955	3.0590629	-1.1720534
H	-7.0224534	4.0270048	-1.2668768
H	-7.3972057	2.7150760	-0.1245989
C	-0.9437143	1.8816262	-7.0498680
H	-0.4223543	0.8946935	-7.0594802
H	-1.8814083	1.7381279	-7.6366879
C	-0.5375779	-3.0783481	-7.3515940
H	-0.4820634	-2.0017809	-7.0628857
H	0.4466827	-3.3187079	-7.8176689
C	3.6214386	-9.0403809	-2.3585750
H	2.6680952	-9.5336970	-2.6623596
H	3.5948171	-8.9828950	-1.2446269
N	-2.3361714	0.0546388	1.8714987
O	-3.1520965	0.5778584	2.5873735
O	-1.7159179	-1.0427057	2.1811528
O	-2.0106381	0.5232565	0.7028934
Th	-0.3801947	-1.2613898	0.0363794
C	-9.0665418	3.2873370	-1.4036928
H	-9.4752073	4.0268075	-0.6817203
H	-9.2654017	3.6752508	-2.4277289
H	-9.6464448	2.3449587	-1.2831215
C	-0.0650359	2.9356524	-7.7350936
H	0.1783358	2.6401719	-8.7785725
H	-0.5755483	3.9236753	-7.7783551
H	0.8970123	3.0787478	-7.1934388
C	-1.6551800	-3.2799570	-8.3822643
H	-1.4879522	-2.6536998	-9.2850260
H	-1.7120532	-4.3396259	-8.7177909
H	-2.6506505	-3.0067816	-7.9646441
C	4.8103031	-9.9017459	-2.8024631
H	4.7544037	-10.9202167	-2.3616545
H	4.8367039	-10.0176208	-3.9088886
H	5.7792822	-9.4532166	-2.4880228
C	5.9396345	-3.9841735	5.9064797
H	5.3681396	-3.7000489	6.8213333

H	5.4168992	-4.8747494	5.4832706
C	2.5254072	4.1160208	4.1430129
H	3.6325143	4.2323735	4.0750868
H	2.1344274	4.3063945	3.1159283
C	7.3744561	-4.3640606	6.2928919
H	7.9085524	-3.5091156	6.7641910
H	7.3843801	-5.2050376	7.0193080
H	7.9658991	-4.6816731	5.4046972
C	1.3813683	-9.5219528	3.3033856
H	1.7241288	-10.4602303	2.8162224
H	2.2828450	-8.9013988	3.5092346
H	0.9361226	-9.8005963	4.2844763
C	-8.1930311	-4.6079257	5.3526661
H	-8.1971569	-5.6874491	5.6232917
H	-8.6312749	-4.0482602	6.2068076
H	-8.8740005	-4.4767550	4.4818140
C	1.9573218	5.1593113	5.1132718
H	2.3585553	5.0198734	6.1422639
H	2.2181089	6.1903855	4.7907332
H	0.8475848	5.0973594	5.1740920

Th(IV)-*iso*-Amyl DGA

C	-6.2112587	-4.7531882	3.7505466
C	-4.7405766	-4.3627248	3.4666970
C	-4.1018823	-5.1372832	2.2997519
N	-2.7026252	-4.7404647	2.0272308
C	-2.3678872	-3.8023259	1.1360606
C	-3.4768203	-3.1385857	0.3084642
O	-2.8473749	-2.1322304	-0.4789764
C	-3.7204564	-1.3845906	-1.3275946
C	-2.8286309	-0.3771811	-2.0657418
N	-3.3788425	0.5921083	-2.7933130
C	-4.8416416	0.7671020	-2.9318291
C	-5.4340447	1.7611413	-1.9170782
C	-6.9626190	1.9642523	-2.0541112
C	-1.6542692	-5.4003580	2.8349678
C	-1.1808496	-6.7295135	2.2225957
C	-0.1347136	-7.4800877	3.0813787
O	-1.1711520	-3.4388822	0.9312587
O	0.1740311	-3.0525918	-1.5933427
C	1.2269715	-3.7242468	-1.8030354
N	1.3511399	-4.5658972	-2.8347045
C	2.5743993	-5.3555924	-3.0978363
C	2.5402244	-6.7713374	-2.4978307
C	3.7802553	-7.6302285	-2.8494795
O	-1.5709150	-0.5178498	-1.9430662
O	1.9270962	-2.8004682	0.2756395
C	2.9663981	-2.3305292	1.1287292
C	2.3340305	-1.3001152	2.0653440

N	3.0152641	-0.8204281	3.1037474
C	4.3888773	-1.2525020	3.4422237
C	4.4332013	-2.3810868	4.4863551
C	5.8656503	-2.8031469	4.8955805
C	2.4043585	-3.5435992	-0.8414582
O	1.1543878	-0.9120441	1.7914557
C	-2.5149661	1.6005608	-3.4534088
C	-2.1786758	1.2485322	-4.9109513
C	-1.3012101	2.3105046	-5.6174501
C	2.3995523	0.2209377	3.9636729
C	2.7281695	1.6467307	3.4885130
C	2.2441795	2.7540537	4.4556092
C	0.2373200	-4.7287818	-3.7949581
C	0.3879774	-3.8438636	-5.0443967
C	-0.7507119	-4.0198676	-6.0776970
H	-4.6854213	-3.2701697	3.2504056
H	2.4510525	-6.6924540	-1.3887334
H	-3.9736591	-3.8852679	-0.3572508
H	-4.2540111	-2.6882931	0.9687047
H	-4.0823467	-6.2264433	2.5121468
H	-4.7046630	-5.0223503	1.3745259
H	-6.7849550	-4.6134905	2.8015830
H	-2.0855764	-5.5552744	3.8453934
H	-0.8095093	-4.6897431	2.9338853
H	-0.7496133	-6.5157650	1.2174906
H	0.7016783	-6.7682804	3.2882076
H	-4.4984484	-0.8672889	-0.7215296
H	-4.2299187	-2.0691419	-2.0487809
H	-5.3388370	-0.2233171	-2.8539541
H	-5.0157231	1.1114662	-3.9725216
H	-4.9239973	2.7461699	-2.0265719
H	-7.4459201	0.9594819	-1.9745941
H	-1.5922751	1.6979365	-2.8472803
H	-3.0624905	2.5630506	-3.3910596
H	-1.6486955	0.2688788	-4.9234124
H	-0.3792359	2.4459361	-5.0015676
H	3.7690712	-1.8401481	0.5247140
H	3.4200631	-3.1795164	1.6905578
H	4.9137448	-0.3485064	3.8150750
H	4.9206670	-1.5511482	2.5135984
H	3.8709520	-2.0640363	5.3960285
H	6.4258337	-3.0493377	3.9598921
H	2.7836785	0.0502791	4.9923089
H	1.3076227	0.0395841	3.9719348
H	2.2762102	1.8082370	2.4818166
H	2.7062314	2.5518983	5.4527069
H	2.8129339	-4.5237218	-0.5041116
H	3.2170666	-2.9777921	-1.3584131
H	3.4612774	-4.7932226	-2.7369602
H	2.6795231	-5.4023334	-4.2011436
H	4.6881667	-7.0429353	-2.5674982

H	-0.7032185	-4.4899659	-3.2593435
H	0.2114553	-5.8046761	-4.0665725
H	0.4283395	-2.7796351	-4.7182592
H	-1.7153886	-3.8166393	-5.5507532
N	1.4630243	0.7047626	-1.1902936
O	1.5900307	-0.5872441	-1.3607105
O	2.2054513	1.5045683	-1.6962371
O	0.4699207	1.0242168	-0.4264368
H	3.8919478	-3.2677475	4.0796607
H	-5.1977477	1.4109102	-0.8851271
H	-4.1354407	-4.5218184	4.3893721
H	-2.0569146	-7.4004796	2.0561749
H	1.6207830	-7.2983704	-2.8458617
H	3.8320608	1.7405118	3.3640589
H	1.3618897	-4.0608478	-5.5441098
C	-6.8102403	-3.8037031	4.8036704
H	-7.8822358	-4.0369940	4.9828306
H	-6.2794974	-3.8996169	5.7781249
H	-6.7450467	-2.7392929	4.4857690
C	0.4429140	-8.6672513	2.2893443
H	0.9038590	-8.3382655	1.3306470
H	1.2240278	-9.1969103	2.8769675
H	-0.3502779	-9.4100946	2.0455248
C	-7.4795344	2.8263459	-0.8884086
H	-7.0291739	3.8444493	-0.9134635
H	-8.5829418	2.9474871	-0.9441534
H	-7.2382523	2.3738533	0.0992988
C	-0.8687749	1.7965937	-7.0023789
H	-0.1967666	2.5258260	-7.5048862
H	-0.3218857	0.8294971	-6.9313964
H	-1.7497487	1.6417752	-7.6665049
C	-0.6019783	-2.9803569	-7.2028060
H	-0.5933424	-1.9404941	-6.8058528
H	0.3451602	-3.1346361	-7.7677293
H	-1.4389819	-3.0586323	-7.9304646
C	3.7793556	-8.9216889	-2.0114416
H	2.8860947	-9.5465316	-2.2395112
H	4.6797032	-9.5360512	-2.2280750
H	3.7744434	-8.7051112	-0.9196394
N	-2.3576642	0.0294657	1.8078431
O	-3.1841830	0.5539758	2.5109464
O	-1.7327234	-1.0598640	2.1336872
O	-2.0252806	0.4888744	0.6374541
Th	-0.3791180	-1.2943295	-0.0007906
C	5.8086922	-4.0783556	5.7559085
H	6.8309212	-4.4177592	6.0300986
H	5.2514279	-3.8986546	6.7035813
H	5.3079946	-4.9160626	5.2204794
C	2.7515325	4.1260854	3.9761327
H	2.3218993	4.3889802	2.9826336
H	2.4606661	4.9272463	4.6897560

H	3.8601359	4.1450156	3.8832700
C	-0.7016889	-7.9518694	4.4332717
H	-1.5559851	-8.6512260	4.2851605
H	0.0733502	-8.4960890	5.0155459
H	-1.0534068	-7.1123095	5.0733579
C	-6.3636152	-6.2224185	4.1850914
H	-6.0289327	-6.9441889	3.4065469
H	-5.7848320	-6.4264951	5.1151710
H	-7.4283086	-6.4574538	4.4011917
C	-7.3601527	2.5766123	-3.4097473
H	-6.8748560	3.5686846	-3.5580556
H	-7.0918978	1.9299701	-4.2749140
H	-8.4590296	2.7362600	-3.4590312
C	-0.8181987	-5.4450723	-6.6575125
H	0.1361898	-5.7162660	-7.1646766
H	-1.0281129	-6.2189702	-5.8859505
H	-1.6269334	-5.5221298	-7.4166665
C	3.8697331	-7.9518319	-4.3525439
H	2.9773982	-8.5262815	-4.6921158
H	3.9551192	-7.0422876	-4.9877411
H	4.7645695	-8.5755628	-4.5657661
H	-3.1214957	1.1124288	-5.4929433
C	-1.9997054	3.6779243	-5.7367498
H	-1.3511983	4.4019679	-6.2760870
H	-2.9511532	3.5945159	-6.3110527
H	-2.2326781	4.1335582	-4.7485310
C	0.7148608	2.7617694	4.6336573
H	0.1989462	2.9229418	3.6588754
H	0.3266903	1.8168426	5.0754529
H	0.4052793	3.5852130	5.3133827
C	6.6272050	-1.6817237	5.6261068
H	6.7639221	-0.7704064	5.0022875
H	6.1000789	-1.3828426	6.5611451
H	7.6436649	-2.0253207	5.9158734

Np(IV)-*n*-Butyl DGA

C	-6.1173837	-4.9165852	3.7502935
C	-4.6966196	-4.3768822	3.5070813
C	-3.9959829	-5.0909773	2.3381129
N	-2.6035526	-4.6449194	2.1114841
C	-2.2742490	-3.6828183	1.2423837
C	-3.3751489	-3.0376227	0.3922407
O	-2.7438957	-2.0162257	-0.3717133
C	-3.5897229	-1.2997739	-1.2713863
C	-2.6741375	-0.3145480	-2.0110240
N	-3.2043019	0.6214664	-2.7999536
C	-4.6591956	0.7638936	-3.0215828
C	-5.3325110	1.7899422	-2.0934212
C	-6.8320221	1.9541816	-2.3993667

C	-1.5540893	-5.2848429	2.9337375
C	-1.0419116	-6.6074391	2.3395736
C	-0.0278368	-7.3066787	3.2616392
O	-1.0821488	-3.2850469	1.0790584
O	-0.0040198	-2.9081047	-1.5254274
C	1.0142306	-3.6182063	-1.7647253
N	1.0867504	-4.4399682	-2.8209202
C	2.2751622	-5.2646510	-3.1288541
C	2.2067360	-6.7009317	-2.5831286
C	3.4185265	-7.5445188	-3.0182432
O	-1.4236069	-0.4334430	-1.8392313
O	1.8032124	-2.7873788	0.3225057
C	2.8911349	-2.3289314	1.1187351
C	2.3256509	-1.2861025	2.0805417
N	3.0503275	-0.8397876	3.1048631
C	4.4249947	-1.3059807	3.3888561
C	4.4974041	-2.4304082	4.4354185
C	5.9481687	-2.8233722	4.7676941
C	2.2184137	-3.5156990	-0.8269044
O	1.1522348	-0.8506459	1.8499080
C	-2.3163819	1.6138564	-3.4503505
C	-1.8679546	1.2086013	-4.8629808
C	-0.9915405	2.2916383	-5.5169894
C	2.4838563	0.1950966	4.0053272
C	2.7886036	1.6308641	3.5476817
C	2.2665914	2.6747864	4.5515308
C	-0.0466204	-4.5283006	-3.7659158
C	0.0999645	-3.5978244	-4.9815173
C	-1.0347825	-3.7927731	-6.0021334
H	-4.7346035	-3.2797067	3.3095602
H	2.1415370	-6.6769623	-1.4693168
H	-3.8387933	-3.7906178	-0.2901788
H	-4.1797311	-2.6079399	1.0338669
H	-3.9529433	-6.1850807	2.5286209
H	-4.5775538	-4.9746436	1.3996547
H	-6.0638191	-6.0137049	3.9422769
H	-6.7218881	-4.7987261	2.8202127
H	-1.9921318	-5.4550145	3.9405327
H	-0.7271155	-4.5558108	3.0467026
H	-0.5788082	-6.4044291	1.3459660
H	-0.5018368	-7.4907729	4.2539510
H	0.8281812	-6.6183342	3.4574834
H	-4.3903346	-0.7662272	-0.7106718
H	-4.0702753	-2.0103996	-1.9870486
H	-5.1433387	-0.2316773	-2.9284948
H	-4.7906532	1.0621634	-4.0843610
H	-4.8200493	2.7732410	-2.1986001
H	-6.9560767	2.2602773	-3.4643929
H	-7.3404931	0.9654206	-2.3052902
H	-1.4414620	1.7620640	-2.7862066
H	-2.8796995	2.5705878	-3.4802158

H	-1.3038483	0.2491930	-4.8040698
H	-0.1050365	2.4856277	-4.8687201
H	-1.5595261	3.2503996	-5.5521031
H	3.6685779	-1.8499218	0.4736426
H	3.3608265	-3.1824076	1.6598692
H	4.9906433	-0.4165585	3.7415613
H	4.9111724	-1.6147020	2.4392823
H	3.9770095	-2.1027724	5.3649295
H	6.4923017	-1.9255179	5.1427468
H	6.4724090	-3.1301374	3.8316251
H	2.9111823	0.0043525	5.0128461
H	1.3898463	0.0266987	4.0633473
H	2.3238644	1.8005035	2.5492812
H	2.7368487	2.4940457	5.5467736
H	1.1710383	2.5273173	4.6978944
H	2.5926707	-4.5214928	-0.5282196
H	3.0425948	-2.9716339	-1.3489428
H	3.1881754	-4.7464846	-2.7672060
H	2.3661048	-5.2840232	-4.2359615
H	3.4641287	-7.5670768	-4.1317926
H	4.3573139	-7.0422043	-2.6850168
H	-0.9710711	-4.2915772	-3.2022299
H	-0.1110237	-5.5887026	-4.0930408
H	0.1209058	-2.5412718	-4.6283295
H	-2.0158238	-3.6126244	-5.5014189
H	-1.0531063	-4.8577616	-6.3320695
N	1.4472375	0.7411811	-1.0190161
O	1.6052426	-0.5530487	-1.1142539
O	2.1953159	1.5330625	-1.5291636
O	0.4117155	1.0638207	-0.3210631
H	3.9383731	-3.3220287	4.0640885
H	-5.1899583	1.4854285	-1.0298290
H	-2.7617572	1.0165367	-5.5023748
H	-4.0877542	-4.4996968	4.4318065
H	-1.9009233	-7.2934477	2.1530857
H	1.2677676	-7.1857919	-2.9374773
H	3.8886434	1.7583982	3.4174091
H	1.0786909	-3.7849380	-5.4818321
C	-6.8294993	-4.2243368	4.9192647
H	-7.8508027	-4.6379002	5.0616063
H	-6.2752731	-4.3648338	5.8736791
H	-6.9315919	-3.1297388	4.7459234
C	0.4923141	-8.6325548	2.6915328
H	1.0100293	-8.4855728	1.7166166
H	1.2154742	-9.1100272	3.3870887
H	-0.3364097	-9.3561846	2.5252445
C	-7.5204473	2.9771259	-1.4867564
H	-7.0630018	3.9860992	-1.5896560
H	-8.5981909	3.0711243	-1.7393430
H	-7.4503161	2.6823369	-0.4158732
C	-0.5272333	1.9205539	-6.9308448

H	0.1030930	2.7252545	-7.3664470
H	0.0773019	0.9857375	-6.9298531
H	-1.3902848	1.7650508	-7.6161142
C	-0.9038346	-2.8804149	-7.2284673
H	-0.9153334	-1.8049132	-6.9411983
H	0.0453265	-3.0707678	-7.7770376
H	-1.7393094	-3.0477848	-7.9414927
C	3.3813380	-8.9789298	-2.4767969
H	2.4732416	-9.5215581	-2.8223458
H	4.2657461	-9.5557412	-2.8222904
H	3.3843078	-8.9970652	-1.3637323
N	-2.3045183	0.1418224	1.8461225
O	-3.1229565	0.6693169	2.5553008
O	-1.6358967	-0.9186183	2.1981388
O	-2.0146491	0.5510230	0.6542047
Np	-0.3683847	-1.2054137	0.1311880
C	6.0413540	-3.9502935	5.8040461
H	7.1012332	-4.2031788	6.0202352
H	5.5648234	-3.6587236	6.7664617
H	5.5421598	-4.8785008	5.4454669
C	2.5379148	4.1185022	4.1096653
H	2.0420315	4.3487394	3.1402417
H	2.1556094	4.8413176	4.8619500
H	3.6273043	4.3090629	3.9862314

Np(IV)-*iso*-Butyl DGA

C	-6.2099757	-4.6210612	3.6699396
C	-4.7676830	-4.1080092	3.5031661
C	-4.0375274	-5.0239071	2.4882963
N	-2.6364514	-4.6534851	2.1779526
C	-2.3216121	-3.7389570	1.2524611
C	-3.4359568	-3.1147039	0.4062273
O	-2.8174977	-2.1108433	-0.3922481
C	-3.6937694	-1.3879461	-1.2593777
C	-2.8044647	-0.3829365	-2.0020178
N	-3.3415004	0.5614217	-2.7767829
C	-4.7967282	0.7172672	-2.9957786
C	-5.4575275	1.8879025	-2.2276014
C	-6.9028611	2.0526044	-2.7318804
C	-1.5439273	-5.2856647	2.9524854
C	-0.8653013	-6.4853373	2.2507429
C	0.2921997	-6.9805182	3.1365016
O	-1.1274526	-3.3785184	1.0250979
O	-0.0339044	-2.9712574	-1.5674985
C	1.0009817	-3.6631140	-1.7918564
N	1.1044174	-4.4757196	-2.8536652
C	2.3067477	-5.3021391	-3.1105383
C	2.3328697	-6.6921816	-2.4283071
C	3.6819636	-7.3650578	-2.7414674

O	-1.5493209	-0.4919326	-1.8457903
O	1.7494318	-2.8041965	0.2999295
C	2.8190571	-2.3343397	1.1149677
C	2.2278946	-1.2983220	2.0680955
N	2.9276753	-0.8573928	3.1150443
C	4.2715271	-1.3833182	3.4505513
C	4.3031941	-2.6726691	4.3100366
C	5.7744198	-3.0776896	4.5179491
C	2.1908104	-3.5332277	-0.8395720
O	1.0666802	-0.8578951	1.7915803
C	-2.4340935	1.5485624	-3.4159345
C	-1.7235634	1.0594473	-4.6987424
C	-0.7433025	2.1547181	-5.1569836
C	2.3839391	0.2375328	3.9573124
C	3.0168086	1.6245453	3.6924239
C	2.4006211	2.6321207	4.6806274
C	-0.0091715	-4.5231072	-3.8291160
C	-0.0204863	-3.3673707	-4.8572842
C	-1.2463618	-3.5413470	-5.7718026
H	-4.8164362	-3.0809542	3.0682543
H	2.2771507	-6.5315789	-1.3244992
H	-3.9064320	-3.8878105	-0.2491855
H	-4.2333367	-2.6693312	1.0440335
H	-4.0105555	-6.0616425	2.8800789
H	-4.6134633	-5.0740785	1.5391196
H	-6.2251173	-5.6389665	4.1208949
H	-6.7534895	-4.6704576	2.7000889
H	-1.9794142	-5.6086188	3.9198525
H	-0.7910809	-4.4991382	3.1642182
H	-0.4341567	-6.1036545	1.2959264
H	-0.0820181	-7.3608975	4.1138450
H	1.0287164	-6.1731262	3.3479924
H	-4.4812787	-0.8704760	-0.6683184
H	-4.1860777	-2.0910739	-1.9741993
H	-5.3072992	-0.2388065	-2.7503443
H	-4.9346762	0.8683002	-4.0873272
H	-4.8994298	2.8164384	-2.4911733
H	-6.9417674	2.2399205	-3.8276388
H	-7.5138875	1.1461661	-2.5173575
H	-1.6804821	1.8394647	-2.6555995
H	-3.0501014	2.4440660	-3.6414348
H	-1.1275431	0.1593817	-4.4211228
H	-0.0014560	2.4019431	-4.3660541
H	-1.2807171	3.0922854	-5.4267773
H	3.5977616	-1.8377722	0.4840543
H	3.2951575	-3.1838846	1.6537558
H	4.7975902	-0.5678719	3.9896306
H	4.8417337	-1.5377868	2.5089517
H	6.3229030	-2.3082522	5.1064660
H	6.3121991	-3.2138414	3.5532344
H	2.5551688	-0.0563952	5.0135485

H	1.2900043	0.2722758	3.7832632
H	2.5405968	2.3151145	5.7378423
H	1.3088768	2.7570422	4.5011128
H	2.5835389	-4.5274670	-0.5290335
H	3.0088699	-2.9760889	-1.3579766
H	3.2096086	-4.7209383	-2.8242068
H	2.3715593	-5.4310384	-4.2104032
H	3.7930544	-7.5546689	-3.8329137
H	4.5456948	-6.7433090	-2.4161894
H	-0.9578714	-4.5198228	-3.2533526
H	0.0650867	-5.4980409	-4.3531876
H	-0.1451974	-2.4201304	-4.2832200
H	-2.1954884	-3.5888292	-5.1919800
H	-1.1721510	-4.4740499	-6.3756413
N	1.3125583	0.6941293	-1.1162421
O	1.4861471	-0.5989947	-1.2082427
O	2.0329570	1.4921479	-1.6576457
O	0.2970966	1.0071509	-0.3886070
H	3.8034759	-3.4852916	3.7284122
H	4.1067140	1.5548551	3.9218059
N	-2.3500771	0.0205803	1.8827040
O	-3.1504255	0.5478136	2.6132041
O	-1.7106464	-1.0666014	2.1902429
O	-2.0536070	0.4685875	0.7034847
Np	-0.4452846	-1.2794053	0.0822196
H	-7.3944268	2.9117421	-2.2277542
H	-0.1804693	1.8254270	-6.0571059
H	-1.3286017	-2.6925214	-6.4847898
H	3.7595150	-8.3454977	-2.2247886
H	5.8404468	-4.0341268	5.0791138
H	0.8353489	-7.8162951	2.6444954
H	-6.7858737	-3.9510472	4.3434021
H	2.8758129	3.6297302	4.5653219
C	3.5617650	-2.5369060	5.6503972
H	4.0007094	-1.7284929	6.2780324
H	2.4772767	-2.3278464	5.5183700
H	3.6445576	-3.4815980	6.2298543
C	2.8631204	2.0876194	2.2359991
H	3.3554175	1.3918877	1.5187714
H	1.7930427	2.1848969	1.9475537
H	3.3402683	3.0813644	2.0943471
C	1.1497456	-7.5888536	-2.8292395
H	0.1684920	-7.1493868	-2.5443810
H	1.1406501	-7.7826774	-3.9259543
H	1.2271019	-8.5757886	-2.3240331
C	1.2773551	-3.2693855	-5.6756769
H	1.4620515	-4.1968491	-6.2649590
H	1.2150858	-2.4298931	-6.4018857
H	2.1677563	-3.0768843	-5.0369448
C	-2.7001339	0.6694442	-5.8206216
H	-3.3393895	1.5304254	-6.1216520

H	-2.1423248	0.3459328	-6.7265249
H	-3.3658679	-0.1743441	-5.5315893
C	-5.4041986	1.7213779	-0.7008723
H	-6.0217329	0.8533842	-0.3692753
H	-4.3679690	1.5949050	-0.3142382
H	-5.8244926	2.6199575	-0.1995483
C	-4.0461844	-3.9981018	4.8563653
H	-3.9515265	-4.9922912	5.3500491
H	-3.0328736	-3.5502219	4.7592749
H	-4.6249504	-3.3450023	5.5445782
C	-1.8415535	-7.6265961	1.9185652
H	-1.3062439	-8.4666509	1.4247893
H	-2.3154885	-8.0379644	2.8387625
H	-2.6504086	-7.3051062	1.2252916

Np(IV)-*n*-Amyl DGA

C	-6.1134866	-4.9621806	3.7355650
C	-4.7081212	-4.3909603	3.4812687
C	-3.9840867	-5.1211653	2.3368037
N	-2.5938512	-4.6640544	2.1177052
C	-2.2658433	-3.7093937	1.2403870
C	-3.3659984	-3.0808802	0.3768512
O	-2.7395814	-2.0558028	-0.3859277
C	-3.5872032	-1.3440647	-1.2877177
C	-2.6744573	-0.3564302	-2.0278020
N	-3.2072835	0.5787816	-2.8156614
C	-4.6634920	0.7242671	-3.0272119
C	-5.3268654	1.7480969	-2.0894982
C	-6.8284636	1.9140838	-2.3788180
C	-1.5458163	-5.2865154	2.9554064
C	-1.0177788	-6.6105213	2.3784004
C	-0.0185193	-7.3003809	3.3218985
O	-1.0754409	-3.3047065	1.0804163
O	-0.0007532	-2.9420055	-1.5264630
C	1.0269821	-3.6349083	-1.7758883
N	1.0972885	-4.4651498	-2.8252862
C	2.3000500	-5.2612787	-3.1523296
C	2.2797877	-6.6963192	-2.5995471
C	3.5061160	-7.5069855	-3.0526640
O	-1.4233422	-0.4740200	-1.8580078
O	1.8201325	-2.7940348	0.3033160
C	2.9034904	-2.3214306	1.0975302
C	2.3194025	-1.3048679	2.0759456
N	3.0280938	-0.8739378	3.1177585
C	4.4075696	-1.3256925	3.4024882
C	4.4897830	-2.4778472	4.4177408
C	5.9435880	-2.8431197	4.7634639
C	2.2421474	-3.5024423	-0.8562489
O	1.1437605	-0.8764278	1.8425756

C	-2.3213839	1.5687578	-3.4725432
C	-1.8911739	1.1646569	-4.8911620
C	-1.0076286	2.2394816	-5.5469402
C	2.4357254	0.1249082	4.0416881
C	2.7391302	1.5794795	3.6467143
C	2.1618740	2.5760593	4.6668232
C	-0.0572271	-4.5974170	-3.7391975
C	0.0174502	-3.6705411	-4.9640491
C	-1.1378619	-3.9241702	-5.9472407
H	-4.7749496	-3.3018357	3.2500988
H	2.2326045	-6.6689994	-1.4851740
H	-3.8147169	-3.8425531	-0.3060334
H	-4.1812410	-2.6575755	1.0090661
H	-3.9297627	-6.2099936	2.5524812
H	-4.5547452	-5.0332583	1.3885520
H	-6.0299793	-6.0476505	3.9808737
H	-6.7146433	-4.9072134	2.7964519
H	-1.9920405	-5.4504851	3.9596894
H	-0.7264685	-4.5490509	3.0687578
H	-0.5387672	-6.4110438	1.3918660
H	-0.5104604	-7.4877513	4.3058755
H	0.8317599	-6.6086121	3.5348874
H	-4.3907381	-0.8134425	-0.7285595
H	-4.0635600	-2.0574155	-2.0035324
H	-5.1487805	-0.2707686	-2.9343616
H	-4.8018541	1.0267717	-4.0877987
H	-4.8140593	2.7307534	-2.1972995
H	-6.9665417	2.2307789	-3.4399315
H	-7.3390424	0.9250963	-2.2873071
H	-1.4383815	1.7096176	-2.8177628
H	-2.8794661	2.5287851	-3.4930680
H	-1.3391599	0.1978121	-4.8420577
H	-0.1103638	2.4191949	-4.9078858
H	-1.5620014	3.2074490	-5.5736652
H	3.6651987	-1.8158385	0.4539046
H	3.3956179	-3.1711044	1.6242086
H	4.9538102	-0.4372500	3.7863010
H	4.9083329	-1.5978387	2.4491684
H	3.9455202	-2.1894310	5.3466314
H	6.4579267	-1.9452071	5.1804063
H	6.4957185	-3.1047482	3.8285014
H	2.8414413	-0.1004225	5.0509713
H	1.3420180	-0.0523614	4.0682567
H	2.3119949	1.7796358	2.6374091
H	2.5793012	2.3542929	5.6782244
H	1.0597323	2.4219071	4.7494444
H	2.6492115	-4.4985889	-0.5685115
H	3.0422682	-2.9307061	-1.3861202
H	3.2059592	-4.7174507	-2.8112135
H	2.3697211	-5.2834507	-4.2610401
H	3.5404111	-7.5259795	-4.1675924

H	4.4384497	-6.9848595	-2.7287216
H	-0.9737229	-4.3919783	-3.1508773
H	-0.0917282	-5.6612447	-4.0594014
H	0.0036051	-2.6114459	-4.6187174
H	-2.1122502	-3.7868593	-5.4187573
H	-1.1177730	-4.9913643	-6.2733375
N	1.4346790	0.7278787	-1.0276229
O	1.5989240	-0.5648697	-1.1279297
O	2.1795961	1.5255503	-1.5336123
O	0.3970811	1.0430616	-0.3292634
H	3.9592351	-3.3713536	4.0115180
H	-5.1724232	1.4401488	-1.0286992
H	-2.7934351	0.9870087	-5.5224836
H	-4.0991836	-4.4690877	4.4105658
H	-1.8713858	-7.3000254	2.1811315
H	1.3482711	-7.2073288	-2.9359774
H	3.8413847	1.7251482	3.5652685
H	0.9883749	-3.8213398	-5.4902881
C	-6.8687052	-4.2421837	4.8658218
H	-6.2616289	-4.2923513	5.7996789
H	-6.9551854	-3.1583793	4.6158950
C	0.5280127	-8.6282942	2.7701145
H	1.0261814	-8.4415032	1.7887232
H	-0.3262258	-9.3108567	2.5511685
C	-7.5168504	2.9298511	-1.4507354
H	-7.0036490	3.9152856	-1.5446700
H	-7.3746344	2.6123463	-0.3907543
C	-0.5551963	1.8762201	-6.9713081
H	-0.0076081	0.9042093	-6.9442171
H	-1.4547407	1.7028408	-7.6078540
C	-1.0988877	-3.0162814	-7.1886026
H	-1.1130044	-1.9490324	-6.8629594
H	-0.1265193	-3.1598799	-7.7150964
C	3.5197403	-8.9499503	-2.5203554
H	2.5854846	-9.4665804	-2.8434557
H	3.4883992	-8.9300451	-1.4051366
N	-2.3155320	0.1214225	1.8238318
O	-3.1314724	0.6543063	2.5320503
O	-1.6425552	-0.9337262	2.1831993
O	-2.0320099	0.5196665	0.6268815
Np	-0.3712314	-1.2305903	0.1198797
C	-9.0130641	3.0978586	-1.7433766
H	-9.4753534	3.8371927	-1.0543590
H	-9.1866294	3.4560581	-2.7827422
H	-9.5630075	2.1375977	-1.6228253
C	0.3312726	2.9491543	-7.6159082
H	0.6421542	2.6518270	-8.6407044
H	-0.2031513	3.9219282	-7.6978646
H	1.2563435	3.1239670	-7.0216970
C	-2.2536745	-3.2755957	-8.1644318
H	-2.1938383	-2.6037324	-9.0477372

H	-2.2393230	-4.3227204	-8.5412955
H	-3.2426946	-3.1078326	-7.6807904
C	4.7402773	-9.7526070	-2.9878157
H	4.7168898	-10.7887297	-2.5871026
H	4.7778347	-9.8245562	-4.0976277
H	5.6912303	-9.2835634	-2.6489321
C	6.0586325	-4.0054260	5.7647626
H	5.5008682	-3.7428275	6.6944438
H	5.5468432	-4.9033545	5.3438587
C	2.4450493	4.0461325	4.3126807
H	3.5471683	4.1979018	4.2357312
H	2.0347272	4.2646171	3.2988312
C	7.5095807	-4.3564232	6.1168102
H	8.0352347	-3.4926628	6.5815080
H	7.5541316	-5.2011577	6.8375419
H	8.0877814	-4.6559581	5.2137600
C	1.5075785	-9.3238083	3.7236007
H	1.8779716	-10.2794259	3.2939911
H	2.3945397	-8.6850718	3.9365758
H	1.0252858	-9.5620577	4.6978547
C	-8.2631701	-4.8252545	5.1257482
H	-8.2075423	-5.8967189	5.4217420
H	-8.7789848	-4.2793181	5.9446606
H	-8.9080615	-4.7591636	4.2209190
C	1.8593479	5.0332138	5.3302198
H	2.2792584	4.8668237	6.3477197
H	2.0836260	6.0836633	5.0448985
H	0.7529535	4.9342377	5.4029580

Np(IV)-*iso*-Amyl DGA

C	-6.1708665	-4.8871018	3.6550078
C	-4.7156230	-4.4161104	3.4158974
C	-3.9936681	-5.1664807	2.2824464
N	-2.6030167	-4.7089896	2.0672340
C	-2.2725836	-3.7582517	1.1869465
C	-3.3699571	-3.1405361	0.3123623
O	-2.7449366	-2.1129786	-0.4483260
C	-3.5927286	-1.4061650	-1.3541269
C	-2.6863635	-0.3936812	-2.0677079
N	-3.2258545	0.5663761	-2.8190893
C	-4.6834582	0.7065205	-3.0262401
C	-5.3479024	1.6865076	-2.0426543
C	-6.8789517	1.8206968	-2.2269308
C	-1.5598119	-5.3239299	2.9162758
C	-1.0230395	-6.6433723	2.3355787
C	0.0348802	-7.3400009	3.2249847
O	-1.0825476	-3.3499447	1.0315813
O	0.0216347	-2.9885907	-1.5566754
C	1.0545271	-3.6826021	-1.7820633

N	1.1385026	-4.5323845	-2.8143295
C	2.3500650	-5.3236777	-3.1208280
C	2.3323738	-6.7447101	-2.5326569
C	3.5787216	-7.5888049	-2.8969019
O	-1.4335425	-0.5148492	-1.9071282
O	1.8216610	-2.8135467	0.2956149
C	2.8916050	-2.3200698	1.0949807
C	2.2879342	-1.2926112	2.0493686
N	2.9841736	-0.8258890	3.0836461
C	4.3644515	-1.2565004	3.3948642
C	4.4317606	-2.3882978	4.4344437
C	5.8734526	-2.7957565	4.8259717
C	2.2606449	-3.5290892	-0.8531472
O	1.1072993	-0.8861501	1.8008114
C	-2.3526004	1.5952104	-3.4317828
C	-1.9224346	1.2540813	-4.8670635
C	-1.0103174	2.3269780	-5.5099516
C	2.3757703	0.1988619	3.9686737
C	2.6669374	1.6354684	3.5022909
C	2.1883852	2.7207339	4.4970122
C	-0.0069480	-4.6923232	-3.7354233
C	0.0692497	-3.7693951	-4.9636287
C	-1.0743396	-3.9955098	-5.9823972
H	-4.7161346	-3.3249624	3.1860064
H	2.2484027	-6.6755999	-1.4223670
H	-3.8072103	-3.9077180	-0.3718290
H	-4.1938102	-2.7208730	0.9356650
H	-3.9349168	-6.2524443	2.5036416
H	-4.5607868	-5.0833954	1.3314850
H	-6.7158128	-4.8025024	2.6830734
H	-2.0177094	-5.4820939	3.9146092
H	-0.7431906	-4.5837139	3.0323217
H	-0.5807227	-6.4295511	1.3351851
H	0.8499366	-6.6001291	3.4175147
H	-4.4134716	-0.8979022	-0.7995681
H	-4.0456292	-2.1191110	-2.0855838
H	-5.1596798	-0.2956389	-2.9686718
H	-4.8183735	1.0444102	-4.0749891
H	-4.8770885	2.6912749	-2.1498051
H	-7.3204355	0.7969393	-2.1411897
H	-1.4685882	1.7144854	-2.7740164
H	-2.9258758	2.5442351	-3.4015864
H	-1.3835315	0.2792644	-4.8494706
H	-0.1328506	2.4669054	-4.8331707
H	3.6567878	-1.8181883	0.4526388
H	3.3849755	-3.1568891	1.6408610
H	4.8931556	-0.3520394	3.7616297
H	4.8789840	-1.5495331	2.4549604
H	3.8772015	-2.0800655	5.3519059
H	6.4267927	-3.0293173	3.8831139
H	2.7897407	0.0240432	4.9848452

H	1.2873528	0.0002282	4.0033534
H	2.1839044	1.8004910	2.5107758
H	2.6897138	2.5208637	5.4754225
H	2.6753812	-4.5180501	-0.5520460
H	3.0592674	-2.9544639	-1.3822597
H	3.2494982	-4.7669845	-2.7830030
H	2.4216702	-5.3608084	-4.2275265
H	4.4814963	-7.0027935	-2.5959370
H	-0.9314933	-4.4920063	-3.1577608
H	-0.0190725	-5.7602668	-4.0377679
H	0.0472890	-2.7140785	-4.6081884
H	-2.0399257	-3.9302064	-5.4227568
N	1.4160043	0.6942011	-1.0734004
O	1.5879827	-0.5981598	-1.1651544
O	2.1589136	1.4928888	-1.5813580
O	0.3742190	1.0082771	-0.3813782
H	3.8949642	-3.2788853	4.0306338
H	-5.1280431	1.3588998	-0.9996488
H	-4.1346674	-4.5290451	4.3605413
H	-1.8691088	-7.3502326	2.1637867
H	1.4158733	-7.2774881	-2.8797239
H	3.7650466	1.7512487	3.3490696
H	1.0468564	-3.9115863	-5.4820558
C	-6.8631168	-3.9518170	4.6627582
H	-7.9243936	-4.2465963	4.8122093
H	-6.3617856	-3.9915528	5.6564333
H	-6.8520522	-2.8934371	4.3192945
C	0.6508613	-8.5333572	2.4720915
H	1.1020767	-8.2215084	1.5030692
H	1.4478742	-9.0187828	3.0763884
H	-0.1183677	-9.3082230	2.2526547
C	-7.4664585	2.6803298	-1.0934233
H	-7.0635230	3.7178704	-1.1283263
H	-8.5724551	2.7484495	-1.1798286
H	-7.2304033	2.2592688	-0.0906614
C	-0.4815623	1.8250769	-6.8656684
H	0.2151638	2.5638227	-7.3182327
H	0.0689752	0.8630098	-6.7634288
H	-1.3146249	1.6659827	-7.5880495
C	-1.0677801	-2.8771330	-7.0393619
H	-1.1628804	-1.8702682	-6.5745409
H	-0.1229373	-2.8890430	-7.6286591
H	-1.9082092	-3.0010304	-7.7565561
C	3.5804336	-8.8988750	-2.0882650
H	2.6947979	-9.5258060	-2.3393627
H	4.4880969	-9.5007700	-2.3096470
H	3.5628215	-8.7071935	-0.9919729
N	-2.3541221	0.0626333	1.7674661
O	-3.1849882	0.5861241	2.4659431
O	-1.6825880	-0.9912895	2.1288957
O	-2.0540048	0.4725725	0.5779883

Np	-0.3863005	-1.2710208	0.0722932
C	5.8407444	-4.0767189	5.6791096
H	6.8699347	-4.4046139	5.9409607
H	5.2908582	-3.9097315	6.6333930
H	5.3454590	-4.9174514	5.1434571
C	2.6433692	4.1101768	4.0153558
H	2.1694017	4.3737726	3.0423255
H	2.3605245	4.8954884	4.7495058
H	3.7467737	4.1581365	3.8805258
C	-0.5304215	-7.7877149	4.5856824
H	-1.3704563	-8.5070714	4.4519616
H	0.2518458	-8.3019876	5.1853039
H	-0.9011604	-6.9387017	5.2021254
C	-6.2529918	-6.3529207	4.1192234
H	-5.8471006	-7.0707133	3.3714256
H	-5.6991569	-6.5012267	5.0745731
H	-7.3096228	-6.6459706	4.3015153
C	-7.2633663	2.3891469	-3.6053494
H	-6.8172076	3.3983703	-3.7607009
H	-6.9423096	1.7380831	-4.4489830
H	-8.3662774	2.4995143	-3.6885671
C	-1.0085422	-5.3795565	-6.6550326
H	-0.0568055	-5.5023112	-7.2209134
H	-1.0871408	-6.2206858	-5.9301066
H	-1.8416103	-5.5044270	-7.3805074
C	3.6801106	-7.8758176	-4.4062128
H	2.7907357	-8.4422645	-4.7662759
H	3.7705863	-6.9519055	-5.0195006
H	4.5767487	-8.4946741	-4.6261916
H	-2.8249814	1.1119862	-5.5084899
C	-1.7112443	3.6890824	-5.6679987
H	-1.0334703	4.4228234	-6.1558915
H	-2.6200176	3.6020256	-6.3072501
H	-2.0169433	4.1345906	-4.6952469
C	0.6665264	2.6873126	4.7278787
H	0.1131394	2.8423148	3.7729715
H	0.3178862	1.7294719	5.1749069
H	0.3595666	3.4973881	5.4246077
C	6.6286032	-1.6696447	5.5559628
H	6.7486369	-0.7528784	4.9366597
H	6.1071803	-1.3828496	6.4979937
H	7.6518634	-2.0027752	5.8337412

Pu(IV)-*n*-Butyl DGA

C	-6.0867590	-5.0211167	3.6960608
C	-4.6748474	-4.4485600	3.4780696
C	-3.9480349	-5.1238664	2.3022537
N	-2.5613941	-4.6485987	2.1031018
C	-2.2337186	-3.6678511	1.2527690

C	-3.3319065	-3.0293582	0.3953867
O	-2.7121016	-1.9912656	-0.3545077
C	-3.5595573	-1.2993740	-1.2702450
C	-2.6591828	-0.2913963	-1.9968351
N	-3.2066578	0.6373352	-2.7852985
C	-4.6629129	0.7490049	-3.0139172
C	-5.3618856	1.7527979	-2.0802763
C	-6.8637604	1.8887549	-2.3882730
C	-1.5119725	-5.2827859	2.9295006
C	-0.9468769	-6.5702442	2.3069912
C	0.0823038	-7.2579390	3.2210207
O	-1.0450168	-3.2525843	1.1175040
O	-0.0801154	-2.9380942	-1.4731190
C	0.9464225	-3.6265584	-1.7245158
N	1.0305171	-4.4411916	-2.7882255
C	2.2136567	-5.2767206	-3.0825829
C	2.1165543	-6.7141020	-2.5442708
C	3.3290299	-7.5727526	-2.9458019
O	-1.4088172	-0.3841630	-1.8214372
O	1.7663082	-2.7435823	0.3343293
C	2.8597817	-2.3439095	1.1529132
C	2.3252688	-1.2672178	2.0956148
N	3.0525824	-0.8272348	3.1195226
C	4.4006337	-1.3469597	3.4375390
C	4.4030307	-2.4436373	4.5158372
C	5.8285796	-2.8883141	4.8906447
C	2.1583403	-3.5182972	-0.7947723
O	1.1710032	-0.7950341	1.8371803
C	-2.3372751	1.6491620	-3.4297196
C	-1.8829284	1.2615154	-4.8454154
C	-1.0205349	2.3608350	-5.4907596
C	2.5213437	0.2589988	3.9804495
C	2.9062487	1.6622282	3.4822427
C	2.4004534	2.7663972	4.4280464
C	-0.0886882	-4.5108782	-3.7508460
C	0.0932729	-3.5700640	-4.9535236
C	-1.0260860	-3.7285230	-5.9967453
H	-4.7324838	-3.3485938	3.3023640
H	2.0192678	-6.6919700	-1.4325380
H	-3.7763420	-3.7835244	-0.2984439
H	-4.1493671	-2.6191068	1.0335068
H	-3.8876775	-6.2211473	2.4690100
H	-4.5206556	-4.9969024	1.3597366
H	-6.0136424	-6.1216981	3.8598017
H	-6.6866962	-4.8904946	2.7647636
H	-1.9656944	-5.4968962	3.9208128
H	-0.7093242	-4.5341293	3.0833273
H	-0.4806040	-6.3232022	1.3249424
H	-0.3959387	-7.4935532	4.2003305
H	0.9069301	-6.5423052	3.4508739
H	-4.3862186	-0.7898431	-0.7245787

H	-4.0072593	-2.0225157	-1.9950175
H	-5.1262768	-0.2574760	-2.9317030
H	-4.7965931	1.0530803	-4.0747347
H	-4.8694917	2.7473816	-2.1753449
H	-6.9920630	2.2037890	-3.4501422
H	-7.3518715	0.8886719	-2.3059314
H	-1.4639294	1.8076718	-2.7657913
H	-2.9166669	2.5965678	-3.4526912
H	-1.3065049	0.3091107	-4.7941720
H	-0.1331071	2.5562481	-4.8442505
H	-1.5984675	3.3140876	-5.5129590
H	3.6803135	-1.9142680	0.5256946
H	3.2697001	-3.2189465	1.7088091
H	5.0011918	-0.4747894	3.7750041
H	4.8853387	-1.7054928	2.5049905
H	3.8786105	-2.0675637	5.4242155
H	6.4036573	-2.0033538	5.2500195
H	6.3580001	-3.2469508	3.9763383
H	2.9213017	0.0784645	5.0009416
H	1.4195341	0.1463124	4.0230929
H	2.4828275	1.8141909	2.4627364
H	2.8171632	2.5962480	5.4485754
H	1.2933275	2.6829304	4.5299931
H	2.5099389	-4.5218791	-0.4622818
H	2.9934946	-3.0097439	-1.3336212
H	3.1278232	-4.7734666	-2.7029286
H	2.3240159	-5.2922440	-4.1879965
H	3.4157757	-7.5831079	-4.0571828
H	4.2634284	-7.0914046	-2.5718315
H	-1.0195530	-4.2672898	-3.2006732
H	-0.1619587	-5.5672099	-4.0891387
H	0.1303041	-2.5186044	-4.5868248
H	-2.0116436	-3.5221387	-5.5152991
H	-1.0685645	-4.7909362	-6.3326902
N	1.4210280	0.6292831	-1.2219849
O	1.4630223	-0.6571625	-1.3861859
O	2.1433998	1.3970654	-1.8038232
O	0.5233228	1.0006167	-0.3662635
H	3.8134876	-3.3204672	4.1567441
H	-5.2165177	1.4424427	-1.0186152
H	-2.7742032	1.0630347	-5.4864370
H	-4.0729653	-4.5786879	4.4064379
H	-1.7792426	-7.2799848	2.0917760
H	1.1822929	-7.1868338	-2.9263273
H	4.0146677	1.7348629	3.3855431
H	1.0767350	-3.7706694	-5.4394813
C	-6.8200813	-4.3734668	4.8773968
H	-7.8347100	-4.8089496	5.0006847
H	-6.2703957	-4.5296545	5.8320676
H	-6.9407243	-3.2766161	4.7326615
C	0.6639103	-8.5421922	2.6160597

H	1.1839783	-8.3421601	1.6516474
H	1.4004366	-9.0105999	3.3037597
H	-0.1314667	-9.2944962	2.4180902
C	-7.5745461	2.8873603	-1.4658110
H	-7.1376739	3.9065238	-1.5570673
H	-8.6537040	2.9621411	-1.7187171
H	-7.4995979	2.5824083	-0.3980630
C	-0.5589933	2.0099037	-6.9106462
H	0.0602606	2.8259895	-7.3409211
H	0.0557440	1.0818666	-6.9222907
H	-1.4237510	1.8518909	-7.5931874
C	-0.8430453	-2.8149726	-7.2154045
H	-0.8248790	-1.7410816	-6.9224077
H	0.1100775	-3.0333371	-7.7465951
H	-1.6693573	-2.9513211	-7.9455978
C	3.2459851	-9.0126723	-2.4242505
H	2.3442389	-9.5351165	-2.8145702
H	4.1342561	-9.6011926	-2.7387122
H	3.2009114	-9.0437357	-1.3122652
N	-2.3064921	0.1995992	1.8283284
O	-3.1109371	0.7616208	2.5264429
O	-1.7254566	-0.9122342	2.1658135
O	-1.9456930	0.6263737	0.6612549
Pu	-0.3634999	-1.1746821	0.1549170
C	5.8499047	-3.9847007	5.9631236
H	6.8928309	-4.2748406	6.2123680
H	5.3646596	-3.6425657	6.9041820
H	5.3198371	-4.9020893	5.6214381
C	2.7700925	4.1766884	3.9503088
H	2.3355332	4.3959566	2.9494808
H	2.3906524	4.9457329	4.6567115
H	3.8729162	4.3056637	3.8763492

Pu(IV)-*iso*-Butyl DGA

C	-6.2345121	-4.7812737	3.5252656
C	-4.8027176	-4.2202450	3.4450856
C	-3.9973551	-5.0763406	2.4353506
N	-2.6007407	-4.6442300	2.1936031
C	-2.2813397	-3.7001536	1.2984214
C	-3.3811354	-3.0996625	0.4179546
O	-2.7691029	-2.0772908	-0.3597371
C	-3.6348965	-1.4013121	-1.2725389
C	-2.7581085	-0.3717024	-1.9962017
N	-3.3106298	0.5532805	-2.7870763
C	-4.7641946	0.6567170	-3.0430948
C	-5.4850337	1.8069311	-2.2981024
C	-6.9263229	1.9102607	-2.8293701
C	-1.5166252	-5.2509125	3.0002141
C	-0.7501791	-6.3937044	2.2948847

C	0.3895967	-6.8641085	3.2164930
O	-1.0914317	-3.2967786	1.1333716
O	-0.1303896	-2.9892197	-1.4741497
C	0.9111693	-3.6535129	-1.7311070
N	1.0100915	-4.4547706	-2.8051850
C	2.2124981	-5.2716446	-3.0852764
C	2.2552260	-6.6680356	-2.4176950
C	3.5995939	-7.3356334	-2.7603854
O	-1.5057791	-0.4401881	-1.8158603
O	1.7127412	-2.7599120	0.3293763
C	2.7968315	-2.3487121	1.1548906
C	2.2468041	-1.2840837	2.1019002
N	2.9625871	-0.8547063	3.1413002
C	4.2827111	-1.4320093	3.4865200
C	4.2545001	-2.7064837	4.3682328
C	5.7047491	-3.1802116	4.5784835
C	2.1224860	-3.5175644	-0.8053410
O	1.1009420	-0.8065020	1.8170108
C	-2.4236991	1.5700718	-3.4062697
C	-1.6748609	1.1121338	-4.6787792
C	-0.7201129	2.2399195	-5.1113991
C	2.4677827	0.2802558	3.9603919
C	3.1592582	1.6320045	3.6581205
C	2.5844570	2.6913671	4.6167286
C	-0.1133440	-4.4928031	-3.7686136
C	-0.1345518	-3.3220617	-4.7791637
C	-1.3817042	-3.4651218	-5.6695710
H	-4.8631831	-3.1804307	3.0428480
H	2.2180255	-6.5183793	-1.3114272
H	-3.8112824	-3.8825496	-0.2534099
H	-4.2090573	-2.6795778	1.0342466
H	-3.9461084	-6.1243297	2.7970939
H	-4.5326700	-5.1183574	1.4624225
H	-6.2382046	-5.8167161	3.9345356
H	-6.7327408	-4.8069551	2.5303515
H	-1.9807804	-5.6255771	3.9349298
H	-0.8122006	-4.4383394	3.2728539
H	-0.2961033	-5.9611474	1.3730957
H	-0.0083658	-7.2946027	4.1630997
H	1.0762302	-6.0307903	3.4872506
H	-4.4675680	-0.9112546	-0.7211674
H	-4.0678270	-2.1323171	-1.9982722
H	-5.2474207	-0.3155768	-2.8060076
H	-4.8820471	0.7980120	-4.1383303
H	-4.9593471	2.7545085	-2.5604082
H	-6.9526693	2.0841009	-3.9277304
H	-7.5059021	0.9831679	-2.6155585
H	-1.6922789	1.8798938	-2.6316502
H	-3.0625105	2.4477197	-3.6382185
H	-1.0571346	0.2285904	-4.3961581
H	0.0026169	2.4993532	-4.3069102

H	-1.2805716	3.1643414	-5.3799088
H	3.6101115	-1.8949718	0.5344069
H	3.2230243	-3.2216799	1.6989041
H	4.8439101	-0.6312373	4.0118041
H	4.8447698	-1.6292482	2.5478285
H	6.2935779	-2.4286253	5.1508444
H	6.2308649	-3.3615655	3.6146988
H	2.6310723	0.0043242	5.0226680
H	1.3757297	0.3584065	3.7888278
H	2.7080047	2.3977399	5.6826927
H	1.4997339	2.8589800	4.4296178
H	2.5061410	-4.5107650	-0.4796666
H	2.9392783	-2.9817805	-1.3464329
H	3.1171500	-4.6896680	-2.8052997
H	2.2647095	-5.3900107	-4.1870391
H	3.6904921	-7.5169503	-3.8551032
H	4.4681942	-6.7143326	-2.4472312
H	-1.0562288	-4.4979294	-3.1832572
H	-0.0450989	-5.4605293	-4.3069730
H	-0.2329197	-2.3824196	-4.1878480
H	-2.3192221	-3.5050163	-5.0704060
H	-1.3358440	-4.3914007	-6.2861419
N	1.3088121	0.6044607	-1.2498633
O	1.3740906	-0.6821611	-1.4044243
O	2.0117430	1.3809327	-1.8450735
O	0.4124775	0.9658341	-0.3900921
H	3.7126268	-3.5027384	3.8019451
H	4.2447090	1.5221173	3.8924853
N	-2.3830860	0.1465851	1.8341032
O	-3.1844431	0.7081696	2.5364783
O	-1.7990040	-0.9643143	2.1676960
O	-2.0280296	0.5741763	0.6655201
Pu	-0.4370764	-1.2220077	0.1489199
H	-7.4596309	2.7552055	-2.3438928
H	-0.1343084	1.9363835	-6.0058287
H	-1.4655000	-2.6062075	-6.3701161
H	3.6891815	-8.3198174	-2.2526925
H	5.7250713	-4.1282807	5.1570671
H	0.9939797	-7.6562169	2.7234615
H	-6.8601992	-4.1562707	4.1975613
H	3.1033095	3.6636714	4.4760646
C	3.5266245	-2.5098174	5.7082608
H	4.0082866	-1.7131483	6.3192426
H	2.4529959	-2.2498697	5.5774123
H	3.5653581	-3.4468090	6.3045811
C	3.0271867	2.0600501	2.1888294
H	3.4940614	1.3269621	1.4921601
H	1.9629091	2.1900983	1.8921532
H	3.5428549	3.0304393	2.0225600
C	1.0671472	-7.5630006	-2.8074173
H	0.0903259	-7.1255785	-2.5050146

H	1.0417318	-7.7477924	-3.9054479
H	1.1521993	-8.5541220	-2.3116188
C	1.1463689	-3.2284331	-5.6245820
H	1.3058140	-4.1494042	-6.2311827
H	1.0804016	-2.3769956	-6.3364411
H	2.0524837	-3.0572626	-5.0022066
C	-2.6177323	0.7016731	-5.8217349
H	-3.2799486	1.5440291	-6.1257263
H	-2.0333736	0.4066492	-6.7206558
H	-3.2601145	-0.1666110	-5.5530330
C	-5.4529548	1.6573708	-0.7691558
H	-6.0414266	0.7688126	-0.4388453
H	-4.4189580	1.5762679	-0.3648070
H	-5.9166779	2.5433601	-0.2840645
C	-4.1496020	-4.1391928	4.8346961
H	-4.0479108	-5.1480603	5.2964059
H	-3.1467129	-3.6598272	4.8034299
H	-4.7795760	-3.5292449	5.5175137
C	-1.6559206	-7.5666654	1.8842694
H	-1.0615119	-8.3644769	1.3880201
H	-2.1484083	-8.0295576	2.7694867
H	-2.4493907	-7.2592291	1.1674528

Pu(IV)-*n*-Amyl DGA

C	-6.0693575	-5.0977067	3.7362411
C	-4.6727018	-4.4978337	3.5010933
C	-3.9428252	-5.1690361	2.3249064
N	-2.5589536	-4.6858969	2.1245361
C	-2.2372487	-3.7031485	1.2744864
C	-3.3392567	-3.0705016	0.4176585
O	-2.7258985	-2.0279740	-0.3313283
C	-3.5745712	-1.3479862	-1.2546244
C	-2.6803643	-0.3330240	-1.9791043
N	-3.2329895	0.5895809	-2.7711716
C	-4.6882990	0.6802557	-3.0147918
C	-5.4136132	1.6755154	-2.0922942
C	-6.9129739	1.7829478	-2.4188908
C	-1.5059337	-5.3158528	2.9499543
C	-0.9431112	-6.6060982	2.3310321
C	0.0780034	-7.2972129	3.2500461
O	-1.0508869	-3.2813579	1.1384952
O	-0.0982861	-2.9612032	-1.4566565
C	0.9286407	-3.6475149	-1.7123840
N	1.0114731	-4.4600450	-2.7778145
C	2.1953227	-5.2938086	-3.0747378
C	2.1037486	-6.7311918	-2.5354134
C	3.3215258	-7.5815786	-2.9350027
O	-1.4301039	-0.4131812	-1.7975822
O	1.7535917	-2.7662245	0.3455365

C	2.8498287	-2.3610582	1.1576218
C	2.3142680	-1.2909739	2.1071600
N	3.0436335	-0.8524714	3.1301124
C	4.3967846	-1.3650047	3.4381300
C	4.4121880	-2.4694698	4.5082528
C	5.8423260	-2.9013058	4.8762051
C	2.1431523	-3.5383238	-0.7861836
O	1.1566713	-0.8229434	1.8557637
C	-2.3709249	1.6127892	-3.4073853
C	-1.9106020	1.2409924	-4.8253212
C	-1.0480887	2.3496552	-5.4521273
C	2.5094499	0.2247226	4.0005577
C	2.8814158	1.6339695	3.5096493
C	2.3768670	2.7257988	4.4687959
C	-0.1089379	-4.5289413	-3.7393054
C	0.0791278	-3.5978952	-4.9487395
C	-1.0434968	-3.7517655	-5.9878592
H	-4.7534826	-3.4009310	3.3162549
H	2.0044390	-6.7085687	-1.4240619
H	-3.7787892	-3.8270006	-0.2767546
H	-4.1593194	-2.6658946	1.0560214
H	-3.8752210	-6.2656742	2.4927509
H	-4.5168708	-5.0466721	1.3827052
H	-5.9720519	-6.1942199	3.9198631
H	-6.6805939	-4.9974094	2.8075120
H	-1.9564929	-5.5260445	3.9435433
H	-0.7035159	-4.5659066	3.0980795
H	-0.4725462	-6.3619128	1.3505258
H	-0.4042418	-7.5287447	4.2294513
H	0.9096395	-6.5889222	3.4818462
H	-4.4097388	-0.8447923	-0.7159858
H	-4.0104345	-2.0782746	-1.9794949
H	-5.1377504	-0.3327253	-2.9351012
H	-4.8149700	0.9796824	-4.0777431
H	-4.9370043	2.6777459	-2.1861125
H	-7.0366226	2.0910511	-3.4842874
H	-7.3874639	0.7752227	-2.3362406
H	-1.5001824	1.7731879	-2.7406384
H	-2.9580054	2.5556155	-3.4239838
H	-1.3333936	0.2888546	-4.7829055
H	-0.1541456	2.5290391	-4.8084982
H	-1.6211282	3.3071703	-5.4530308
H	3.6628701	-1.9238403	0.5258858
H	3.2696998	-3.2346394	1.7083122
H	4.9923575	-0.4909069	3.7792971
H	4.8796674	-1.7129442	2.5006363
H	3.8854163	-2.1050065	5.4199020
H	6.4083559	-2.0154557	5.2501288
H	6.3786774	-3.2419136	3.9578295
H	2.9165058	0.0404511	5.0175304
H	1.4087697	0.1037144	4.0485900

H	2.4482098	1.7904222	2.4951188
H	2.8074645	2.5551094	5.4844732
H	1.2708180	2.6339788	4.5844666
H	2.4978115	-4.5417216	-0.4564961
H	2.9754183	-3.0272450	-1.3270952
H	3.1094241	-4.7882792	-2.6979777
H	2.3028029	-5.3098221	-4.1803115
H	3.4122215	-7.5928296	-4.0469468
H	4.2542326	-7.0964328	-2.5587100
H	-1.0372818	-4.2747805	-3.1898180
H	-0.1899342	-5.5871435	-4.0700128
H	0.1281050	-2.5447008	-4.5890338
H	-2.0271652	-3.5219077	-5.5108424
H	-1.1050299	-4.8177452	-6.3126749
N	1.3969545	0.6083698	-1.2039638
O	1.4445700	-0.6780894	-1.3661997
O	2.1142887	1.3783655	-1.7893984
O	0.5000749	0.9771682	-0.3465579
H	3.8306953	-3.3490775	4.1433760
H	-5.2747816	1.3712140	-1.0281957
H	-2.7991498	1.0491275	-5.4718027
H	-4.0598707	-4.6080638	4.4246595
H	-1.7779780	-7.3119602	2.1133793
H	1.1724309	-7.2082058	-2.9189040
H	3.9883807	1.7136704	3.4039781
H	1.0592132	-3.8119996	-5.4354026
C	-6.8198534	-4.4504944	4.9126426
H	-6.2025543	-4.5481485	5.8360173
H	-6.9185989	-3.3550539	4.7262588
C	0.6591778	-8.5916395	2.6558687
H	1.1421849	-8.3614976	1.6758778
H	-0.1760558	-9.2930858	2.4243309
C	-7.6629207	2.7743979	-1.5124378
H	-7.1859673	3.7786468	-1.5983967
H	-7.5350126	2.4665729	-0.4478028
C	-0.5905662	2.0343571	-6.8861368
H	-0.0249967	1.0723156	-6.8867400
H	-1.4878109	1.8621766	-7.5261803
C	-0.8529869	-2.8573620	-7.2248114
H	-0.7770214	-1.7926377	-6.8992737
H	0.1263285	-3.0991484	-7.7005387
C	3.2554194	-9.0282408	-2.4169470
H	2.3241576	-9.5094121	-2.7981839
H	3.1599628	-9.0153684	-1.3050819
N	-2.3213350	0.1686991	1.8539369
O	-3.1207361	0.7322547	2.5566123
O	-1.7402449	-0.9441020	2.1883635
O	-1.9657968	0.5951528	0.6851936
Pu	-0.3802020	-1.2016549	0.1759223
C	-9.1567825	2.8830200	-1.8429273
H	-9.6638814	3.6083711	-1.1708215

H	-9.3179637	3.2279063	-2.8887924
H	-9.6727874	1.9031989	-1.7290050
C	0.2745511	3.1413646	-7.5013791
H	0.5845650	2.8814539	-8.5365887
H	-0.2766044	4.1070853	-7.5502245
H	1.1999136	3.3131450	-6.9067666
C	-1.9747967	-3.0027781	-8.2600978
H	-1.7976584	-2.3476205	-9.1402276
H	-2.0503400	-4.0485459	-8.6333710
H	-2.9653030	-2.7280332	-7.8316387
C	4.4722342	-9.8704820	-2.8200381
H	4.3891638	-10.9079546	-2.4306617
H	4.5721307	-9.9363618	-3.9263944
H	5.4176025	-9.4377293	-2.4224568
C	5.8863299	-4.0166259	5.9349072
H	5.3438716	-3.6743843	6.8474009
H	5.3223294	-4.9024056	5.5568970
C	2.7240003	4.1503739	4.0025561
H	3.8295180	4.2365864	3.8834645
H	2.2927454	4.3184276	2.9876790
C	7.3130105	-4.4356917	6.3110729
H	7.8890680	-3.5827102	6.7341809
H	7.3044250	-5.2433793	7.0743836
H	7.8737294	-4.8155403	5.4275346
C	1.6685573	-9.2844093	3.5798761
H	2.0627105	-10.2159633	3.1196009
H	2.5383105	-8.6257109	3.8029465
H	1.2036579	-9.5649091	4.5513206
C	-8.2060379	-5.0609540	5.1528198
H	-8.1376794	-6.1478492	5.3826688
H	-8.7164102	-4.5703137	6.0092435
H	-8.8624712	-4.9463247	4.2612504
C	2.2235058	5.2368865	4.9626145
H	2.6686724	5.1213441	5.9762503
H	2.4914072	6.2506933	4.5945383
H	1.1166863	5.2023682	5.0753958

Pu(IV)-iso-Amyl DGA

C	-6.1382121	-5.0045040	3.6077255
C	-4.6892783	-4.5003831	3.4007000
C	-3.9403976	-5.1979353	2.2512736
N	-2.5578288	-4.7046445	2.0671272
C	-2.2328826	-3.7276327	1.2122262
C	-3.3288386	-3.1163742	0.3325254
O	-2.7209405	-2.0629639	-0.4053195
C	-3.5685806	-1.3905566	-1.3355767
C	-2.6817845	-0.3522403	-2.0353994
N	-3.2409107	0.5879273	-2.8008094
C	-4.6969810	0.6738236	-3.0432476

C	-5.4210604	1.6304209	-2.0788488
C	-6.9501282	1.7148280	-2.3044803
C	-1.5142637	-5.3122109	2.9207987
C	-0.9209764	-6.5960206	2.3157327
C	0.1409979	-7.2807666	3.2098375
O	-1.0488187	-3.2947091	1.0897651
O	-0.0742341	-2.9872947	-1.4898788
C	0.9622123	-3.6651657	-1.7301070
N	1.0541119	-4.5062274	-2.7720377
C	2.2548022	-5.3197736	-3.0586116
C	2.1924282	-6.7418669	-2.4756935
C	3.4486972	-7.6000135	-2.7631755
O	-1.4303020	-0.4311278	-1.8573285
O	1.7683485	-2.7470900	0.3175684
C	2.8522885	-2.3180778	1.1337445
C	2.2883623	-1.2590035	2.0786763
N	2.9988268	-0.8048469	3.1077798
C	4.3564358	-1.2939145	3.4330572
C	4.3639528	-2.3993196	4.5029815
C	5.7789889	-2.9097044	4.8703298
C	2.1773759	-3.5147486	-0.8103387
O	1.1243304	-0.8134145	1.8153266
C	-2.3901189	1.6404113	-3.4036942
C	-1.9145740	1.3016511	-4.8253848
C	-1.0149452	2.3936836	-5.4531579
C	2.4347895	0.2648780	3.9687793
C	2.7992897	1.6749290	3.4723237
C	2.3461130	2.8060585	4.4271648
C	-0.0759055	-4.6387465	-3.7153036
C	0.0705269	-3.7371006	-4.9531382
C	-1.0705894	-3.8956965	-5.9862171
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H	-3.7397875	-3.8820954	-0.3693908
H	-4.1692520	-2.7262280	0.9529967
H	-3.8610623	-6.2893059	2.4370179
H	-4.4994604	-5.0950423	1.2975535
H	-6.6788397	-4.8828645	2.6372758
H	-1.9877524	-5.5147995	3.9037203
H	-0.7243812	-4.5506802	3.0774466
H	-0.4650480	-6.3393384	1.3316530
H	0.9212620	-6.5169143	3.4475903
H	-4.4213448	-0.9099064	-0.8043210
H	-3.9785348	-2.1215508	-2.0747859
H	-5.1380280	-0.3449618	-2.9951664
H	-4.8196280	1.0049528	-4.0956657
H	-4.9802050	2.6501751	-2.1723704
H	-7.3599254	0.6768070	-2.2333231
H	-1.5254377	1.7957150	-2.7276395
H	-2.9956241	2.5697430	-3.3958049
H	-1.3505488	0.3418319	-4.7870812

H	-0.1537494	2.5537988	-4.7603169
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H	3.2884745	-3.1820266	1.6868453
H	4.9300292	-0.4075411	3.7757221
H	4.8548510	-1.6397647	2.5026941
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H	6.2713088	-3.2481223	3.9257303
H	2.8336826	0.0917672	4.9911280
H	1.3378085	0.1198527	4.0003971
H	2.3465560	1.8339326	2.4656193
H	2.8013395	2.6023355	5.4269658
H	2.5617454	-4.5048935	-0.4743456
H	2.9923686	-2.9831988	-1.3579092
H	3.1595919	-4.7852024	-2.6994391
H	2.3504398	-5.3548246	-4.1633753
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H	-1.0039320	-4.3912406	-3.1619884
H	-0.1262261	-5.7097540	-4.0027945
H	0.1147449	-2.6785262	-4.6096939
H	-2.0355167	-3.7160111	-5.4508556
N	1.3781708	0.6083040	-1.2540696
O	1.4347112	-0.6777067	-1.4155172
O	2.0894218	1.3830371	-1.8410451
O	0.4801854	0.9718086	-0.3956496
H	3.7489084	-3.2555220	4.1381934
H	-5.2206359	1.3084959	-1.0300701
H	-4.1172052	-4.6356061	4.3479670
H	-1.7388545	-7.3251920	2.1061973
H	1.2932249	-7.2652117	-2.8780649
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H	1.0426803	-3.9484650	-5.4586639
C	-6.8503784	-4.1280875	4.6537336
H	-7.9089452	-4.4427382	4.7795980
H	-6.3563164	-4.2100274	5.6485267
H	-6.8497892	-3.0541802	4.3623358
C	0.8227955	-8.4243355	2.4368469
H	1.2915269	-8.0634896	1.4932045
H	1.6184095	-8.9022709	3.0490140
H	0.0893389	-9.2177868	2.1673690
C	-7.5959888	2.5508001	-1.1850479
H	-7.2269751	3.6012724	-1.2066578
H	-8.7009968	2.5826311	-1.3007065
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C	-0.4499576	1.9009612	-6.7975498
H	0.2397132	2.6533659	-7.2382782
H	0.1188638	0.9509746	-6.6824095
H	-1.2655424	1.7230646	-7.5352223
C	-0.9363889	-2.8255847	-7.0840481
H	-0.9363780	-1.7969468	-6.6591959
H	0.0107448	-2.9553211	-7.6550716
H	-1.7744769	-2.8925574	-7.8117500

C	3.3481684	-8.9407466	-2.0134417
H	2.4873942	-9.5430586	-2.3840807
H	4.2672101	-9.5480171	-2.1601042
H	3.2131178	-8.7924165	-0.9184763
N	-2.3610405	0.1401251	1.7830903
O	-3.1761749	0.6957659	2.4743765
O	-1.7753622	-0.9673601	2.1241806
O	-1.9925769	0.5719174	0.6200198
Pu	-0.3896798	-1.2134294	0.1237249
C	5.6654976	-4.1300790	5.8017548
H	6.6702555	-4.5410974	6.0400865
H	5.1804597	-3.8546503	6.7658743
H	5.0676941	-4.9482050	5.3406441
C	2.8926648	4.1576315	3.9327244
H	2.4745621	4.4197609	2.9341567
H	2.6199445	4.9748291	4.6351730
H	4.0017077	4.1456413	3.8453659
C	-0.4404871	-7.7939347	4.5404080
H	-1.2469180	-8.5411472	4.3615372
H	0.3460974	-8.2958415	5.1448646
H	-0.8609858	-6.9802347	5.1723452
C	-6.2002356	-6.4915463	4.0024486
H	-5.7853265	-7.1676591	3.2214242
H	-5.6438841	-6.6776798	4.9498026
H	-7.2526830	-6.8070780	4.1709599
C	-7.3157054	2.2752910	-3.6912633
H	-6.8988831	3.2990419	-3.8320162
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H	-8.4190082	2.3497944	-3.8038906
C	-1.1265929	-5.3056194	-6.6035526
H	-0.1729511	-5.5511127	-7.1250372
H	-1.3204138	-6.1023597	-5.8513002
H	-1.9403726	-5.3724293	-7.3583195
C	3.6826634	-7.8286697	-4.2677620
H	2.8088747	-8.3365613	-4.7366557
H	3.8719191	-6.8847144	-4.8257983
H	4.5690328	-8.4792789	-4.4300403
H	-2.7967771	1.1310357	-5.4879976
C	-1.7430572	3.7393995	-5.6270710
H	-1.0752372	4.4858366	-6.1094735
H	-2.6411803	3.6296944	-6.2778812
H	-2.0714842	4.1822166	-4.6605372
C	0.8173919	2.8589143	4.6027725
H	0.3074647	3.0234042	3.6253426
H	0.4019704	1.9309793	5.0556687
H	0.5303181	3.6987422	5.2722070
C	6.6597390	-1.8158001	5.5017229
H	6.8469414	-0.9588407	4.8168730
H	6.1980730	-1.4182346	6.4344500
H	7.6551242	-2.2271163	5.7763082