Electronic Supplementary Material (ESI) for RSC Advances

Sparkle/RM1 Parameters for the Semiempirical Quantum Chemical Calculation of Lanthanide Complexes

Supplementary Information

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1. How to run lanthanide complexes Sparkle calculations with MOPAC2012

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MOPAC2012 is the new software released by Prof. James J. P. Stewart from *Stewart Computational Chemistry* of Colorado Springs, CO, and represents the most recent version of the MOPAC series of molecular modeling softwares, which started in 1981.

MOPAC2012 has Sparkle/AM1, Sparkle/PM3, Sparkle/PM6, and Sparkle/RM1 fully implemented. Instructions on how to use the Sparkle Model in MOPAC2012, and on how to visualize the complexes with graphical user interfaces, can be found at http://www.sparkle.pro.br.

A MOPAC2012 executable can be obtained from http://openmopac.net and is presently free for academics.

In order to be acquainted with the software, users are encouraged to read the MOPAC2012 manual at http://openmopac.net/manual/.

As the MOPAC2012 manual says:

MOPAC is written with the non-theoretician in mind.

While MOPAC calls upon many concepts in quantum theory and thermodynamics and uses some fairly advanced mathematics, the users need not be familiar with these specialized topics.

At present, the most recent version of MOPAC2012 is 12.301W.

To run a Sparkle calculation in MOPAC 2012, proceed as follows:

i. Create a data-file with extension .mop which describes a molecular system and specifies the type of calculation that is to be carried out.

a. Use the lanthanide sparkles as you would use any atom in MOPAC.

b. Do not forget to set the charge n of the complex with keyword CHARGE=n such as CHARGE=+3

c. For a Sparkle/AM1 calculation, use the keywords AM1 SPARKLE in the keyword line.

d. For a Sparkle/PM3 calculation, use the keywords PM3 SPARKLE.

e. For a Sparkle/PM6 calculation, use the keywords PM6 SPARKLE.

f. For a **Sparkle/RM1** calculation, use the keywords RM1 SPARKLE

ii. Command MOPAC to run the calculation using that data-file.

iii. Get the desired output on the system from the output files created by MOPAC.

Attention: sparkles are overall neutral species

Please notice that when one uses a lanthanide as an element symbol in MOPAC2012, and the keyword SPARKLE, one is actually introducing an overall neutral species in the calculation, that is: a +3 charged sparkle plus three electrons which will be donated to the molecular orbitals of the organic part of the complex. If the whole complex is charged, then this must be indicated with the appropriate CHARGE keyword.

2. MOPAC2012 Input (.mop) and output (.arc) files

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Sample input and output files for all Sparkle Models can be found in http://www.sparkle.pro.br.

As examples, we are providing in the appendix of this supplementary material the content of a MOPAC2012 input and the corresponding Sparkle/RM1 output file for one complex for each lanthanide ion.

In order to reproduce the calculation, please request a password and download MOPAC2012.exe from http://openmopac.net, which is presently free for academics. Then, copy the contents of one of the sample inputs to a text file, name it something like sample.mop, and simply open it with MOPAC2012.

Warning: MOPAC2012 output files with extension .arc may be confused with some types of compressed files in some Windows systems. Be sure to open them with notepad, or a similar text editor.

3. Graphical User Interfaces for MOPAC2012

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A large number of graphical user interfaces, GUIs, that can be used with MOPAC2012, both commercial and free, can be found here.

Warning: the bond connection algorithm of some of the Graphical User Interfaces may not work efficiently with some high coordination number lanthanide complexes. Some coordinating bonds may not appear, while sometimes some other spurious bond connections may also appear. However, the positions of the atoms are always correct.

4. Additional Tables and Figures

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Table S1: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 65 lanthanum (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	UME (Å)		$UME_{(Ln-L)}$s (Å)	UME (Å)
ABXALA	0.0614	0.4227	POHDUL	0.0788	0.2504
ALANIC	0.0695	0.1970	PUHYAS	0.0861	0.2334
APBNLA	0.0577	0.1542	PUWZIQ	0.0702	0.1176
BEQPOC	0.0721	0.2441	PUZHOH	0.0420	0.1221
BIZTIN	0.0640	0.2010	QAKWEE	0.0856	0.2138
BUVVIX01	0.0756	0.1270	QAPXAG	0.0734	0.1719
CABLAS01	0.0533	0.1430	QUBWIT	0.0304	0.0982
CEFQOT	0.0575	0.1270	SIXBIK	0.0612	0.1193
DUBWEC	0.0747	0.1538	SUXLIG	0.0517	0.0847
DUCBOS	0.0485	0.2356	SUZXIU	0.0585	0.1166
EBEGOH	0.0653	0.1218	TEQBIA	0.0551	0.2839
EPAILA	0.0734	0.0988	TEQBOG	0.0703	0.2329
FICJEG	0.0550	0.2160	TUPWEG	0.0101	0.0887
FIVCIW	0.0420	0.1194	WAVNAI	0.0579	0.1486
GIMMIY	0.0577	0.2556	WEHTAE	0.0515	0.2331
GOJQAX	0.1363	0.2535	XALSOS	0.0519	0.1114
GOZBEC	0.0923	0.5602	XAWVUM	0.0912	0.1460
GULFOI	0.0863	0.4283	XECQEB	0.0963	0.1303
HELHOV	0.0619	0.1116	XEMNUY	0.0542	0.3330
HELMIU	0.0621	0.2106	XERCAY	0.0870	0.1180
HETALA11	0.0540	0.1369	XONXUT	0.0376	0.0595
KIXHAA	0.0598	0.1467	YUCXAV	0.0572	0.2448
LANITA	0.0593	0.1409	ZAMHEA	0.0432	0.3050
LAPTEB10	0.1730	0.2328	ZAZQAS	0.0387	0.0560
LIWQEN	0.0736	0.1150	ZEHTUB	0.0492	0.0725
MENQOL	0.0737	0.1326	ZEJFOJ	0.1196	0.1871
MILWEJ	0.0901	0.1326	ZEQVUM	0.0876	0.1676
NASTOQ	0.0273	0.0697	ZIDSOX	0.2040	0.2746
NEHDAF	0.1101	0.1151	ZIQXIG	0.0851	0.1834
NOHNIH	0.0332	0.1596	ZULFOB	0.0803	0.2009
OFEGIP	0.0614	0.1329	ZUWFOM	0.0430	0.1136
PAFNEP	0.0211	0.1783			
PIBGOW	0.0717	0.2961			

Table S2: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database, [(1)-(3)] for each of the 32 cerium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	**UME (Å)**		**$UME_{(Ln-L)}$s (Å)**	**UME (Å)**
AFURUO	0.0937	0.1676	LIFHUD	0.0436	0.1340
APSBCE	0.0780	0.2146	MIPTAG	0.1409	0.1365
BABZIN	0.0920	0.2764	NOJTAH	0.0962	0.2056
CIBSAH	0.0763	0.1232	NOJTEL	0.2329	0.3692
CUMCIW	0.0658	0.1447	OXDACE	0.0820	0.1599
FILKEQ	0.0354	0.0814	PEKWEH	0.0870	0.1460
FUHFEZ	0.0425	0.2847	PIDBAF	0.0543	0.2209
GACJIE	0.1630	0.1357	PUTQAW	0.0964	0.2804
GAPFIM	0.0794	0.3754	TIJCIY	0.0794	0.1641
GINNUM	0.0714	0.1289	UKAPEB	0.0499	0.1638
HIDLUB	0.0504	0.1064	VAKJAS	0.0594	0.1542
HIXWEQ	0.0774	0.1193	VAPCAQ	0.0538	0.1902
HUMDOI	0.0604	0.1902	XEXCUY	0.0840	0.2109
HURRAN	0.0646	0.1252	XOLMAM	0.0333	0.2480
JAPPUL	0.0398	0.3163	XONYAA	0.0392	0.0600
JEXXOZ	0.0754	0.1820	ZUNMAW	0.0512	0.1493

Table S3: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 45 Praseodymium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	**UME (Å)**		**$UME_{(Ln-L)}$s (Å)**	**UME (Å)**
ACURLB	0.0455	0.1242	LEJSOI	0.0487	0.0891
BABZOT	0.0667	0.2492	MIPTEK	0.0769	0.2121
BAFYOX	0.1687	0.3176	NPYPRP10	0.1088	0.0987
BIFYUK	0.0425	0.3075	PEHHIP	0.1211	0.1724
BUVWIY01	0.0856	0.1934	PEHXIJ	0.0578	0.1287
CAZGUF	0.0573	0.2387	PELGOC	0.0378	0.1731
CUMCOC	0.0724	0.1615	POGWIR	0.0788	0.1901
DIYMUT	0.0891	0.2661	POPJAF	0.1835	0.2488
DORDIX	0.0406	0.2713	QIMRIN	0.0321	0.0712
DUCHAK	0.0540	0.2363	QOBBIS	0.0818	0.2267
ECABAL	0.0196	0.1562	QOVXII	0.0730	0.1563
EFUJEU	0.0228	0.0838	QOZVEG	0.0813	0.2497
FAGYIW	0.0913	0.1865	RASROS	0.0857	0.1861
FATWOM	0.0495	0.1618	RUGQUF	0.0356	0.1847
FEDYAO	0.0988	0.1140	SERWOB01	0.0516	0.2371
GIWWEO	0.0713	0.1095	VELRUZ	0.0580	0.1219
HEDBOH	0.0767	0.1615	XAVWUM	0.1125	0.1437
HEDKAC	0.0477	0.1411	XIZRAZ	0.0436	0.1415
JERWOS	0.0693	0.2213	XOKYIF	0.0773	0.2904
JEXXUF	0.1036	0.2196	YOTYUB	0.1009	0.1722
KAHGEF	0.0282	0.1188	ZAXSEW	0.0803	0.1378
KAWBIT	0.0538	0.0865	ZULRED	0.0704	0.2605
KOBRUO	0.0487	0.0891			

Table S4: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database, [(1)-(3)] for each of the 48 neodymium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	**UME (Å)**		**$UME_{(Ln-L)}$s (Å)**	**UME (Å)**
ANTNND10	0.0933	0.1911	QAJHEO	0.0548	0.1307
BAFYUD	0.0695	0.1374	QAYWOC	0.2207	0.2779
BAWDIM10	0.0444	0.2401	QOZVIK	0.0605	0.2034
BEXQIE	0.0674	0.1866	QOZWAD	0.0415	0.1265
BILSIY	0.1142	0.1545	QQQCGM01	0.0603	0.1447
BUVWOE01	0.0640	0.0768	QUBWOZ	0.0600	0.2907
CAHJAX	0.0576	0.2015	RAMXAE	0.0806	0.2641
CANBOI	0.1039	0.1019	RICNOG	0.0909	0.3493
DODVAT	0.0710	0.2965	RIMQIN	0.1184	0.3727
DUCMAP	0.0805	0.2076	RUGRAM	0.0835	0.2449
FAHFID	0.0628	0.1606	SOKBAV	0.0405	0.1593
FIBXET	0.0801	0.2370	SOTXEE	0.1020	0.2143
FUHQII	0.1079	0.2055	SUCRIR	0.0862	0.2940
GUHJAU	0.0402	0.1797	SUXCAP	0.0475	0.1788
HEBCIA	0.0775	0.3721	TAZYOI	0.0657	0.1400
HERWAC	0.0566	0.1914	TUPYOS	0.0847	0.1672
HOXNND01	0.0769	0.1364	WEFVUY	0.0544	0.0766
JIRHAT	0.0291	0.0602	XIFMAA	0.0745	0.1688
LEJSUO	0.0477	0.1541	XIPKIQ	0.0704	0.2475
LUDQIK	0.0352	0.0740	XONYII	0.0345	0.0488
MINLIE	0.0952	0.1642	YENKOR	0.0426	0.2764
MIPTIO	0.1151	0.1187	YODYEV	0.0409	0.1549
NATPAZ01	0.0547	0.2146	YURMUT	0.0419	0.1459
NIPREJ	0.0822	0.1021	ZAMHIE	0.0424	0.2999

Table S5: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective values, obtained by ab initio calculations for each of the 15 promethium (III) complexes, using as starting point the geometries of the corresponding experimental crystallographic samarium complexes indicated by their respective CSD codes.[4]

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	**UME (Å)**		**$UME_{(Ln-L)}$s (Å)**	**UME (Å)**
BUVWUK01{Pm}	0.0252	0.1655	NOWTUO{Pm}	0.0787	0.1486
CAZHAM{Pm}	0.0880	0.3895	NUQYUT{Pm}	0.0599	0.1086
FINDOV{Pm}	0.0127	0.0579	QALFAK{Pm}	0.0241	0.1577
FUHQOO{Pm}	0.0502	0.1878	QIPQOV{Pm}	0.0069	0.0547
FUJYEO{Pm}	0.0672	0.1782	SOXKAR{Pm}	0.0600	0.2185
GUPHUU{Pm}	0.0391	0.1181	XEXJAL{Pm}	0.1066	0.1423
KUYBAH{Pm}	0.0347	0.1800	XILGOO{Pm}	0.1136	0.1679
LUHFEZ{Pm}	0.0361	0.2131			

Table S6: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 34 samarium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	**UME (Å)**		**$UME_{(Ln-L)}$s (Å)**	**UME (Å)**
ADELAW	0.1207	0.0988	NAFKIO	0.1438	0.1939
BUVWUK01	0.0620	0.1655	NOWTUO	0.0341	0.1985
CAZHAM	0.0345	0.1887	NSMEDT01	0.0346	0.2780
CORKEZ	0.0418	0.2162	QALFAK	0.0576	0.3195
ECABIT	0.0709	0.1496	QIPQOV	0.0738	0.1467
FINDOV	0.0395	0.0643	QOCKIC	0.0266	0.0727
FUHQOO	0.0613	0.1510	QQQEMA01	0.0691	0.1691
FUJYEO	0.0596	0.2309	SOXKAR	0.0724	0.1917
GINPEY	0.0373	0.0892	XAXYAW	0.0767	0.1559
GUPHUU	0.0474	0.1575	XEPLAF	0.0452	0.1929
HAWMUN	0.0518	0.2096	XEXJAL	0.1090	0.0955
JIZVOD	0.1312	0.2146	XILGOO	0.0710	0.1021
KIWROX	0.0996	0.1764	XIVFIR	0.0952	0.2503
KUYBAH	0.0358	0.1687	XOWGAR	0.0740	0.1563
LIXDUR	0.1085	0.1367	YENHOO	0.1153	0.2245
LUHFEZ	0.0603	0.1934	YUBPAM	0.0707	0.1042
MOXJEO	0.1017	0.1370	ZALDUL	0.1686	0.2058

Table S7: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 90 europium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	UME (Å)		$UME_{(Ln-L)}$s (Å)	UME (Å)
ACPNEU	0.0732	0.1970	LOWBEE	0.0950	0.1298
AMEWEU	0.0586	0.1390	LUHFUP	0.0818	0.1288
AZEBAI	0.0429	0.2698	LUHGAW	0.0684	0.1148
AZEBEM	0.0713	0.1649	MASKAS	0.0693	0.2180
BAFZEO	0.0428	0.1226	MEBDUS	0.0945	0.1415
BAPXAR	0.0733	0.1646	MIHNOG	0.0716	0.1918
BEKQOY	0.0777	0.1965	MIHPOI	0.0483	0.1378
BILSEV	0.0785	0.1702	MOYJUF	0.0713	0.1187
BUVXAR11	0.0770	0.1878	MUHROW	0.0853	0.1463
CEXKUL01	0.0551	0.1339	MUHRUC	0.0650	0.1453
CEYRON	0.0385	0.2295	NOHLOL	0.0646	0.1115
CIRKET	0.0681	0.2767	NOHLUR	0.0505	0.1345
COSSIM03	0.0753	0.3471	PHASEU	0.0329	0.0708
COZLEI10	0.0737	0.3674	PIEUAC01	0.0571	0.1964
DADMAX	0.0578	0.2644	PITCUQ	0.0736	0.3442
DIWNOM	0.0434	0.3483	PUHYEW01	0.0781	0.2016
DOFXIF	0.0728	0.1558	QAKWUU	0.0638	0.1892
DOPCEQ	0.0749	0.2145	QALFEO	0.0406	0.3015
DUCNAQ	0.0576	0.1694	QALFOY	0.0852	0.3374
ECABOZ	0.0195	0.1454	QECGOU	0.1128	0.2419
FALTIW	0.0437	0.1769	QHDOEU	0.0967	0.2036
FETGUG	0.0654	0.2496	QIGJAR	0.2168	0.2383
FEWQAA	0.0440	0.1784	QIQHAZ	0.1508	0.5313
FOCQOD	0.0716	0.2483	QUBWUF	0.0315	0.0944
FOCQUJ	0.0666	0.0983	SOPFUY	0.0404	0.1201
FOCREU	0.0795	0.3030	SUXXIS	0.0514	0.0805
FUXPOD	0.0511	0.2200	TMHPEU10	0.0968	0.1485
GACJOJ	0.0960	0.4687	TOKMUB	0.0658	0.1441
GAPRUK	0.0237	0.0546	VUSGOF	0.0796	0.2015
GEBYAN	0.0441	0.1149	WOMCIK	0.0610	0.0996
GINPIC	0.0548	0.1229	XECLEW	0.0809	0.2760
HANBIH	0.0623	0.2139	XIHQIO	0.1209	0.4147
HUWMUH	0.0315	0.2250	XILGII	0.0719	0.1029
JAXXOV	0.0911	0.1715	XIWTAY	0.0912	0.1726
JUCZIQ	0.0747	0.2217	XIWTUS	0.0828	0.1639
JUDBOZ	0.1181	0.2458	YEZFAK	0.0681	0.2323
JUGBUI	0.0450	0.1230	YICSEI	0.0737	0.1580
KAFDOK	0.0423	0.2590	YODYIZ	0.0765	0.4107
KAKPAN	0.0817	0.4013	YOJDIK	0.0715	0.1825
KELNOE	0.0565	0.2691	YUXREO	0.0826	0.1987
KIFKOZ02	0.0468	0.0889	ZACXAC	0.0532	0.1183

KIHSEZ	0.0549	0.0992	ZAMHOK	0.0477	0.3036
LAPJAN	0.0415	0.0837	ZESSUL	0.0926	0.1754
LEJTAV	0.0741	0.2140	ZEXJUH	0.0855	0.4377
LELRUP	0.1002	0.1905	ZIDCUK	0.0701	0.1980

Table S8: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 60 gadolinium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	**UME (Å)**		**$UME_{(Ln-L)}$s (Å)**	**UME (Å)**
ACAQGD	0.0770	0.1611	NAVWIQ	0.0989	0.1434
ADUPEU	0.1166	0.1004	NIGHEQ	0.0351	0.0985
BIFZEV	0.0362	0.3406	NIGXAC	0.0416	0.1097
BUVVOD	0.0564	0.0954	NIVQEO	0.0548	0.1767
BUVVOD01	0.0533	0.0908	PADEGA10	0.0746	0.1337
CULNIG10	0.0615	0.2656	PEBDOP	0.0458	0.2913
DIYNEE	0.0182	0.1621	PROPGD	0.0574	0.1479
DUFBEL	0.0259	0.1560	PUZHUN	0.1060	0.1503
EHAXEQ	0.0659	0.0830	TUFLUB	0.0646	0.2832
FONMEA	0.0634	0.1869	UDOMIJ	0.0349	0.1313
FUHQUU	0.0529	0.1562	UDOMOP	0.0369	0.0993
FUXPUJ	0.0362	0.1645	VEDSEC	0.0685	0.0978
GAKYAS	0.0227	0.1563	VETDON	0.0225	0.1181
GAWBEL	0.0196	0.0567	VIGBOC	0.0420	0.1133
GEGCIE	0.0308	0.0684	WALQAB	0.0233	0.1401
GIDQUF	0.0293	0.0889	WAVPAK	0.0567	0.2326
GINPOI	0.0369	0.0785	WAXCIH	0.0784	0.1545
GIRKUN	0.1063	0.2096	WEWNOB	0.0399	0.0558
GODMER	0.0996	0.2114	WUCCOM	0.0680	0.1839
HEDMIM	0.0665	0.2025	YEWGEM	0.0809	0.1636
JARBUZ	0.0744	0.3095	YIYLAT	0.0485	0.1285
JOPJIH	0.0538	0.1457	YOVFIY01	0.0230	0.1310
JOPJIH01	0.0232	0.0909	YUWZOF	0.0470	0.1592
LANITB	0.0716	0.3114	ZAXQAQ	0.0394	0.1823
LASZIO	0.0478	0.1640	ZAZQEW	0.0213	0.0877
LASZOU	0.0249	0.1327	ZENGUU	0.0884	0.1225
LEJVEB	0.0327	0.1043	ZIPJIR	0.0228	0.1433
LOKNEE	0.0475	0.1496	ZIZNUR	0.0543	0.1676
LOQKEH	0.0235	0.0928	ZUNCAM	0.1000	0.1042
MIPTOU	0.1034	0.0883	ZZZARA01	0.0487	0.0954

Table S9: Unsigned mean errors, $UME_{(Ln-L)}s$ and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 32 terbium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}s$ (Å)	**UME (Å)**		**$UME_{(Ln-L)}s$ (Å)**	**UME (Å)**
BAFWUB	0.0333	0.1435	LIFJEP	0.0756	0.1386
BAFZOY	0.0873	0.1391	MIWTAN	0.0663	0.1069
BUVXEV01	0.0595	0.1619	NASTUW	0.0787	0.1019
CULSEH	0.0693	0.1334	NIGYUX	0.0445	0.1135
DUCQEX	0.0756	0.1431	PEJZAF	0.0313	0.2235
FAGZAP	0.0354	0.1925	QALFUE	0.0243	0.1923
FOPPUV	0.0293	0.0836	SEGVEF	0.0181	0.0507
HANBUT	0.0230	0.1397	TOKVIY	0.0932	0.1517
IDOZEG	0.0921	0.1315	VAPTEL01	0.1433	0.1975
JAXWOU01	0.1009	0.2769	VAPTEL	0.1540	0.2121
JAXWOU	0.0894	0.3005	XARXET	0.0551	0.2106
JEXWOY	0.0398	0.1283	XAXXUP	0.0807	0.1718
KITGAV	0.0246	0.1804	XEXJIT	0.0954	0.1110
KUYBEL	0.0338	0.2856	XORGAM	0.0520	0.3006
LEJTEZ	0.0333	0.1147	XUGBUW	0.0872	0.1777
LEYHOM	0.0340	0.2350	ZZZARD01	0.0576	0.1656

Table S10: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 29 dysprosium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	UME (Å)		$UME_{(Ln-L)}$s (Å)	UME (Å)
AMAQDY	0.0771	0.1743	MANHOY	0.1046	0.1740
BAFZUE	0.0687	0.1353	PALBIN	0.0331	0.4337
BIHLIN	0.0362	0.1062	QQQEMM01	0.0627	0.1455
BUVXIZ01	0.0715	0.1635	SETADY	0.0732	0.2889
CECLIF	0.0238	0.1272	TISQUH	0.0575	0.1209
CECLIF10	0.0225	0.1194	TUQTUU	0.0389	0.0764
DIBTIR	0.0702	0.1984	TUQTUU01	0.0392	0.0768
DIDBOH	0.0713	0.1424	VOSBOU	0.0565	0.1436
FOPNAZ	0.0294	0.1577	XAWVIA	0.0608	0.1422
FUXRAR	0.0265	0.1594	XEQMAH	0.1013	0.1031
GAKYEW	0.0421	0.2087	XIVFUD	0.1025	0.2502
GINPUO	0.0370	0.0892	YAVSOD	0.1074	0.1046
HANCAA	0.0470	0.1770	ZAXSAS	0.0901	0.1759
KITGEZ	0.0460	0.1865	ZZZARG01	0.0660	0.1698
LEYHUS	0.0280	0.2726			

Table S11: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 26 holmium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	UME (Å)		$UME_{(Ln-L)}$s (Å)	UME (Å)
BAGBAN	0.0674	0.1306	IDOZIK	0.0463	0.1094
BEYSAZ	0.0481	0.2354	KITGOJ	0.0336	0.1748
BUVXOF01	0.0653	0.0963	LEYJEE	0.0317	0.2592
CAQFUV	0.0592	0.1150	LIZPAL	0.0632	0.2985
COZHEE	0.0510	0.1434	NIHRIF	0.0426	0.0965
CUSYUK	0.0452	0.2782	NUJBAV	0.0488	0.1223
ECOJEL	0.1121	0.2246	QOZVOQ	0.0441	0.1312
FAGYOC	0.0379	0.3434	SIFZIQ	0.0400	0.2647
GAKYIA	0.0361	0.2178	XARVOB	0.0590	0.1461
GINREA	0.0294	0.0825	XAWVOG	0.0757	0.1308
GODKOZ	0.0238	0.0864	XEQMEL	0.1022	0.0855
HANCII	0.0294	0.1253	XEWVIE	0.0776	0.1332
HOESUL02	0.0638	0.0969	XORGEQ	0.0440	0.2632

Table S12: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 37 erbium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	UME (Å)		$UME_{(Ln-L)}$s (Å)	UME (Å)
AERETS02	0.0641	0.1162	SEGVAB	0.1003	0.1793
BAGBER	0.0713	0.1353	SOKBID	0.0531	0.1913
BOWXOA	0.0618	0.1344	TACERB0	0.0668	0.1353
DIBTAJ	0.0629	0.1809	TEPKOO	0.0565	0.1006
DIDCAU	0.0760	0.1447	TMHDER	0.1242	0.2311
DIJQAO	0.0378	0.0886	TUMJEQ	0.0585	0.0975
DIJQIW	0.0226	0.0735	UFIRIK	0.0486	0.0861
DIYNII	0.0316	0.1696	VEQFOM	0.0944	0.0966
DOGKEP	0.0594	0.0971	VOSNOG	0.0704	0.1465
GAKYOG	0.0369	0.1576	VUSGUL	0.1272	0.1792
GINRIE	0.0340	0.0762	VUSHEW	0.0674	0.1545
HAGSAJ	0.0703	0.2069	WEFVIM	0.0504	0.0897
HANCOO	0.0414	0.1642	XEWVOK	0.0502	0.1424
HENAEB	0.0592	0.2051	XEWWUR	0.0542	0.1124
KITGUP	0.0350	0.1728	XOYXIS	0.0845	0.2370
KOZBUW	0.0581	0.1979	YEGFEV	0.0682	0.0966
LEYJII	0.0398	0.2811	YICCIW	0.0298	0.2230
NIVQUE	0.0599	0.2608	ZUFSAU	0.0340	0.1161
RUNQOG	0.1094	0.1874			

Table S13: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 14 thulium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	UME (Å)		$UME_{(Ln-L)}$s (Å)	UME (Å)
BAGBIV	0.0784	0.1386	MEDNAK	0.0741	0.1706
COZHII	0.0618	0.1408	MIHPAU	0.0450	0.1843
FAGYUI	0.0411	0.2890	NIHZUZ	0.0470	0.1122
FENWOK	0.0721	0.2666	TUPYUY	0.1217	0.1261
HANCUU	0.0261	0.2539	TUTXOV	0.0865	0.0956
KITHAW	0.0357	0.1344	VEQFUS	0.1001	0.0868
LEYJOO	0.0612	0.2395	ZZZARJ01	0.0724	0.1646

Table S14: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 32 ytterbium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	**UME (Å)**		**$UME_{(Ln-L)}$s (Å)**	**UME (Å)**
BEQTAS	0.0652	0.0899	KITHEA	0.0213	0.1517
BUVYEW01	0.0957	0.1163	KOLGIB	0.0502	0.1100
CAQGAC	0.0626	0.0988	LOEAYB10	0.0523	0.2179
CETAYB	0.0398	0.1742	METSAF	0.0931	0.2500
DIBKUU	0.1106	0.1581	MIPTUA	0.1080	0.0937
DIYNOO	0.0219	0.2468	POHFAT	0.1494	0.1494
EBUWAZ	0.1193	0.1578	QAKXIJ	0.0596	0.1917
ECOJAH	0.0481	0.1232	QALFIS	0.0520	0.2493
EFIZUO	0.0803	0.1163	QAXYAP	0.0795	0.0877
FEBGAU	0.1071	0.3263	QOZVUW	0.0496	0.1423
FONQUU01	0.0873	0.1408	RAMXEI	0.1015	0.2299
GAKYUM	0.0266	0.2417	RENXIR	0.0336	0.1318
GEIAYB10	0.0241	0.1825	ROGRIO	0.0323	0.1524
HOYKIP	0.0345	0.1136	XEWVUQ	0.0532	0.1186
IBIFII	0.2044	0.2419	XOHVEV	0.0405	0.0697
IBIGAB	0.2096	0.2632	YENRAK	0.0811	0.1540
JEMROI	0.1610	0.2143			

Table S15: Unsigned mean errors, $UME_{(Ln-L)}$s and UMEs, for Sparkle/RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 32 lutetium (III) complexes.

Structure	Sparkle/RM1 Model		Structure	Sparkle/RM1 Model	
	$UME_{(Ln-L)}$s (Å)	UME (Å)		$UME_{(Ln-L)}$s (Å)	UME (Å)
BAGBUH	0.0724	0.1122	QQQENA01	0.0761	0.1340
BORQEE	0.0929	0.1604	RADRIX	0.0828	0.1225
BUVVUJ	0.0947	0.1148	RADROD	0.0590	0.1142
DICBUM	0.0091	0.0435	SUDDOK	0.0327	0.2652
DICCAT	0.0327	0.1188	UFIROQ	0.0451	0.0768
DIHZID	0.0196	0.0343	VEQGAZ	0.1057	0.0998
EFIZEY	0.0356	0.0793	XAWVAS	0.0796	0.1108
EFIZOI	0.0591	0.1418	XECQUR	0.0649	0.1188
FEWKEX	0.0609	0.2000	XECRIG	0.1089	0.2622
FOPPOP	0.0241	0.0442	XEPLUZ	0.0168	0.0667
HELGUA	0.0673	0.3086	XEWRAS	0.0950	0.1212
NIJHAP	0.0496	0.2526	XEWREW	0.0625	0.1260
POGWEN	0.1991	0.2729	XEWWAX	0.0852	0.1654
POHDIZ	0.0609	0.3513			

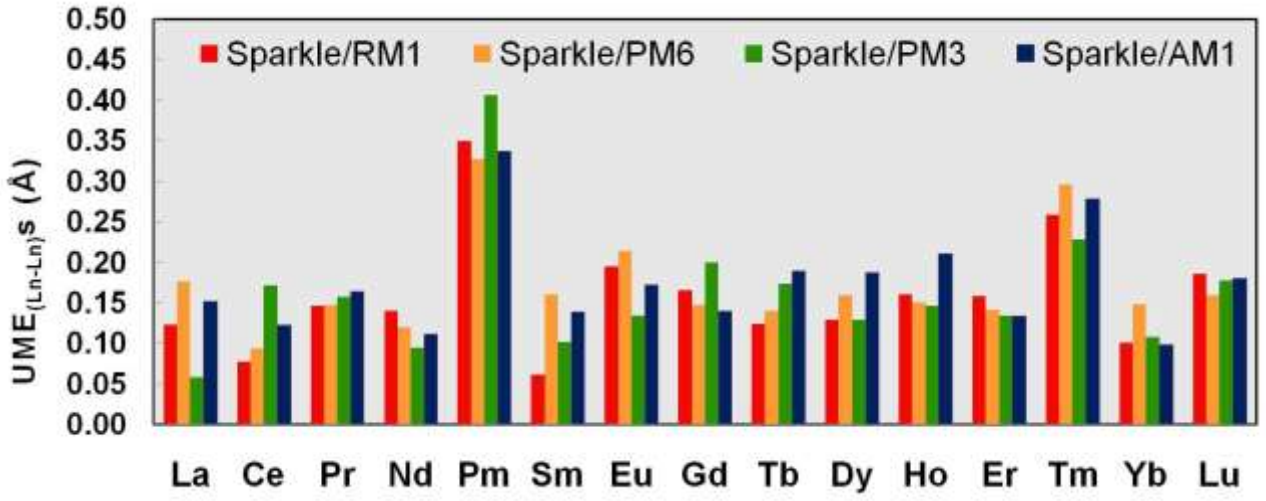

Figure S1 - $UME_{(Ln-Ln)}$s obtained using all four versions of the Sparkle Model: Sparkle/AM1, Sparkle/PM3, Sparkle/PM6 and Sparkle/RM1 for all dilanthanide(III) complexes of the validation set, for all lanthanide trications, from La(III) to Lu(III). The UMEs are calculated as the absolute value of the difference between the experimental and calculated interatomic distances between the two lanthanide ions, all summed for all complexes, for each of the lanthanides.

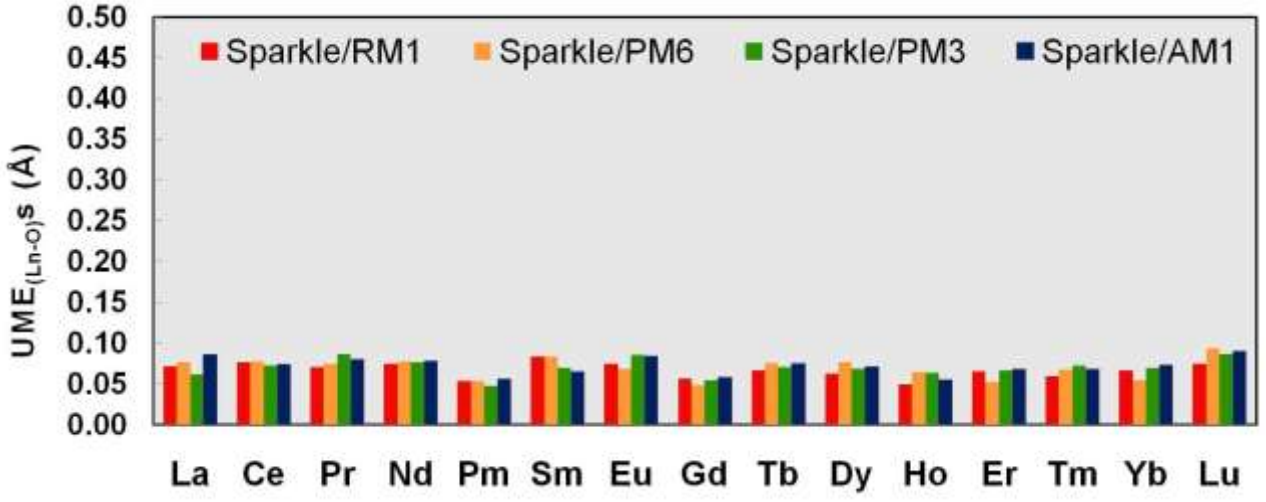

Figure S2 - $UME_{(Ln-O)}$s obtained using all four versions of the Sparkle Model: Sparkle/AM1, Sparkle/PM3, Sparkle/PM6 and Sparkle/RM1 for all complexes of the validation set, for all lanthanide trications, from La(III) to Lu(III). The UMEs are calculated as the absolute value of the difference between the experimental and calculated interatomic distances between the lanthanide ion and the directly coordinating oxygen atoms, summed for all complexes, for each of the lanthanides.

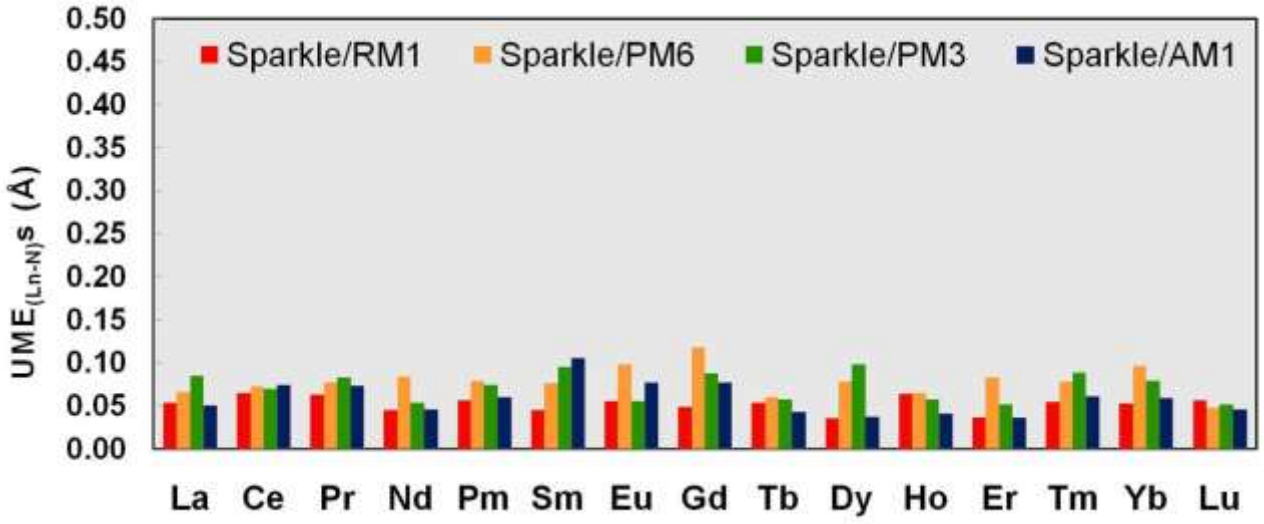

Figure S3 - $UME_{(Ln-N)}$s obtained using all four versions of the Sparkle Model: Sparkle/AM1, Sparkle/PM3, Sparkle/PM6 and Sparkle/RM1 for all complexes of the validation set, for all lanthanide trications, from La(III) to Lu(III). The UMEs are calculated as the absolute value of the difference between the experimental and calculated interatomic distances between the lanthanide ion and the directly coordinating nitrogen atoms, summed for all complexes, for each of the lanthanides.

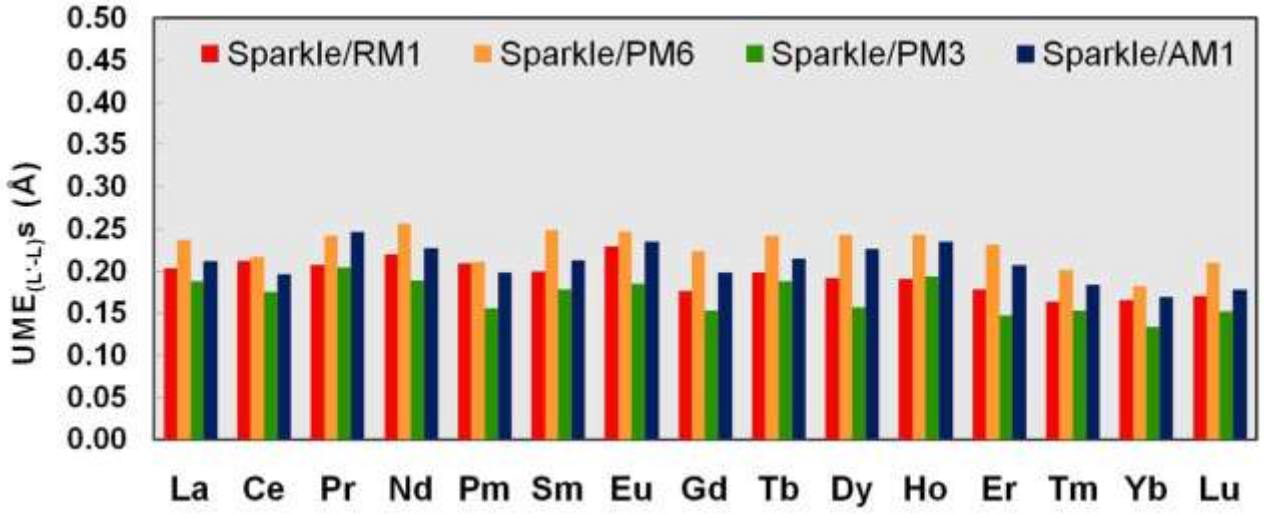

Figure S4 - $UME_{(L-L')}$s obtained using all four versions of the Sparkle Model: Sparkle/AM1, Sparkle/PM3, Sparkle/PM6 and Sparkle/RM1 for all complexes of the validation set, for all lanthanide trications, from La(III) to Lu(III). The UMEs are calculated as the average of the absolute value of the difference between the experimental and calculated interatomic distances, summed over all interatomic distances between all atoms of the coordination polyhedra, for all complexes, for each of the lanthanides.

5. Sample Input and Output Files

(back to contents)

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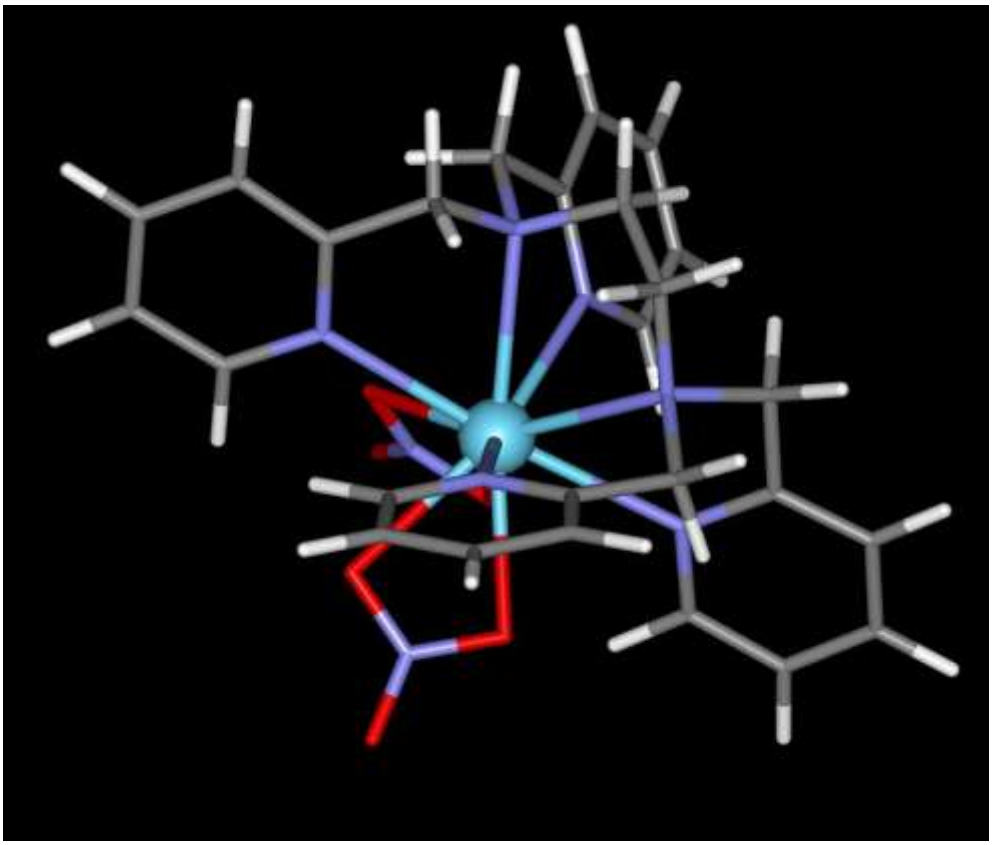

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---------- Begin of file **NASTOQ.arc**----------

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                                                Wed Nov 21 16:10:12 2012
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 NUMERO DE COORDENAÇÃO = 10



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     SCF FIELD WAS ACHIEVED

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ELECTRONIC ENERGY       =     -75840.59673 EV
CORE-CORE REPULSION     =      68582.03359 EV
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COSMO VOLUME            =        646.44 CUBIC ANGSTROMS

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            H    61    H    55    12.55182
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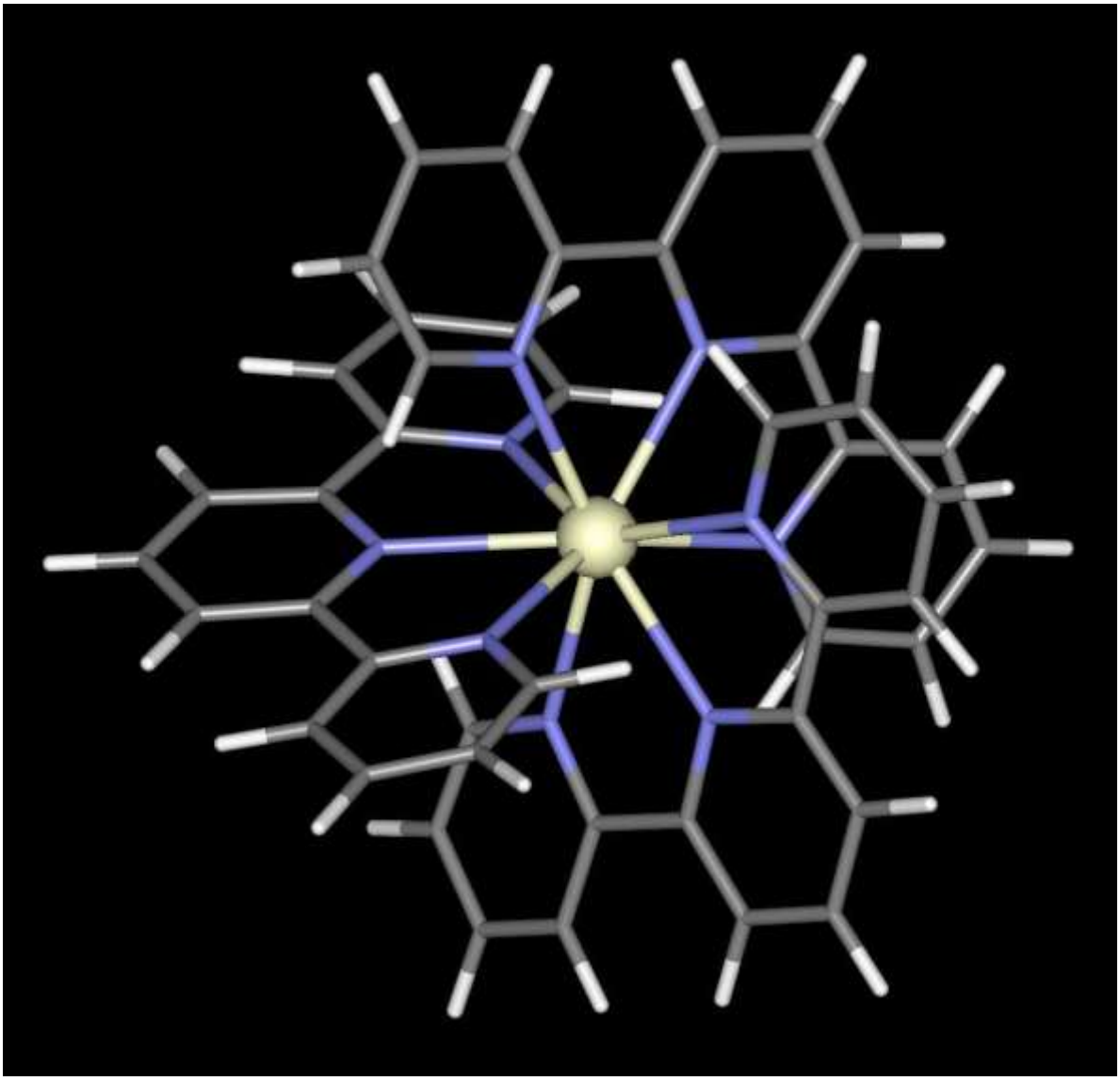
  O     0.62885346 +1  -1.88047320 +1  -2.02796042 +1    -0.6513
  O     0.45555956 +1   0.04673787 +1  -2.85403904 +1    -0.6664
  N    -1.36073955 +1   1.46357840 +1   1.37989575 +1    -0.4489
  N    -1.63989931 +1  -1.45720057 +1   1.10365500 +1    -0.4489
  N     0.96043686 +1  -2.36201778 +1   0.73466118 +1    -0.5085
  N    -2.05819945 +1  -0.67786308 +1  -1.51036941 +1    -0.5075
  N     1.17406949 +1   0.66097336 +1   2.11340732 +1    -0.5078
  N    -0.67698907 +1   2.33025777 +1  -1.16801374 +1    -0.5084
  O     0.77016729 +1  -1.63547825 +1  -4.16634287 +1    -0.2281
  O     4.15816053 +1   1.55412153 +1  -0.38205831 +1    -0.2283
```

N	3.04892945 +1	1.11263951 +1	-0.37238530 +1	0.5477
N	0.63141629 +1	-1.18062449 +1	-3.07127272 +1	0.5477
C	-2.10750015 +1	0.62798963 +1	2.39853369 +1	-0.0509
C	-2.72742583 +1	-0.60049774 +1	1.71770657 +1	-0.0509
C	-0.99780388 +1	-2.26106575 +1	2.21803218 +1	-0.0199
C	0.20059047 +1	-3.00378011 +1	1.68527215 +1	0.0613
C	0.49158789 +1	-4.26361498 +1	2.19069193 +1	-0.1697
C	1.61631430 +1	-4.93821805 +1	1.71015816 +1	0.0101
C	2.39729753 +1	-4.33106358 +1	0.74490920 +1	-0.1686
C	2.04015759 +1	-3.05618202 +1	0.28184665 +1	0.1273
C	-2.32477406 +1	-2.44980454 +1	0.18141240 +1	-0.0302
C	-2.78834745 +1	-1.75577852 +1	-1.07322534 +1	0.0863
C	-3.89277704 +1	-2.27223951 +1	-1.74591286 +1	-0.1689
C	-4.29622068 +1	-1.67382703 +1	-2.93705841 +1	0.0180
C	-3.59562288 +1	-0.57153750 +1	-3.40141727 +1	-0.1662
C	-2.50025441 +1	-0.10800637 +1	-2.66795542 +1	0.0904
C	-0.51384001 +1	2.45651627 +1	2.15550494 +1	-0.0302
C	0.67159307 +1	1.75777044 +1	2.76952042 +1	0.0866
C	1.22256001 +1	2.28889652 +1	3.93284362 +1	-0.1689
C	2.35092208 +1	1.68372653 +1	4.48059599 +1	0.0182
C	2.87417318 +1	0.56009717 +1	3.85984478 +1	-0.1661
C	2.26408102 +1	0.08438294 +1	2.69627310 +1	0.0904
C	-2.38303658 +1	2.26915784 +1	0.60139526 +1	-0.0199
C	-1.70445633 +1	2.99061803 +1	-0.53462886 +1	0.0613
C	-2.15847321 +1	4.25098047 +1	-0.89884149 +1	-0.1697
C	-1.53951046 +1	4.90671772 +1	-1.96557811 +1	0.0101
C	-0.49394975 +1	4.28099842 +1	-2.61795363 +1	-0.1687
C	-0.09073777 +1	3.00641719 +1	-2.19355936 +1	0.1272
H	-1.41807720 +1	0.31610323 +1	3.21952924 +1	0.1041
H	-2.91183072 +1	1.19370268 +1	2.93080554 +1	0.0939
H	-3.45890711 +1	-0.28776833 +1	0.93421274 +1	0.1040
H	-3.35660152 +1	-1.14966489 +1	2.46123176 +1	0.0940
H	-1.70933173 +1	-2.96614600 +1	2.71401786 +1	0.0976
H	-0.66666470 +1	-1.58250973 +1	3.04163591 +1	0.1052
H	-0.13958296 +1	-4.73363418 +1	2.95127383 +1	0.1402
H	1.86779984 +1	-5.93442843 +1	2.09272693 +1	0.1357
H	3.28249330 +1	-4.82934134 +1	0.33369637 +1	0.1568
H	2.66185318 +1	-2.58437220 +1	-0.50187463 +1	0.1815
H	-1.62031592 +1	-3.26913232 +1	-0.11082762 +1	0.1338
H	-3.17516182 +1	-2.98286338 +1	0.67338258 +1	0.0983
H	-4.43318433 +1	-3.14392036 +1	-1.36258258 +1	0.1444
H	-5.15170618 +1	-2.07120319 +1	-3.49625780 +1	0.1374
H	-3.87898007 +1	-0.07482479 +1	-4.33577536 +1	0.1535
H	-1.94053572 +1	0.76586695 +1	-3.04381240 +1	0.1616
H	-0.13366325 +1	3.26455664 +1	1.48067453 +1	0.1337
H	-1.09543391 +1	3.00436248 +1	2.93714047 +1	0.0983
H	0.79369725 +1	3.17687627 +1	4.40867825 +1	0.1445
H	2.81587907 +1	2.09247399 +1	5.38564772 +1	0.1374
H	3.76146138 +1	0.05627584 +1	4.25841524 +1	0.1534
H	2.68797518 +1	-0.80538758 +1	2.19950491 +1	0.1614
H	-3.16925193 +1	1.59388324 +1	0.18380341 +1	0.1051
H	-2.95165854 +1	2.98840304 +1	1.24080466 +1	0.0977
H	-2.98462810 +1	4.73550796 +1	-0.36921291 +1	0.1402
H	-1.87864413 +1	5.90302305 +1	-2.27277591 +1	0.1357
H	0.02598727 +1	4.76440022 +1	-3.45277004 +1	0.1568
H	0.75663114 +1	2.51942285 +1	-2.71145096 +1	0.1816

---------- End of file **NASTOQ.arc**----------

Cerium: XONYAA



---------- Begin of file **XONYAA.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 charge=+3
NUMERO DE COORDENAÇÃO = 10

Ce       -0.012302  1     0.028260  1    -0.026665  1
 N        2.600798  1     0.028260  1    -0.026665  1
 N        1.232784  1     2.374794  1    -0.026665  1
 N       -1.493001  1     2.195446  1    -0.123295  1
 N        0.514928  1     0.769486  1     2.509660  1
 N        0.790485  1    -1.822998  1     1.717104  1
 N       -2.151749  1    -1.063710  1     1.001992  1
 N       -2.012282  1    -0.577131  1    -1.666541  1
 N        0.256410  1     0.656214  1    -2.562798  1
 N        0.244726  1    -2.521224  1    -0.859572  1
 C        3.277568  1    -1.143098  1    -0.107106  1
```

H	2.798085	1	-1.920809	1	-0.274784	1
C	4.636650	1	-1.230678	1	0.048838	1
H	5.063577	1	-2.053209	1	-0.026688	1
C	5.360778	1	-0.095619	1	0.317930	1
H	6.279990	1	-0.140723	1	0.446824	1
C	4.702122	1	1.113710	1	0.394669	1
H	5.175465	1	1.896317	1	0.562559	1
C	3.315732	1	1.154795	1	0.214693	1
C	2.572548	1	2.442234	1	0.222473	1
C	3.216009	1	3.660523	1	0.459401	1
H	4.131382	1	3.685710	1	0.624028	1
C	2.477438	1	4.822289	1	0.448663	1
H	2.889622	1	5.639358	1	0.620273	1
C	1.116255	1	4.770427	1	0.181100	1
H	0.609402	1	5.549554	1	0.161039	1
C	0.523805	1	3.530420	1	-0.056418	1
C	-0.941158	1	3.424502	1	-0.292945	1
C	-1.699135	1	4.543122	1	-0.645611	1
H	-1.290441	1	5.367963	1	-0.779317	1
C	-3.052765	1	4.410007	1	-0.791869	1
H	-3.571119	1	5.145145	1	-1.026071	1
C	-3.646683	1	3.181605	1	-0.596931	1
H	-4.565804	1	3.073359	1	-0.680068	1
C	-2.828651	1	2.115552	1	-0.269492	1
H	-3.229455	1	1.285662	1	-0.139716	1
C	0.445932	1	2.054602	1	2.892843	1
H	-0.177507	1	2.600461	1	2.470193	1
C	1.237227	1	2.621540	1	3.875390	1
H	1.132806	1	3.515796	1	4.110009	1
C	2.182805	1	1.842469	1	4.499534	1
H	2.767575	1	2.207082	1	5.123439	1
C	2.240005	1	0.494902	1	4.171490	1
H	2.848400	1	-0.064671	1	4.599200	1
C	1.385601	1	-0.019136	1	3.203036	1
C	1.324640	1	-1.468432	1	2.905267	1
C	1.742554	1	-2.416119	1	3.837661	1
H	2.096592	1	-2.150135	1	4.656264	1
C	1.625702	1	-3.749099	1	3.531367	1
H	1.905975	1	-4.395433	1	4.140175	1
C	-2.248014	1	-1.231022	1	2.343375	1
H	-1.596417	1	-0.850212	1	2.884910	1
C	-3.262810	1	-1.937380	1	2.935271	1
H	-3.298352	1	-2.017395	1	3.860939	1
C	-4.224134	1	-2.525452	1	2.150953	1
H	-4.907175	1	-3.024969	1	2.535058	1
C	-4.160027	1	-2.363729	1	0.782768	1
H	-4.808560	1	-2.742343	1	0.234344	1
C	-3.112901	1	-1.622456	1	0.225812	1
C	-3.039362	1	-1.365641	1	-1.236488	1
C	-0.775842	1	0.535003	1	-3.436672	1
C	-1.926445	1	-0.295757	1	-2.990349	1
C	-2.836236	1	-0.803959	1	-3.917129	1
C	-3.867087	1	-1.617580	1	-3.467168	1
C	-3.982070	1	-1.893838	1	-2.123381	1
H	-4.677277	1	-2.426740	1	-1.809778	1
H	-4.478480	1	-1.975258	1	-4.071496	1
H	-2.754738	1	-0.602193	1	-4.821005	1
C	-0.761523	1	1.131299	1	-4.699382	1
H	-1.493493	1	1.051949	1	-5.267885	1
C	0.344865	1	1.834567	1	-5.090206	1
H	0.369876	1	2.237107	1	-5.927647	1

```
 C        1.421248  1     1.950382  1    -4.237154  1
 H        2.186321  1     2.413872  1    -4.488656  1
 C        1.325848  1     1.350006  1    -2.994852  1
 H        2.051921  1     1.429810  1    -2.418092  1
 C       -0.085008  1    -2.886853  1    -2.108853  1
 H        0.030953  1    -2.262448  1    -2.788517  1
 C       -0.583059  1    -4.130031  1    -2.454423  1
 H       -0.778925  1    -4.331814  1    -3.341308  1
 C       -0.786003  1    -5.063508  1    -1.465455  1
 H       -1.171580  1    -5.887475  1    -1.656676  1
 C       -0.398808  1    -4.740738  1    -0.172118  1
 H       -0.494731  1    -5.362950  1     0.513340  1
 C        0.134358  1    -3.485902  1     0.098543  1
 C        0.672727  1    -3.137670  1     1.433307  1
 C        1.093583  1    -4.124288  1     2.322903  1
 H        1.014780  1    -5.024993  1     2.102168  1
0
```

---------- End of file **XONYAA.mop**----------

---------- Begin of file **XONYAA.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No: 3560

                                        MOPAC2012 (Version: 12.290W)
                                        Wed Nov 21 16:10:12 2012
                                        No. of days left = 329
           Empirical Formula: C45 H33 N9 Ce  =    88 atoms

 RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 charge=+3
 NUMERO DE COORDENAÇÃO = 10



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =        834.53527 KCAL/MOL =    3491.69556 KJ/MOL
TOTAL ENERGY            =      -8001.43137 EV
ELECTRONIC ENERGY       =    -103902.97946 EV
CORE-CORE REPULSION     =      95901.54809 EV
GRADIENT NORM           =          0.23613
DIPOLE                  =          0.00777 DEBYE    POINT GROUP:       D3
NO. OF FILLED LEVELS    =        129
CHARGE ON SYSTEM        =          3
IONIZATION POTENTIAL    =         16.692758 EV
HOMO LUMO ENERGIES (EV) =        -16.693 -8.357
MOLECULAR WEIGHT        =        839.932
COSMO AREA              =        550.06 SQUARE ANGSTROMS
COSMO VOLUME            =        829.89 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    67    H    16    12.43713
            H    82    H    32    12.22003
            H    72    H    54    11.66276
```

```
          SCF CALCULATIONS        =        543
          COMPUTATION TIME =  3 MINUTES AND  34.406 SECONDS

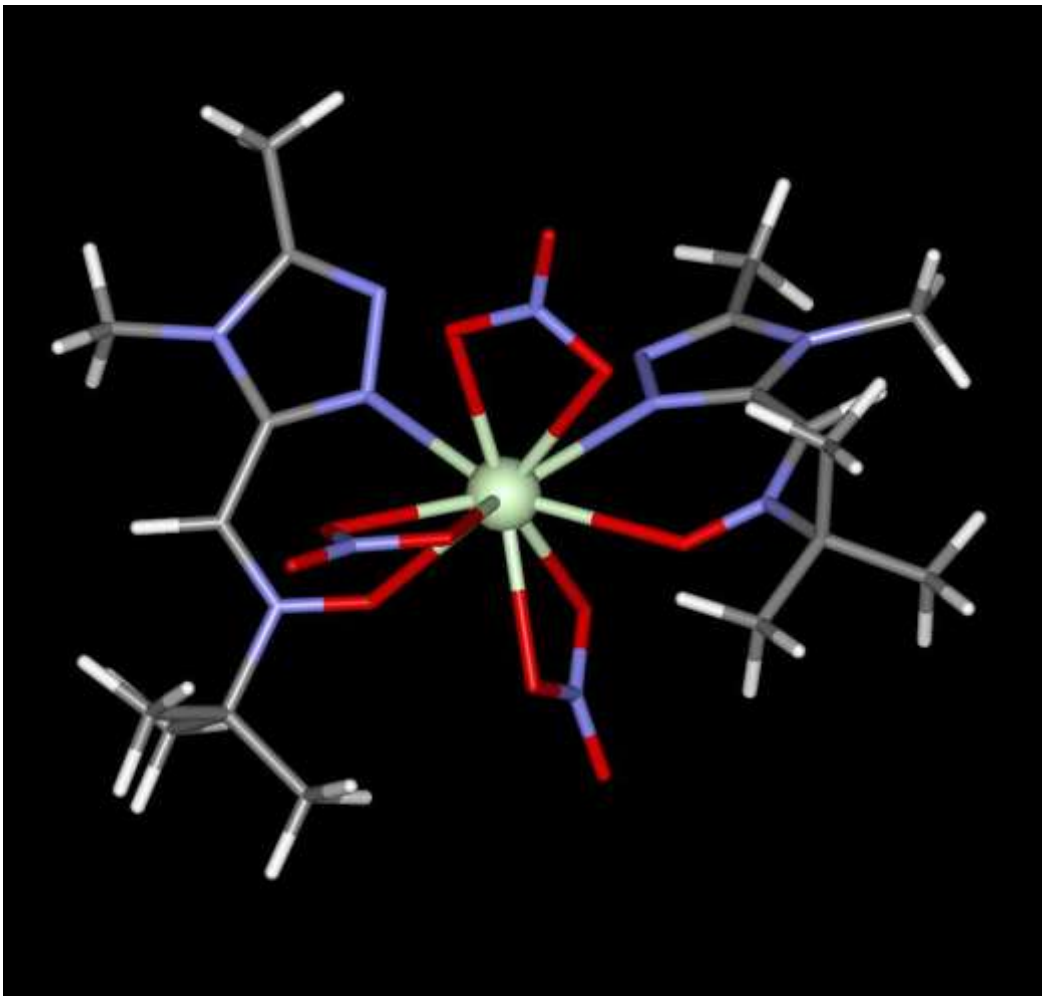

          FINAL GEOMETRY OBTAINED                                      CHARGE
RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 charge=+3
NUMERO DE COORDENAÇÃO = 10

Ce     0.05828652 +1  -0.01102757 +1  -0.05241838 +1      3.0000
 N     2.67102824 +1  -0.03809755 +1  -0.18706394 +1     -0.5275
 N     1.26635746 +1   2.28664200 +1  -0.25030187 +1     -0.5215
 N    -1.44193534 +1   2.13188248 +1  -0.09892795 +1     -0.5277
 N     0.57031793 +1   0.81146192 +1   2.37822847 +1     -0.5274
 N     0.89977144 +1  -1.78653933 +1   1.65552595 +1     -0.5214
 N    -2.04701916 +1  -1.04649305 +1   1.10614337 +1     -0.5273
 N    -1.99494541 +1  -0.54168113 +1  -1.56261484 +1     -0.5213
 N     0.26921733 +1   0.54257981 +1  -2.60108245 +1     -0.5274
 N     0.32943189 +1  -2.46749367 +1  -0.91187384 +1     -0.5274
 C     3.44422038 +1  -1.16502421 +1  -0.20340956 +1      0.0689
 H     2.92627379 +1  -2.13349263 +1  -0.28968597 +1      0.1409
 C     4.84011048 +1  -1.19038277 +1  -0.12655958 +1     -0.1443
 H     5.37721180 +1  -2.14739655 +1  -0.14863286 +1      0.1674
 C     5.52663557 +1   0.00731150 +1  -0.02521957 +1      0.0289
 H     6.62284009 +1   0.02967285 +1   0.05480630 +1      0.1636
 C     4.79109966 +1   1.19235408 +1  -0.04012306 +1     -0.1332
 H     5.32146298 +1   2.15418798 +1   0.02048033 +1      0.1607
 C     3.40405928 +1   1.14100444 +1  -0.14101277 +1      0.0873
 C     2.63837383 +1   2.40586635 +1  -0.23650218 +1      0.1268
 C     3.31639776 +1   3.62297259 +1  -0.33574060 +1     -0.1430
 H     4.41553389 +1   3.66390831 +1  -0.30855074 +1      0.1665
 C     2.58703047 +1   4.79707390 +1  -0.47321585 +1      0.0305
 H     3.09762570 +1   5.76738288 +1  -0.56008026 +1      0.1655
 C     1.20024203 +1   4.72155861 +1  -0.49877958 +1     -0.1430
 H     0.60615540 +1   5.64073419 +1  -0.61087534 +1      0.1664
 C     0.58191868 +1   3.47486606 +1  -0.37895195 +1      0.1268
 C    -0.89681506 +1   3.38400919 +1  -0.35367046 +1      0.0874
 C    -1.65175889 +1   4.53573193 +1  -0.55439520 +1     -0.1332
 H    -1.17057333 +1   5.49908169 +1  -0.77906581 +1      0.1607
 C    -3.04209418 +1   4.47510087 +1  -0.46042812 +1      0.0289
 H    -3.65398766 +1   5.37475891 +1  -0.61784545 +1      0.1636
 C    -3.62486851 +1   3.25788395 +1  -0.15259675 +1     -0.1443
 H    -4.71291402 +1   3.16705867 +1  -0.03946857 +1      0.1674
 C    -2.80390654 +1   2.13866604 +1   0.01574558 +1      0.0689
 H    -3.29592046 +1   1.18533591 +1   0.26650498 +1      0.1409
 C     0.38921999 +1   2.08896689 +1   2.82905210 +1      0.0688
 H    -0.12580056 +1   2.79462869 +1   2.15795624 +1      0.1408
 C     0.79707374 +1   2.57309623 +1   4.07578553 +1     -0.1444
 H     0.60638332 +1   3.61817162 +1   4.35181499 +1      0.1674
 C     1.43937592 +1   1.71341142 +1   4.95009014 +1      0.0289
 H     1.79111856 +1   2.05933351 +1   5.93254097 +1      0.1636
 C     1.61885531 +1   0.38693390 +1   4.55791241 +1     -0.1332
 H     2.10999866 +1  -0.31490771 +1   5.24796816 +1      0.1607
 C     1.16673432 +1  -0.02946831 +1   3.30935490 +1      0.0874
 C     1.28891301 +1  -1.45783081 +1   2.93508856 +1      0.1268
 C     1.74924279 +1  -2.38527072 +1   3.87252069 +1     -0.1430
 H     2.05817791 +1  -2.06800313 +1   4.87962872 +1      0.1664
 C     1.81377377 +1  -3.72827281 +1   3.52374099 +1      0.0304
 H     2.16678671 +1  -4.47882264 +1   4.24608045 +1      0.1655
 C    -2.16681533 +1  -1.28755450 +1   2.44615071 +1      0.0688
 H    -1.37099079 +1  -0.90260280 +1   3.10344424 +1      0.1409
```

C	-3.22063803 +1	-1.97702874 +1	3.05370936 +1	-0.1445
H	-3.23182229 +1	-2.12136421 +1	4.14175967 +1	0.1674
C	-4.24381566 +1	-2.46853418 +1	2.26153178 +1	0.0289
H	-5.08092085 +1	-3.03173672 +1	2.69812882 +1	0.1636
C	-4.19365331 +1	-2.21943330 +1	0.89006372 +1	-0.1333
H	-5.00829647 +1	-2.58534499 +1	0.24781835 +1	0.1607
C	-3.12362572 +1	-1.50613101 +1	0.35818411 +1	0.0874
C	-3.12048727 +1	-1.17650145 +1	-1.08627372 +1	0.1268
C	-0.82470891 +1	0.43724866 +1	-3.45082671 +1	0.0874
C	-2.03737863 +1	-0.21069434 +1	-2.89878661 +1	0.1268
C	-3.12468753 +1	-0.47716350 +1	-3.73407728 +1	-0.1430
C	-4.23665836 +1	-1.12744691 +1	-3.21435844 +1	0.0304
C	-4.23300204 +1	-1.48534823 +1	-1.87222918 +1	-0.1430
H	-5.10366444 +1	-2.00392434 +1	-1.44396553 +1	0.1664
H	-5.10312897 +1	-1.35408039 +1	-3.85275396 +1	0.1655
H	-3.11165018 +1	-0.18156810 +1	-4.79376530 +1	0.1664
C	-0.82965934 +1	0.87416265 +1	-4.77207942 +1	-0.1332
H	-1.73291201 +1	0.79208828 +1	-5.39450981 +1	0.1607
C	0.33067289 +1	1.41671702 +1	-5.32416124 +1	0.0289
H	0.34388559 +1	1.76807304 +1	-6.36577620 +1	0.1636
C	1.46226027 +1	1.48712122 +1	-4.53003662 +1	-0.1445
H	2.40687060 +1	1.87852826 +1	-4.92915633 +1	0.1674
C	1.38648674 +1	1.04792183 +1	-3.20473114 +1	0.0688
H	2.30509267 +1	1.10931721 +1	-2.59983758 +1	0.1408
C	0.10751077 +1	-2.87891339 +1	-2.19623156 +1	0.0688
H	-0.07607618 +1	-2.09982660 +1	-2.95315054 +1	0.1409
C	0.10107187 +1	-4.20783367 +1	-2.63100195 +1	-0.1445
H	-0.08577810 +1	-4.44274660 +1	-3.68686172 +1	0.1674
C	0.33604259 +1	-5.21422533 +1	-1.71009200 +1	0.0288
H	0.32151058 +1	-6.27234479 +1	-2.00788585 +1	0.1635
C	0.60631489 +1	-4.85119455 +1	-0.39071139 +1	-0.1332
H	0.81496387 +1	-5.63679226 +1	0.35051568 +1	0.1607
C	0.61819868 +1	-3.50577218 +1	-0.03527901 +1	0.0874
C	0.98749311 +1	-3.12623564 +1	1.34849950 +1	0.1269
C	1.42370296 +1	-4.10457514 +1	2.24482416 +1	-0.1430
H	1.46424997 +1	-5.16432680 +1	1.95217263 +1	0.1664

---------- End of file **XONYAA.arc**----------

Praseodymium: QIMRIN



---------- Begin of file **QIMRIN.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO = 10

Pr       -0.111340  1     0.195498  1     0.862793  1
 O        2.323360  1     0.195498  1     0.862793  1
 O        0.616330  1     2.628616  1     0.862793  1
 O        0.583779  1    -2.174791  1     1.819735  1
 O        0.523603  1    -1.994236  1    -0.304356  1
 O        0.618032  1     0.548446  1     3.207429  1
 O       -1.412477  1    -0.284696  1     3.090495  1
 O       -2.084046  1    -1.266404  1     0.687439  1
 O       -1.252773  1     2.436325  1     1.872119  1
 N        0.906239  1     0.529846  1    -1.571095  1
 N       -2.011721  1     1.087814  1    -0.719782  1
 O       -0.175963  1     4.392131  1     1.919171  1
 O        0.831627  1    -3.943556  1     0.614066  1
 O       -0.541356  1     0.137188  1     4.994948  1
 N        2.326122  1     0.692904  1    -3.317014  1
 N        3.385559  1     0.001391  1     0.136903  1
 N        0.193623  1     0.708642  1    -2.649992  1
```

```
 N        -0.320188  1     3.131328  1     1.543900  1
 N         0.779580  1    -2.748070  1     0.731840  1
 N        -2.902341  1     1.015607  1    -2.757472  1
 N        -1.836873  1     2.331177  1    -1.299340  1
 N        -2.754898  1    -1.727413  1    -0.366026  1
 N        -0.397055  1     0.195203  1     3.844110  1
 C         2.277822  1     0.568705  1    -1.971999  1
 C         3.316155  1     0.228813  1    -1.118579  1
 C         1.156237  1     0.894494  1    -3.729355  1
 C         4.176522  1    -1.546512  1     1.872352  1
 C         4.653396  1    -0.499184  1     1.007565  1
 C         3.535000  1     0.761555  1    -4.033835  1
 C         4.966591  1     0.706815  1     1.755989  1
 C         5.786347  1    -0.704634  1     0.193046  1
 C        -2.420222  1     2.188085  1    -2.525943  1
 C        -2.644883  1     0.394460  1    -1.578780  1
 C        -3.537086  1     0.532651  1    -3.989065  1
 C        -3.124351  1    -3.212459  1    -0.233973  1
 C         0.801112  1     1.164298  1    -5.089290  1
 C        -3.079907  1    -1.163130  1    -1.425738  1
 C        -2.597369  1     3.428263  1    -3.473234  1
 C        -2.336329  1    -4.002148  1    -1.085245  1
 C        -4.610061  1    -3.461766  1    -0.613284  1
 C        -2.901110  1    -3.687151  1     1.115026  1
 H         4.135287  1     0.148988  1    -1.551651  1
 H         4.009598  1    -2.336795  1     1.354443  1
 H         3.363083  1    -1.264787  1     2.297488  1
 H         4.838847  1    -1.736758  1     2.540157  1
 H         4.267980  1     0.569100  1    -3.444512  1
 H         3.641011  1     1.642128  1    -4.400410  1
 H         3.521811  1     0.119117  1    -4.745316  1
 H         4.233225  1     0.922575  1     2.337028  1
 H         5.115163  1     1.432933  1     1.145528  1
 H         5.758091  1     0.561784  1     2.279161  1
 H         5.673824  1    -1.512034  1    -0.313570  1
 H         6.567586  1    -0.782240  1     0.745360  1
 H         5.889150  1     0.037258  1    -0.406038  1
 H        -3.753383  1    -0.396864  1    -3.892718  1
 H        -2.932558  1     0.645871  1    -4.726954  1
 H        -4.339874  1     1.033469  1    -4.153632  1
 H        -0.150467  1     1.271064  1    -5.156418  1
 H         1.081627  1     0.433191  1    -5.644277  1
 H         1.234840  1     1.969961  1    -5.379785  1
 H        -3.546626  1    -1.608146  1    -2.093616  1
 H        -2.170293  1     4.193018  1    -3.082558  1
 H        -3.532553  1     3.609301  1    -3.591828  1
 H        -2.197420  1     3.239804  1    -4.325814  1
 H        -2.538170  1    -3.785917  1    -1.998749  1
 H        -2.523937  1    -4.929485  1    -0.926194  1
 H        -1.408480  1    -3.829481  1    -0.913375  1
 H        -5.181033  1    -3.034161  1     0.029168  1
 H        -4.784799  1    -4.405419  1    -0.616330  1
 H        -4.782893  1    -3.100125  1    -1.485606  1
 H        -3.495928  1    -3.232628  1     1.716345  1
 H        -1.992699  1    -3.511541  1     1.369172  1
 H        -3.066446  1    -4.631998  1     1.154122  1
0
```

---------- End of file **QIMRIN.mop**----------

---------- Begin of file **QIMRIN.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No: 3560

                                    MOPAC2012 (Version: 12.290W)
                                    Wed Nov 21 16:10:12 2012
                                    No. of days left = 329
           Empirical Formula: C18 H32 N11 O11 Pr  =    73 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO = 10



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =        -58.66920 KCAL/MOL =    -245.47192 KJ/MOL
TOTAL ENERGY            =      -8524.62768 EV
ELECTRONIC ENERGY       =     -84464.47271 EV
CORE-CORE REPULSION     =      75939.84503 EV
GRADIENT NORM           =          0.23454
DIPOLE                  =         12.24555 DEBYE    POINT GROUP:       C1
NO. OF FILLED LEVELS    =        114
IONIZATION POTENTIAL    =          9.718233 EV
HOMO LUMO ENERGIES (EV) =         -9.718 -0.954
MOLECULAR WEIGHT        =        719.426
COSMO AREA              =        521.27 SQUARE ANGSTROMS
COSMO VOLUME            =        692.25 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    47    H    66    12.74066
            H    64    H    45    11.95319
            H    59    O    14     7.59451
          SCF CALCULATIONS        =        761
          COMPUTATION TIME =  3 MINUTES AND  19.250 SECONDS

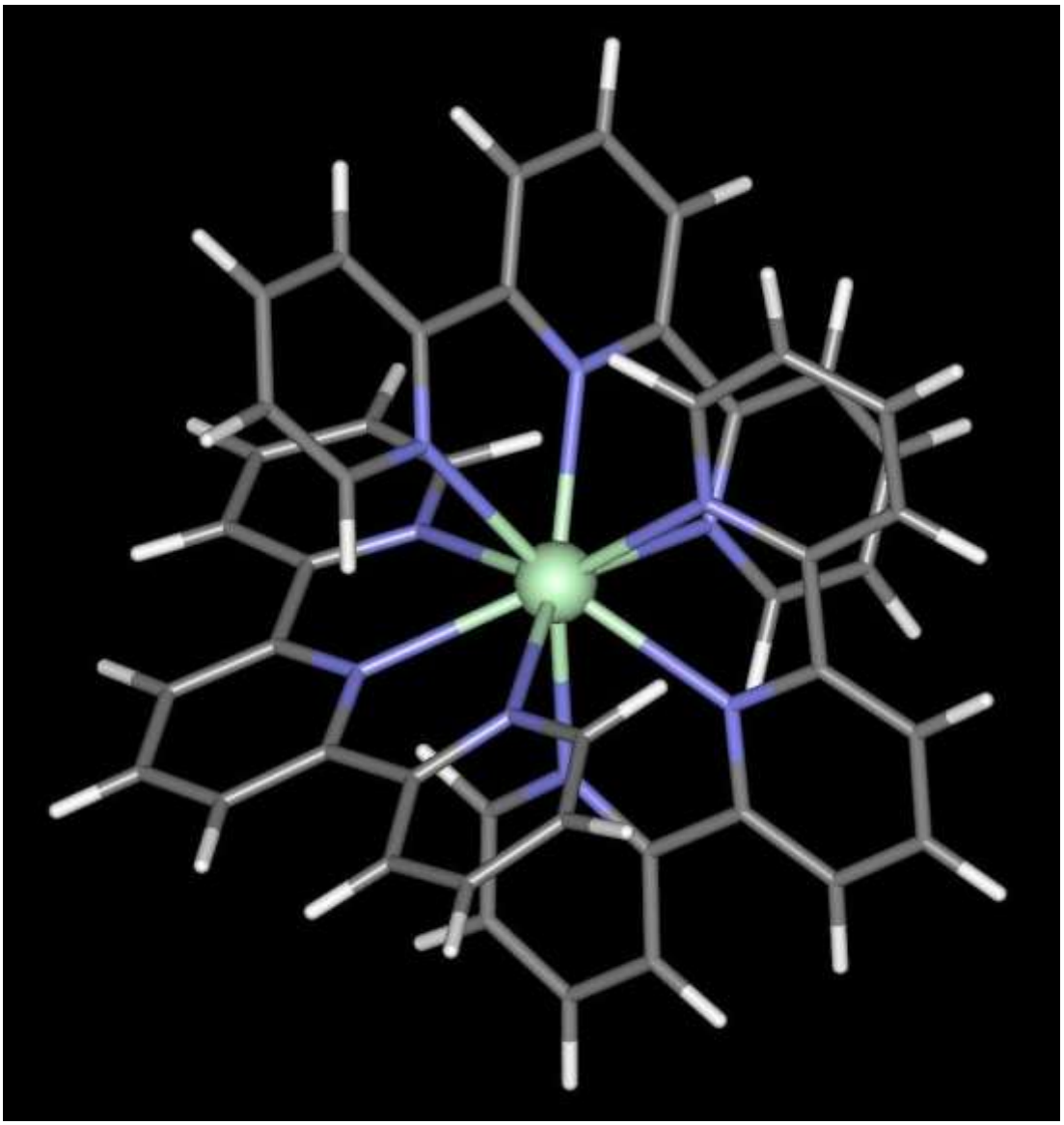

          FINAL GEOMETRY OBTAINED                                      CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO = 10

 Pr     0.02704493 +1  -0.29912643 +1  -0.17074261 +1         3.0000
  O     2.52227958 +1  -0.64735045 +1   0.39217278 +1        -0.5264
  O     1.50062831 +1   1.70615074 +1   0.42193322 +1        -0.6615
  O     0.53838552 +1  -2.67119532 +1   0.57647515 +1        -0.6255
  O     0.86103823 +1  -2.31169722 +1  -1.46776464 +1        -0.6385
  O    -0.26684496 +1  -0.03962823 +1   2.33820243 +1        -0.6186
  O    -2.04950870 +1  -0.40915074 +1   1.29346269 +1        -0.6628
  O    -1.82055520 +1  -2.07068850 +1  -0.64559575 +1        -0.5198
  O    -0.55199909 +1   2.12587232 +1   0.37098747 +1        -0.6122
  N     1.69860323 +1   0.40318756 +1  -2.04241265 +1        -0.4053
  N    -2.02951497 +1   0.46393747 +1  -1.57594062 +1        -0.4164
  O     0.83213292 +1   3.70233205 +1   0.89330596 +1        -0.2821
  O     1.23992619 +1  -4.28281986 +1  -0.67572948 +1        -0.2914
```

O	-2.12875801 +1	-0.13778700 +1	3.43083966 +1	-0.2766
N	3.50018046 +1	0.94048108 +1	-3.26511799 +1	-0.2455
N	3.60000224 +1	-0.05519339 +1	0.27968343 +1	0.2313
N	1.29221689 +1	0.56089117 +1	-3.33165616 +1	-0.1348
N	0.59823961 +1	2.56837986 +1	0.58298056 +1	0.5561
N	0.89643252 +1	-3.14237695 +1	-0.52800818 +1	0.5563
N	-4.12558197 +1	0.95369574 +1	-2.20942899 +1	-0.2448
N	-1.98742270 +1	1.62500478 +1	-2.28626938 +1	-0.1236
N	-3.04847393 +1	-2.16518757 +1	-0.55169827 +1	0.2282
N	-1.50762258 +1	-0.18581368 +1	2.40738604 +1	0.5584
C	3.05053203 +1	0.63272115 +1	-1.97724436 +1	0.1954
C	3.93941301 +1	0.58845490 +1	-0.83214994 +1	-0.1299
C	2.36454685 +1	0.88859918 +1	-4.09400287 +1	0.1014
C	3.91942027 +1	-0.88015129 +1	2.63071682 +1	-0.2185
C	4.54258149 +1	-0.05523115 +1	1.50568236 +1	0.1732
C	4.86999797 +1	1.25525775 +1	-3.64928106 +1	-0.0083
C	4.70372990 +1	1.39856813 +1	1.94376645 +1	-0.2369
C	5.86861198 +1	-0.67539361 +1	1.07207193 +1	-0.2326
C	-3.24538669 +1	1.95224890 +1	-2.66934353 +1	0.1035
C	-3.33160522 +1	0.02713902 +1	-1.52899491 +1	0.1889
C	-5.57479004 +1	0.90799013 +1	-2.35324224 +1	-0.0084
C	-3.62742393 +1	-3.45782250 +1	0.06939805 +1	0.1731
C	2.37055563 +1	1.14803617 +1	-5.54732694 +1	-0.1399
C	-3.86121742 +1	-1.18871579 +1	-0.94554508 +1	-0.1333
C	-3.65356052 +1	3.14785194 +1	-3.43322611 +1	-0.1406
C	-4.54082335 +1	-4.09975380 +1	-0.97289760 +1	-0.2318
C	-4.39268603 +1	-3.05091761 +1	1.32648933 +1	-0.2364
C	-2.49009901 +1	-4.41165744 +1	0.42797571 +1	-0.2210
H	4.88929638 +1	1.13211005 +1	-0.89221443 +1	0.1661
H	3.72795003 +1	-1.92430396 +1	2.33999328 +1	0.1042
H	2.95681423 +1	-0.46953748 +1	2.97478991 +1	0.1158
H	4.58350414 +1	-0.90711876 +1	3.50690593 +1	0.0812
H	5.57004948 +1	0.47342464 +1	-3.30182395 +1	0.0878
H	5.19310315 +1	2.22195600 +1	-3.22030171 +1	0.0858
H	4.97074491 +1	1.32578858 +1	-4.74662907 +1	0.0944
H	3.73367360 +1	1.89891741 +1	2.10433660 +1	0.1268
H	5.26727891 +1	2.01720283 +1	1.23156922 +1	0.0726
H	5.24706334 +1	1.45588448 +1	2.89908412 +1	0.0917
H	5.74645063 +1	-1.69238181 +1	0.66938986 +1	0.0962
H	6.54988794 +1	-0.76086945 +1	1.93284391 +1	0.0947
H	6.41053382 +1	-0.08984886 +1	0.31643358 +1	0.0697
H	-6.07640184 +1	0.96030216 +1	-1.36890362 +1	0.0907
H	-5.89547923 +1	-0.02370181 +1	-2.85415586 +1	0.0827
H	-5.94270826 +1	1.75520369 +1	-2.95831592 +1	0.0948
H	1.35364920 +1	1.08217089 +1	-5.96790905 +1	0.1131
H	2.98878459 +1	0.41524204 +1	-6.08964226 +1	0.0897
H	2.75142245 +1	2.15401550 +1	-5.78285239 +1	0.0866
H	-4.94508671 +1	-1.27640475 +1	-0.81068704 +1	0.1669
H	-2.78315312 +1	3.77823508 +1	-3.67998469 +1	0.1157
H	-4.34980741 +1	3.77912699 +1	-2.85860161 +1	0.0924
H	-4.14047767 +1	2.88257626 +1	-4.38438259 +1	0.0836
H	-5.42443410 +1	-3.49741051 +1	-1.22573695 +1	0.0696
H	-4.92692789 +1	-5.06138883 +1	-0.60068625 +1	0.0947
H	-4.01632984 +1	-4.31900251 +1	-1.91516858 +1	0.0939
H	-3.78104188 +1	-2.44277166 +1	2.01388413 +1	0.1257
H	-4.70648555 +1	-3.94112747 +1	1.89252161 +1	0.0919
H	-5.30856469 +1	-2.47832579 +1	1.12425178 +1	0.0723
H	-1.78675798 +1	-3.98110421 +1	1.15907610 +1	0.1211
H	-1.88792279 +1	-4.70662325 +1	-0.44479754 +1	0.1036
H	-2.88307846 +1	-5.33737822 +1	0.87285063 +1	0.0815

---------- End of file **QIMRIN.arc**----------

Neodymium: XONYII



---------- Begin of file **XONYII.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=+3
NUMERO DE COORDENAÇÃO = 9

Nd       -0.011544  1     0.026163  1    -0.024981  1
 N        2.575456  1     0.026163  1    -0.024981  1
 N        1.192120  1     2.350828  1    -0.024981  1
 N       -1.536976  1     2.149556  1    -0.129163  1
 N       -2.119361  1    -1.058159  1     1.011321  1
 N       -1.966611  1    -0.598368  1    -1.650060  1
 N        0.299546  1     0.650272  1    -2.546946  1
 N        0.271278  1    -2.498443  1    -0.867444  1
 N        0.478630  1     0.801568  1     2.489297  1
 N        0.791032  1    -1.789846  1     1.710763  1
 C        3.260782  1    -1.133046  1    -0.097677  1
 H        2.786579  1    -1.914520  1    -0.270021  1
```

C	4.626615	1	-1.219632	1	0.067442	1
H	5.058209	1	-2.040073	1	0.002622	1
C	5.340489	1	-0.071135	1	0.331398	1
H	6.261217	1	-0.102707	1	0.459986	1
C	4.659743	1	1.129717	1	0.400235	1
H	5.125526	1	1.918236	1	0.563764	1
C	3.284550	1	1.162087	1	0.228171	1
C	2.521291	1	2.443137	1	0.224888	1
C	3.155217	1	3.657134	1	0.458354	1
H	4.067371	1	3.690143	1	0.628092	1
C	2.400643	1	4.824507	1	0.435663	1
H	2.800994	1	5.647035	1	0.602084	1
C	1.053876	1	4.749086	1	0.160285	1
H	0.536740	1	5.521225	1	0.133578	1
C	0.474591	1	3.507054	1	-0.072393	1
C	-0.987283	1	3.373762	1	-0.317451	1
C	-1.761928	1	4.475304	1	-0.674575	1
H	-1.361307	1	5.302207	1	-0.808861	1
C	-3.123635	1	4.333489	1	-0.828529	1
H	-3.650574	1	5.059417	1	-1.075524	1
C	-3.693279	1	3.093954	1	-0.611623	1
H	-4.611734	1	2.974530	1	-0.700066	1
C	-2.875562	1	2.029819	1	-0.258091	1
H	-3.265868	1	1.199741	1	-0.104085	1
C	0.367367	1	2.086855	1	2.859646	1
H	-0.259838	1	2.616274	1	2.422986	1
C	1.136791	1	2.671569	1	3.859161	1
H	1.005500	1	3.561423	1	4.099721	1
C	2.102141	1	1.904944	1	4.486119	1
H	2.678461	1	2.283017	1	5.109279	1
C	2.193053	1	0.559539	1	4.163194	1
H	2.810957	1	0.017164	1	4.595489	1
C	1.355961	1	0.024605	1	3.191523	1
C	1.314565	1	-1.427230	1	2.899293	1
C	1.745062	1	-2.362139	1	3.836906	1
H	2.098688	1	-2.081801	1	4.649742	1
C	1.639276	1	-3.709163	1	3.545210	1
H	1.922524	1	-4.350055	1	4.157772	1
C	-2.221006	1	-1.219662	1	2.346352	1
H	-1.576144	1	-0.824343	1	2.887784	1
C	-3.231405	1	-1.937327	1	2.949935	1
H	-3.265150	1	-2.017110	1	3.875188	1
C	-4.188673	1	-2.535088	1	2.159585	1
H	-4.874107	1	-3.035923	1	2.539870	1
C	-4.109759	1	-2.374157	1	0.789156	1
H	-4.754245	1	-2.758319	1	0.239143	1
C	-3.071794	1	-1.643474	1	0.231896	1
C	-2.988168	1	-1.386726	1	-1.234652	1
C	-0.736856	1	0.527355	1	-3.411271	1
C	-1.885592	1	-0.314341	1	-2.979240	1
C	-2.784916	1	-0.831973	1	-3.904105	1
C	-3.803514	1	-1.649954	1	-3.469745	1
C	-3.919966	1	-1.926718	1	-2.112329	1
H	-4.608997	1	-2.464595	1	-1.799516	1
H	-4.407841	1	-2.010986	1	-4.077176	1
H	-2.697952	1	-0.630798	1	-4.807602	1
C	-0.710457	1	1.118888	1	-4.672381	1
H	-1.437245	1	1.030011	1	-5.243501	1
C	0.396778	1	1.836500	1	-5.068764	1
H	0.422904	1	2.243775	1	-5.904879	1
C	1.467325	1	1.942631	1	-4.202360	1

```
 H        2.230274  1     2.413922  1    -4.450227  1
 C        1.388719  1     1.334362  1    -2.957425  1
 H        2.116333  1     1.401203  1    -2.381929  1
 C       -0.028410  1    -2.853866  1    -2.126555  1
 H        0.085794  1    -2.222503  1    -2.799371  1
 C       -0.499978  1    -4.112556  1    -2.481881  1
 H       -0.669602  1    -4.321523  1    -3.373233  1
 C       -0.714040  1    -5.045896  1    -1.484011  1
 H       -1.092431  1    -5.871833  1    -1.679101  1
 C       -0.353576  1    -4.721827  1    -0.184894  1
 H       -0.456522  1    -5.344666  1     0.496523  1
 C        0.163421  1    -3.462586  1     0.094480  1
 C        0.688556  1    -3.105338  1     1.432982  1
 C        1.105304  1    -4.087491  1     2.327633  1
 H        1.025317  1    -4.986980  1     2.106579  1
0
```

---------- End of file **XONYII.mop**----------

---------- Begin of file **XONYII.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No: 3560

                                                MOPAC2012 (Version: 12.203W)
                                                Tue Oct 30 11:08:58 2012
                                                No. of days left = 264

           Empirical Formula: C45 H33 N9 Nd  =    88 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=+3
 NUMERO DE COORDENAÇÃO = 9



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

     HEAT OF FORMATION       =        643.34714 KCAL/MOL =    2691.76445 KJ/MOL
     TOTAL ENERGY            =      -8010.50697 EV
     ELECTRONIC ENERGY       =    -104147.70814 EV
     CORE-CORE REPULSION     =      96137.20117 EV
     GRADIENT NORM           =          0.22988
     DIPOLE                  =          0.00549 DEBYE    POINT GROUP:       D3
     NO. OF FILLED LEVELS    =        129
     CHARGE ON SYSTEM        =          3
     IONIZATION POTENTIAL    =         16.710001 EV
      HOMO LUMO ENERGIES (EV) =        -16.710 -8.373
      MOLECULAR WEIGHT        =        844.056
      COSMO AREA              =        544.85 SQUARE ANGSTROMS
      COSMO VOLUME            =        826.51 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    50    H    32    12.40956
            H    56    H    16    12.15809
            H    42    H    80    11.65101
```

```
          SCF CALCULATIONS        =        524
          COMPUTATION TIME =  4 MINUTES AND  30.287 SECONDS

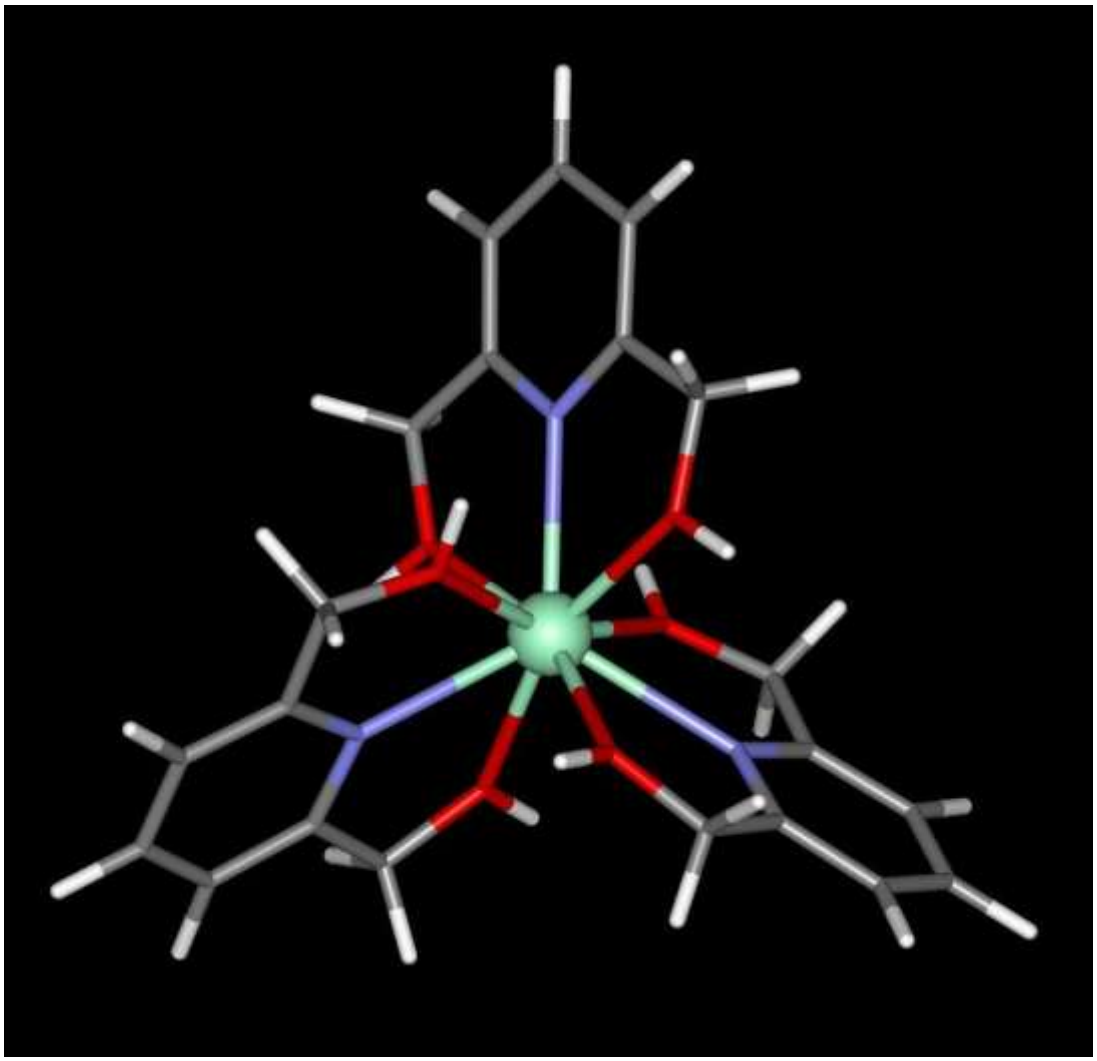

          FINAL GEOMETRY OBTAINED                                      CHARGE
RM1 SPARKLE EXTERNAL=spk.inp    PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=+3
NUMERO DE COORDENAÇÃO = 9

Nd     0.06029304 +1  -0.00931249 +1  -0.04791614 +1                 3.0000
 N     2.67296596 +1  -0.03093056 +1  -0.15163089 +1                -0.5266
 N     1.23642379 +1   2.28102393 +1  -0.23779364 +1                -0.5281
 N    -1.47797835 +1   2.10409086 +1  -0.11547545 +1                -0.5266
 N    -2.03417533 +1  -1.06354501 +1   1.11006233 +1                -0.5263
 N    -1.95499675 +1  -0.55970242 +1  -1.56435534 +1                -0.5280
 N     0.31032001 +1   0.54984348 +1  -2.59002627 +1                -0.5266
 N     0.35524403 +1  -2.45828952 +1  -0.91642350 +1                -0.5264
 N     0.53268807 +1   0.84389012 +1   2.37803615 +1                -0.5267
 N     0.89558248 +1  -1.75712159 +1   1.65850815 +1                -0.5280
 C     3.45150687 +1  -1.15083162 +1  -0.15665861 +1                 0.0697
 H     2.93907286 +1  -2.11994070 +1  -0.26138264 +1                 0.1418
 C     4.84574922 +1  -1.16085912 +1  -0.04778875 +1                -0.1426
 H     5.39481504 +1  -2.11113864 +1  -0.06321872 +1                 0.1675
 C     5.51474572 +1   0.04498872 +1   0.07651213 +1                 0.0265
 H     6.60850167 +1   0.07915559 +1   0.18266066 +1                 0.1636
 C     4.76761784 +1   1.22288216 +1   0.05018850 +1                -0.1311
 H     5.28574554 +1   2.19002974 +1   0.12760537 +1                 0.1604
 C     3.38359806 +1   1.15618265 +1  -0.08419932 +1                 0.0844
 C     2.60456288 +1   2.41034004 +1  -0.19835585 +1                 0.1288
 C     3.27066736 +1   3.63480890 +1  -0.29168297 +1                -0.1429
 H     4.36844471 +1   3.68865388 +1  -0.24294178 +1                 0.1667
 C     2.53047908 +1   4.79949775 +1  -0.45135605 +1                 0.0302
 H     3.03187429 +1   5.77499290 +1  -0.53430936 +1                 0.1657
 C     1.14522418 +1   4.70885631 +1  -0.50414759 +1                -0.1428
 H     0.54370378 +1   5.62078819 +1  -0.63456602 +1                 0.1667
 C     0.53830301 +1   3.45594949 +1  -0.38715452 +1                 0.1289
 C    -0.93883039 +1   3.35124704 +1  -0.38520462 +1                 0.0844
 C    -1.70369428 +1   4.49120091 +1  -0.61650190 +1                -0.1311
 H    -1.23062845 +1   5.45504364 +1  -0.85512487 +1                 0.1604
 C    -3.09436381 +1   4.41608207 +1  -0.53443669 +1                 0.0265
 H    -3.71374022 +1   5.30646856 +1  -0.71405985 +1                 0.1636
 C    -3.66895169 +1   3.19916270 +1  -0.20883505 +1                -0.1426
 H    -4.75687220 +1   3.09992533 +1  -0.10299100 +1                 0.1675
 C    -2.83796486 +1   2.09149790 +1  -0.01284174 +1                 0.0697
 H    -3.31403161 +1   1.13434415 +1   0.25170321 +1                 0.1418
 C     0.33093742 +1   2.11923596 +1   2.81738900 +1                 0.0696
 H    -0.20066043 +1   2.80669527 +1   2.14103415 +1                 0.1418
 C     0.73807638 +1   2.61487816 +1   4.06012633 +1                -0.1428
 H     0.53199872 +1   3.65751815 +1   4.33423219 +1                 0.1675
 C     1.39957180 +1   1.76769912 +1   4.93293239 +1                 0.0265
 H     1.75256017 +1   2.12359491 +1   5.91135255 +1                 0.1636
 C     1.59689692 +1   0.44154032 +1   4.54728904 +1                -0.1311
 H     2.10171269 +1  -0.24983286 +1   5.23794489 +1                 0.1604
 C     1.14308080 +1   0.01282211 +1   3.30302373 +1                 0.0845
 C     1.27570827 +1  -1.41534353 +1   2.93471411 +1                 0.1289
 C     1.73583684 +1  -2.33589180 +1   3.87952284 +1                -0.1428
 H     2.04021734 +1  -2.01184285 +1   4.88586571 +1                 0.1667
 C     1.80515990 +1  -3.68083289 +1   3.53850419 +1                 0.0302
 H     2.15651450 +1  -4.42626261 +1   4.26703726 +1                 0.1657
 C    -2.16019260 +1  -1.29823706 +1   2.44767012 +1                 0.0695
 H    -1.38088238 +1  -0.88561329 +1   3.10722695 +1                 0.1418
```

C	-3.20451657 +1	-2.01275995 +1	3.04327250 +1	-0.1429
H	-3.22914713 +1	-2.15182777 +1	4.13175866 +1	0.1675
C	-4.20133123 +1	-2.53546209 +1	2.23694269 +1	0.0264
H	-5.02903189 +1	-3.11960161 +1	2.66385616 +1	0.1636
C	-4.13957619 +1	-2.29123529 +1	0.86477830 +1	-0.1311
H	-4.93425951 +1	-2.68221021 +1	0.21264449 +1	0.1604
C	-3.08220422 +1	-1.54935605 +1	0.34563569 +1	0.0844
C	-3.06942329 +1	-1.21502140 +1	-1.09681771 +1	0.1289
C	-0.78042841 +1	0.44549826 +1	-3.43751176 +1	0.0845
C	-1.98762957 +1	-0.21962232 +1	-2.89600448 +1	0.1288
C	-3.06536984 +1	-0.49670795 +1	-3.74063990 +1	-0.1428
C	-4.16958060 +1	-1.17002983 +1	-3.23331532 +1	0.0302
C	-4.17018819 +1	-1.53853286 +1	-1.89389055 +1	-0.1428
H	-5.03438762 +1	-2.07626460 +1	-1.47637783 +1	0.1667
H	-5.02727644 +1	-1.40684594 +1	-3.87989513 +1	0.1657
H	-3.05033422 +1	-0.19228925 +1	-4.79771432 +1	0.1666
C	-0.78283062 +1	0.89661765 +1	-4.75451659 +1	-0.1312
H	-1.68290467 +1	0.81687734 +1	-5.38169994 +1	0.1604
C	0.37813352 +1	1.44999406 +1	-5.29516972 +1	0.0265
H	0.39353429 +1	1.81272609 +1	-6.33289059 +1	0.1636
C	1.50796641 +1	1.51687928 +1	-4.49757932 +1	-0.1427
H	2.45225793 +1	1.91564769 +1	-4.89004202 +1	0.1675
C	1.42919327 +1	1.06364302 +1	-3.17691130 +1	0.0696
H	2.34101715 +1	1.11736808 +1	-2.56180790 +1	0.1417
C	0.14769980 +1	-2.86881386 +1	-2.20042243 +1	0.0696
H	-0.02233677 +1	-2.08768665 +1	-2.95777618 +1	0.1418
C	0.14360976 +1	-4.20046379 +1	-2.62761621 +1	-0.1428
H	-0.03044680 +1	-4.44188612 +1	-3.68406857 +1	0.1675
C	0.36498578 +1	-5.20129589 +1	-1.69685669 +1	0.0264
H	0.35166603 +1	-6.26110607 +1	-1.98882601 +1	0.1636
C	0.62073989 +1	-4.83259539 +1	-0.37591655 +1	-0.1312
H	0.81956829 +1	-5.61464228 +1	0.37149404 +1	0.1604
C	0.63115054 +1	-3.48467276 +1	-0.02808890 +1	0.0845
C	0.98805193 +1	-3.09485232 +1	1.35520168 +1	0.1289
C	1.42231265 +1	-4.06664907 +1	2.26001681 +1	-0.1428
H	1.46700426 +1	-5.12814571 +1	1.97432954 +1	0.1666

---------- End of file **XONYII.arc**----------

Promecium: QIPQOV



---------- Begin of file **QIPQOV.mop**----------

```
RM1 SPARKLE PRECISE XYZ EXTERNAL=spk.inp T=10D BFGS GNORM=0.25 +
GEO-OK SCFCRT=1.D-10 CHARGE=+3
NUMERO DE COORDENAÇÃO = 9

 Pm       -0.000053  1    -0.000385  1     0.000024  1
  N       -2.251901  1    -1.202259  1     0.000522  1
  N        0.084669  1     2.550741  1    -0.000105  1
  N        2.167448  1    -1.348432  1    -0.000395  1
  O        1.309353  1     1.063283  1     1.779669  1
  O        1.611287  1     0.495673  1    -1.780671  1
  O       -1.236732  1     1.147597  1    -1.779061  1
  O       -1.575226  1     0.601373  1     1.780410  1
  O       -0.376569  1    -1.645438  1    -1.778928  1
  O        0.266765  1    -1.666745  1     1.778914  1
  C       -3.284713  1    -0.769025  1     0.782504  1
  C       -4.516950  1    -1.402311  1     0.808160  1
  C       -4.718329  1    -2.517076  1    -0.000225  1
  C       -3.680153  1    -2.971103  1    -0.808197  1
```

C	-2.467528	1	-2.301075	1	-0.781792	1
C	-3.010012	1	0.478459	1	1.625189	1
C	-1.278225	1	-2.768290	1	-1.623839	1
C	1.919380	1	2.367759	1	1.624629	1
C	0.975766	1	3.228951	1	0.782165	1
C	1.042497	1	4.612765	1	0.808267	1
C	0.177309	1	5.344233	1	0.000068	1
C	-0.734440	1	4.671801	1	-0.808183	1
C	-0.759546	1	3.286582	1	-0.782246	1
C	-1.758257	1	2.489983	1	-1.624766	1
C	3.034822	1	0.278176	1	-1.625498	1
C	3.226501	1	-0.984646	1	-0.782688	1
C	4.414079	1	-1.698154	1	-0.808562	1
C	4.541382	1	-2.823730	1	-0.000089	1
C	3.475607	1	-3.207926	1	0.808162	1
C	2.310006	1	-2.459061	1	0.781968	1
C	1.092579	1	-2.846551	1	1.624297	1
H	-5.308231	1	-1.028073	1	1.447568	1
H	-5.678928	1	-3.029151	1	-0.000524	1
H	-3.810194	1	-3.836543	1	-1.447825	1
H	1.761872	1	5.111200	1	1.447863	1
H	0.213394	1	6.432200	1	0.000135	1
H	-1.419231	1	5.216871	1	-1.447699	1
H	5.228250	1	-1.377215	1	-1.448206	1
H	5.465957	1	-3.398303	1	0.000046	1
H	3.548188	1	-4.080028	1	1.447842	1
H	1.908340	1	0.509570	1	2.321722	1
H	-1.870982	1	0.634990	1	-2.321425	1
H	-1.394699	1	1.396643	1	2.322779	1
H	0.384691	1	-1.938815	1	-2.320791	1
H	-0.512176	1	-1.909196	1	2.320823	1
H	1.483748	1	1.301199	1	-2.322953	1
H	-3.407611	1	1.375338	1	1.129812	1
H	-3.486673	1	0.389519	1	2.605624	1
H	-0.755284	1	-3.598076	1	-1.127997	1
H	-1.617220	1	-3.114780	1	-2.604346	1
H	2.894942	1	2.264417	1	1.129183	1
H	2.080432	1	2.824953	1	2.605143	1
H	-2.738725	1	2.452300	1	-1.129670	1
H	-1.888029	1	2.956510	1	-2.605527	1
H	3.490877	1	1.146869	1	-1.130261	1
H	3.504501	1	0.157797	1	-2.605946	1
H	0.516143	1	-3.640369	1	1.128879	1
H	1.408116	1	-3.214139	1	2.604955	1

---------- End of file **QIPQOV.mop**----------

---------- Begin of file **QIPQOV.arc**----------

```
          SUMMARY OF RM1 CALCULATION, Site No: 3560

                                MOPAC2012 (Version: 12.203W)
                                Tue Oct 30 11:26:48 2012
                                No. of days left = 264

          Empirical Formula: C21 H27 N3 O6 Pm  =    58 atoms
```

```
 RM1 SPARKLE PRECISE XYZ EXTERNAL=spk.inp T=10D BFGS GNORM=0.25 +
 GEO-OK SCFCRT=1.D-10 CHARGE=+3
 NUMERO DE COORDENAÇÃO = 9


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =        343.48411 KCAL/MOL =    1437.13750 KJ/MOL
TOTAL ENERGY            =      -5559.94502 EV
ELECTRONIC ENERGY       =     -49417.99120 EV
CORE-CORE REPULSION     =      43858.04619 EV
GRADIENT NORM           =          0.22253
DIPOLE                  =          0.01248 DEBYE    POINT GROUP:       D3
NO. OF FILLED LEVELS    =         81
CHARGE ON SYSTEM        =          3
IONIZATION POTENTIAL    =         18.241449 EV
HOMO LUMO ENERGIES (EV) =        -18.241 -8.826
MOLECULAR WEIGHT        =        562.461
COSMO AREA              =        400.88 SQUARE ANGSTROMS
COSMO VOLUME            =        516.56 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    33    H    36    11.29914
            H    39    H    32    10.35214
            H    54    H    58     6.93481
          SCF CALCULATIONS        =        162
          COMPUTATION TIME        =         27.971 SECONDS

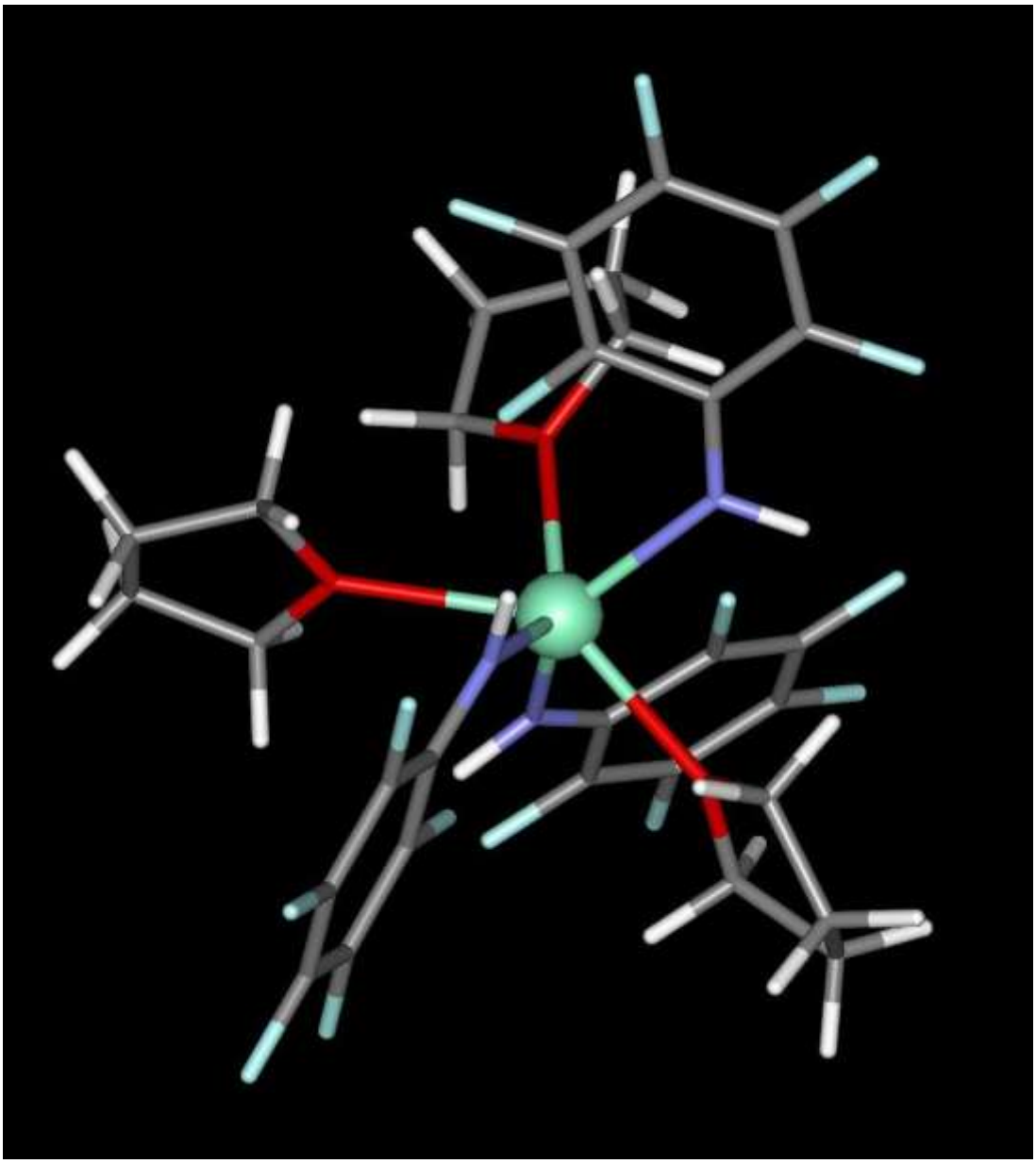

          FINAL GEOMETRY OBTAINED                                      CHARGE
 RM1 SPARKLE PRECISE XYZ EXTERNAL=spk.inp T=10D BFGS GNORM=0.25 +
 GEO-OK SCFCRT=1.D-10 CHARGE=+3
 NUMERO DE COORDENAÇÃO = 9

 Pm    -0.00094583 +1  -0.00694023 +1  -0.00225862 +1              3.0000
  N    -2.24977721 +1  -1.19923299 +1   0.01230265 +1             -0.5905
  N     0.08477680 +1   2.53703486 +1   0.00375481 +1             -0.5900
  N     2.16594993 +1  -1.34240867 +1  -0.01209684 +1             -0.5904
  O     1.19761320 +1   1.14367212 +1   1.81034776 +1             -0.5620
  O     1.61246337 +1   0.34745119 +1  -1.82347745 +1             -0.5622
  O    -1.12137783 +1   1.22977225 +1  -1.80834196 +1             -0.5623
  O    -1.58972667 +1   0.46142769 +1   1.81442282 +1             -0.5621
  O    -0.52238422 +1  -1.59540490 +1  -1.80525314 +1             -0.5625
  O     0.41408047 +1  -1.62314787 +1   1.80351125 +1             -0.5624
  C    -3.23278122 +1  -1.00014797 +1   0.97729153 +1              0.0839
  C    -4.47219481 +1  -1.62672004 +1   1.01859585 +1             -0.1451
  C    -4.80042896 +1  -2.54525301 +1   0.02539540 +1              0.0731
  C    -3.86454342 +1  -2.79750352 +1  -0.97383190 +1             -0.1451
  C    -2.64725510 +1  -2.12816842 +1  -0.94484864 +1              0.0838
  C    -2.91993429 +1  -0.00948260 +1   2.07658402 +1              0.0668
  C    -1.66108447 +1  -2.43448448 +1  -2.05001157 +1              0.0666
  C     1.45074894 +1   2.53285951 +1   2.06768700 +1              0.0665
  C     0.74513984 +1   3.29369817 +1   0.96728234 +1              0.0836
  C     0.81495564 +1   4.68081250 +1   1.00626259 +1             -0.1450
  C     0.18113928 +1   5.41932736 +1   0.01083471 +1              0.0730
  C    -0.50029041 +1   4.72969724 +1  -0.98812512 +1             -0.1450
```

C	-0.52320883 +1	3.34079829 +1	-0.95596844 +1	0.0837
C	-1.27758677 +1	2.63427807 +1	-2.06026855 +1	0.0665
C	2.91046042 +1	-0.20814263 +1	-2.08198614 +1	0.0666
C	3.16024947 +1	-1.21015517 +1	-0.97690009 +1	0.0840
C	4.35815451 +1	-1.91322291 +1	-1.01361735 +1	-0.1451
C	4.62632911 +1	-2.84703364 +1	-0.01666372 +1	0.0731
C	3.67479046 +1	-3.03646049 +1	0.98172467 +1	-0.1450
C	2.50241186 +1	-2.29152654 +1	0.94865944 +1	0.0836
C	1.49682421 +1	-2.53198252 +1	2.05264537 +1	0.0666
H	-5.18936791 +1	-1.40355332 +1	1.82187190 +1	0.1795
H	-5.77497248 +1	-3.05869127 +1	0.03019740 +1	0.1771
H	-4.09152803 +1	-3.51881960 +1	-1.77229633 +1	0.1795
H	1.36290733 +1	5.19471501 +1	1.80938233 +1	0.1795
H	0.21789474 +1	6.52023303 +1	0.01355184 +1	0.1771
H	-1.01240365 +1	5.28281455 +1	-1.78884704 +1	0.1795
H	5.08940042 +1	-1.73840562 +1	-1.81621235 +1	0.1796
H	5.56659065 +1	-3.42083379 +1	-0.01805491 +1	0.1771
H	3.85455739 +1	-3.76802633 +1	1.78285761 +1	0.1795
H	1.69842024 +1	0.64805970 +1	2.47337984 +1	0.2857
H	-1.65799480 +1	0.77331409 +1	-2.47152749 +1	0.2858
H	-1.40719103 +1	1.14498761 +1	2.47413365 +1	0.2857
H	0.13689677 +1	-1.82989159 +1	-2.47338447 +1	0.2858
H	-0.26084924 +1	-1.81433735 +1	2.46978121 +1	0.2858
H	1.47278556 +1	1.03443330 +1	-2.49020499 +1	0.2857
H	-3.65082837 +1	0.83534288 +1	2.07162034 +1	0.1334
H	-2.97278531 +1	-0.49158071 +1	3.08238771 +1	0.1282
H	-1.37169359 +1	-3.51345913 +1	-2.03826138 +1	0.1337
H	-2.09850260 +1	-2.21695085 +1	-3.05415131 +1	0.1283
H	2.54717336 +1	2.74693212 +1	2.06016777 +1	0.1336
H	1.06067735 +1	2.82163989 +1	3.07335870 +1	0.1280
H	-2.35656664 +1	2.92367594 +1	-2.05396933 +1	0.1337
H	-0.86639382 +1	2.89896573 +1	-3.06414808 +1	0.1280
H	3.69304976 +1	0.58903814 +1	-2.08223823 +1	0.1335
H	2.93295074 +1	-0.69893671 +1	-3.08477159 +1	0.1283
H	1.13970048 +1	-3.59049878 +1	2.04258312 +1	0.1337
H	1.94503924 +1	-2.34010427 +1	3.05722426 +1	0.1281

---------- End of file **QIPQOV.arc**----------

Samarium: FINDOV



---------- Begin of file **FINDOV.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp   PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO = 6

 Sm         0.000000  1     0.000000  1     0.000000  1
  O         0.085057  1     0.336864  1     2.418471  1
  O         0.541910  1     1.192277  1    -2.129862  1
  O        -1.611442  1    -0.884164  1    -1.696764  1
  N         2.351602  1     0.109344  1     0.171752  1
  N        -1.616139  1     1.722033  1     0.218313  1
  N        -0.080667  1    -2.218343  1     0.778005  1
  C         3.148624  1     1.197875  1     0.203462  1
  C         4.553198  1     1.205254  1     0.110446  1
```

C	5.306190	1	2.347807	1	0.123587	1
C	4.711374	1	3.572398	1	0.237843	1
C	3.347184	1	3.630882	1	0.326253	1
C	2.611720	1	2.491899	1	0.324581	1
C	-2.944482	1	1.578395	1	0.443917	1
C	-3.917733	1	2.576413	1	0.305028	1
C	-5.269328	1	2.357875	1	0.500354	1
C	-5.721733	1	1.120567	1	0.858139	1
C	-4.819392	1	0.116773	1	1.013827	1
C	-3.473619	1	0.349644	1	0.830901	1
C	0.458161	1	-3.324905	1	0.213645	1
C	0.412830	1	-4.621132	1	0.768696	1
C	1.013308	1	-5.710662	1	0.126188	1
C	1.652012	1	-5.567208	1	-1.064903	1
C	1.726946	1	-4.328906	1	-1.635766	1
C	1.128446	1	-3.259804	1	-1.011604	1
C	-0.459027	1	1.440809	1	3.186084	1
C	0.113335	1	1.285945	1	4.580665	1
C	1.375108	1	0.510327	1	4.370754	1
C	0.980656	1	-0.437592	1	3.273903	1
C	0.152480	1	2.525202	1	-2.530905	1
C	0.262973	1	2.554684	1	-4.012699	1
C	1.383809	1	1.608743	1	-4.282141	1
C	1.422322	1	0.679432	1	-3.135802	1
C	-2.199922	1	-2.201487	1	-1.679034	1
C	-3.533678	1	-2.051850	1	-2.312013	1
C	-3.385428	1	-0.955681	1	-3.203065	1
C	-2.278893	1	-0.122999	1	-2.721124	1
F	5.178300	1	0.000000	1	0.000000	1
F	6.640758	1	2.272365	1	0.000000	1
F	5.451368	1	4.691853	1	0.216398	1
F	2.732531	1	4.826500	1	0.402149	1
F	1.245010	1	2.555914	1	0.429969	1
F	-3.503093	1	3.817255	1	-0.049223	1
F	-6.126290	1	3.380506	1	0.350634	1
F	-7.033275	1	0.894080	1	1.021971	1
F	-5.232310	1	-1.114327	1	1.347544	1
F	-2.594424	1	-0.661777	1	1.035090	1
F	-0.194856	1	-4.795177	1	1.952613	1
F	0.950975	1	-6.913890	1	0.719941	1
F	2.282783	1	-6.624012	1	-1.624786	1
F	2.362219	1	-4.155307	1	-2.794837	1
F	1.201764	1	-2.032640	1	-1.590657	1
H	2.724610	1	-0.474140	1	0.048529	1
H	-1.331376	1	2.428920	1	0.284981	1
H	-0.566749	1	-2.321160	1	1.541120	1
H	-1.426688	1	1.398852	1	3.207163	1
H	-0.191043	1	2.290628	1	2.799790	1
H	0.298821	1	2.151171	1	4.977759	1
H	-0.500338	1	0.801360	1	5.154671	1
H	1.634986	1	0.034760	1	5.174518	1
H	2.102504	1	1.089493	1	4.093017	1
H	1.760263	1	-0.735715	1	2.777546	1
H	0.524946	1	-1.213350	1	3.636434	1
H	0.741264	1	3.185148	1	-2.132041	1
H	-0.757990	1	2.712205	1	-2.253811	1
H	0.474231	1	3.445211	1	-4.330356	1
H	-0.558237	1	2.252517	1	-4.431048	1
H	1.227192	1	1.125377	1	-5.107005	1
H	2.223191	1	2.089719	1	-4.356856	1
H	1.134139	1	-0.205700	1	-3.413138	1

```
 H        2.325856  1     0.613081  1    -2.788375  1
 H       -2.288235  1    -2.524335  1    -0.768611  1
 H       -1.652201  1    -2.827896  1    -2.178712  1
 H       -3.776766  1    -2.858232  1    -2.794222  1
 H       -4.213343  1    -1.868217  1    -1.645773  1
 H       -4.204517  1    -0.435513  1    -3.230920  1
 H       -3.195684  1    -1.275829  1    -4.098618  1
 H       -1.666516  1     0.077985  1    -3.445101  1
 H       -2.614390  1     0.711492  1    -2.357584  1
0
```

---------- End of file **FINDOV.mop**----------

---------- Begin of file **FINDOV.arc**----------

```
          SUMMARY OF RM1 CALCULATION, Site No: 3560

                                                MOPAC2012 (Version: 12.203W)
                                                Tue Oct 30 11:30:04 2012
                                                No. of days left = 264

          Empirical Formula: C30 H27 N3 O3 Sm F15  =    79 atoms

 RM1 SPARKLE EXTERNAL=spk.inp   PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 GEO-OK SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO = 6



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

    HEAT OF FORMATION       =       -772.34416 KCAL/MOL =   -3231.48796 KJ/MOL
    TOTAL ENERGY            =     -13073.07764 EV
    ELECTRONIC ENERGY       =    -123666.23841 EV
    CORE-CORE REPULSION     =     110593.16077 EV
    GRADIENT NORM           =          0.23997
    DIPOLE                  =          5.44921 DEBYE    POINT GROUP:       C1
    NO. OF FILLED LEVELS    =        144
    IONIZATION POTENTIAL    =          8.659877 EV
    HOMO LUMO ENERGIES (EV) =         -8.660 -0.800
    MOLECULAR WEIGHT        =        912.898
    COSMO AREA              =        576.76 SQUARE ANGSTROMS
    COSMO VOLUME            =        808.30 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            F    50    F    44    13.15179
            F    50    F    44    12.88064
            H    68    H    60    10.59411
          SCF CALCULATIONS        =        361
          COMPUTATION TIME =  2 MINUTES AND  41.726 SECONDS


          FINAL GEOMETRY OBTAINED                                  CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp   PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
```

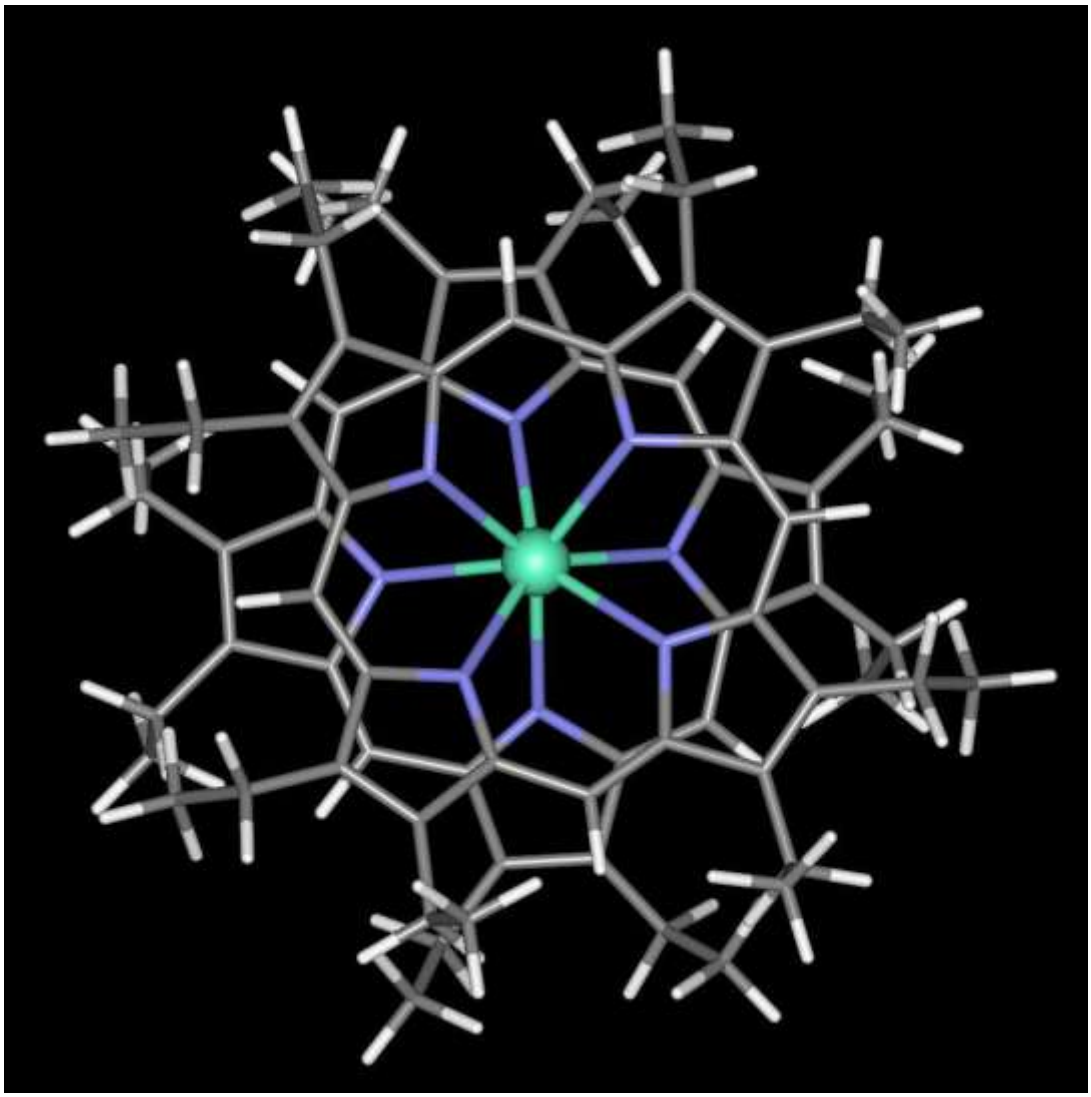
```
GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO = 6

Sm    -0.02833473 +1  -0.00605413 +1  -0.01870755 +1                3.0000
 O     0.21368161 +1   0.48960779 +1   2.47044363 +1               -0.4979
 O     0.54512958 +1   1.04393917 +1  -2.27600474 +1               -0.5001
 O    -1.76328311 +1  -1.01007313 +1  -1.60317807 +1               -0.4922
 N     2.32714658 +1   0.06783238 +1   0.07296948 +1               -0.9482
 N    -1.64224937 +1   1.71094619 +1   0.01615283 +1               -0.9658
 N    -0.02449119 +1  -2.22185689 +1   0.78699123 +1               -0.9504
 C     3.16028451 +1   1.12437779 +1   0.26456580 +1                0.2623
 C     4.57720066 +1   1.16309334 +1   0.31716016 +1               -0.0478
 C     5.25709485 +1   2.36529915 +1   0.52259593 +1                0.2148
 C     4.55424090 +1   3.57763428 +1   0.68318012 +1               -0.0364
 C     3.15288620 +1   3.57938741 +1   0.63867770 +1                0.2303
 C     2.49124567 +1   2.37325791 +1   0.43241820 +1               -0.1082
 C    -2.93100231 +1   1.68127217 +1   0.46472763 +1                0.2484
 C    -3.91377512 +1   2.70030021 +1   0.44103514 +1               -0.0432
 C    -5.20030871 +1   2.47228504 +1   0.93868990 +1                0.2118
 C    -5.55682136 +1   1.21869138 +1   1.47433742 +1               -0.0266
 C    -4.60867319 +1   0.18495445 +1   1.51628591 +1                0.2279
 C    -3.33077251 +1   0.43268676 +1   1.02499110 +1               -0.0951
 C     0.47999870 +1  -3.34824737 +1   0.21418114 +1                0.2621
 C     0.55207661 +1  -4.66837086 +1   0.72814977 +1               -0.0436
 C     1.11520896 +1  -5.70335525 +1  -0.02105227 +1                0.2162
 C     1.62685192 +1  -5.46723279 +1  -1.31469056 +1               -0.0314
 C     1.57663696 +1  -4.17545432 +1  -1.85564495 +1                0.2319
 C     1.00731562 +1  -3.15655275 +1  -1.09731577 +1               -0.1116
 C    -0.51259496 +1   1.48710702 +1   3.19407793 +1                0.0506
 C    -0.18508300 +1   1.33747577 +1   4.67691807 +1               -0.1527
 C     1.15475800 +1   0.61441810 +1   4.67497299 +1               -0.1530
 C     1.15950123 +1  -0.13544755 +1   3.34522712 +1                0.0503
 C     0.09123532 +1   2.31828246 +1  -2.74308918 +1                0.0439
 C     0.61575724 +1   2.52963401 +1  -4.16148761 +1               -0.1524
 C     1.80384960 +1   1.58209369 +1  -4.24583001 +1               -0.1541
 C     1.46526594 +1   0.49577072 +1  -3.22877676 +1                0.0461
 C    -2.26747813 +1  -2.34967681 +1  -1.55953538 +1                0.0500
 C    -3.59468021 +1  -2.36818919 +1  -2.31226166 +1               -0.1547
 C    -3.45096057 +1  -1.22710543 +1  -3.30964159 +1               -0.1511
 C    -2.39834269 +1  -0.31544758 +1  -2.67955398 +1                0.0473
 F     5.26665539 +1   0.04046238 +1   0.16928456 +1               -0.1396
 F     6.57568662 +1   2.37555738 +1   0.56683631 +1               -0.1307
 F     5.21804641 +1   4.70677405 +1   0.87566870 +1               -0.1317
 F     2.47652511 +1   4.70230338 +1   0.78708668 +1               -0.1349
 F     1.14963090 +1   2.29476184 +1   0.38052030 +1               -0.2355
 F    -3.61217606 +1   3.88914330 +1  -0.06242439 +1               -0.1407
 F    -6.09832190 +1   3.43794359 +1   0.90322324 +1               -0.1289
 F    -6.78153075 +1   1.01945116 +1   1.93474572 +1               -0.1292
 F    -4.92387824 +1  -0.99504159 +1   2.01343696 +1               -0.1304
 F    -2.36899428 +1  -0.50603768 +1   1.03234520 +1               -0.2279
 F     0.08045953 +1  -4.92268920 +1   1.94076941 +1               -0.1401
 F     1.17063612 +1  -6.92253562 +1   0.47968871 +1               -0.1296
 F     2.15253078 +1  -6.46337520 +1  -2.00999403 +1               -0.1305
 F     2.04843218 +1  -3.93103892 +1  -3.06318783 +1               -0.1356
 F     0.92111735 +1  -1.89381699 +1  -1.55420068 +1               -0.2388
 H     2.81862915 +1  -0.81610179 +1  -0.02193112 +1                0.2082
 H    -1.36429267 +1   2.63976645 +1  -0.28770084 +1                0.2020
 H    -0.42993949 +1  -2.39178587 +1   1.70257180 +1                0.2044
 H    -1.59116065 +1   1.34374577 +1   2.97254809 +1                0.0814
 H    -0.21639055 +1   2.47854036 +1   2.78827688 +1                0.0831
 H    -0.15038863 +1   2.31360418 +1   5.19763772 +1                0.0945
```

H	-0.96490947 +1	0.76011762 +1	5.21342691 +1	0.0877
H	1.28047259 +1	-0.06611199 +1	5.53885064 +1	0.0939
H	2.00507918 +1	1.32215022 +1	4.74951792 +1	0.0892
H	2.15099710 +1	-0.11767134 +1	2.84440796 +1	0.0906
H	0.85830961 +1	-1.19925867 +1	3.45411564 +1	0.0796
H	0.46588424 +1	3.09155149 +1	-2.03824495 +1	0.0860
H	-1.01797408 +1	2.32222541 +1	-2.69055140 +1	0.0799
H	0.88867721 +1	3.58525869 +1	-4.35309443 +1	0.0980
H	-0.15440763 +1	2.29615060 +1	-4.92399939 +1	0.0835
H	1.96117362 +1	1.17012538 +1	-5.26104088 +1	0.0955
H	2.75691044 +1	2.09273743 +1	-3.99932369 +1	0.0939
H	0.97292902 +1	-0.38366503 +1	-3.69714895 +1	0.0777
H	2.35882503 +1	0.13217570 +1	-2.67777553 +1	0.1008
H	-2.37253548 +1	-2.64983894 +1	-0.49608724 +1	0.0999
H	-1.50786915 +1	-3.01759313 +1	-2.02059530 +1	0.0789
H	-3.78745365 +1	-3.34581801 +1	-2.79403885 +1	0.0952
H	-4.45575472 +1	-2.21577281 +1	-1.63045780 +1	0.0918
H	-4.40489844 +1	-0.69695456 +1	-3.49593438 +1	0.0928
H	-3.13378805 +1	-1.58902777 +1	-4.30834640 +1	0.0851
H	-1.60689500 +1	-0.01687835 +1	-3.39944438 +1	0.0687
H	-2.84130525 +1	0.61178642 +1	-2.25592329 +1	0.0842

---------- End of file **FINDOV.arc**----------

Europium: GAPRUK



---------- Begin of file **GAPRUK.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ  T=10D GNORM=0.25 +
NOLOG GEO-OK BFGS SCFCRT=1.D-10 CHARGE=3.0
NUMERO DE COORDENAÇÃO = 8

Eu          -0.0585  1     -0.0021  1      0.0377  1
 N           2.4990  1     -0.0021  1      0.0377  1
 N           0.8285  1     -2.3038  1     -0.4604  1
 N          -0.9332  1     -0.6985  1     -2.1679  1
 N           0.7631  1      1.6341  1     -1.6795  1
 N           0.3738  1      1.9627  1      1.5436  1
 N           0.3122  1     -0.8499  1      2.3526  1
 N          -2.0991  1     -1.2505  1      0.7310  1
 N          -2.0325  1      1.5730  1     -0.0406  1
 C           3.2376  1      1.1704  1      0.0377  1
 C           4.4562  1      0.9898  1      0.7993  1
 C           4.4797  1     -0.3221  1      1.1854  1
 C           3.2587  1     -0.9205  1      0.6981  1
```

C	2.9287	1	-2.2769	1	0.8200	1
C	1.8388	1	-2.9193	1	0.2439	1
C	1.6436	1	-4.3742	1	0.2353	1
C	0.5411	1	-4.6140	1	-0.4989	1
C	0.0406	1	-3.3120	1	-0.9571	1
C	-1.0002	1	-3.1239	1	-1.8342	1
C	-1.4087	1	-1.9418	1	-2.4645	1
C	-2.3270	1	-1.8774	1	-3.5672	1
C	-2.3774	1	-0.5718	1	-3.9665	1
C	-1.4777	1	0.1528	1	-3.0796	1
C	-1.1071	1	1.4939	1	-3.2464	1
C	-0.0231	1	2.1559	1	-2.6740	1
C	0.5269	1	3.4156	1	-3.1554	1
C	1.6941	1	3.5917	1	-2.4939	1
C	1.8240	1	2.4839	1	-1.5698	1
C	2.9171	1	2.3005	1	-0.7032	1
C	5.4592	1	2.0549	1	1.0884	1
C	6.6184	1	2.1115	1	0.1310	1
C	5.5554	1	-1.0503	1	1.9268	1
C	6.4381	1	-1.8663	1	0.9961	1
C	2.5227	1	-5.3707	1	0.9282	1
C	2.0927	1	-5.6134	1	2.3635	1
C	-0.1177	1	-5.9240	1	-0.7858	1
C	-1.3857	1	-6.1538	1	0.0136	1
C	-3.0036	1	-3.0511	1	-4.2346	1
C	-2.1809	1	-3.6623	1	-5.3397	1
C	-3.0555	1	-0.0043	1	-5.1763	1
C	-2.1157	1	0.0632	1	-6.3654	1
C	-0.0729	1	4.3030	1	-4.2027	1
C	0.5713	1	4.2097	1	-5.5579	1
C	2.7570	1	4.6223	1	-2.7468	1
C	3.9062	1	4.0394	1	-3.5638	1
C	0.1672	1	3.2602	1	1.1685	1
C	1.1450	1	4.1293	1	1.7830	1
C	1.8957	1	3.3467	1	2.6220	1
C	1.3890	1	1.9823	1	2.4709	1
C	1.7802	1	0.9066	1	3.2382	1
C	1.2358	1	-0.3843	1	3.2528	1
C	1.4458	1	-1.3576	1	4.3143	1
C	0.6377	1	-2.4182	1	4.0342	1
C	-0.0712	1	-2.0760	1	2.8134	1
C	-1.1166	1	-2.8310	1	2.3153	1
C	-2.0912	1	-2.4400	1	1.4038	1
C	-3.3559	1	-3.1585	1	1.1578	1
C	-4.1061	1	-2.3611	1	0.3642	1
C	-3.3147	1	-1.1576	1	0.1241	1
C	-3.8144	1	-0.0201	1	-0.5063	1
C	-3.2635	1	1.2479	1	-0.5266	1
C	-3.9768	1	2.4605	1	-0.9567	1
C	-3.1577	1	3.5047	1	-0.6976	1
C	-1.9514	1	2.9366	1	-0.0943	1
C	-0.9022	1	3.7013	1	0.3814	1
C	1.2383	1	5.6004	1	1.5928	1
C	1.7462	1	5.9925	1	0.2134	1
C	2.9889	1	3.7713	1	3.5500	1
C	2.4521	1	4.2344	1	4.9037	1
C	2.2948	1	-1.1361	1	5.5323	1
C	3.7302	1	-1.4858	1	5.3606	1
C	0.3736	1	-3.5944	1	4.9154	1
C	-0.7377	1	-3.3149	1	5.9083	1
C	-3.7523	1	-4.4445	1	1.8386	1

C	-4.4095	1	-4.1934	1	3.1863	1
C	-5.4923	1	-2.6318	1	-0.1161	1
C	-5.5161	1	-3.2700	1	-1.4776	1
C	-5.3530	1	2.4758	1	-1.5319	1
C	-5.3616	1	2.1625	1	-2.9865	1
C	-3.3844	1	4.9626	1	-0.8969	1
C	-2.5767	1	5.5105	1	-2.0763	1
H	3.5113	1	-2.8120	1	1.3479	1
H	-1.5102	1	-3.8964	1	-2.0368	1
H	-1.6606	1	2.0124	1	-3.8191	1
H	3.5070	1	3.0385	1	-0.6138	1
H	5.8071	1	1.9041	1	1.9615	1
H	5.0138	1	2.8928	1	1.0643	1
H	7.2065	1	2.8128	1	0.3878	1
H	7.0848	1	1.2837	1	0.1500	1
H	6.4626	1	2.4253	1	-0.9543	1
H	5.1520	1	-1.6369	1	2.5580	1
H	6.0952	1	-0.4182	1	2.3845	1
H	7.1044	1	-2.3138	1	1.5051	1
H	5.9090	1	-2.5082	1	0.5415	1
H	6.8539	1	-1.2899	1	0.3675	1
H	3.4174	1	-5.0453	1	0.9281	1
H	2.4854	1	-6.1926	1	0.4552	1
H	2.6743	1	-6.2475	1	2.7658	1
H	2.1351	1	-4.7961	1	2.8492	1
H	1.2040	1	-5.9435	1	2.3768	1
H	0.4984	1	-6.6198	1	-0.5821	1
H	-0.3338	1	-5.9550	1	-1.7106	1
H	-1.7546	1	-7.0002	1	-0.2130	1
H	-1.1829	1	-6.1362	1	0.9414	1
H	-2.0130	1	-5.4688	1	-0.1866	1
H	-3.8276	1	-2.7528	1	-4.6018	1
H	-3.2540	1	-3.7917	1	-3.4734	1
H	-2.6550	1	-4.3924	1	-5.7194	1
H	-2.0133	1	-3.0108	1	-6.0053	1
H	-1.3552	1	-3.9718	1	-4.9840	1
H	-3.3599	1	0.8708	1	-4.9736	1
H	-3.8259	1	-0.4500	1	-5.3462	1
H	-2.5736	1	0.4256	1	-7.1117	1
H	-1.3709	1	0.6151	1	-6.1501	1
H	-1.8067	1	-0.8110	1	-6.5740	1
H	0.0000	1	5.2009	1	-3.9047	1
H	-0.9864	1	4.0713	1	-4.2946	1
H	0.1358	1	4.7983	1	-6.1566	1
H	1.4892	1	4.4475	1	-5.4876	1
H	0.5009	1	3.3187	1	-5.8799	1
H	3.0925	1	4.9307	1	-1.9143	1
H	2.3747	1	5.3479	1	-3.2253	1
H	4.5636	1	4.7094	1	-3.7085	1
H	4.2960	1	3.3135	1	-3.0869	1
H	3.5776	1	3.7301	1	-4.3973	1
H	2.5092	1	1.0592	1	3.8297	1
H	-1.1740	1	-3.7246	1	2.6344	1
H	-4.6314	1	-0.1299	1	-0.9779	1
H	-0.9053	1	4.6207	1	0.1493	1
H	1.8359	1	5.9493	1	2.2469	1
H	0.3775	1	5.9752	1	1.7196	1
H	1.7871	1	6.9383	1	0.1494	1
H	2.6125	1	5.6271	1	0.0803	1
H	1.1544	1	5.6522	1	-0.4475	1
H	3.4700	1	4.4851	1	3.1514	1

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H           3.5747  1       3.0350  1       3.6905  1
H           3.1797  1       4.4931  1       5.4593  1
H           1.8726  1       4.9740  1       4.7767  1
H           1.9775  1       3.5230  1       5.3154  1
H           1.9427  1      -1.6603  1       6.2393  1
H           2.2455  1      -0.2143  1       5.7632  1
H           4.1921  1      -1.3193  1       6.1739  1
H           3.8040  1      -2.4094  1       5.1438  1
H           4.1062  1      -0.9640  1       4.6683  1
H           1.1688  1      -3.8044  1       5.3952  1
H           0.1275  1      -4.3348  1       4.3740  1
H          -0.8770  1      -4.0841  1       6.4479  1
H          -0.4941  1      -2.5814  1       6.4574  1
H          -1.5359  1      -3.1100  1       5.4370  1
H          -2.9729  1      -4.9747  1       1.9692  1
H          -4.3630  1      -4.9117  1       1.2812  1
H          -4.6418  1      -5.0243  1       3.5856  1
H          -3.8018  1      -3.7318  1       3.7534  1
H          -5.1905  1      -3.6684  1       3.0654  1
H          -5.9652  1      -1.8105  1      -0.1586  1
H          -5.9176  1      -3.2151  1       0.4996  1
H          -6.4138  1      -3.4214  1      -1.7397  1
H          -5.0926  1      -2.6920  1      -2.1046  1
H          -5.0477  1      -4.0978  1      -1.4480  1
H          -5.7273  1       3.3389  1      -1.4039  1
H          -5.8811  1       1.8304  1      -1.0783  1
H          -6.2519  1       2.1815  1      -3.3116  1
H          -4.8390  1       2.8048  1      -3.4513  1
H          -4.9928  1       1.2964  1      -3.1256  1
H          -3.1271  1       5.4243  1      -0.1073  1
H          -4.3062  1       5.1080  1      -1.0641  1
H          -2.7467  1       6.4380  1      -2.1710  1
H          -1.6496  1       5.3731  1      -1.9151  1
H          -2.8293  1       5.0564  1      -2.8713  1
0
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---------- End of file **GAPRUK.mop**----------

---------- Begin of file **GAPRUK.arc**----------

```
           SUMMARY OF RM1 CALCULATION, Site No: 3560

                                MOPAC2012 (Version: 12.203W)
                                Tue Oct 30 13:20:59 2012
                                No. of days left = 264

           Empirical Formula: C72 H88 N8 Eu  =   169 atoms

 RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ  T=10D GNORM=0.25 +
 NOLOG GEO-OK BFGS SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO = 8


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED
```

```
HEAT OF FORMATION        =        889.65273 KCAL/MOL =    3722.30704 KJ/MOL
TOTAL ENERGY             =     -11956.34138 EV
ELECTRONIC ENERGY        =    -221278.80037 EV
CORE-CORE REPULSION      =     209322.45899 EV
GRADIENT NORM            =          0.23683
DIPOLE                   =          0.62641 DEBYE    POINT GROUP:       C1
NO. OF FILLED LEVELS     =        208
CHARGE ON SYSTEM         =          3
IONIZATION POTENTIAL     =         16.182454 EV
HOMO LUMO ENERGIES (EV)  =        -16.182 -9.825
MOLECULAR WEIGHT         =       1217.505
COSMO AREA               =        829.02 SQUARE ANGSTROMS
COSMO VOLUME             =       1446.26 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H   137    H   108    15.77443
            H   147    H   118    15.23892
            H   160    H    93    13.98485
          SCF CALCULATIONS         =       1055
          COMPUTATION TIME = 33 MINUTES AND   4.239 SECONDS


          FINAL GEOMETRY OBTAINED                                      CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ  T=10D GNORM=0.25 +
 NOLOG GEO-OK BFGS SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO = 8

 Eu    -0.06528998 +1   0.04015238 +1   0.08599108 +1                3.0000
  N     2.41802044 +1  -0.08337394 +1   0.22014529 +1               -0.6307
  N     0.61370621 +1  -2.31048522 +1  -0.38353377 +1               -0.6315
  N    -0.92902025 +1  -0.58049251 +1  -2.16593784 +1               -0.6340
  N     0.88442897 +1   1.63928406 +1  -1.57164149 +1               -0.6315
  N     0.33997293 +1   2.07802606 +1   1.45860551 +1               -0.6320
  N     0.34675872 +1  -0.67902449 +1   2.43517668 +1               -0.6311
  N    -2.05469058 +1  -1.24545713 +1   0.85701437 +1               -0.6335
  N    -2.06267349 +1   1.51491464 +1  -0.11787080 +1               -0.6332
  C     3.33482625 +1   1.05195705 +1   0.09062295 +1                0.1167
  C     4.63063229 +1   0.70071398 +1   0.72199792 +1                0.0085
  C     4.58740648 +1  -0.62870277 +1   0.98328369 +1               -0.1402
  C     3.22807084 +1  -1.08495830 +1   0.64271131 +1                0.2984
  C     2.84667252 +1  -2.47248435 +1   0.74449395 +1               -0.1422
  C     1.73641109 +1  -3.02330517 +1   0.23170445 +1                0.1208
  C     1.55178270 +1  -4.48287261 +1   0.03345256 +1                0.0132
  C     0.51060217 +1  -4.63225194 +1  -0.82069309 +1               -0.1405
  C    -0.02792295 +1  -3.28534151 +1  -1.07396972 +1                0.2974
  C    -1.10885476 +1  -3.07274560 +1  -2.00561561 +1               -0.1427
  C    -1.45379789 +1  -1.89448964 +1  -2.54494392 +1                0.1181
  C    -2.29541558 +1  -1.74997982 +1  -3.75811342 +1                0.0114
  C    -2.11105965 +1  -0.48587389 +1  -4.21112325 +1               -0.1411
  C    -1.24587248 +1   0.19557316 +1  -3.23216030 +1                0.3001
  C    -0.78536899 +1   1.54710227 +1  -3.43943517 +1               -0.1420
  C     0.19270238 +1   2.15796053 +1  -2.75440644 +1                0.1191
  C     0.86862605 +1   3.39997975 +1  -3.20503852 +1                0.0104
  C     2.01946847 +1   3.49609250 +1  -2.49567124 +1               -0.1414
  C     2.01196375 +1   2.39140503 +1  -1.52085803 +1                0.2996
  C     3.12385267 +1   2.16368906 +1  -0.62904023 +1               -0.1407
  C     5.72883985 +1   1.66058847 +1   0.94731301 +1               -0.1023
  C     6.66772129 +1   1.68953986 +1  -0.25246194 +1               -0.1864
  C     5.65978918 +1  -1.50002969 +1   1.50879180 +1               -0.0759
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C	2.41636849	-5.51516853	0.63655656	-0.1097
C	2.15845890	-5.61294988	2.13398290	-0.1802
C	-0.03032923	-5.87859918	-1.40354266	-0.0802
C	-1.22494240	-6.36599713	-0.59547409	-0.1850
C	-3.10056527	-2.84313297	-4.33665920	-0.1052
C	-2.25208099	-3.69063891	-5.27749247	-0.1856
C	-2.64854468	0.14121964	-5.43726328	-0.0752
C	-1.58873090	0.16887247	-6.53045389	-0.1906
C	0.35238456	4.28530237	-4.26716684	-0.1046
C	0.87333568	3.84415730	-5.62957942	-0.1862
C	3.10427659	4.49140716	-2.62999102	-0.0753
C	4.28479527	3.89418121	-3.38443953	-0.1908
C	-0.04964926	3.36220457	1.26205594	0.2987
C	0.72064815	4.33182117	2.05841735	-0.1413
C	1.59600059	3.61710756	2.80630816	0.0102
C	1.29050300	2.18565330	2.56847991	0.1184
C	1.69664594	1.18887928	3.36822451	-0.1411
C	1.15522352	-0.14834352	3.38642254	0.2987
C	1.41993562	-1.06779544	4.50484005	-0.1427
C	0.71710604	-2.19934830	4.25642919	0.0115
C	-0.08309362	-1.94534242	3.03374006	0.1203
C	-1.13494977	-2.68867194	2.66047807	-0.1411
C	-2.13718990	-2.30841563	1.69559334	0.2986
C	-3.40473622	-3.04758145	1.57603259	-0.1427
C	-4.17253844	-2.36878925	0.68985730	0.0135
C	-3.40560076	-1.16075141	0.29581012	0.1212
C	-3.94019823	-0.10144385	-0.32904047	-0.1440
C	-3.34938976	1.21134972	-0.42050533	0.2986
C	-4.14687234	2.38270300	-0.82136497	-0.1405
C	-3.33534696	3.46281260	-0.71795635	0.0137
C	-2.05214080	2.98015066	-0.14918670	0.1214
C	-1.12804227	3.78154605	0.40079423	-0.1433
C	0.55365749	5.79971741	2.00914350	-0.0814
C	1.28917958	6.37919832	0.80911711	-0.1849
C	2.61855589	4.11046958	3.74877593	-0.1048
C	2.02038121	4.25583019	5.14330691	-0.1862
C	2.30709417	-0.78225951	5.65218383	-0.0810
C	3.76019374	-1.03203195	5.27364399	-0.1849
C	0.66241854	-3.43960500	5.05401856	-0.1064
C	-0.43821392	-3.33980765	6.10377853	-0.1864
C	-3.73013427	-4.28663797	2.31420313	-0.0761
C	-4.29980048	-3.94661952	3.68467975	-0.1908
C	-5.53809045	-2.67419275	0.22163699	-0.1106
C	-5.51686453	-3.11635224	-1.23464843	-0.1807
C	-5.55726889	2.33078355	-1.26137067	-0.0804
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C	-3.62341127	4.87607699	-1.02835587	-0.1099
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H	-1.62032184	-3.98541303	-2.35380855	0.1811
H	-1.23228991	2.07266930	-4.29973705	0.1809
H	3.89626895	2.95048623	-0.62142641	0.1807
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H	5.33189206	2.67551045	1.16714879	0.0820
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H	-0.66949161 +1	0.68658429 +1	-6.22285944 +1	0.0576
H	-1.29030620 +1	-0.84090355 +1	-6.84810842 +1	0.0842
H	0.64464812 +1	5.34132269 +1	-4.06852161 +1	0.1083
H	-0.75947472 +1	4.31502956 +1	-4.25690994 +1	0.0839
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H	1.96888645 +1	3.90972158 +1	-5.69848365 +1	0.0864
H	0.59726974 +1	2.80872879 +1	-5.87330760 +1	0.0634
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H	0.92615228 +1	6.26319520 +1	2.95097328 +1	0.1092
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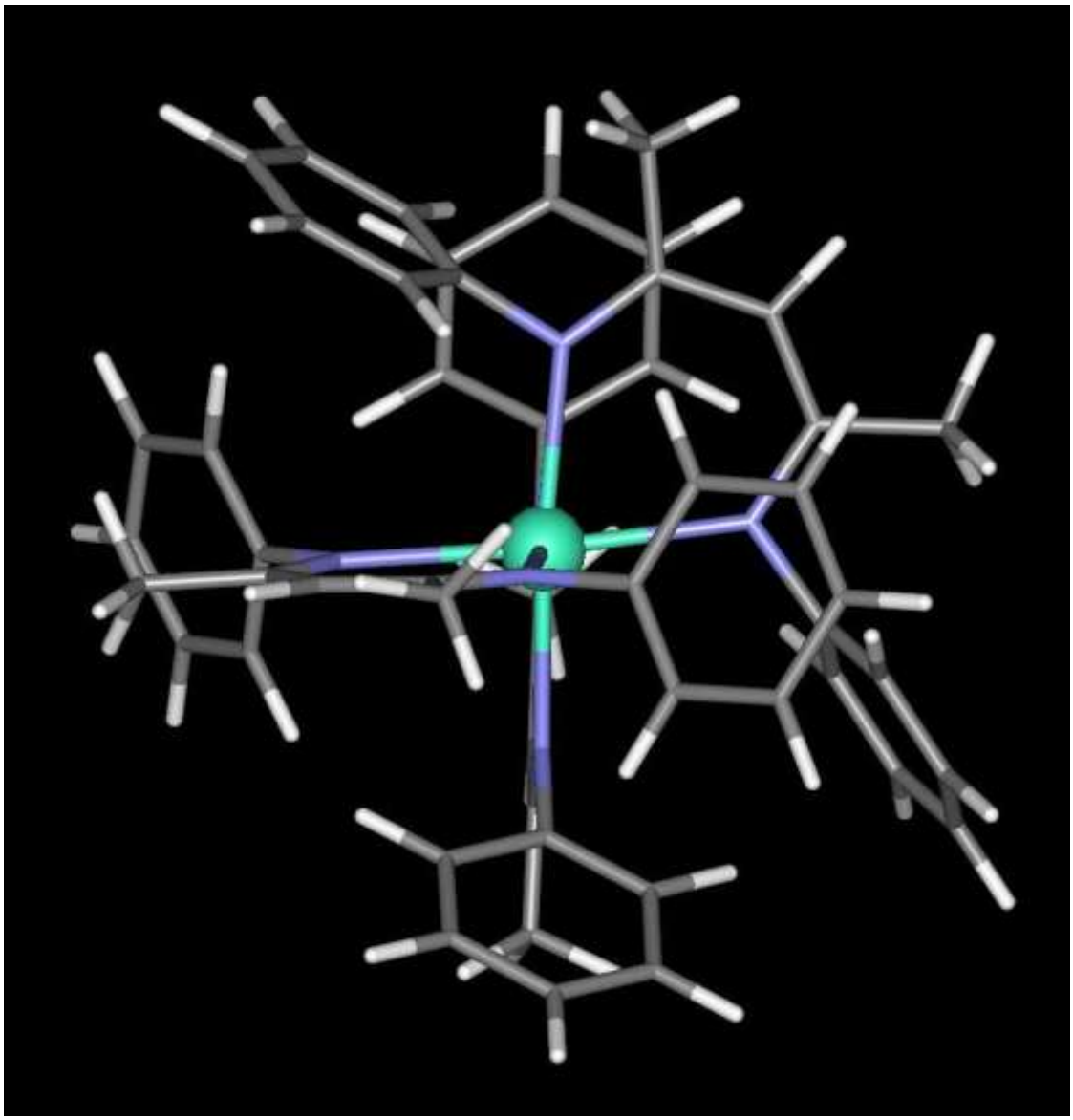
H	1.16281294 +1	7.47140092 +1	0.75062133 +1	0.1006
H	2.37211511 +1	6.19353714 +1	0.85752169 +1	0.0709
H	0.93485083 +1	5.96772294 +1	-0.14649468 +1	0.0479
H	3.02405316 +1	5.08717278 +1	3.39916889 +1	0.1102
H	3.50720333 +1	3.44311242 +1	3.76178381 +1	0.0840
H	2.76701852 +1	4.62892647 +1	5.86132509 +1	0.1020
H	1.18297513 +1	4.96868175 +1	5.16641231 +1	0.0854
H	1.64310325 +1	3.30422363 +1	5.54350012 +1	0.0628
H	2.02264052 +1	-1.41029016 +1	6.52696923 +1	0.1091
H	2.15674635 +1	0.25518754 +1	6.02337404 +1	0.0894
H	4.43706907 +1	-0.81264617 +1	6.11388002 +1	0.1005
H	3.94104633 +1	-2.08014538 +1	4.99358267 +1	0.0713
H	4.09224432 +1	-0.41204835 +1	4.42897840 +1	0.0476
H	1.64641715 +1	-3.62488121 +1	5.54211369 +1	0.1100
H	0.51652312 +1	-4.33019347 +1	4.40441653 +1	0.0856
H	-0.48906349 +1	-4.25275774 +1	6.71703406 +1	0.1018
H	-0.27654870 +1	-2.50480729 +1	6.80125173 +1	0.0850
H	-1.43416688 +1	-3.19947836 +1	5.66022990 +1	0.0634
H	-2.83765368 +1	-4.94440223 +1	2.40084018 +1	0.0768
H	-4.45127719 +1	-4.90719154 +1	1.73669182 +1	0.1026
H	-4.53970534 +1	-4.85532172 +1	4.25787521 +1	0.0990
H	-3.60239080 +1	-3.35854394 +1	4.29818841 +1	0.0600
H	-5.23216398 +1	-3.36733619 +1	3.61493648 +1	0.0834

H	-6.20542303 +1	-1.79502874 +1	0.36673228 +1	0.1016
H	-6.01015030 +1	-3.45851641 +1	0.85609558 +1	0.1168
H	-6.53081874 +1	-3.35320907 +1	-1.59348392 +1	0.1030
H	-5.11616051 +1	-2.34422294 +1	-1.90653491 +1	0.0500
H	-4.91424546 +1	-4.02423342 +1	-1.38313276 +1	0.0705
H	-6.05426884 +1	3.31456315 +1	-1.10332526 +1	0.1082
H	-6.14963507 +1	1.64276304 +1	-0.61900112 +1	0.0888
H	-6.68394365 +1	1.87912157 +1	-3.07183505 +1	0.1003
H	-5.12971094 +1	2.65080341 +1	-3.38337008 +1	0.0729
H	-5.19296073 +1	0.94461176 +1	-2.92403120 +1	0.0476
H	-3.41461116 +1	5.52065215 +1	-0.14523337 +1	0.1019
H	-4.71097998 +1	5.03208318 +1	-1.21093355 +1	0.1162
H	-3.02342218 +1	6.38257468 +1	-2.48180724 +1	0.1026
H	-1.73884501 +1	5.23359082 +1	-2.09776909 +1	0.0492
H	-3.08335208 +1	4.74982780 +1	-3.14433092 +1	0.0706

---------- End of file **GAPRUK.arc**----------

Gadolinium: WEWNOB



---------- Begin of file **WEWNOB.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO = 6

 Gd    0.0000000  1     0.0000000  1     0.0000000  1
  N    2.4364000  1     0.0000000  1     0.0000000  1
  N    0.5398890  1     2.3823920  1     0.0000000  1
  N    0.1766930  1    -0.3603580  1    -2.4111251  1
  N   -0.2799994  1    -2.4158153  1    -0.2317017  1
  N   -0.3326020  1     0.1642715  1     2.4185163  1
  N   -2.4170414  1     0.1866013  1     0.2431783  1
  C    2.9878730  1    -1.3247279  1     0.0140927  1
  C    3.5021272  1    -1.8720126  1     1.1757901  1
  C    4.0422509  1    -3.1502251  1     1.1551003  1
  C    4.0462945  1    -3.8813484  1    -0.0141231  1
```

C	3.4988594	1	-3.3522855	1	-1.1452904	1
C	2.9759118	1	-2.0813121	1	-1.1339878	1
C	3.2988168	1	1.0053396	1	-0.0523920	1
C	2.9485481	1	2.3601776	1	-0.1237155	1
C	1.7038839	1	3.0009340	1	-0.1276400	1
C	-0.6498706	1	3.1953885	1	0.0656897	1
C	-1.3604602	1	3.2415553	1	1.2536106	1
C	-2.5362279	1	3.9689281	1	1.3466888	1
C	-3.0092859	1	4.6648515	1	0.2593725	1
C	-2.3104161	1	4.6344094	1	-0.9057607	1
C	-1.1416167	1	3.8988210	1	-1.0256284	1
C	4.7889761	1	0.7228573	1	-0.0700369	1
C	1.7811519	1	4.5127479	1	-0.2766151	1
C	0.4802517	1	0.8655556	1	-3.0983345	1
C	-0.5146990	1	1.6345524	1	-3.6856875	1
C	-0.1989911	1	2.8324383	1	-4.2890167	1
C	1.0849677	1	3.2928232	1	-4.3121949	1
C	2.0760969	1	2.5375559	1	-3.7311748	1
C	1.7791292	1	1.3268561	1	-3.1368619	1
C	0.0135937	1	-1.4551540	1	-3.1468745	1
C	-0.2129955	1	-2.7276827	1	-2.6290852	1
C	-0.3324367	1	-3.1837372	1	-1.3065180	1
C	-0.4172682	1	-3.0452743	1	1.0568118	1
C	-1.5465189	1	-2.8044565	1	1.8247550	1
C	-1.6959780	1	-3.3750082	1	3.0730294	1
C	-0.7055197	1	-4.1899160	1	3.5814483	1
C	0.4255411	1	-4.4236268	1	2.8449480	1
C	0.5816195	1	-3.8493360	1	1.5910048	1
C	0.1202633	1	-1.3747844	1	-4.6535666	1
C	-0.6037198	1	-4.6690914	1	-1.1720513	1
C	0.9129930	1	0.0438845	1	3.1323906	1
C	1.1921296	1	-1.0940898	1	3.8883329	1
C	2.3831212	1	-1.2011517	1	4.5789569	1
C	3.3159292	1	-0.2018335	1	4.5133955	1
C	3.0607582	1	0.9144158	1	3.7436895	1
C	1.8678125	1	1.0342363	1	3.0506439	1
C	-1.4254162	1	0.3582674	1	3.1409380	1
C	-2.7242505	1	0.4335836	1	2.6268581	1
C	-3.1963902	1	0.3679074	1	1.3043025	1
C	-3.0357572	1	0.1584013	1	-1.0537177	1
C	-3.5063855	1	1.3157581	1	-1.6571997	1
C	-4.0518878	1	1.2749751	1	-2.9281795	1
C	-4.1174792	1	0.0970498	1	-3.6191392	1
C	-3.6507837	1	-1.0666924	1	-3.0322297	1
C	-3.1182310	1	-1.0367871	1	-1.7514480	1
C	-1.3214047	1	0.5589848	1	4.6419092	1
C	-4.6953157	1	0.5278223	1	1.1442950	1
H	3.4867981	1	-1.3851120	1	1.9668235	1
H	4.4012333	1	-3.5136309	1	1.9332112	1
H	4.4210615	1	-4.7313494	1	-0.0306996	1
H	3.4804578	1	-3.8553366	1	-1.9272756	1
H	2.6106881	1	-1.7289108	1	-1.9130597	1
H	3.6737177	1	2.9402683	1	-0.1775286	1
H	-1.0447833	1	2.7784134	1	1.9964862	1
H	-3.0069201	1	3.9868968	1	2.1482298	1
H	-3.7988239	1	5.1518389	1	0.3180526	1
H	-2.6216614	1	5.1165422	1	-1.6370817	1
H	-0.6867303	1	3.8761795	1	-1.8362416	1
H	5.2705388	1	1.5468389	1	-0.1709125	1
H	4.9948603	1	0.1408247	1	-0.8045367	1
H	5.0452188	1	0.3021063	1	0.7548539	1

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H     1.1021735  1      4.9228609  1      0.2632330  1
H     1.6463299  1      4.7498719  1     -1.1961085  1
H     2.6464593  1      4.8168230  1      0.0092623  1
H    -1.3979376  1      1.3409093  1     -3.6702540  1
H    -0.8736538  1      3.3343746  1     -4.6864789  1
H     1.2859770  1      4.1071879  1     -4.7161335  1
H     2.9546665  1      2.8458118  1     -3.7375781  1
H     2.4606848  1      0.8182924  1     -2.7611135  1
H    -0.2965137  1     -3.3941651  1     -3.2727342  1
H    -2.2151341  1     -2.2492782  1      1.4936495  1
H    -2.4640208  1     -3.2099853  1      3.5706152  1
H    -0.8065833  1     -4.5778770  1      4.4205981  1
H     1.0956041  1     -4.9708666  1      3.1880904  1
H     1.3589064  1     -4.0027478  1      1.1053214  1
H     0.9781886  1     -1.0226473  1     -4.8950258  1
H    -0.5688384  1     -0.7970317  1     -4.9924791  1
H     0.0154203  1     -2.2516413  1     -5.0282483  1
H    -1.3761310  1     -4.8069439  1     -0.6192460  1
H     0.1573993  1     -5.0999078  1     -0.7730618  1
H    -0.7624754  1     -5.0458127  1     -2.0415422  1
H     0.5717325  1     -1.7868471  1      3.9281242  1
H     2.5507441  1     -1.9564112  1      5.0949023  1
H     4.1139248  1     -0.2740651  1      4.9823435  1
H     3.6965873  1      1.5905657  1      3.6882758  1
H     1.7076821  1      1.7881582  1      2.5287734  1
H    -3.3883874  1      0.5450216  1      3.2678306  1
H    -3.4549032  1      2.1242310  1     -1.2049452  1
H    -4.3753945  1      2.0540328  1     -3.3163940  1
H    -4.4749376  1      0.0767037  1     -4.4775654  1
H    -3.6916606  1     -1.8698090  1     -3.4981881  1
H    -2.8157576  1     -1.8225944  1     -1.3582366  1
H    -2.1451206  1      0.9271584  1      4.9715949  1
H    -0.6013229  1      1.1629603  1      4.8341392  1
H    -1.1545749  1     -0.2845131  1      5.0677254  1
H    -5.0093944  1     -0.0638790  1      0.4580552  1
H    -4.8974049  1      1.4362652  1      0.9011014  1
H    -5.1299827  1      0.3167400  1      1.9746283  1
```

---------- End of file **WEWNOB.mop**----------

---------- Begin of file **WEWNOB.arc**----------

```
                  SUMMARY OF RM1 CALCULATION, Site No: 3560

                MOPAC2012 (Version: 12.290W)
                Wed Nov 21 16:11:22 2012
                No. of days left = 329

         Empirical Formula: C51 H51 N6 Gd  =   109 atoms

RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO = 6
```

```
    PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
    SCF FIELD WAS ACHIEVED

EAT OF FORMATION       =        115.05581 KCAL/MOL =     481.39349 KJ/MOL
OTAL ENERGY            =      -8412.31910 EV
LECTRONIC ENERGY       =    -122385.88358 EV
ORE-CORE REPULSION     =     113973.56448 EV
RADIENT NORM           =          0.23597
IPOLE                  =          0.01612 DEBYE    POINT GROUP:       C3
O. OF FILLED LEVELS    =        144
ONIZATION POTENTIAL    =          8.111636 EV
OMO LUMO ENERGIES (EV) =         -8.112  0.407
OLECULAR WEIGHT        =        905.254
OSMO AREA              =        571.84 SQUARE ANGSTROMS
OSMO VOLUME            =        994.99 CUBIC ANGSTROMS

         MOLECULAR DIMENSIONS (Angstroms)

           Atom       Atom       Distance
           H    84    H    78    13.39892
           H    95    H   101    11.93030
           H    62    H    67    11.39585
         SCF CALCULATIONS        =        448
         COMPUTATION TIME =  4 MINUTES AND  15.344 SECONDS


         FINAL GEOMETRY OBTAINED                                    CHARGE
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO = 6

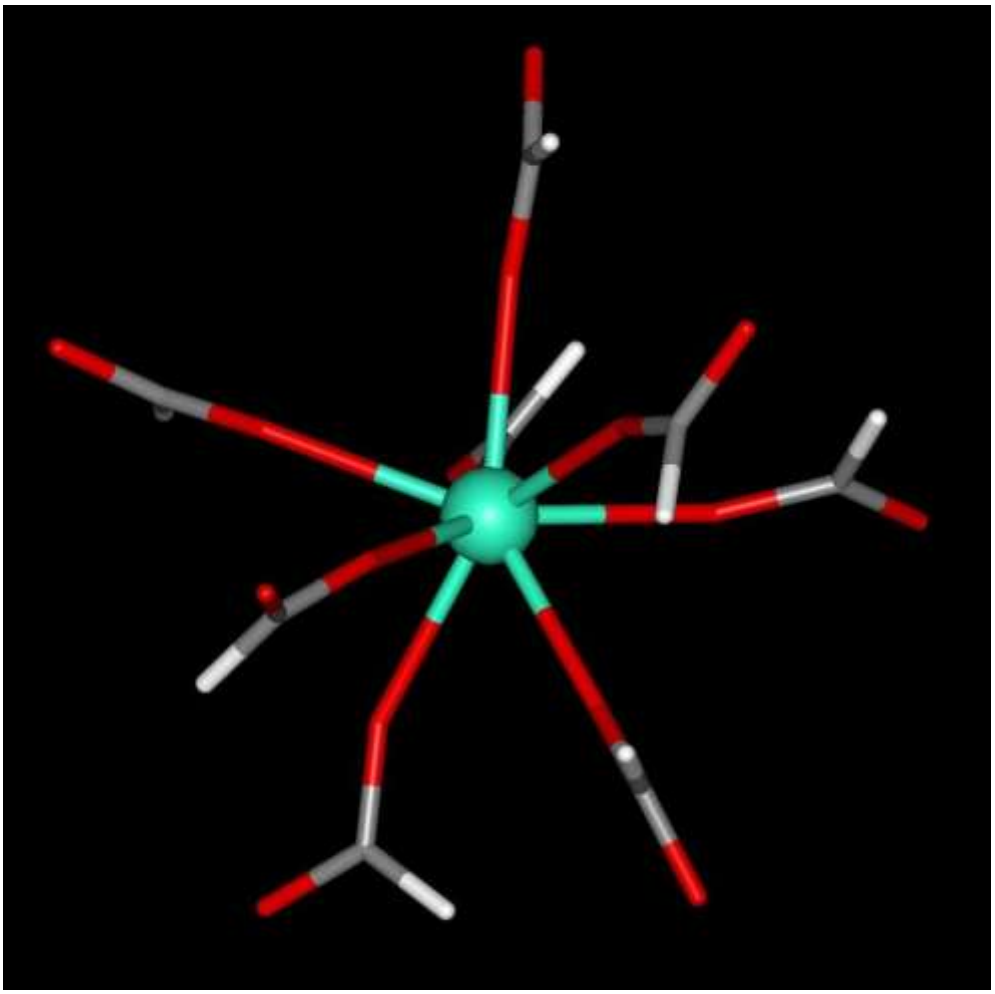
Gd     0.03718224 +1   0.00565421 +1  -0.00409803 +1           3.0000
 N     2.43887156 +1  -0.01490261 +1   0.02357019 +1          -0.7699
 N     0.56339589 +1   2.34887909 +1   0.01118719 +1          -0.7704
 N     0.13736002 +1  -0.30722938 +1  -2.38329249 +1          -0.7702
 N    -0.27514959 +1  -2.36559622 +1  -0.21925653 +1          -0.7701
 N    -0.28580871 +1   0.13919908 +1   2.37242121 +1          -0.7699
 N    -2.34742700 +1   0.22602415 +1   0.17227312 +1          -0.7706
 C     3.11489195 +1  -1.30371763 +1   0.07368939 +1           0.0593
 C     3.63553583 +1  -1.76932597 +1   1.28167275 +1          -0.1299
 C     4.23220746 +1  -3.02219820 +1   1.33045724 +1          -0.0949
 C     4.30700376 +1  -3.80848277 +1   0.18653462 +1          -0.1219
 C     3.78093364 +1  -3.34240385 +1  -1.01217209 +1          -0.0920
 C     3.18769148 +1  -2.08806876 +1  -1.07794854 +1          -0.1224
 C     3.33941935 +1   0.99880867 +1  -0.02560055 +1           0.3695
 C     2.99861133 +1   2.35542926 +1  -0.02688894 +1          -0.5161
 C     1.75562127 +1   2.99603308 +1   0.01185371 +1           0.3705
 C    -0.54072875 +1   3.29786405 +1   0.04261652 +1           0.0587
 C    -1.19442312 +1   3.54967759 +1   1.24941464 +1          -0.1201
 C    -2.29155691 +1   4.40112629 +1   1.26641106 +1          -0.0900
 C    -2.72936229 +1   5.00506241 +1   0.09394797 +1          -0.1198
 C    -2.07008857 +1   4.75598286 +1  -1.10393101 +1          -0.0969
 C    -0.97466642 +1   3.90278516 +1  -1.13720422 +1          -0.1316
 C     4.82266716 +1   0.73270274 +1  -0.07968144 +1          -0.2415
 C     1.83344548 +1   4.50126303 +1   0.05002435 +1          -0.2415
 C     0.38268426 +1   0.86160264 +1  -3.21643470 +1           0.0586
 C    -0.68294641 +1   1.50772817 +1  -3.84349687 +1          -0.1315
 C    -0.44337709 +1   2.65879594 +1  -4.58283086 +1          -0.0970
 C     0.84646760 +1   3.16373644 +1  -4.69688081 +1          -0.1200
 C     1.90425327 +1   2.51505458 +1  -4.07127911 +1          -0.0901
```

C	1.68078701	1.36010059	-3.33295920	-0.1200
C	0.02016206	-1.42474175	-3.14331852	0.3705
C	-0.23150010	-2.70193434	-2.63110050	-0.5161
C	-0.37398649	-3.15759978	-1.31637300	0.3697
C	-0.41347994	-3.15038009	0.99931840	0.0585
C	-1.61984809	-3.12717043	1.69993098	-0.1221
C	-1.72690588	-3.82539482	2.89595154	-0.0918
C	-0.64692971	-4.55005487	3.38521537	-0.1218
C	0.55136267	-4.57198616	2.68103400	-0.0949
C	0.67582006	-3.87257446	1.48798677	-0.1299
C	0.15085631	-1.37247825	-4.64447880	-0.2415
C	-0.64757394	-4.63571989	-1.19829357	-0.2415
C	0.88564171	0.03606195	3.23126622	0.0593
C	1.17119240	-1.16732540	3.87727980	-0.1299
C	2.31926499	-1.27098759	4.65148941	-0.0949
C	3.18029141	-0.18706440	4.77810135	-0.1219
C	2.89401269	1.00687122	4.12740649	-0.0917
C	1.74485655	1.12823740	3.35653886	-0.1223
C	-1.40880002	0.32507518	3.11087034	0.3696
C	-2.69784408	0.41369312	2.57503919	-0.5159
C	-3.15538594	0.35334553	1.25452123	0.3705
C	-3.12783871	0.20870792	-1.05700693	0.0586
C	-3.55240269	1.40740682	-1.63060557	-0.1315
C	-4.24155035	1.38084657	-2.83613652	-0.0970
C	-4.50631904	0.17073602	-3.46631359	-0.1199
C	-4.08147749	-1.02030945	-2.89003411	-0.0901
C	-3.39525857	-1.00959103	-1.68260140	-0.1200
C	-1.35227527	0.44957959	4.61255448	-0.2415
C	-4.65326418	0.44801668	1.11080272	-0.2415
H	3.56418304	-1.15732409	2.18877289	0.1278
H	4.64453698	-3.39074705	2.27435299	0.1039
H	4.78052145	-4.79322688	0.22986731	0.1051
H	3.83637933	-3.96339947	-1.91124551	0.1058
H	2.77944674	-1.72506343	-2.02706514	0.1230
H	3.85746185	3.03787914	-0.05906038	0.1332
H	-0.85344736	3.07710707	2.17647875	0.1223
H	-2.81177401	4.59645949	2.20884403	0.1058
H	-3.59150572	5.67754436	0.11420159	0.1050
H	-2.41394887	5.23403127	-2.02589351	0.1037
H	-0.46311543	3.70116918	-2.08553479	0.1269
H	5.41888230	1.62185407	-0.33500762	0.0823
H	5.09096837	-0.02812699	-0.82912658	0.0926
H	5.19827805	0.38087015	0.89339655	0.0942
H	1.21425867	4.93576022	0.85022191	0.0928
H	1.49587519	4.94128417	-0.90097818	0.0944
H	2.85069927	4.88487720	0.22081928	0.0823
H	-1.70295968	1.11795698	-3.74744322	0.1268
H	-1.27497170	3.16899417	-5.07770036	0.1037
H	1.02927138	4.07055890	-5.28011643	0.1050
H	2.91913804	2.91397495	-4.16009504	0.1058
H	2.51830738	0.85282496	-2.84268680	0.1225
H	-0.33071022	-3.48377881	-3.39482202	0.1332
H	-2.47647420	-2.56217165	1.31754599	0.1229
H	-2.66868958	-3.80585283	3.45236842	0.1057
H	-0.74010979	-5.10394596	4.32346410	0.1051
H	1.40155784	-5.14183312	3.06729730	0.1040
H	1.62694880	-3.87872180	0.94220274	0.1279
H	1.05166648	-0.83044480	-4.97187284	0.0928
H	-0.71674357	-0.87227905	-5.10161480	0.0943
H	0.21510522	-2.36520364	-5.11503913	0.0823
H	-1.47839022	-4.86085253	-0.51157907	0.0926

H	0.23831236 +1	-5.17416314 +1	-0.82803914 +1	0.0941
H	-0.91747794 +1	-5.10975827 +1	-2.15412102 +1	0.0823
H	0.50232948 +1	-2.02911993 +1	3.76581091 +1	0.1277
H	2.54618068 +1	-2.21106021 +1	5.16289676 +1	0.1039
H	4.08219661 +1	-0.27366286 +1	5.39039920 +1	0.1051
H	3.57413575 +1	1.85839883 +1	4.22418587 +1	0.1057
H	1.52282525 +1	2.07389491 +1	2.85094974 +1	0.1228
H	-3.48994462 +1	0.55193598 +1	3.32191697 +1	0.1332
H	-3.33751456 +1	2.36420992 +1	-1.14078412 +1	0.1268
H	-4.57771858 +1	2.31777075 +1	-3.28994612 +1	0.1037
H	-5.05070930 +1	0.15565488 +1	-4.41460948 +1	0.1050
H	-4.28829322 +1	-1.97243066 +1	-3.38774868 +1	0.1058
H	-3.06326171 +1	-1.95116563 +1	-1.23279639 +1	0.1225
H	-2.29274270 +1	0.80650896 +1	5.05905004 +1	0.0823
H	-0.57765084 +1	1.15502174 +1	4.95138600 +1	0.0926
H	-1.13907234 +1	-0.52227336 +1	5.08353825 +1	0.0942
H	-5.06740091 +1	-0.34626969 +1	0.47038581 +1	0.0928
H	-4.94996050 +1	1.41220201 +1	0.66996930 +1	0.0943
H	-5.19276579 +1	0.36941190 +1	2.06673805 +1	0.0823

---------- End of file **WEWNOB.arc**----------

Terbium: SEGVEF



---------- Begin of file **SEGVEF.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=-5.0
NUMERO DE COORDENAÇÃO = 8

 Tb     0.0000000  1     0.0000000  1     0.0000000  1
  O     2.3893000  1     0.0000000  1     0.0000000  1
  O     0.2737100  1     1.5713989  1     1.8135544  1
  O     0.7765669  1    -0.7118557  1    -2.1949354  1
  O     0.4163310  1     2.2029450  1    -0.8880043  1
  O    -1.9944908  1     0.0239848  1     1.3153652  1
  O     0.7856180  1    -1.5072775  1     1.7157001  1
  O    -1.8636181  1     0.6462704  1    -1.4270737  1
  O    -0.8144106  1    -2.2268781  1    -0.4383116  1
  O     4.5905660  1     0.3721345  1     0.0000000  1
  O     1.0742794  1    -0.7375371  1    -4.4088604  1
  O     1.2194569  1     3.9432486  1    -1.8800524  1
  O     1.0236420  1     2.5242982  1     3.6714486  1
  C     3.4143389  1     0.7625632  1     0.0941034  1
  C     1.0991487  1     1.7122570  1     2.8063641  1
  C     0.6480822  1    -0.2585714  1    -3.4026618  1
  C     1.3082324  1     2.8249676  1    -1.5105071  1
```

```
 H     3.2447664  1     1.7785434  1     0.2580502  1
 H     1.7007501  1     1.6870740  1     2.8941928  1
 H     0.1076396  1     0.6410957  1    -3.5061126  1
 H     2.2016843  1     2.3153725  1    -1.7210933  1
 C    -2.7907141  1    -0.7247341  1     1.9835040  1
 C     0.6445050  1    -1.6067402  1     3.0028737  1
 C    -2.4168129  1     0.1519013  1    -2.4901953  1
 C    -1.8954465  1    -2.8603707  1    -0.4458975  1
 O    -3.8282838  1    -0.3259270  1     2.5395637  1
 H    -2.5487673  1    -1.7363434  1     2.0606875  1
 O     1.1918882  1    -2.3902863  1     3.7099172  1
 H     0.1904131  1    -1.5726485  1     3.4064956  1
 O    -3.3312996  1     0.6013804  1    -3.1108162  1
 H    -2.0136452  1    -0.7560553  1    -2.8441045  1
 O    -2.0136331  1    -3.9912576  1    -0.7658352  1
 H    -2.7622828  1    -2.3491687  1    -0.1466362  1
```

---------- End of file **SEGVEF.mop**----------

---------- Begin of file **SEGVEF.arc**----------

```
           SUMMARY OF RM1 CALCULATION, Site No: 3560

                                MOPAC2012 (Version: 12.203W)
                                Tue Oct 30 13:57:30 2012
                                No. of days left = 264

            Empirical Formula: C8 H8 O16 Tb  =    33 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=-5.0
 NUMERO DE COORDENAÇÃO = 8


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =       -461.59602 KCAL/MOL =   -1931.31776 KJ/MOL
TOTAL ENERGY            =      -6213.28977 EV
ELECTRONIC ENERGY       =     -36875.35436 EV
CORE-CORE REPULSION     =      30662.06459 EV
GRADIENT NORM           =          1.63180
DIPOLE                  =          2.99316 DEBYE    POINT GROUP:       C1
NO. OF FILLED LEVELS    =         72
CHARGE ON SYSTEM        =         -5
IONIZATION POTENTIAL    =         -4.299210 EV
HOMO LUMO ENERGIES (EV) =          4.299 16.474
MOLECULAR WEIGHT        =        519.067
COSMO AREA              =        360.24 SQUARE ANGSTROMS
COSMO VOLUME            =        440.49 CUBIC ANGSTROMS
```

MOLECULAR DIMENSIONS (Angstroms)

Atom		Atom		Distance
O	32	O	12	11.63464
O	32	O	12	8.71463
O	11	H	19	2.95081

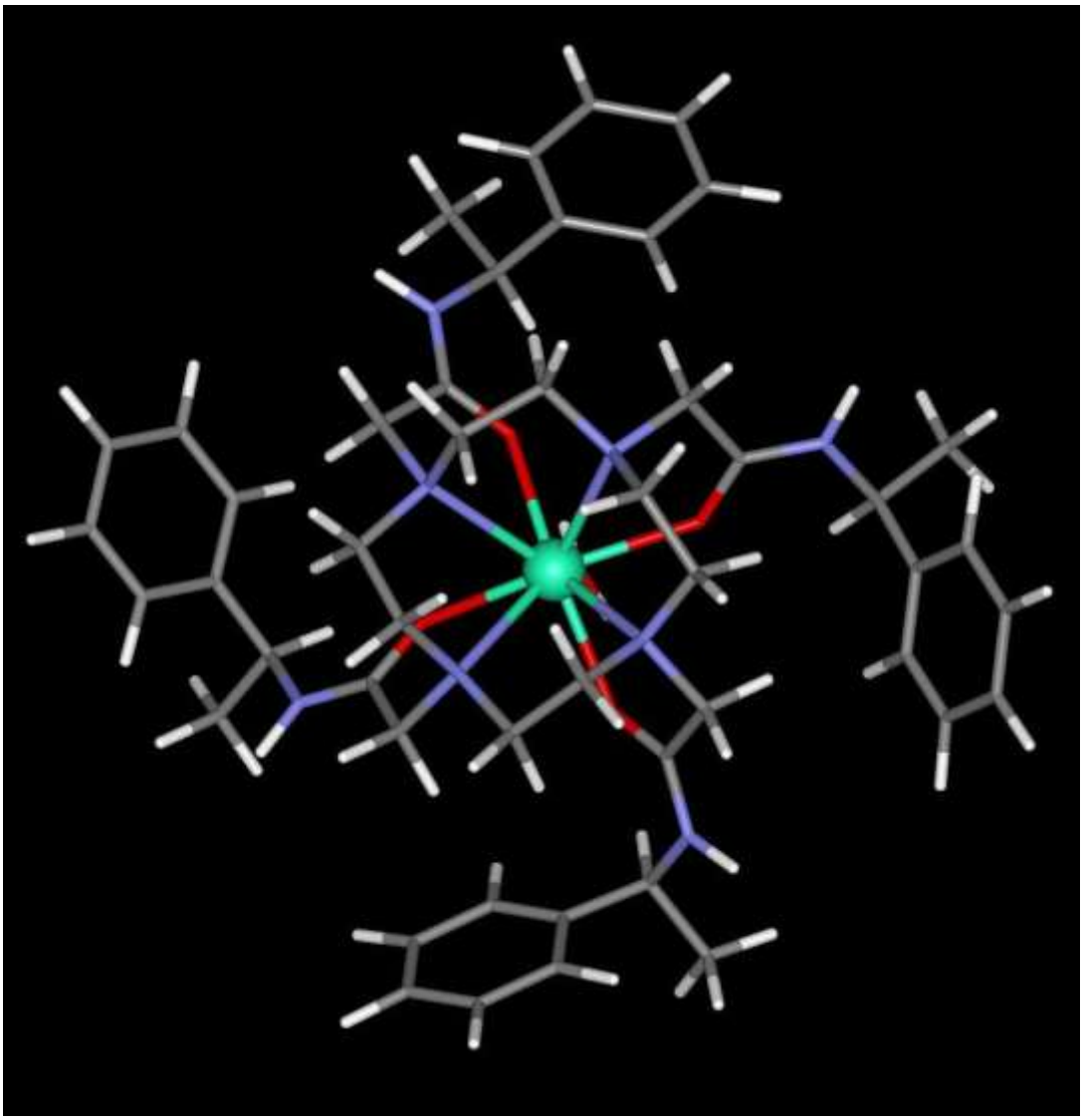
SCF CALCULATIONS = 838
COMPUTATION TIME = 48.953 SECONDS

FINAL GEOMETRY OBTAINED CHARGE
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=-5.0
NUMERO DE COORDENAÇÃO = 8

Tb	0.11770788 +1	-0.02394856 +1	-0.16254403 +1	3.0000
O	2.53303933 +1	-0.25085723 +1	-0.21465758 +1	-0.7552
O	0.89124650 +1	1.49462433 +1	1.57019166 +1	-0.7481
O	0.77143723 +1	-0.64994465 +1	-2.41190632 +1	-0.7608
O	0.59899111 +1	2.15347690 +1	-1.11606922 +1	-0.7599
O	-1.71748586 +1	0.24275858 +1	1.40435998 +1	-0.7525
O	0.67835588 +1	-1.46457610 +1	1.71497135 +1	-0.7435
O	-1.83203021 +1	0.59991405 +1	-1.46331557 +1	-0.7572
O	-0.93360616 +1	-2.20298243 +1	-0.32821812 +1	-0.7621
O	4.73534382 +1	-0.59560945 +1	-0.33569040 +1	-0.6619
O	1.28442701 +1	-1.30757919 +1	-4.48211726 +1	-0.6649
O	1.13113211 +1	4.08246903 +1	-2.10076852 +1	-0.6667
O	1.66010564 +1	3.00548179 +1	3.02227118 +1	-0.6645
C	3.73342362 +1	0.05452446 +1	0.05900934 +1	0.4413
C	1.05942367 +1	1.93463943 +1	2.74696723 +1	0.4421
C	1.42988439 +1	-0.54502557 +1	-3.49201298 +1	0.4478
C	0.78685762 +1	3.40872604 +1	-1.09477217 +1	0.4405
H	3.90484493 +1	0.96083254 +1	0.69052014 +1	-0.0242
H	0.65017714 +1	1.32708934 +1	3.59218655 +1	-0.0292
H	2.18145941 +1	0.27872917 +1	-3.56192779 +1	-0.0221
H	0.63050859 +1	3.93954823 +1	-0.12501681 +1	-0.0140
C	-2.83967454 +1	-0.01018209 +1	1.93750676 +1	0.4445
C	0.71889505 +1	-1.84103258 +1	2.92425856 +1	0.4370
C	-2.57389961 +1	0.64911624 +1	-2.49119121 +1	0.4445
C	-1.17205820 +1	-3.39372153 +1	0.04397932 +1	0.4319
O	-3.31711873 +1	0.62256136 +1	2.91438646 +1	-0.6637
H	-3.43650106 +1	-0.85412903 +1	1.51120716 +1	-0.0282
O	1.22016620 +1	-2.92719890 +1	3.31349818 +1	-0.6617
H	0.27741721 +1	-1.15943458 +1	3.69437304 +1	-0.0313
O	-3.67238640 +1	1.26067331 +1	-2.53985276 +1	-0.6647
H	-2.22433141 +1	0.11276483 +1	-3.40707903 +1	-0.0227
O	-2.00648625 +1	-4.14929450 +1	-0.51909909 +1	-0.6652
H	-0.60476793 +1	-3.78385493 +1	0.92271935 +1	-0.0051

---------- End of file **SEGVEF.arc**----------

Dysprosium: TUQTUU



---------- Begin of file **TUQTUU.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
NUMERO DE COORDENAÇÃO= 9

 Dy     0.0000000  1      0.0000000  1      0.0000000  1
  O     2.3433000  1      0.0000000  1      0.0000000  1
  O     0.2380334  1      2.3137883  1      0.0000000  1
  O    -1.8569542  1      0.4814148  1     -1.2836464  1
  O     0.1795788  1     -1.9596941  1     -1.3428255  1
  O     0.7761963  1      0.7187132  1     -2.1787736  1
  N    -2.1047519  1     -1.4943444  1      0.5906424  1
  N    -1.7432635  1      1.2606860  1      1.5907666  1
  N     1.0573863  1      0.6685125  1      2.3439588  1
  N     0.7030414  1     -2.1090847  1      1.3640835  1
  N    -0.4590173  1      4.4369249  1      0.3634656  1
```

H	-1.0344338	1	4.9504715	1	0.7430415	1
N	0.7137801	1	-4.1469008	1	-1.6420903	1
H	1.0901770	1	-4.8386547	1	-1.2972919	1
N	-3.8599251	1	0.0324038	1	-2.2006523	1
H	-4.5275817	1	-0.5098515	1	-2.2395743	1
N	4.3491712	1	0.4575573	1	0.8979137	1
H	4.7932961	1	0.8098294	1	1.5455725	1
C	3.0364119	1	0.5075392	1	0.9087079	1
C	-1.2359234	1	1.2975902	1	2.9992233	1
H	-1.3700716	1	0.4267116	1	3.4083530	1
H	-1.7476219	1	1.9465762	1	3.5055142	1
C	-0.5921491	1	3.1427819	1	0.4567797	1
C	0.6768616	1	5.0368073	1	-0.3903463	1
H	0.7108250	1	4.6252228	1	-1.2794092	1
C	1.2226164	1	-0.5495490	1	3.2027517	1
H	0.3785374	1	-0.7412629	1	3.6418882	1
H	1.8754465	1	-0.3590533	1	3.8945740	1
C	-0.4777514	1	-2.7950651	1	1.9573647	1
H	-0.7386838	1	-2.3279776	1	2.7663452	1
H	-0.2248782	1	-3.6978253	1	2.2074870	1
C	-1.8841377	1	2.6188941	1	1.0909347	1
H	-2.1365746	1	3.2039479	1	1.8230905	1
H	-2.5938227	1	2.6434016	1	0.4310235	1
C	0.2365407	1	1.6582280	1	3.0684978	1
H	0.3717696	1	2.5371256	1	2.6787557	1
H	0.5190003	1	1.6953088	1	3.9955111	1
C	1.6633977	1	-1.7794165	1	2.4398916	1
H	2.5379933	1	-1.6214803	1	2.0540083	1
H	1.7347165	1	-2.5292782	1	3.0507377	1
C	3.4443857	1	4.9347908	1	2.2301658	1
H	3.5761688	1	5.2019135	1	3.1118092	1
C	-3.0647405	1	0.5982673	1	1.5743057	1
H	-3.5267233	1	0.8282847	1	0.7512164	1
H	-3.5953774	1	0.9274644	1	2.3156533	1
C	-2.8940136	1	-1.5862517	1	-0.6647155	1
H	-3.8142878	1	-1.8118444	1	-0.4557049	1
H	-2.5327807	1	-2.2898345	1	-1.2263043	1
C	2.0044324	1	4.7759603	1	0.3104934	1
C	-1.3887047	1	-4.1814967	1	-2.9141589	1
C	-3.4709769	1	-3.1874815	1	-3.7244346	1
H	-3.9139421	1	-2.5771875	1	-4.2681855	1
C	-4.1913073	1	-4.0323137	1	-2.8594737	1
H	-5.1211984	1	-4.0064455	1	-2.8499172	1
C	-3.5229931	1	-4.8911013	1	-2.0345917	1
H	-4.0036416	1	-5.4138330	1	-1.4343778	1
C	2.2284140	1	5.1380329	1	1.6176031	1
H	1.5391901	1	5.5308311	1	2.1043089	1
C	0.1152624	1	-4.2663397	1	-2.9725869	1
H	0.4415630	1	-3.5263332	1	-3.5253386	1
C	-2.8527334	1	-0.2648825	1	-1.4119628	1
C	-1.6786877	1	-2.8598429	1	1.0141404	1
H	-1.4443484	1	-3.3825187	1	0.2307086	1
H	-2.4149069	1	-3.3037005	1	1.4619285	1
C	0.5888987	1	-5.5747869	1	-3.6003943	1
H	1.5474102	1	-5.5903582	1	-3.6228072	1
H	0.2476013	1	-5.6430137	1	-4.4957231	1
H	0.2661038	1	-6.3133134	1	-3.0803495	1
C	2.3746097	1	1.2536057	1	2.0377062	1
H	2.9380582	1	1.2138955	1	2.8271411	1
H	2.2673455	1	2.1864616	1	1.7928586	1
C	-2.0780094	1	-3.2835897	1	-3.7492739	1

```
H   -1.5966699  1    -2.7435072  1    -4.3314432  1
C    1.3962805  1    -3.0495112  1     0.4028946  1
H    1.3744296  1    -3.9528943  1     0.7541093  1
H    2.3243796  1    -2.7853833  1     0.3002072  1
C    0.3840581  1     6.5132237  1    -0.5590885  1
H   -0.4585346  1     6.6236489  1    -1.0069682  1
H    1.0778780  1     6.9198191  1    -1.0824759  1
H    0.3460291  1     6.9319582  1     0.3030483  1
C   -2.1336047  1    -4.9962467  1    -2.0789386  1
H   -1.7030769  1    -5.6196799  1    -1.5394362  1
C    0.7001596  1    -3.0043651  1    -0.9401565  1
C    4.2746154  1     3.9596566  1     0.2119076  1
H    4.9688450  1     3.5609896  1    -0.2611927  1
C    4.4718177  1     4.3312113  1     1.5293769  1
H    5.2900647  1     4.1766546  1     1.9391986  1
C   -4.4689781  1     4.3624061  1    -0.8856403  1
H   -3.9633141  1     5.0491237  1    -0.5131632  1
C   -3.8915643  1     1.2586887  1    -3.0234820  1
H   -2.9671669  1     1.5411641  1    -3.1886291  1
C   -3.8575072  1     3.3942067  1    -1.7139580  1
H   -2.9506790  1     3.4533300  1    -1.9082916  1
C   -4.5984198  1     2.3718797  1    -2.2255803  1
C   -4.5373068  1     0.9355632  1    -4.3618149  1
H   -4.0424141  1     0.2358358  1    -4.7945444  1
H   -4.5359108  1     1.7180213  1    -4.9157670  1
H   -5.4414224  1     0.6441900  1    -4.2188843  1
C    6.5062274  1     0.3570955  1    -0.2147535  1
H    6.4753428  1     1.3164737  1    -0.2816008  1
H    6.9918892  1     0.0016169  1    -0.9624056  1
H    6.9439139  1     0.1072601  1     0.6020872  1
C    5.2173090  1    -2.3520045  1     1.0841566  1
H    5.3666317  1    -1.8578102  1     1.8575833  1
C   -2.9465487  1    -0.9075858  1     1.6761064  1
H   -2.5589407  1    -1.1369244  1     2.5360031  1
H   -3.8324707  1    -1.2991342  1     1.6365044  1
C    5.0775005  1    -0.2002592  1    -0.2196171  1
H    4.6499662  1     0.0639729  1    -1.0611560  1
C    5.1886320  1    -3.7419586  1     1.1431253  1
H    5.3006575  1    -4.1805305  1     1.9555323  1
C    5.0241157  1    -1.7045491  1    -0.1185479  1
C   -5.8057619  1     4.2797934  1    -0.6349158  1
H   -6.2046582  1     4.9054186  1    -0.0727328  1
C   -5.9505092  1     2.3104251  1    -1.9913699  1
H   -6.4521230  1     1.6174327  1    -2.3584121  1
C   -6.5821054  1     3.2834287  1    -1.1988902  1
H   -7.5018241  1     3.2589011  1    -1.0584683  1
C    3.0259419  1     4.1764338  1    -0.4243832  1
H    2.8935774  1     3.9260364  1    -1.3101003  1
C    4.8397196  1    -2.4291338  1    -1.2658192  1
H    4.7022677  1    -2.0138030  1    -2.0867207  1
C    4.9969485  1    -4.4362148  1     0.0171744  1
H    4.9538839  1    -5.3646247  1     0.0661937  1
C    4.8676154  1    -3.8658102  1    -1.1416937  1
H    4.7938231  1    -4.3904621  1    -1.9054118  1
H    0.5339177  1     1.7229262  1    -2.7812967  1
H    1.3955082  1     0.0821286  1    -3.4222778  1
0
```

---------- End of file **TUQTUU.mop**----------

---------- Begin of file **TUQTUU.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No: 3560

                              MOPAC2012 (Version: 12.290W)
                              Wed Nov 21 16:23:08 2012
                              No. of days left = 329

           Empirical Formula: C48 H66 N8 O5 Dy  =   128 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO= 9


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =        305.12044 KCAL/MOL =    1276.62392 KJ/MOL
TOTAL ENERGY            =     -10235.06570 EV
ELECTRONIC ENERGY       =    -149466.99194 EV
CORE-CORE REPULSION     =     139231.92624 EV
GRADIENT NORM           =          0.24909
DIPOLE                  =          8.42248 DEBYE    POINT GROUP:       C1
NO. OF FILLED LEVELS    =        164
CHARGE ON SYSTEM        =          3
IONIZATION POTENTIAL    =         15.665750 EV
HOMO LUMO ENERGIES (EV) =        -15.666 -6.979
MOLECULAR WEIGHT        =        997.600
COSMO AREA              =        674.90 SQUARE ANGSTROMS
COSMO VOLUME            =       1099.30 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H   124    H   114    16.18489
            H   124    H   114    16.16730
            H    79    H   106     6.84848
          SCF CALCULATIONS        =       1383
          COMPUTATION TIME = 16 MINUTES AND   7.375 SECONDS


          FINAL GEOMETRY OBTAINED                                      CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO= 9

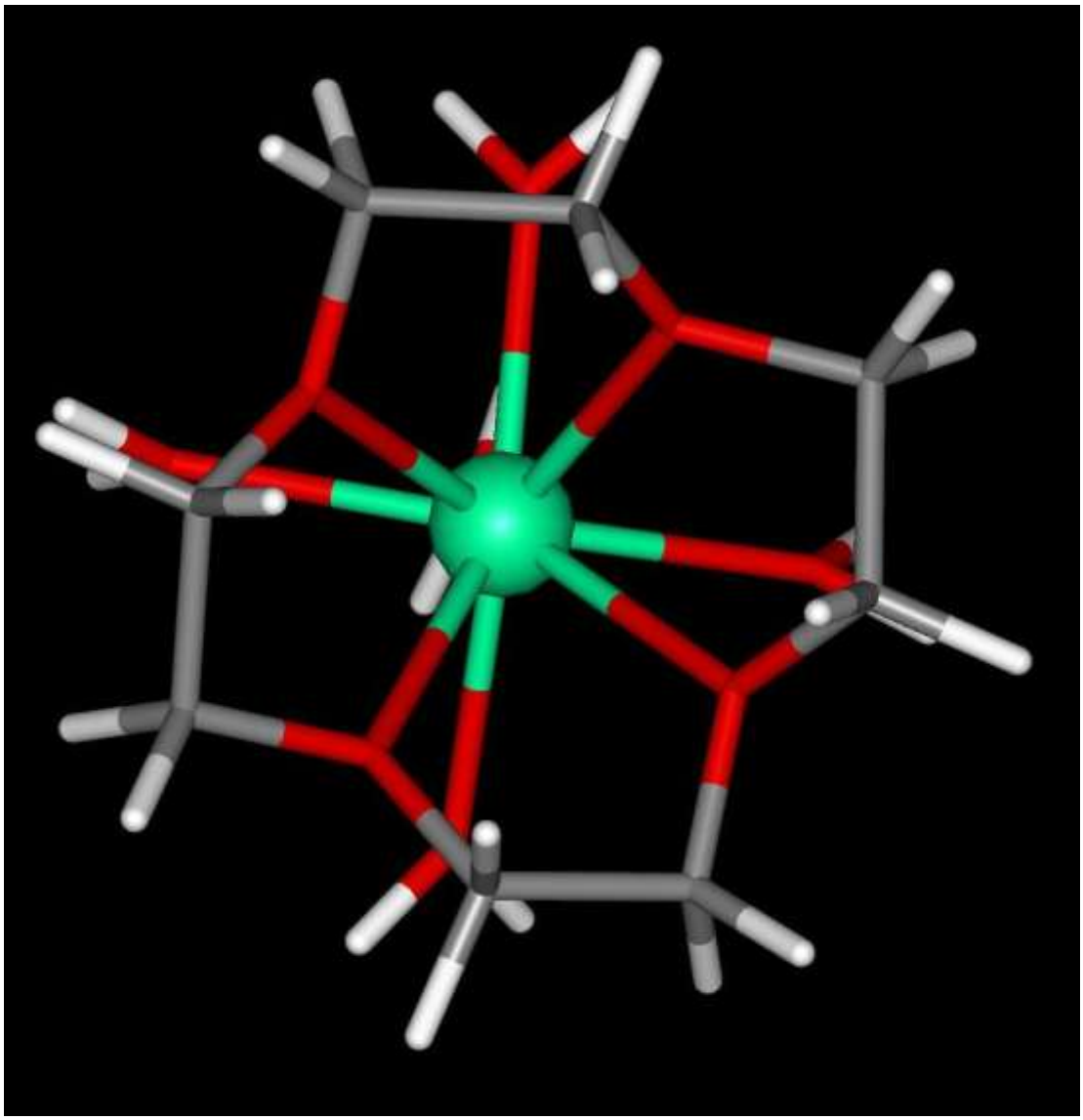
 Dy     0.01956531 +1   0.05951876 +1  -0.24579157 +1              3.0000
  O     2.42430398 +1   0.00336780 +1  -0.16886429 +1             -0.7202
  O     0.19920889 +1   2.45880516 +1  -0.25003700 +1             -0.7287
  O    -2.04848079 +1   0.40178476 +1  -1.42772513 +1             -0.7210
  O     0.19650578 +1  -2.03332910 +1  -1.41481493 +1             -0.7273
  O     0.72033630 +1   0.76372344 +1  -2.44703597 +1             -0.5803
  N    -2.10950452 +1  -1.34792104 +1   0.49990303 +1             -0.4625
```

N	-1.56503091	+1	1.43093259 +1	1.38840576 +1	-0.4621
N	1.22597105	+1	0.67865078 +1	2.04175600 +1	-0.4624
N	0.68061414	+1	-2.10077359 +1	1.15485182 +1	-0.4620
N	-0.23132130	+1	4.67342442 +1	0.18467635 +1	-0.3456
H	-0.85814384	+1	5.36637999 +1	0.59932028 +1	0.2775
N	0.65021280	+1	-4.23726716 +1	-1.87772201 +1	-0.3458
H	1.05611208	+1	-5.12065971 +1	-1.56217106 +1	0.2772
N	-4.19276275	+1	0.10836143 +1	-2.20088942 +1	-0.3468
H	-5.04073047	+1	-0.46204926 +1	-2.19784269 +1	0.2767
N	4.59209439	+1	0.30947899 +1	0.52937999 +1	-0.3469
H	5.22641314	+1	0.69386211 +1	1.23242905 +1	0.2766
C	3.26887355	+1	0.44122275 +1	0.67218421 +1	0.4362
C	-1.00950196	+1	1.48409186 +1	2.80696572 +1	-0.0729
H	-1.19907847	+1	0.50628408 +1	3.32312788 +1	0.1010
H	-1.52503246	+1	2.22680862 +1	3.46585250 +1	0.1227
C	-0.52530917	+1	3.37122086 +1	0.25873681 +1	0.4374
C	1.02533153	+1	5.18493033 +1	-0.44399603 +1	0.1503
H	1.30738554	+1	4.49492324 +1	-1.28810035 +1	0.1007
C	1.28076937	+1	-0.51403316 +1	2.98965622 +1	-0.0722
H	0.27644214	+1	-0.66217231 +1	3.46673298 +1	0.1002
H	1.96087370	+1	-0.36269922 +1	3.86499342 +1	0.1225
C	-0.52333522	+1	-2.70723578 +1	1.86646300 +1	-0.0727
H	-0.76848436	+1	-2.10036117 +1	2.77750842 +1	0.1006
H	-0.33478124	+1	-3.72906702 +1	2.28111111 +1	0.1226
C	-1.79822405	+1	2.87481708 +1	0.93641902 +1	-0.1173
H	-2.14503211	+1	3.55017328 +1	1.75436354 +1	0.1289
H	-2.61779948	+1	2.93579366 +1	0.16964473 +1	0.1570
C	0.49402735	+1	1.78536358 +1	2.79558761 +1	-0.0586
H	0.70516200	+1	2.78029743 +1	2.33842036 +1	0.1170
H	0.85225593	+1	1.90820927 +1	3.84901533 +1	0.1187
C	1.70078660	+1	-1.78856729 +1	2.24694114 +1	-0.0578
H	2.72458299	+1	-1.68954495 +1	1.81631219 +1	0.1184
H	1.81795907	+1	-2.62133214 +1	2.98598381 +1	0.1181
C	2.92811116	+1	6.07490707 +1	2.70553597 +1	-0.0917
H	2.78739334	+1	6.68029194 +1	3.60883621 +1	0.1376
C	-2.95298454	+1	0.80494008 +1	1.50375675 +1	-0.0577
H	-3.57363542	+1	1.04959241 +1	0.61025457 +1	0.1185
H	-3.55268267	+1	1.22607749 +1	2.35013821 +1	0.1181
C	-3.15046802	+1	-1.51512468 +1	-0.60999019 +1	-0.1186
H	-4.16880312	+1	-1.77500839 +1	-0.23464919 +1	0.1290
H	-2.88796816	+1	-2.36809470 +1	-1.29270465 +1	0.1554
C	2.09635795	+1	5.23171266 +1	0.60829523 +1	-0.1330
C	-1.45086478	+1	-4.55068701 +1	-3.06195763 +1	-0.1318
C	-3.75865686	+1	-4.02783107 +1	-3.50319055 +1	-0.1246
H	-4.51326931	+1	-3.37779491 +1	-3.95788031 +1	0.1189
C	-4.14788141	+1	-5.21222303 +1	-2.88831129 +1	-0.0707
H	-5.20802570	+1	-5.48813648 +1	-2.84502175 +1	0.1350
C	-3.18633696	+1	-6.06316330 +1	-2.35372426 +1	-0.0932
H	-3.49163198	+1	-7.00665448 +1	-1.88600776 +1	0.1371
C	1.90654287	+1	5.97793567 +1	1.76804667 +1	-0.0894
H	0.97250254	+1	6.51935214 +1	1.94796201 +1	0.1114
C	0.00666517	+1	-4.22668855 +1	-3.22730602 +1	0.1497
H	0.15307858	+1	-3.20653656 +1	-3.68162221 +1	0.1035
C	-3.13861091	+1	-0.24876760 +1	-1.45944463 +1	0.4369
C	-1.73902736	+1	-2.76335784 +1	0.93370342 +1	-0.0584
H	-1.53983135	+1	-3.40826576 +1	0.04592995 +1	0.1175
H	-2.57638963	+1	-3.29524065 +1	1.45227197 +1	0.1186
C	0.68854056	+1	-5.26895656 +1	-4.11184352 +1	-0.2417
H	1.75595710	+1	-5.05656695 +1	-4.27388457 +1	0.0918
H	0.21949357	+1	-5.28653974 +1	-5.10981177 +1	0.1232
H	0.61716437	+1	-6.29937419 +1	-3.73189729 +1	0.0979

C	2.66089716 +1	1.18023689 +1	1.85974568 +1	-0.1183
H	3.28371402 +1	1.10298212 +1	2.78254430 +1	0.1290
H	2.68343163 +1	2.27536549 +1	1.61002826 +1	0.1545
C	-2.41217572 +1	-3.69369946 +1	-3.58916592 +1	-0.1014
H	-2.11829720 +1	-2.77664884 +1	-4.10956113 +1	0.1088
C	1.31026438 +1	-3.20640203 +1	0.30341889 +1	-0.1179
H	1.25981303 +1	-4.21740712 +1	0.77313491 +1	0.1288
H	2.41061116 +1	-3.03171818 +1	0.15530966 +1	0.1567
C	0.76768447 +1	6.58094535 +1	-1.00830845 +1	-0.2417
H	0.00350686 +1	6.58511285 +1	-1.79983366 +1	0.0915
H	1.68862941 +1	6.98398072 +1	-1.46186649 +1	0.1233
H	0.45840702 +1	7.32226495 +1	-0.25608390 +1	0.0984
C	-1.83862821 +1	-5.73543195 +1	-2.44216515 +1	-0.0902
H	-1.09754329 +1	-6.43588212 +1	-2.04449869 +1	0.1115
C	0.66893092 +1	-3.16447023 +1	-1.07979598 +1	0.4379
C	4.32668717 +1	4.68259442 +1	1.32831695 +1	-0.1224
H	5.29437009 +1	4.20703177 +1	1.13837291 +1	0.1190
C	4.14145691 +1	5.43202504 +1	2.48445006 +1	-0.0688
H	4.95671450 +1	5.53571696 +1	3.21021208 +1	0.1358
C	-4.37720698 +1	4.72663246 +1	-1.31203908 +1	-0.1236
H	-3.79751494 +1	5.65458622 +1	-1.27391460 +1	0.1186
C	-4.21411887 +1	1.35802736 +1	-3.02076497 +1	0.1487
H	-3.17497692 +1	1.54092610 +1	-3.41509015 +1	0.1054
C	-3.91355258 +1	3.64844313 +1	-2.05669201 +1	-0.1036
H	-2.96683625 +1	3.73680453 +1	-2.59890351 +1	0.1077
C	-4.67969638 +1	2.49059776 +1	-2.15030972 +1	-0.1303
C	-5.16825500 +1	1.16441375 +1	-4.19805355 +1	-0.2411
H	-4.85491519 +1	0.35141658 +1	-4.87000054 +1	0.0915
H	-5.20535665 +1	2.07932656 +1	-4.81261593 +1	0.1226
H	-6.20934862 +1	0.96049404 +1	-3.90534154 +1	0.0977
C	6.60108824 +1	0.13027153 +1	-0.88106218 +1	-0.2410
H	6.57875451 +1	1.19039755 +1	-1.17463230 +1	0.0913
H	7.07776981 +1	-0.41356086 +1	-1.71366344 +1	0.1227
H	7.29630272 +1	0.04300889 +1	-0.03245109 +1	0.0977
C	5.97303324 +1	-2.27190569 +1	0.92221360 +1	-0.0911
H	6.42636315 +1	-1.52968608 +1	1.58667280 +1	0.1111
C	-2.81628174 +1	-0.71125546 +1	1.69111460 +1	-0.0722
H	-2.24369246 +1	-0.93106412 +1	2.63026947 +1	0.1001
H	-3.82672587 +1	-1.14407701 +1	1.89932258 +1	0.1226
C	5.20872877 +1	-0.43676157 +1	-0.60986252 +1	0.1487
H	4.56563287 +1	-0.28599611 +1	-1.52223079 +1	0.1054
C	6.11184331 +1	-3.62013714 +1	1.22965390 +1	-0.0923
H	6.66149183 +1	-3.92360438 +1	2.12850464 +1	0.1370
C	5.29887756 +1	-1.88855133 +1	-0.23388971 +1	-0.1307
C	-5.60100157 +1	4.65019167 +1	-0.65722315 +1	-0.0708
H	-5.97851695 +1	5.51090751 +1	-0.09274511 +1	0.1352
C	-5.90373116 +1	2.41033423 +1	-1.49201974 +1	-0.0910
H	-6.53420174 +1	1.51947537 +1	-1.57423417 +1	0.1113
C	-6.36124451 +1	3.48876855 +1	-0.74420276 +1	-0.0923
H	-7.33517011 +1	3.43481164 +1	-0.24352575 +1	0.1370
C	3.30594760 +1	4.57878904 +1	0.39081969 +1	-0.1038
H	3.47987454 +1	4.01746937 +1	-0.53256998 +1	0.1069
C	4.76269644 +1	-2.85462768 +1	-1.07980494 +1	-0.1037
H	4.26305118 +1	-2.56692991 +1	-2.01028912 +1	0.1083
C	5.58353948 +1	-4.58725582 +1	0.38112092 +1	-0.0705
H	5.72091583 +1	-5.65064825 +1	0.60990304 +1	0.1353
C	4.90814844 +1	-4.20210552 +1	-0.77116822 +1	-0.1234
H	4.52624581 +1	-4.96483853 +1	-1.45749501 +1	0.1187
H	0.83744862 +1	1.68440150 +1	-2.69060053 +1	0.2864
H	0.94440910 +1	0.26342857 +1	-3.23641208 +1	0.2926

---------- End of file **TUQTUU.arc**----------

Holmium: GINREA



---------- Begin of file GINREA**.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
NUMERO DE COORDENAÇÃO = 9

 Ho     0.0000000  1     0.0000000  1     0.0000000  1
  O     2.4921000  1     0.0000000  1     0.0000000  1
  O     0.7798406  1     2.2106837  1     0.0000000  1
  O     0.8583639  1    -0.0270662  1    -2.2366975  1
  O     0.8597800  1    -2.2204043  1    -0.0510084  1
  O     0.7312169  1    -0.0683079  1     2.2186088  1
  O    -1.7007602  1    -1.0545348  1     1.4946159  1
  O    -1.6056121  1    -1.5533589  1    -1.1147182  1
  O    -1.6011334  1     1.0930086  1    -1.6220269  1
  O    -1.6904883  1     1.6016852  1     0.9890703  1
  C    -2.1403516  1    -2.3378414  1     0.9835156  1
```

```
 C   -2.6474590  1    -2.2368890  1    -0.2806285  1
 C   -2.0773915  1    -1.1672761  1    -2.3836804  1
 C   -2.6037075  1     0.2929275  1    -2.2216002  1
 C   -2.6865329  1     2.2012119  1     0.2930187  1
 C   -2.0799850  1     2.3808673  1    -1.2168388  1
 C   -2.2455017  1     1.1620083  1     2.2731939  1
 C   -2.7808924  1    -0.2582406  1     2.1192933  1
 H   -1.4280628  1    -2.9688394  1     1.0229114  1
 H   -2.8581888  1    -2.6271326  1     1.5411405  1
 H   -2.8164158  1    -3.1032051  1    -0.6322535  1
 H   -3.4476700  1    -1.7292187  1    -0.3017856  1
 H   -1.3605383  1    -1.1708474  1    -3.0191902  1
 H   -2.7697393  1    -1.7359891  1    -2.6865956  1
 H   -3.3702484  1     0.2726242  1    -1.6848519  1
 H   -2.8095099  1     0.6571958  1    -3.0706092  1
 H   -1.3728304  1     3.0062461  1    -1.2042528  1
 H   -2.7632462  1     2.6836986  1    -1.8142613  1
 H   -3.4757036  1     1.6688699  1     0.2818120  1
 H   -2.8929331  1     3.0507552  1     0.6693143  1
 H   -1.5560491  1     1.1766202  1     2.9216483  1
 H   -2.9316542  1     1.7538034  1     2.5386875  1
 H   -3.5484147  1    -0.2673340  1     1.5721903  1
 H   -2.9866677  1    -0.6155354  1     2.9745986  1
 H    2.8120997  1    -0.9050968  1     0.0000000  1
 H    0.0327451  1     2.8135504  1     0.0000007  1
 H    0.1280652  1    -0.0346029  1    -2.8596060  1
 H    0.1313176  1    -2.8453398  1    -0.0653645  1
 H   -0.0283157  1    -0.0863720  1     2.8054511  1
 H    3.3347976  1     0.5328883  1    -0.1756264  1
 H    1.7888572  1     2.6042936  1    -0.0875010  1
 H    1.4926668  1    -0.4177187  1     2.4920969  1
 H    1.6650217  1    -2.6124146  1     0.2335084  1
 H    1.6587323  1     0.4319939  1    -2.3810703  1
```

---------- End of file GINREA**.mop**----------

---------- Begin of file GINREA**.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No: 3560

                              MOPAC2012 (Version: 12.290W)
                              Wed Nov 21 16:06:51 2012
                              No. of days left = 329

          Empirical Formula: C8 H26 O9 Ho  =    44 atoms

 RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO = 9



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED
```

```
HEAT OF FORMATION        =        158.59001 KCAL/MOL =     663.54061 KJ/MOL
TOTAL ENERGY             =      -4240.45468 EV
ELECTRONIC ENERGY        =     -29592.20910 EV
CORE-CORE REPULSION      =      25351.75442 EV
GRADIENT NORM            =          0.23817
DIPOLE                   =          4.09371 DEBYE    POINT GROUP:       C2
NO. OF FILLED LEVELS     =         56
CHARGE ON SYSTEM         =          3
IONIZATION POTENTIAL     =         21.075543 EV
HOMO LUMO ENERGIES (EV)  =        -21.076 -8.131
MOLECULAR WEIGHT         =        431.218
COSMO AREA               =        276.45 SQUARE ANGSTROMS
COSMO VOLUME             =        364.96 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    43    H    30     9.60356
            H    43    H    30     7.07194
            H    42    H    26     2.64943
          SCF CALCULATIONS         =        186
          COMPUTATION TIME         =          8.906 SECONDS

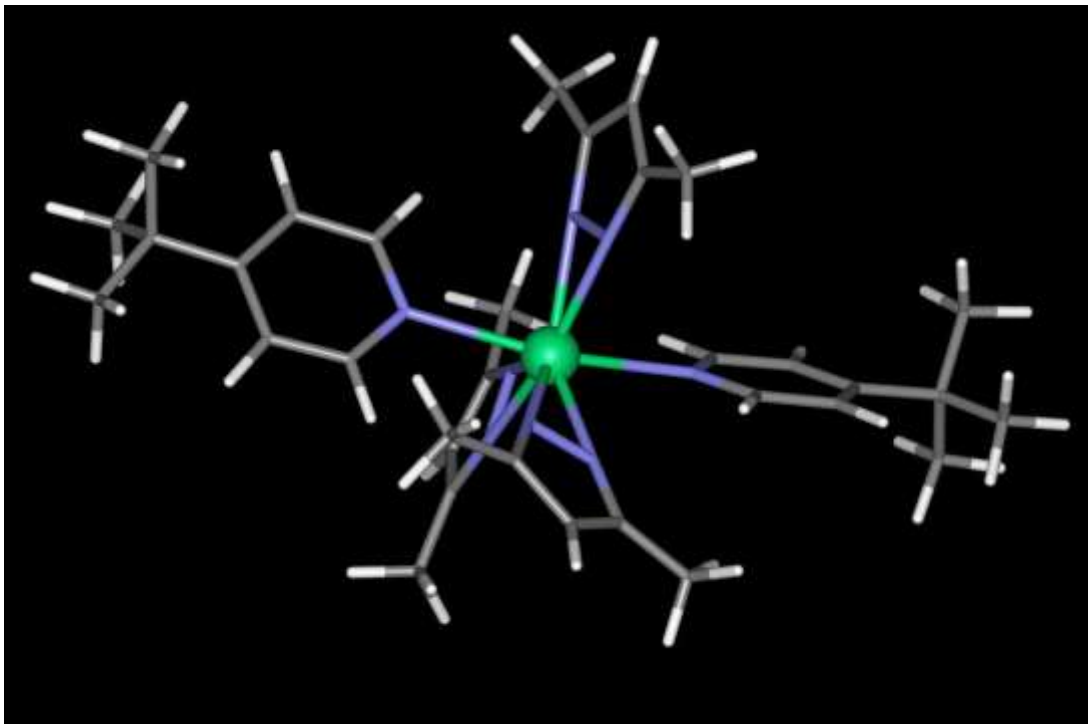

          FINAL GEOMETRY OBTAINED                                      CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp  PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO = 9

 Ho     0.05742131 +1  -0.00410378 +1   0.00750183 +1            3.0000
  O     2.45663124 +1  -0.00125113 +1   0.07505513 +1           -0.6216
  O     0.85179757 +1   2.23231898 +1   0.27275448 +1           -0.6305
  O     0.95450585 +1   0.36266583 +1  -2.17093868 +1           -0.6318
  O     0.87236886 +1  -2.23732845 +1  -0.21977235 +1           -0.6307
  O     0.83033724 +1  -0.35958883 +1   2.23472998 +1           -0.6319
  O    -1.74645879 +1  -1.01457378 +1   1.41155573 +1           -0.5308
  O    -1.67117971 +1  -1.46394137 +1  -1.05571401 +1           -0.5304
  O    -1.66942714 +1   1.00329453 +1  -1.49217601 +1           -0.5308
  O    -1.72869816 +1   1.45286178 +1   0.97523569 +1           -0.5303
  C    -2.18474896 +1  -2.33806406 +1   1.09327129 +1           -0.0027
  C    -2.62186900 +1  -2.30055604 +1  -0.37870628 +1            0.0068
  C    -2.09347955 +1  -1.15380727 +1  -2.38607883 +1           -0.0056
  C    -2.58276970 +1   0.30164490 +1  -2.34870447 +1            0.0047
  C    -2.64230936 +1   2.28834325 +1   0.24773294 +1            0.0067
  C    -2.12587152 +1   2.32630135 +1  -1.19832387 +1           -0.0026
  C    -2.22183040 +1   1.14189660 +1   2.28079681 +1           -0.0055
  C    -2.70628814 +1  -0.31424949 +1   2.21691798 +1            0.0047
  H    -1.32399012 +1  -3.01670233 +1   1.28903358 +1            0.1073
  H    -3.00454878 +1  -2.73572796 +1   1.74073995 +1            0.1619
  H    -2.63077147 +1  -3.32385190 +1  -0.82299578 +1            0.1388
  H    -3.65430045 +1  -1.89091631 +1  -0.48363538 +1            0.1219
  H    -1.21387745 +1  -1.31668121 +1  -3.04901709 +1            0.1067
  H    -2.88182474 +1  -1.82717147 +1  -2.80418554 +1            0.1631
  H    -3.62443683 +1   0.36983758 +1  -1.95533498 +1            0.1227
  H    -2.59125319 +1   0.75099335 +1  -3.36978046 +1            0.1387
  H    -1.25626305 +1   3.00561837 +1  -1.34710647 +1            0.1071
  H    -2.90961589 +1   2.72311887 +1  -1.88936688 +1            0.1619
  H    -3.67850623 +1   1.87764631 +1   0.29657055 +1            0.1220
  H    -2.67634539 +1   3.31168430 +1   0.69068263 +1            0.1387
  H    -1.37941075 +1   1.30592580 +1   2.99014745 +1            0.1067
```

H	-3.03244144 +1	1.81424366 +1	2.65584944 +1	0.1631
H	-3.72502265 +1	-0.38385417 +1	1.76744420 +1	0.1227
H	-2.76978644 +1	-0.76396111 +1	3.23593080 +1	0.1387
H	3.07154450 +1	-0.70426017 +1	-0.18569043 +1	0.3110
H	0.50055332 +1	2.86330256 +1	0.91881678 +1	0.3131
H	0.46719346 +1	0.73575442 +1	-2.92073968 +1	0.3132
H	0.56254750 +1	-2.86550563 +1	-0.88929893 +1	0.3131
H	0.30562417 +1	-0.74002524 +1	2.95505650 +1	0.3133
H	3.05384392 +1	0.70313524 +1	0.37077117 +1	0.3108
H	1.49410444 +1	2.76385367 +1	-0.22300024 +1	0.3165
H	1.69055131 +1	-0.19948216 +1	2.65219298 +1	0.3162
H	1.48528345 +1	-2.77014785 +1	0.31072289 +1	0.3167
H	1.84005428 +1	0.21577675 +1	-2.53740814 +1	0.3162

---------- End of file GINREA**.arc**----------

Erbium: DIJQIW



---------- Begin of file DIJQIW**.mop**----------

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RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO= 8

 Er    0.0000000  1     0.0000000  1     0.0000000  1
  N    2.3667000  1     0.0000000  1     0.0000000  1
  N    1.9119859  1     1.3114035  1     0.0000000  1
  N    0.0551489  1    -2.2657939  1     0.5619865  1
  N   -0.1319398  1     0.4394134  1     2.4335293  1
  N   -2.2263218  1     0.8028827  1    -0.0118068  1
  N   -1.3536962  1     1.8816937  1    -0.0469567  1
  N   -0.8233225  1    -2.1277768  1    -0.4973553  1
  N    0.2610464  1     0.2989682  1    -2.4443874  1
  C    2.9744179  1     2.1206220  1    -0.0586349  1
  C    4.1105501  1     1.3514257  1    -0.1015988  1
  H    4.9966164  1     1.6619321  1    -0.1491413  1
  C    3.7013633  1     0.0349614  1    -0.0649499  1
  C    2.7848297  1     3.6030434  1    -0.0549698  1
  H    1.8364638  1     3.8085318  1    -0.0173954  1
  H    3.1652915  1     3.9798829  1    -0.8647188  1
  H    3.2288448  1     3.9842371  1     0.7178680  1
  C    4.5119260  1    -1.2316212  1    -0.0518707  1
  H    3.9149634  1    -1.9953350  1    -0.0220558  1
  H    5.0854771  1    -1.2391494  1     0.7294903  1
  H    5.0557495  1    -1.2758326  1    -0.8537480  1
  C    0.1032253  1    -3.5697844  1     0.8897035  1
  C   -0.7471651  1    -4.2733962  1     0.0628520  1
  H   -0.9092840  1    -5.2006316  1     0.0764876  1
  C    1.0346935  1    -4.0321351  1     1.9636331  1
```

H	1.4874022	1	-3.2664075	1	2.3499338	1
H	1.6908077	1	-4.6381641	1	1.5842663	1
H	0.5305635	1	-4.4910822	1	2.6537885	1
C	-0.8689479	1	-0.3503854	1	3.2233495	1
H	-1.2348928	1	-1.1329289	1	2.8540658	1
C	-1.1182397	1	-0.0758046	1	4.5496748	1
H	-1.6673823	1	-0.6579706	1	5.0442754	1
C	-0.5782578	1	1.0335604	1	5.1678405	1
C	0.1886355	1	1.8567393	1	4.3477965	1
H	0.5688400	1	2.6443852	1	4.6936269	1
C	0.3903785	1	1.5152047	1	3.0262188	1
H	0.9322540	1	2.0796626	1	2.5069240	1
C	-0.8378609	1	1.3784938	1	6.6303545	1
C	-1.2971427	1	0.1697416	1	7.4004216	1
H	-0.6204531	1	-0.5242306	1	7.3443801	1
H	-2.1282902	1	-0.1575914	1	7.0225950	1
H	-1.4357455	1	0.4112947	1	8.3285393	1
C	0.4429278	1	1.8959125	1	7.3008903	1
H	0.7648302	1	2.6776112	1	6.8254621	1
H	1.1205070	1	1.2032674	1	7.2790334	1
H	0.2518114	1	2.1328200	1	8.2215789	1
C	-1.8755534	1	2.4707000	1	6.7028030	1
H	-1.5672647	1	3.2427465	1	6.2024188	1
H	-2.0180575	1	2.7217978	1	7.6289437	1
H	-2.7091278	1	2.1506385	1	6.3233265	1
C	0.6824466	1	-0.7162204	1	-3.2076654	1
H	0.7630400	1	-1.5656287	1	-2.8143838	1
C	1.0034869	1	-0.5804601	1	-4.5400250	1
H	1.3200804	1	-1.3282615	1	-5.0150685	1
C	0.8688161	1	0.6281882	1	-5.1922772	1
C	0.4307789	1	1.6857638	1	-4.3998896	1
H	0.3386198	1	2.5454768	1	-4.7699445	1
C	0.1317283	1	1.4707828	1	-3.0701280	1
H	-0.1839136	1	2.2001730	1	-2.5698592	1
C	1.2227444	1	0.8227142	1	-6.6627242	1
C	1.2408574	1	-0.4916142	1	-7.3956893	1
H	0.3691520	1	-0.9129555	1	-7.3232464	1
H	1.9135348	1	-1.0705875	1	-7.0045358	1
H	1.4485567	1	-0.3379947	1	-8.3296181	1
C	0.1901269	1	1.7246114	1	-7.3541306	1
H	0.1548913	1	2.5823847	1	-6.9028109	1
H	-0.6821358	1	1.3038443	1	-7.3159002	1
H	0.4456856	1	1.8562590	1	-8.2802389	1
C	2.5690609	1	1.4955569	1	-6.7611289	1
H	2.5434814	1	2.3403480	1	-6.2845203	1
H	2.7836780	1	1.6568837	1	-7.6933344	1
H	3.2464963	1	0.9226444	1	-6.3685215	1
C	-1.3125503	1	-3.3469168	1	-0.7879667	1
C	-2.3509792	1	-3.4962995	1	-1.8528969	1
H	-2.5189984	1	-2.6337562	1	-2.2631415	1
H	-3.1718727	1	-3.8327233	1	-1.4596680	1
H	-2.0358899	1	-4.1185457	1	-2.5271539	1
C	-2.0782982	1	3.0046687	1	-0.0167361	1
C	-3.4077709	1	2.6680683	1	0.0424895	1
H	-4.1357073	1	3.2619740	1	0.0767320	1
C	-3.4696366	1	1.2903822	1	0.0454600	1
C	-4.6618643	1	0.3740604	1	0.0644821	1
H	-4.3595421	1	-0.5473993	1	0.0594489	1
H	-5.2078478	1	0.5392596	1	-0.7191975	1
H	-5.1844294	1	0.5398575	1	0.8645715	1
C	-1.3970747	1	4.3341191	1	-0.0617518	1

```
 H    -0.4354374  1     4.2045359  1    -0.1004426  1
 H    -1.6230905  1     4.8406217  1     0.7350070  1
 H    -1.6892924  1     4.8211198  1    -0.8473571  1
 0
```

---------- End of file DIJQIW**.mop**----------

---------- Begin of file DIJQIW**.arc**----------

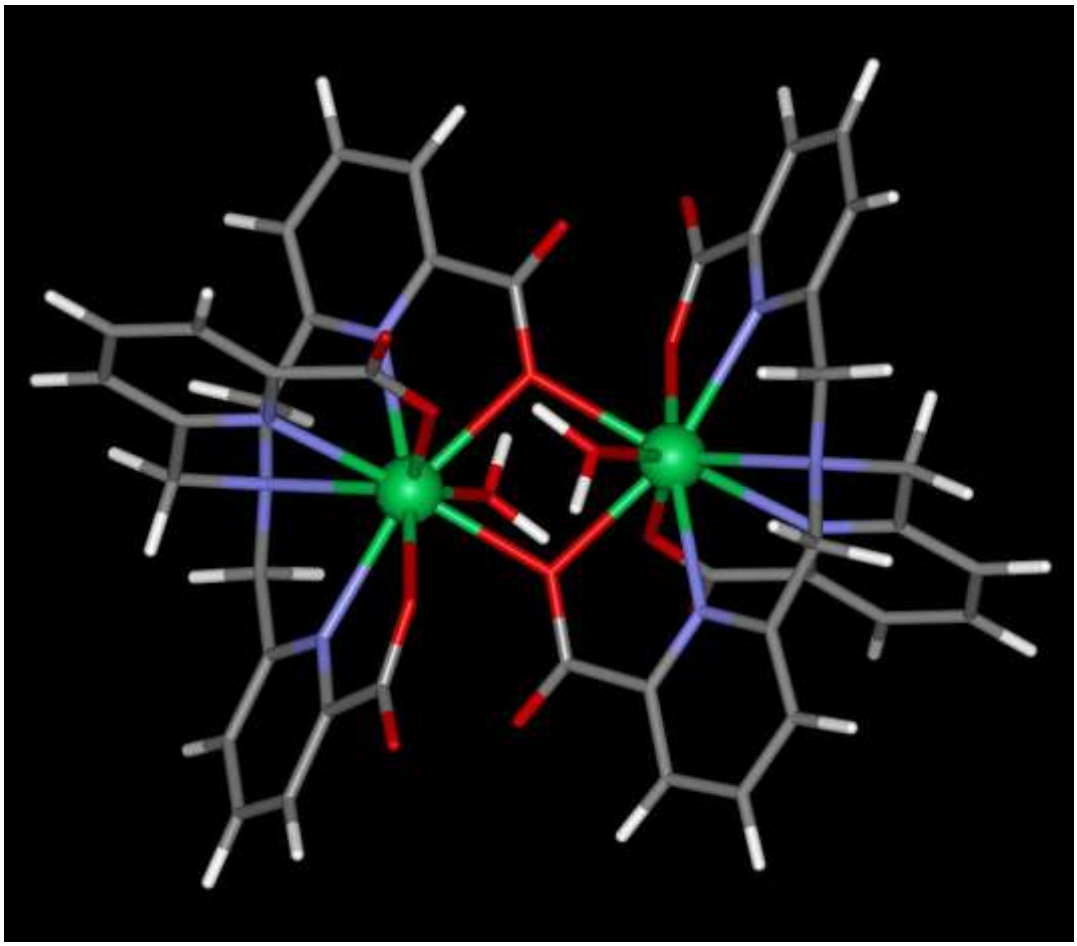
```
           SUMMARY OF RM1 CALCULATION, Site No: 3560

                          MOPAC2012 (Version: 12.290W)
                          Wed Nov 21 16:10:15 2012
                          No. of days left = 329

           Empirical Formula: C33 H47 N8 Er  =    89 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO= 8



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =        -39.76115 KCAL/MOL =    -166.36067 KJ/MOL
TOTAL ENERGY            =      -6528.20145 EV
ELECTRONIC ENERGY       =     -72528.18047 EV
CORE-CORE REPULSION     =      65999.97902 EV
GRADIENT NORM           =          0.21961
DIPOLE                  =          1.67621 DEBYE    POINT GROUP:       C1
NO. OF FILLED LEVELS    =        111
IONIZATION POTENTIAL    =          8.599763 EV
HOMO LUMO ENERGIES (EV) =         -8.600 -0.327
MOLECULAR WEIGHT        =        723.048
COSMO AREA              =        599.27 SQUARE ANGSTROMS
COSMO VOLUME            =        789.30 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    64    H    42    17.44325
            H    84    H    12    10.61586
            H    24    H    88    10.51945
          SCF CALCULATIONS        =        760
          COMPUTATION TIME =  3 MINUTES AND  41.953 SECONDS


          FINAL GEOMETRY OBTAINED                                  CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO= 8

 Er     0.01238931 +1   0.06227558 +1   0.00349902 +1            3.0000
```

N	2.34937566 +1	0.08301213 +1	-0.02658805 +1	-0.5878
N	1.93785881 +1	1.37382914 +1	0.19956279 +1	-0.5985
N	-0.18877576 +1	-2.16046635 +1	0.70133999 +1	-0.5939
N	-0.18985680 +1	0.47956980 +1	2.47535319 +1	-0.5133
N	-2.18139914 +1	0.86918561 +1	0.01191084 +1	-0.5881
N	-1.35878911 +1	1.94043528 +1	-0.23806383 +1	-0.5988
N	-0.52980723 +1	-2.12237660 +1	-0.62933955 +1	-0.5936
N	0.33140288 +1	0.30495205 +1	-2.47941419 +1	-0.5131
C	3.04649016 +1	2.17399013 +1	0.29379757 +1	0.1090
C	4.19933702 +1	1.37718276 +1	0.12628724 +1	-0.3233
H	5.22746610 +1	1.69988250 +1	0.14618200 +1	0.1327
C	3.71721782 +1	0.06325189 +1	-0.07377926 +1	0.1236
C	2.98432952 +1	3.62769678 +1	0.53589884 +1	-0.1380
H	1.95621840 +1	4.01846366 +1	0.57564309 +1	0.0690
H	3.50966051 +1	4.18222983 +1	-0.25660046 +1	0.0717
H	3.46993537 +1	3.89105384 +1	1.48803005 +1	0.0674
C	4.51176343 +1	-1.15879114 +1	-0.29851820 +1	-0.1395
H	3.89656022 +1	-2.06474959 +1	-0.40308869 +1	0.0756
H	5.20678249 +1	-1.33553089 +1	0.53644542 +1	0.0716
H	5.11995441 +1	-1.07153817 +1	-1.21172556 +1	0.0685
C	-0.28336065 +1	-3.45578292 +1	1.13756721 +1	0.1158
C	-0.70515572 +1	-4.26999670 +1	0.06364931 +1	-0.3184
H	-0.87789252 +1	-5.33391196 +1	0.07743717 +1	0.1336
C	0.01827405 +1	-3.88263879 +1	2.51685822 +1	-0.1393
H	0.42963481 +1	-3.07697521 +1	3.14292796 +1	0.0680
H	0.75427301 +1	-4.70112090 +1	2.52289196 +1	0.0751
H	-0.88521815 +1	-4.25869844 +1	3.02090610 +1	0.0679
C	-0.91680492 +1	-0.32677970 +1	3.31200720 +1	0.0883
H	-1.39775600 +1	-1.21683225 +1	2.86950048 +1	0.1504
C	-1.08932983 +1	-0.10428044 +1	4.67782108 +1	-0.2012
H	-1.69642723 +1	-0.82160349 +1	5.23609919 +1	0.1382
C	-0.49777746 +1	1.00276078 +1	5.27584662 +1	0.0766
C	0.25657268 +1	1.84196790 +1	4.45715532 +1	-0.2015
H	0.75813246 +1	2.73072443 +1	4.85136895 +1	0.1367
C	0.38476204 +1	1.55838180 +1	3.10059330 +1	0.0889
H	0.98987813 +1	2.24388280 +1	2.48128480 +1	0.1526
C	-0.63344262 +1	1.32936323 +1	6.73909735 +1	0.0349
C	-1.49667264 +1	0.32031930 +1	7.49650734 +1	-0.1905
H	-1.08041046 +1	-0.69688511 +1	7.46749760 +1	0.0668
H	-2.52561469 +1	0.27319600 +1	7.11190524 +1	0.0678
H	-1.58408446 +1	0.58024194 +1	8.56255130 +1	0.0694
C	0.76167127 +1	1.33638687 +1	7.36845942 +1	-0.1885
H	1.42216269 +1	2.10791832 +1	6.94927677 +1	0.0665
H	1.27539920 +1	0.37335207 +1	7.23641899 +1	0.0693
H	0.71935434 +1	1.52886362 +1	8.45063858 +1	0.0686
C	-1.28113017 +1	2.70993922 +1	6.87157984 +1	-0.1886
H	-0.67101240 +1	3.51782461 +1	6.44453908 +1	0.0662
H	-1.44951420 +1	2.98185486 +1	7.92399907 +1	0.0684
H	-2.25925846 +1	2.75296871 +1	6.37128156 +1	0.0706
C	0.77357538 +1	-0.71749782 +1	-3.27802628 +1	0.0895
H	0.95938650 +1	-1.69418509 +1	-2.79751833 +1	0.1502
C	1.00259488 +1	-0.61200961 +1	-4.64960965 +1	-0.2014
H	1.35824595 +1	-1.50229139 +1	-5.17457621 +1	0.1382
C	0.77840095 +1	0.59904814 +1	-5.29457376 +1	0.0765
C	0.32266539 +1	1.66120062 +1	-4.51488100 +1	-0.2015
H	0.11916800 +1	2.64553240 +1	-4.94674960 +1	0.1366
C	0.11661883 +1	1.48354208 +1	-3.14999180 +1	0.0878
H	-0.24546504 +1	2.34585647 +1	-2.56279071 +1	0.1528
C	1.00152684 +1	0.81025549 +1	-6.76825673 +1	0.0348
C	1.50435864 +1	-0.44557335 +1	-7.48034006 +1	-0.1905
H	0.79337071 +1	-1.28156608 +1	-7.41402196 +1	0.0668

H	2.47047231 +1	-0.79440907 +1	-7.08820803 +1	0.0678
H	1.66131916 +1	-0.26731455 +1	-8.55515677 +1	0.0694
C	-0.32550635 +1	1.22597630 +1	-7.40754621 +1	-0.1885
H	-0.71152270 +1	2.18022919 +1	-7.02329633 +1	0.0665
H	-1.11231885 +1	0.47605321 +1	-7.24225691 +1	0.0693
H	-0.23086765 +1	1.35357417 +1	-8.49596950 +1	0.0686
C	2.04543248 +1	1.91497178 +1	-6.94907528 +1	-0.1886
H	1.72018129 +1	2.88744599 +1	-6.55439858 +1	0.0662
H	2.28174014 +1	2.08245841 +1	-8.01021303 +1	0.0684
H	2.99228517 +1	1.66977693 +1	-6.44682047 +1	0.0705
C	-0.85154288 +1	-3.39158848 +1	-1.03237573 +1	0.1157
C	-1.27829791 +1	-3.73572401 +1	-2.40168741 +1	-0.1392
H	-1.37361764 +1	-2.86095794 +1	-3.06201460 +1	0.0678
H	-2.25701920 +1	-4.23947133 +1	-2.39333003 +1	0.0751
H	-0.56472917 +1	-4.42678899 +1	-2.87600355 +1	0.0680
C	-2.13314101 +1	3.06439729 +1	-0.36315664 +1	0.1089
C	-3.48736500 +1	2.70618886 +1	-0.19103810 +1	-0.3232
H	-4.34713075 +1	3.35502938 +1	-0.22976676 +1	0.1327
C	-3.47620867 +1	1.31206084 +1	0.04402637 +1	0.1238
C	-4.63653422 +1	0.43558816 +1	0.29009538 +1	-0.1397
H	-4.36922445 +1	-0.62884134 +1	0.36521389 +1	0.0760
H	-5.37798038 +1	0.52612664 +1	-0.51821073 +1	0.0714
H	-5.14534108 +1	0.70972783 +1	1.22690958 +1	0.0688
C	-1.58418001 +1	4.40486515 +1	-0.64183721 +1	-0.1381
H	-0.48713724 +1	4.44910761 +1	-0.56623784 +1	0.0701
H	-1.98691122 +1	5.15103154 +1	0.05965055 +1	0.0716
H	-1.85351216 +1	4.73923798 +1	-1.65560261 +1	0.0667

---------- End of file DIJQIW**.arc**----------

Tulium: NIHZUZ



---------- Begin of file NIHZUZ**.mop**----------

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RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK  SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO= 9

 Tm    0.0000000  1     0.0000000  1     0.0000000  1
  O    2.3911000  1     0.0000000  1     0.0000000  1
  O   -1.3143605  1     1.6227374  1    -0.9978111  1
  O    0.6397541  1    -2.2207720  1    -0.1161137  1
  N    1.0676423  1     2.0773908  1     0.8925175  1
  N   -2.2987411  1    -0.7845872  1     0.7526970  1
  N    0.4314909  1    -1.0146083  1     2.2163011  1
  N   -1.1162116  1     1.2971609  1     2.1580843  1
 Tm   -0.5923729  1    -1.1624094  1    -3.8564232  1
  O   -1.2974407  1    -1.2834530  1    -1.6312942  1
  O    0.7050686  1     0.1210343  1    -2.2251293  1
  O   -2.9826728  1    -1.1625781  1    -3.8570039  1
  O    0.7220182  1    -2.7851155  1    -2.8586014  1
  O   -1.2313142  1     1.0582251  1    -3.7408093  1
  N   -1.6600500  1    -3.2398311  1    -4.7489375  1
  N    1.7063670  1    -0.3778377  1    -4.6090932  1
  N   -1.0238435  1    -0.1478089  1    -6.0725708  1
  N    0.5237825  1    -2.4595578  1    -6.0145145  1
  H   -1.2892134  1     1.6360771  1    -1.8738488  1
```

H	-1.8186840	1	1.7345940	1	-0.9447219	1
O	4.3325141	1	1.1353028	1	0.0000000	1
O	1.4398226	1	-4.0897793	1	0.7967720	1
O	1.6725995	1	2.1388172	1	-2.1447409	1
O	-2.0313729	1	2.9272018	1	-4.6536596	1
O	-4.9241024	1	-2.2979187	1	-3.8569963	1
O	-2.2642119	1	-3.3014632	1	-1.7122704	1
C	-1.0386423	1	2.7553019	1	1.8492736	1
H	-1.2403951	1	3.1960964	1	2.7266571	1
H	-1.6308084	1	2.9129221	1	1.2662876	1
C	0.3591278	1	3.0985494	1	1.4008030	1
C	0.8992767	1	4.3602749	1	1.5512039	1
H	0.3720513	1	5.0142656	1	1.9649363	1
C	2.2184468	1	4.5829951	1	1.2106658	1
H	2.6585276	1	5.4618825	1	1.3652972	1
C	2.9742974	1	3.5147696	1	0.7643848	1
H	3.8843263	1	3.5814986	1	0.5851955	1
C	2.3640260	1	2.2732401	1	0.6123232	1
C	3.1066387	1	1.0427636	1	0.1526152	1
C	-2.5116065	1	0.9297717	1	2.4734050	1
H	-2.6141174	1	0.9328915	1	3.6492409	1
H	-2.9724642	1	1.4716688	1	2.1486256	1
C	-2.9962044	1	-0.3106065	1	1.8035890	1
C	-4.1869226	1	-0.9105903	1	2.2113661	1
H	-4.5569158	1	-0.5797914	1	2.9539854	1
C	-4.6682398	1	-2.0114966	1	1.5492116	1
H	-5.4522219	1	-2.4521191	1	1.7294327	1
C	-3.9779850	1	-2.4846138	1	0.4554162	1
H	-4.2768031	1	-3.2434003	1	-0.0202681	1
C	-2.7989316	1	-1.8377589	1	0.0869543	1
C	-2.0749400	1	-2.2141552	1	-1.1756539	1
C	-0.2555861	1	1.0199189	1	3.3386052	1
H	0.4398935	1	1.5914280	1	3.3855877	1
H	-0.7516395	1	1.2236669	1	4.2039039	1
C	0.2556087	1	-0.3757580	1	3.3846855	1
C	0.6097194	1	-0.9766963	1	4.6024746	1
H	0.5039344	1	-0.5391935	1	5.4587827	1
C	1.1513674	1	-2.2452759	1	4.5775863	1
H	1.3622703	1	-2.5892346	1	5.2013754	1
C	1.2958425	1	-2.9184873	1	3.3883265	1
H	1.6165696	1	-3.8247151	1	3.3312803	1
C	0.9291627	1	-2.2792045	1	2.2156854	1
C	1.0298202	1	-2.9450407	1	0.8740388	1
C	-3.6989757	1	-2.2052313	1	-4.0090416	1
C	-2.9564285	1	-3.4357107	1	-4.4687404	1
H	0.6968701	1	-2.7984509	1	-1.9825637	1
H	1.2271802	1	-2.8970922	1	-2.9122726	1
C	1.4833290	1	1.0515088	1	-2.6813571	1
C	2.2065592	1	0.6753360	1	-3.9433547	1
C	-1.6221654	1	1.7825657	1	-4.7303508	1
C	-1.5215218	1	1.1167847	1	-6.0719572	1
C	0.4462482	1	-3.9176987	1	-5.7056945	1
H	0.6488291	1	-4.3586501	1	-6.5837225	1
H	1.0392344	1	-4.0754265	1	-5.1232811	1
C	-0.9507298	1	-4.2610706	1	-5.2577861	1
C	-1.4908561	1	-5.5228046	1	-5.4081972	1
H	-0.9644246	1	-6.1766575	1	-5.8213480	1
C	-2.8100247	1	-5.7455491	1	-5.0676692	1
H	-3.2500897	1	-6.6244429	1	-5.2223091	1
C	-3.5658963	1	-4.6773390	1	-4.6213865	1
H	-4.4767396	1	-4.7439608	1	-4.4416240	1

```
 C     1.9199223  1    -2.0922718  1    -6.3304062  1
 H     2.0224336  1    -2.0953985  1    -7.5062420  1
 H     2.3799993  1    -2.6340454  1    -6.0050365  1
 C     2.4038306  1    -0.8518232  1    -5.6599828  1
 C     3.5953517  1    -0.2519682  1    -6.0683397  1
 H     3.9653459  1    -0.5827708  1    -6.8109567  1
 C     4.0766704  1     0.8489404  1    -5.4061899  1
 H     4.8598005  1     1.2896546  1    -5.5858207  1
 C     3.3856118  1     1.3221882  1    -4.3118252  1
 H     3.6852178  1     2.0808001  1    -3.8367554  1
 C    -0.3368508  1    -2.1823528  1    -7.1950384  1
 H    -1.0323150  1    -2.7538813  1    -7.2420139  1
 H     0.1592083  1    -2.3860959  1    -8.0603349  1
 C    -0.8471467  1    -0.7867957  1    -7.2415624  1
 C    -1.2020610  1    -0.1857083  1    -8.4588133  1
 H    -1.0954711  1    -0.6233055  1    -9.3156513  1
 C    -1.7429098  1     1.0827885  1    -8.4345049  1
 H    -1.9538019  1     1.4267511  1    -9.0582955  1
 C    -1.8881953  1     1.7560964  1    -7.2447050  1
 H    -2.2081144  1     2.6622211  1    -7.1882374  1
```

---------- End of file NIHZUZ**.mop**----------

---------- Begin of file NIHZUZ**.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No: 3560

                                 MOPAC2012 (Version: 12.203W)
                                 Tue Oct 30 13:34:26 2012
                                 No. of days left = 264

          Empirical Formula: C42 H34 N8 O14 Tm2  =   100 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK  SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO= 9


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =       -534.43251 KCAL/MOL =   -2236.06561 KJ/MOL
TOTAL ENERGY            =     -11941.59271 EV
ELECTRONIC ENERGY       =    -159876.86476 EV
CORE-CORE REPULSION     =     147935.27206 EV
GRADIENT NORM           =          0.22122
DIPOLE                  =          0.00152 DEBYE    POINT GROUP:       Ci
NO. OF FILLED LEVELS    =        166
IONIZATION POTENTIAL    =          9.380496 EV
HOMO LUMO ENERGIES (EV) =         -9.380 -0.729
MOLECULAR WEIGHT        =       1212.644
COSMO AREA              =        616.56 SQUARE ANGSTROMS
COSMO VOLUME            =        963.59 CUBIC ANGSTROMS
```

MOLECULAR DIMENSIONS (Angstroms)

Atom		Atom		Distance
H	98	H	58	15.67692
H	78	H	34	14.82275
H	86	H	44	10.38555

SCF CALCULATIONS = 389
COMPUTATION TIME = 5 MINUTES AND 5.918 SECONDS

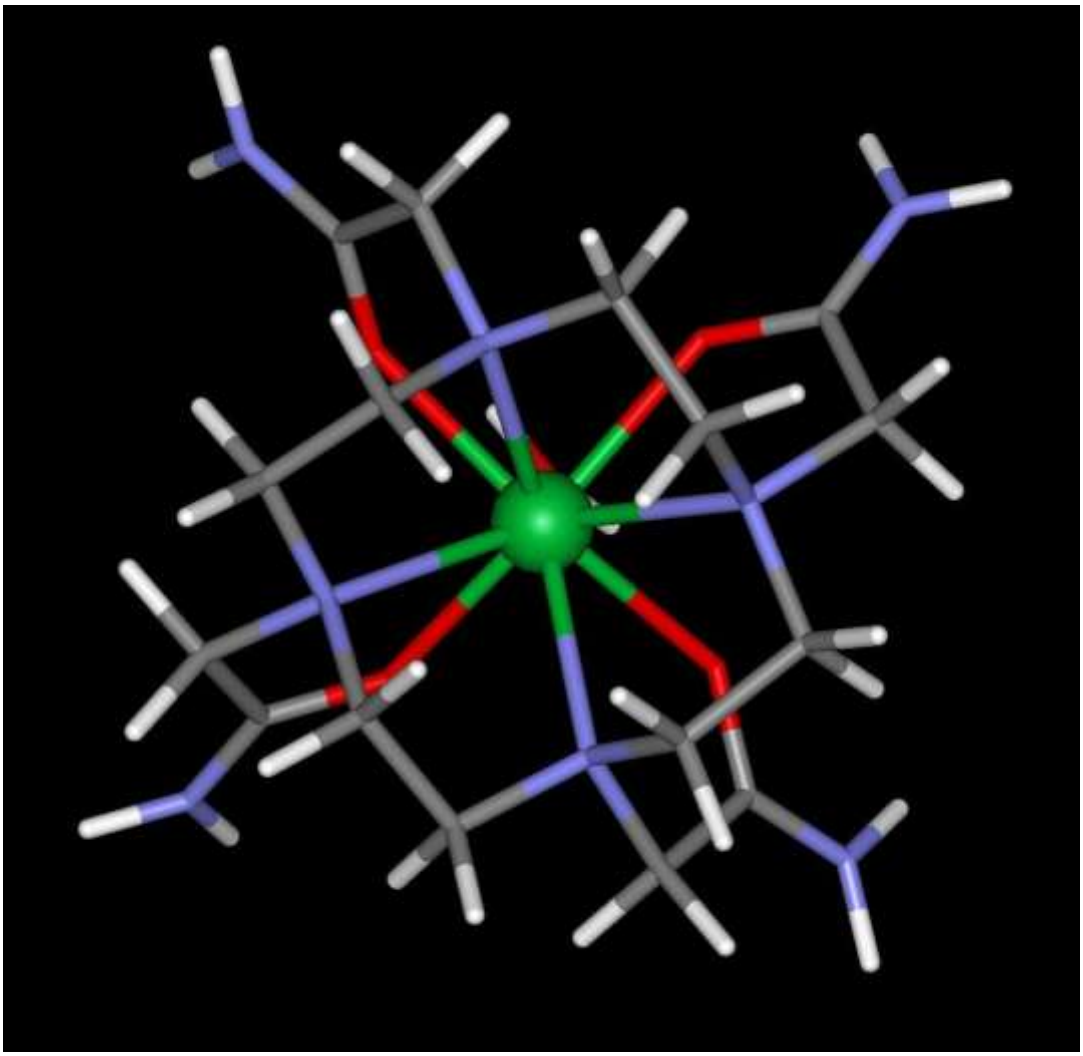
FINAL GEOMETRY OBTAINED CHARG
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO= 9

Tm	-0.06257153 +1	0.02707761 +1	-0.13378629 +1	3.0000
O	2.27135556 +1	0.08205819 +1	-0.46918769 +1	-0.8012
O	-1.70286328 +1	1.26535328 +1	-1.25786502 +1	-0.6782
O	0.73267832 +1	-2.22888937 +1	-0.20783995 +1	-0.7789
N	1.17911631 +1	2.05089030 +1	0.64502489 +1	-0.5083
N	-2.22952613 +1	-0.83716201 +1	0.71956548 +1	-0.4894
N	0.32758718 +1	-1.07605926 +1	2.04754244 +1	-0.4986
N	-1.03666267 +1	1.32495211 +1	1.88769434 +1	-0.4388
Tm	-0.53263986 +1	-1.19008336 +1	-3.72241938 +1	3.0000
O	-1.19300516 +1	-1.60328324 +1	-1.49734561 +1	-0.9810
O	0.59793872 +1	0.44013773 +1	-2.35883827 +1	-0.9810
O	-2.86648829 +1	-1.24469159 +1	-3.38673166 +1	-0.8012
O	1.10759693 +1	-2.42834309 +1	-2.59825830 +1	-0.6782
O	-1.32773251 +1	1.06595781 +1	-3.64833913 +1	-0.7789
N	-1.77461471 +1	-3.21368189 +1	-4.50120158 +1	-0.5083
N	1.63450774 +1	-0.32620916 +1	-4.57560425 +1	-0.4894
N	-0.92241100 +1	-0.08674542 +1	-5.90372932 +1	-0.4986
N	0.44138616 +1	-2.48811888 +1	-5.74384706 +1	-0.4389
H	-1.53641026 +1	1.68498813 +1	-2.15987615 +1	0.3405
H	-2.58837839 +1	0.91593173 +1	-1.34663053 +1	0.2633
O	4.32153180 +1	1.00530660 +1	-0.64806399 +1	-0.4306
O	1.55109828 +1	-4.12862883 +1	0.66319985 +1	-0.4097
O	1.62164298 +1	2.42956710 +1	-2.35438887 +1	-0.3899
O	-2.14584096 +1	2.96588330 +1	-4.51934499 +1	-0.4097
O	-4.91685803 +1	-2.16753306 +1	-3.20826853 +1	-0.4306
O	-2.21660680 +1	-3.59273480 +1	-1.50203492 +1	-0.3899
C	-0.85044951 +1	2.83647708 +1	1.70674654 +1	-0.0230
H	-1.14500763 +1	3.42648069 +1	2.60511018 +1	0.0865
H	-1.50674467 +1	3.20882145 +1	0.88139752 +1	0.1254
C	0.58538493 +1	3.08306314 +1	1.32990345 +1	0.0755
C	1.22238814 +1	4.26932491 +1	1.66204009 +1	-0.1778
H	0.69131600 +1	5.06745950 +1	2.18616814 +1	0.1267
C	2.56235174 +1	4.42871717 +1	1.30050847 +1	-0.0114
H	3.08339494 +1	5.36358358 +1	1.53089261 +1	0.1166
C	3.21995230 +1	3.39280647 +1	0.66107220 +1	-0.1289
H	4.27537481 +1	3.45841985 +1	0.37481116 +1	0.1574
C	2.50484711 +1	2.23098651 +1	0.36085627 +1	0.0758
C	3.14417803 +1	1.00730276 +1	-0.32321929 +1	0.4800
C	-2.52644211 +1	1.12039023 +1	2.12139880 +1	-0.0189
H	-2.84958459 +1	1.36263537 +1	3.16218444 +1	0.0882
H	-3.12989448 +1	1.81324142 +1	1.48086879 +1	0.1150
C	-2.94264764 +1	-0.27145525 +1	1.73751787 +1	0.1004
C	-4.06357770 +1	-0.85828692 +1	2.32421845 +1	-0.1752
H	-4.58265085 +1	-0.37091058 +1	3.15377297 +1	0.1314
C	-4.52488227 +1	-2.06989900 +1	1.82021241 +1	-0.0060
H	-5.40118331 +1	-2.55513397 +1	2.26325234 +1	0.1243

C	-3.87816399 +1	-2.64561534 +1	0.73282331 +1	-0.1094
H	-4.23407332 +1	-3.57277103 +1	0.26836738 +1	0.1657
C	-2.75796878 +1	-2.00018655 +1	0.21961026 +1	0.0763
C	-2.03887224 +1	-2.49552390 +1	-1.00477078 +1	0.5098
C	-0.33139137 +1	0.97554930 +1	3.19835488 +1	-0.0199
H	0.61371584 +1	1.56264050 +1	3.31556881 +1	0.1165
H	-0.93062852 +1	1.25181649 +1	4.09942452 +1	0.0861
C	0.05868201 +1	-0.47843136 +1	3.24926930 +1	0.0981
C	0.20624050 +1	-1.11104033 +1	4.48144976 +1	-0.1849
H	-0.03162198 +1	-0.59135458 +1	5.41321141 +1	0.1290
C	0.67752398 +1	-2.42077830 +1	4.50923848 +1	-0.0083
H	0.80910745 +1	-2.93823901 +1	5.46541310 +1	0.1201
C	0.98245457 +1	-3.05918806 +1	3.31582190 +1	-0.1330
H	1.36838188 +1	-4.08490627 +1	3.28827203 +1	0.1624
C	0.79015754 +1	-2.36643916 +1	2.12274967 +1	0.0641
C	1.07454288 +1	-3.00957671 +1	0.76376672 +1	0.4662
C	-3.73944620 +1	-2.16977248 +1	-3.53290990 +1	0.4800
C	-3.10037069 +1	-3.39356749 +1	-4.21700961 +1	0.0758
H	0.94140369 +1	-2.84811171 +1	-1.69623531 +1	0.3405
H	1.99296126 +1	-2.07863635 +1	-2.50961496 +1	0.2632
C	1.44393179 +1	1.33226262 +1	-2.85142722 +1	0.5098
C	2.16316019 +1	0.83669779 +1	-4.07560039 +1	0.0763
C	-1.66939942 +1	1.84677883 +1	-4.61989704 +1	0.4662
C	-1.38475598 +1	1.20370491 +1	-5.97885555 +1	0.0641
C	0.25485522 +1	-3.99960588 +1	-5.56292845 +1	-0.0230
H	0.54933372 +1	-4.58961482 +1	-6.46133350 +1	0.0865
H	0.91105385 +1	-4.37205261 +1	-4.73748774 +1	0.1254
C	-1.18106301 +1	-4.24590208 +1	-5.18614549 +1	0.0755
C	-1.81838358 +1	-5.43195048 +1	-5.51846899 +1	-0.1778
H	-1.28768249 +1	-6.23016386 +1	-6.04283299 +1	0.1267
C	-3.15837080 +1	-5.59109500 +1	-5.15691617 +1	-0.0114
H	-3.67970255 +1	-6.52571536 +1	-5.38760505 +1	0.1166
C	-3.81575022 +1	-4.55520212 +1	-4.51725486 +1	-0.1288
H	-4.87112915 +1	-4.62068092 +1	-4.23079103 +1	0.1574
C	1.93127071 +1	-2.28386252 +1	-5.97734959 +1	-0.0189
H	2.25443443 +1	-2.52612557 +1	-7.01815021 +1	0.0882
H	2.53447472 +1	-2.97691329 +1	-5.33682977 +1	0.1150
C	2.34770564 +1	-0.89214474 +1	-5.59337286 +1	0.1004
C	3.46886416 +1	-0.30558650 +1	-6.17989419 +1	-0.1752
H	3.98793309 +1	-0.79310598 +1	-7.00937374 +1	0.1314
C	3.93044950 +1	0.90587349 +1	-5.67578823 +1	-0.0060
H	4.80694929 +1	1.39088511 +1	-6.11867532 +1	0.1243
C	3.28365832 +1	1.48181247 +1	-4.58856758 +1	-0.1093
H	3.63981201 +1	2.40886162 +1	-4.12407775 +1	0.1657
C	-0.26365586 +1	-2.13841423 +1	-7.05454222 +1	-0.0198
H	-1.20890983 +1	-2.72525178 +1	-7.17201308 +1	0.1165
H	0.33569328 +1	-2.41475873 +1	-7.95550268 +1	0.0861
C	-0.65337507 +1	-0.68431022 +1	-7.10544678 +1	0.0981
C	-0.80052384 +1	-0.05145485 +1	-8.33752644 +1	-0.1849
H	-0.56250623 +1	-0.57092828 +1	-9.26932911 +1	0.1290
C	-1.27152406 +1	1.25838893 +1	-8.36532630 +1	-0.0083
H	-1.40284759 +1	1.77594888 +1	-9.32139384 +1	0.1201
C	-1.57653772 +1	1.89671919 +1	-7.17188984 +1	-0.1330
H	-1.96235701 +1	2.92247677 +1	-7.14429512 +1	0.1624

---------- End of file **NIHZUZ.arc**----------

Yterbium: XOHVEV



---------- Begin of file **XOHVEV.mop**----------

```
RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
NUMERO DE COORDENAÇÃO = 9

 Yb         0.398708  1     -0.014066  1      0.029495  1
  O         2.733708  1     -0.014066  1      0.029495  1
  O         1.134739  1     -1.637017  1     -1.441616  1
  O         1.073719  1     -1.537539  1      1.618309  1
  O         1.114191  1      1.600657  1      1.482828  1
  O         1.226015  1      1.424931  1     -1.569540  1
  N        -1.124363  1     -0.256360  1     -2.107901  1
  N        -1.228309  1     -2.023724  1      0.247451  1
  N        -1.197958  1      0.310751  1      2.057962  1
  N        -1.111430  1      2.073564  1     -0.311244  1
  H         3.133881  1      0.761139  1      0.029495  1
  H         3.142633  1     -0.436446  1      0.515540  1
  C        -2.249300  1     -1.194109  1     -1.846378  1
  H        -2.637531  1     -1.484304  1     -2.708115  1
```

```
 H        -2.953285  1     -0.717604  1     -1.341917  1
 C        -1.818646  1     -2.408522  1     -1.065042  1
 H        -2.601705  1     -2.993358  1     -0.912389  1
 H        -1.154223  1     -2.917030  1     -1.590500  1
 C        -2.335107  1     -1.709051  1      1.197681  1
 H        -2.777255  1     -2.551383  1      1.468056  1
 H        -3.006653  1     -1.150020  1      0.735252  1
 C        -1.853641  1     -0.974081  1      2.437641  1
 H        -2.620865  1     -0.793090  1      3.034082  1
 H        -1.208878  1     -1.541907  1      2.927311  1
 C        -2.267458  1      1.310950  1      1.754657  1
 H        -2.662657  1      1.632341  1      2.602620  1
 H        -2.983485  1      0.871405  1      1.235564  1
 C        -1.743154  1      2.499709  1      0.969621  1
 H        -2.490420  1      3.117092  1      0.773272  1
 H        -1.081477  1      2.986791  1      1.518869  1
 C        -2.171596  1      1.845740  1     -1.326847  1
 H        -2.517548  1      2.719315  1     -1.634923  1
 H        -2.921343  1      1.355519  1     -0.905111  1
 C        -1.680445  1      1.054452  1     -2.529526  1
 H        -2.426917  1      0.911759  1     -3.161782  1
 H        -0.978396  1      1.573238  1     -2.995039  1
 C        -0.256530  1     -0.780174  1     -3.192030  1
 H         0.154090  1     -0.024132  1     -3.679591  1
 H        -0.807214  1     -1.294364  1     -3.833950  1
 C         0.833932  1     -1.667650  1     -2.643981  1
 N         1.476818  1     -2.419080  1     -3.518461  1
 C        -0.437910  1     -3.163317  1      0.746428  1
 H        -0.021749  1     -3.633257  1     -0.016664  1
 H        -1.036696  1     -3.801025  1      1.207417  1
 C         0.642183  1     -2.706020  1      1.696940  1
 N         1.115995  1     -3.584547  1      2.540087  1
 C        -0.360131  1      0.794114  1      3.184741  1
 H         0.011395  1      0.022394  1      3.678248  1
 H        -0.923116  1      1.314309  1      3.810483  1
 C         0.769686  1      1.664972  1      2.679569  1
 N         1.387882  1      2.434259  1      3.548472  1
 C        -0.208779  1      3.155737  1     -0.766096  1
 H         0.223608  1      3.577262  1      0.015763  1
 H        -0.735892  1      3.848666  1     -1.234424  1
 C         0.851549  1      2.624393  1     -1.697948  1
 N         1.377162  1      3.437477  1     -2.568333  1
 H         1.190941  1     -2.423021  1     -4.310010  1
 H         2.134147  1     -2.891216  1     -3.240561  1
 H         0.778791  1     -4.254000  1      2.509663  1
 H         1.761783  1     -3.368854  1      2.978873  1
 H         2.064828  1      2.894623  1      3.343179  1
 H         1.076914  1      2.508517  1      4.284863  1
 H         1.085280  1      4.180433  1     -2.600921  1
 H         1.928192  1      3.193465  1     -3.013445  1
0
```

---------- End of file XOHVEV.**mop**----------

---------- Begin of file XOHVEV**.arc**----------

```
            SUMMARY OF RM1 CALCULATION, Site No: 3560

                          MOPAC2012 (Version: 12.290W)
                          Wed Nov 21 16:07:49 2012
                          No. of days left = 329

          Empirical Formula: C16 H34 N8 O5 Yb  =    64 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO = 9



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =        284.77982 KCAL/MOL =    1191.51879 KJ/MOL
TOTAL ENERGY            =      -5773.65180 EV
ELECTRONIC ENERGY       =     -55614.30012 EV
CORE-CORE REPULSION     =      49840.64831 EV
GRADIENT NORM           =          0.24595
DIPOLE                  =          1.87998 DEBYE    POINT GROUP:       C2
NO. OF FILLED LEVELS    =         84
CHARGE ON SYSTEM        =          3
IONIZATION POTENTIAL    =         19.787821 EV
HOMO LUMO ENERGIES (EV) =        -19.788 -7.861
MOLECULAR WEIGHT        =        591.535
COSMO AREA              =        371.57 SQUARE ANGSTROMS
COSMO VOLUME            =        516.69 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    57    H    62    10.70904
            H    63    H    59    10.70388
            H    33    H    12     6.42003
          SCF CALCULATIONS        =        251
          COMPUTATION TIME        =         32.922 SECONDS

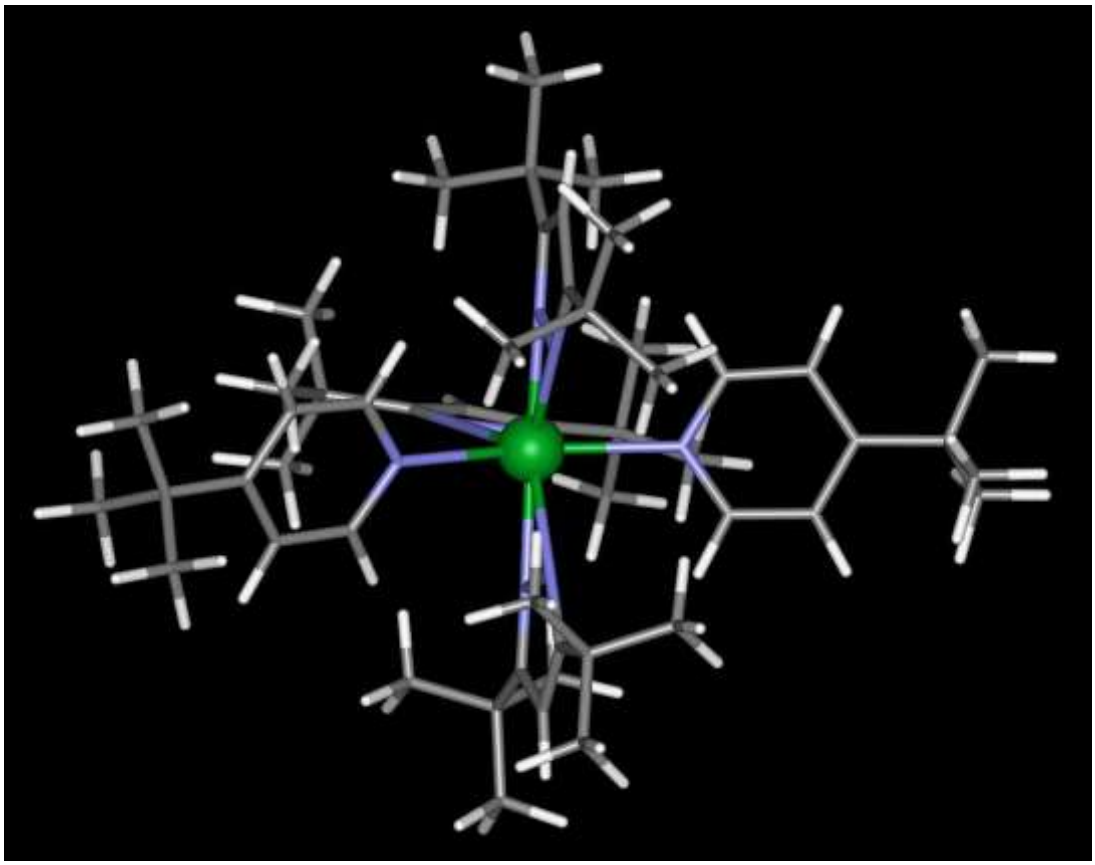

          FINAL GEOMETRY OBTAINED                                    CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3.0
 NUMERO DE COORDENAÇÃO = 9

 Yb     0.39085097 +1   0.01357908 +1  -0.00593088 +1             3.0000
  O     2.73736516 +1  -0.01723838 +1   0.04298969 +1            -0.5884
  O     1.09678323 +1  -1.52938603 +1  -1.62465108 +1            -0.7181
  O     1.07576484 +1  -1.65099118 +1   1.49617163 +1            -0.7251
  O     1.08565711 +1   1.53350400 +1   1.63933011 +1            -0.7178
  O     1.18683928 +1   1.65424044 +1  -1.47931789 +1            -0.7251
  N    -1.09748346 +1  -0.28345814 +1  -2.07182267 +1            -0.4814
  N    -1.17371192 +1  -1.99503410 +1   0.28954448 +1            -0.4804
  N    -1.16407624 +1   0.36064626 +1   2.00244483 +1            -0.4813
  N    -1.09435705 +1   2.07264428 +1  -0.35896245 +1            -0.4804
  H     3.34341485 +1   0.56716118 +1  -0.42400560 +1             0.2931
```

H	3.31059661 +1	-0.61325904 +1	0.53606745 +1	0.2932
C	-2.29075782 +1	-1.20895565 +1	-1.79792775 +1	-0.0770
H	-2.83682530 +1	-1.53052663 +1	-2.72041035 +1	0.1338
H	-3.07756151 +1	-0.66056990 +1	-1.21809989 +1	0.1063
C	-1.81977746 +1	-2.44711772 +1	-1.02864695 +1	-0.0568
H	-2.67943694 +1	-3.14836901 +1	-0.88158596 +1	0.1297
H	-1.09924170 +1	-3.04488930 +1	-1.63515776 +1	0.1135
C	-2.35050412 +1	-1.68691128 +1	1.22515714 +1	-0.0775
H	-2.92428724 +1	-2.59194613 +1	1.54786975 +1	0.1339
H	-3.12187218 +1	-1.07752054 +1	0.68684321 +1	0.1069
C	-1.84386392 +1	-0.93721329 +1	2.46102081 +1	-0.0577
H	-2.69059327 +1	-0.76607294 +1	3.17223708 +1	0.1303
H	-1.13346656 +1	-1.56635608 +1	3.04744861 +1	0.1125
C	-2.31493501 +1	1.32499541 +1	1.68444065 +1	-0.0770
H	-2.88448019 +1	1.66521451 +1	2.58579671 +1	0.1338
H	-3.09706465 +1	0.80240611 +1	1.07520635 +1	0.1063
C	-1.77462631 +1	2.54640884 +1	0.93418061 +1	-0.0568
H	-2.60448642 +1	3.27545604 +1	0.75500340 +1	0.1297
H	-1.05821910 +1	3.12026807 +1	1.56809662 +1	0.1134
C	-2.24419694 +1	1.80296693 +1	-1.33891354 +1	-0.0775
H	-2.77498966 +1	2.72629859 +1	-1.68263789 +1	0.1339
H	-3.05527977 +1	1.21979408 +1	-0.83089193 +1	0.1069
C	-1.71565717 +1	1.03612989 +1	-2.55495501 +1	-0.0577
H	-2.53955123 +1	0.89308304 +1	-3.29842700 +1	0.1303
H	-0.96247827 +1	1.64087866 +1	-3.11304336 +1	0.1124
C	-0.39587658 +1	-0.86658001 +1	-3.31775653 +1	-0.1062
H	0.03087800 +1	-0.05996729 +1	-3.96694632 +1	0.1496
H	-1.07983459 +1	-1.42407368 +1	-4.00275227 +1	0.1437
C	0.76382122 +1	-1.72523076 +1	-2.83524290 +1	0.4469
N	1.40122986 +1	-2.59537496 +1	-3.61997011 +1	-0.3519
C	-0.51236628 +1	-3.26962144 +1	0.85729595 +1	-0.1049
H	-0.12394852 +1	-3.93132830 +1	0.04102201 +1	0.1508
H	-1.21467201 +1	-3.92941312 +1	1.42244119 +1	0.1436
C	0.68123716 +1	-2.84299142 +1	1.69884438 +1	0.4488
N	1.28806805 +1	-3.65663572 +1	2.56398141 +1	-0.3510
C	-0.49061448 +1	0.92028975 +1	3.27433025 +1	-0.1061
H	-0.11423356 +1	0.09988397 +1	3.93729139 +1	0.1496
H	-1.18105322 +1	1.49939979 +1	3.93436562 +1	0.1437
C	0.71354813 +1	1.74089774 +1	2.83647660 +1	0.4467
N	1.34859108 +1	2.59057196 +1	3.64522156 +1	-0.3520
C	-0.37038857 +1	3.32455288 +1	-0.90015065 +1	-0.1049
H	0.00780318 +1	3.97363451 +1	-0.06903385 +1	0.1508
H	-1.02855293 +1	4.00666988 +1	-1.49123188 +1	0.1436
C	0.83963776 +1	2.85845817 +1	-1.69592662 +1	0.4488
N	1.50533907 +1	3.65118034 +1	-2.53682067 +1	-0.3509
H	1.14585146 +1	-2.74564897 +1	-4.58816451 +1	0.2828
H	2.20458885 +1	-3.11864416 +1	-3.28539850 +1	0.2863
H	0.98557570 +1	-4.61057769 +1	2.71981054 +1	0.2836
H	2.11105255 +1	-3.36219393 +1	3.08089281 +1	0.2859
H	2.18004555 +1	3.08807234 +1	3.34139912 +1	0.2862
H	1.06176352 +1	2.74947745 +1	4.60313687 +1	0.2828
H	1.24065966 +1	4.61443058 +1	-2.70357080 +1	0.2837
H	2.33696416 +1	3.32929542 +1	-3.02251920 +1	0.2859

---------- End of file XOHVEV.**arc**----------

Lutecium: DIHZID



---------- Begin of file DIHZID**.mop**----------

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RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10
NUMERO DE COORDENAÇÃO = 8

 Lu         0.024728  1     0.021865  1     0.045770  1
  N         2.479928  1     0.021865  1     0.045770  1
  N        -2.169362  1    -0.197566  1     1.139303  1
  N         0.310561  1    -2.040498  1     1.181308  1
  N         0.082873  1    -2.260209  1    -0.180779  1
  N         0.187974  1     0.302993  1    -2.231645  1
  N        -1.154818  1     0.335917  1    -1.903254  1
  N         0.399068  1     1.674884  1     1.662650  1
  N         0.049940  1     2.279287  1     0.451318  1
  C         3.169510  1     1.160886  1     0.045770  1
  H         2.712228  1     1.947111  1     0.232469  1
  C         4.517143  1     1.248360  1    -0.209050  1
  H         4.936225  1     2.078303  1    -0.192288  1
  C         5.243304  1     0.130790  1    -0.490198  1
  C         4.537394  1    -1.067308  1    -0.456542  1
  H         4.981634  1    -1.867766  1    -0.619735  1
  C         3.198278  1    -1.079492  1    -0.186061  1
  H         2.762758  1    -1.900118  1    -0.163849  1
  C         6.720142  1     0.174310  1    -0.849327  1
  C         7.143994  1     1.557865  1    -1.339219  1
  H         7.135823  1     2.174545  1    -0.604835  1
  H         6.531560  1     1.858683  1    -2.016510  1
  H         8.028914  1     1.510923  1    -1.707904  1
```

C	7.526290	1	0.055356	1	0.412290	1
H	7.086755	1	0.532869	1	1.115323	1
H	8.400722	1	0.424376	1	0.267425	1
H	7.605207	1	-0.870265	1	0.651970	1
C	7.050004	1	-0.779439	1	-1.864020	1
H	6.291331	1	-0.913445	1	-2.434937	1
H	7.301985	1	-1.606822	1	-1.455565	1
H	7.787006	1	-0.450328	1	-2.383006	1
C	-2.839073	1	0.840207	1	1.628345	1
H	-2.413275	1	1.664896	1	1.670898	1
C	-4.146280	1	0.749063	1	2.080818	1
H	-4.570891	1	1.506257	1	2.415770	1
C	-4.819978	1	-0.449264	1	2.034529	1
C	-4.100768	1	-1.528220	1	1.537736	1
H	-4.496208	1	-2.368366	1	1.495881	1
C	-2.812100	1	-1.355841	1	1.113891	1
H	-2.357352	1	-2.097640	1	0.782962	1
C	-6.283945	1	-0.626156	1	2.466914	1
C	-7.124167	1	-0.883572	1	1.259434	1
H	-8.047879	1	-0.927254	1	1.514214	1
H	-6.861157	1	-1.716683	1	0.859333	1
H	-7.000873	1	-0.173484	1	0.623902	1
C	-6.814454	1	0.606443	1	3.195812	1
H	-7.719332	1	0.449564	1	3.475771	1
H	-6.789198	1	1.365536	1	2.605891	1
H	-6.268976	1	0.782488	1	3.964795	1
C	-6.370773	1	-1.773083	1	3.441685	1
H	-7.194452	1	-1.716415	1	3.931721	1
H	-5.632210	1	-1.726216	1	4.056317	1
H	-6.337966	1	-2.602490	1	2.964387	1
C	0.221957	1	-3.230836	1	1.804665	1
C	-0.025924	1	-4.212096	1	0.854078	1
H	-0.117694	1	-5.124428	1	1.008212	1
C	-0.111925	1	-3.566372	1	-0.368614	1
C	0.411227	1	-3.343909	1	3.294035	1
C	1.780661	1	-2.917269	1	3.655099	1
H	1.959121	1	-3.153960	1	4.568082	1
H	1.857219	1	-1.967109	1	3.551982	1
H	2.412197	1	-3.353882	1	3.080292	1
C	-0.610644	1	-2.561493	1	3.981054	1
H	-0.315252	1	-2.357567	1	4.872825	1
H	-1.426776	1	-3.066533	1	4.021262	1
H	-0.766019	1	-1.744876	1	3.500651	1
C	0.306087	1	-4.803097	1	3.714522	1
H	-0.609415	1	-5.086101	1	3.663550	1
H	0.620127	1	-4.897993	1	4.619705	1
H	0.842576	1	-5.343766	1	3.132482	1
C	-0.391617	1	-4.105792	1	-1.755117	1
C	-1.421462	1	-3.233176	1	-2.438142	1
H	-1.624821	1	-3.596042	1	-3.304231	1
H	-1.072867	1	-2.343700	1	-2.535560	1
H	-2.221114	1	-3.204356	1	-1.907560	1
C	-0.929354	1	-5.503649	1	-1.682070	1
H	-1.267845	1	-5.761779	1	-2.542642	1
H	-1.638841	1	-5.541320	1	-1.035720	1
H	-0.227193	1	-6.103022	1	-1.421714	1
C	0.838964	1	-4.064200	1	-2.577021	1
H	0.610061	1	-4.170605	1	-3.503862	1
H	1.426693	1	-4.772626	1	-2.310476	1
H	1.278060	1	-3.219754	1	-2.450940	1
C	0.309999	1	0.459694	1	-3.548856	1

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 C       -0.961866  1     0.594247  1    -4.103877  1
 H       -1.174658  1     0.704548  1    -5.002358  1
 C       -1.852809  1     0.523925  1    -3.033928  1
 C        1.619387  1     0.479096  1    -4.287936  1
 C        2.704999  1     0.246817  1    -3.483319  1
 H        2.880482  1     1.025833  1    -2.953166  1
 H        3.470813  1     0.051801  1    -4.031373  1
 H        2.524626  1    -0.498893  1    -2.909272  1
 C        1.698084  1     1.699980  1    -5.105771  1
 H        0.810357  1     1.985570  1    -5.339589  1
 H        2.197723  1     1.520558  1    -5.904066  1
 H        2.134405  1     2.393300  1    -4.604282  1
 C        1.573075  1    -0.565316  1    -5.369035  1
 H        0.707117  1    -0.554767  1    -5.786061  1
 H        1.732162  1    -1.430767  1    -4.987766  1
 H        2.245922  1    -0.375674  1    -6.026850  1
 C       -3.358442  1     0.614801  1    -3.083858  1
 C       -4.003380  1     0.188235  1    -1.858893  1
 H       -3.569909  1     0.601194  1    -1.108448  1
 H       -3.939610  1    -0.765433  1    -1.776989  1
 H       -4.927307  1     0.445097  1    -1.874828  1
 C       -3.876107  1    -0.204126  1    -4.211932  1
 H       -4.831428  1    -0.265120  1    -4.149495  1
 H       -3.493236  1    -1.083758  1    -4.169106  1
 H       -3.634791  1     0.211098  1    -5.044094  1
 C       -3.743350  1     1.961272  1    -3.433525  1
 H       -3.172428  1     2.287708  1    -4.133834  1
 H       -3.659333  1     2.530221  1    -2.662618  1
 H       -4.656274  1     1.967503  1    -3.735526  1
 C        0.205628  1     3.596535  1     0.590513  1
 C        0.646991  1     3.858731  1     1.880301  1
 H        0.833222  1     4.693112  1     2.246395  1
 C        0.755188  1     2.637831  1     2.512670  1
 C       -0.158071  1     4.534453  1    -0.531038  1
 C        0.298404  1     3.981788  1    -1.871068  1
 H        0.065208  1     4.599833  1    -2.568761  1
 H       -0.130813  1     3.139996  1    -2.032542  1
 H        1.251168  1     3.859002  1    -1.860625  1
 C        0.473951  1     5.905609  1    -0.302548  1
 H        0.083041  1     6.314279  1     0.471835  1
 H        0.318960  1     6.460117  1    -1.071227  1
 H        1.419882  1     5.801654  1    -0.167933  1
 C       -1.669549  1     4.704584  1    -0.560049  1
 H       -2.084084  1     3.855040  1    -0.725181  1
 H       -1.907954  1     5.317340  1    -1.260367  1
 H       -1.969433  1     5.049790  1     0.283140  1
 C        1.177401  1     2.291620  1     3.929180  1
 C        2.338683  1     1.329181  1     3.897416  1
 H        2.187799  1     0.669101  1     3.216599  1
 H        2.416905  1     0.896906  1     4.751345  1
 H        3.147665  1     1.809881  1     3.706470  1
 C       -0.001984  1     1.706080  1     4.661327  1
 H        0.260812  1     1.469148  1     5.552987  1
 H       -0.308524  1     0.923325  1     4.198968  1
 H       -0.709408  1     2.353268  1     4.697914  1
 C        1.616369  1     3.561912  1     4.672380  1
 H        1.905305  1     3.331826  1     5.556640  1
 H        0.876132  1     4.173183  1     4.727795  1
 H        2.338852  1     3.977700  1     4.196209  1
0
```

---------- End of file DIHZID**.mop**----------

---------- Begin of file DIHZID**.arc**----------

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           SUMMARY OF RM1 CALCULATION, Site No: 3560

                          MOPAC2012 (Version: 12.290W)
                          Wed Nov 21 16:21:16 2012
                          No. of days left = 329

           Empirical Formula: C51 H83 N8 Lu  =   143 atoms

 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO = 8



     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

HEAT OF FORMATION       =       -125.30654 KCAL/MOL =    -524.28258 KJ/MOL
TOTAL ENERGY            =      -9299.48611 EV
ELECTRONIC ENERGY       =    -145160.54397 EV
CORE-CORE REPULSION     =     135861.05786 EV
GRADIENT NORM           =          0.21129
DIPOLE                  =          3.90258 DEBYE    POINT GROUP:       C1
NO. OF FILLED LEVELS    =        165
IONIZATION POTENTIAL    =          8.425464 EV
HOMO LUMO ENERGIES (EV) =         -8.425 -0.377
MOLECULAR WEIGHT        =        983.237
COSMO AREA              =        737.47 SQUARE ANGSTROMS
COSMO VOLUME            =       1205.56 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    43    H    31    16.96302
            H   125    H    77    13.13288
            H    69    H    98    11.33061
          SCF CALCULATIONS        =       1148
          COMPUTATION TIME = 14 MINUTES AND  47.656 SECONDS


          FINAL GEOMETRY OBTAINED                                    CHARGE
 RM1 SPARKLE EXTERNAL=spk.inp PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
 NOLOG GEO-OK SCFCRT=1.D-10
 NUMERO DE COORDENAÇÃO = 8

 Lu    -0.05978816 +1   0.03521676 +1  -0.17185462 +1             3.0000
  N     2.42097704 +1   0.07606809 +1  -0.18969907 +1            -0.5251
  N    -2.24225463 +1  -0.17867463 +1   0.99001316 +1            -0.5250
  N     0.25255393 +1  -2.01134082 +1   0.90642488 +1            -0.5919
  N    -0.14293365 +1  -2.26158042 +1  -0.38261966 +1            -0.5953
  N     0.04551192 +1   0.27726924 +1  -2.47543889 +1            -0.5838
  N    -1.26789891 +1   0.44405684 +1  -2.10798192 +1            -0.5840
  N     0.33264157 +1   1.66572403 +1   1.45179840 +1            -0.5918
  N     0.08165334 +1   2.29788427 +1   0.26092521 +1            -0.5956
  C     3.13349532 +1   1.23639169 +1  -0.35178040 +1             0.0929
  H     2.56227407 +1   2.17026671 +1  -0.50392544 +1             0.1578
  C     4.52580527 +1   1.32254911 +1  -0.34049061 +1            -0.2017
```

H	4.97300533	2.31088399	-0.47589638	0.1401
C	5.28669754	0.17352400	-0.16121101	0.0772
C	4.59664953	-1.02838334	-0.00689083	-0.2040
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H	6.93163775	-0.37176364	-2.25118573	0.0698
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C	0.13777836 +1	0.40924874 +1	-3.83878282 +1	0.0989
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C	-3.48019033 +1	0.92385708 +1	-3.26894584 +1	0.0708
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H	-4.82510965 +1	2.47314156 +1	-4.04096881 +1	0.0543
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C	0.46979641 +1	3.90074205 +1	1.80264353 +1	-0.3098
H	0.60205122 +1	4.86123543 +1	2.27529246 +1	0.1369
C	0.57094988 +1	2.62786038 +1	2.40683934 +1	0.0901
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H	0.88314782 +1	5.10978317 +1	-2.57585709 +1	0.0601
H	0.94170111 +1	3.39404015 +1	-2.18032159 +1	0.0767
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H	-1.68291998 +1	5.09621176 +1	-2.06553909 +1	0.0574
H	-2.24927784 +1	4.51208233 +1	-0.49798191 +1	0.0577
C	0.86297382 +1	2.30442654 +1	3.83248227 +1	0.0719
C	2.00051128 +1	1.28667712 +1	3.90306105 +1	-0.1792
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H	2.25906106 +1	1.02911048 +1	4.94043526 +1	0.0564

H	2.91791013 +1	1.66460157 +1	3.42996103 +1	0.0614
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H	-0.23945688 +1	1.46120010 +1	5.52794197 +1	0.0593
H	-0.74699544 +1	0.81630036 +1	3.96520523 +1	0.0634
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C	1.27761205 +1	3.56549024 +1	4.59105377 +1	-0.1844
H	1.54500305 +1	3.34429028 +1	5.63474832 +1	0.0581
H	0.47455024 +1	4.31524503 +1	4.62950197 +1	0.0637
H	2.15192274 +1	4.05268907 +1	4.13658395 +1	0.0656

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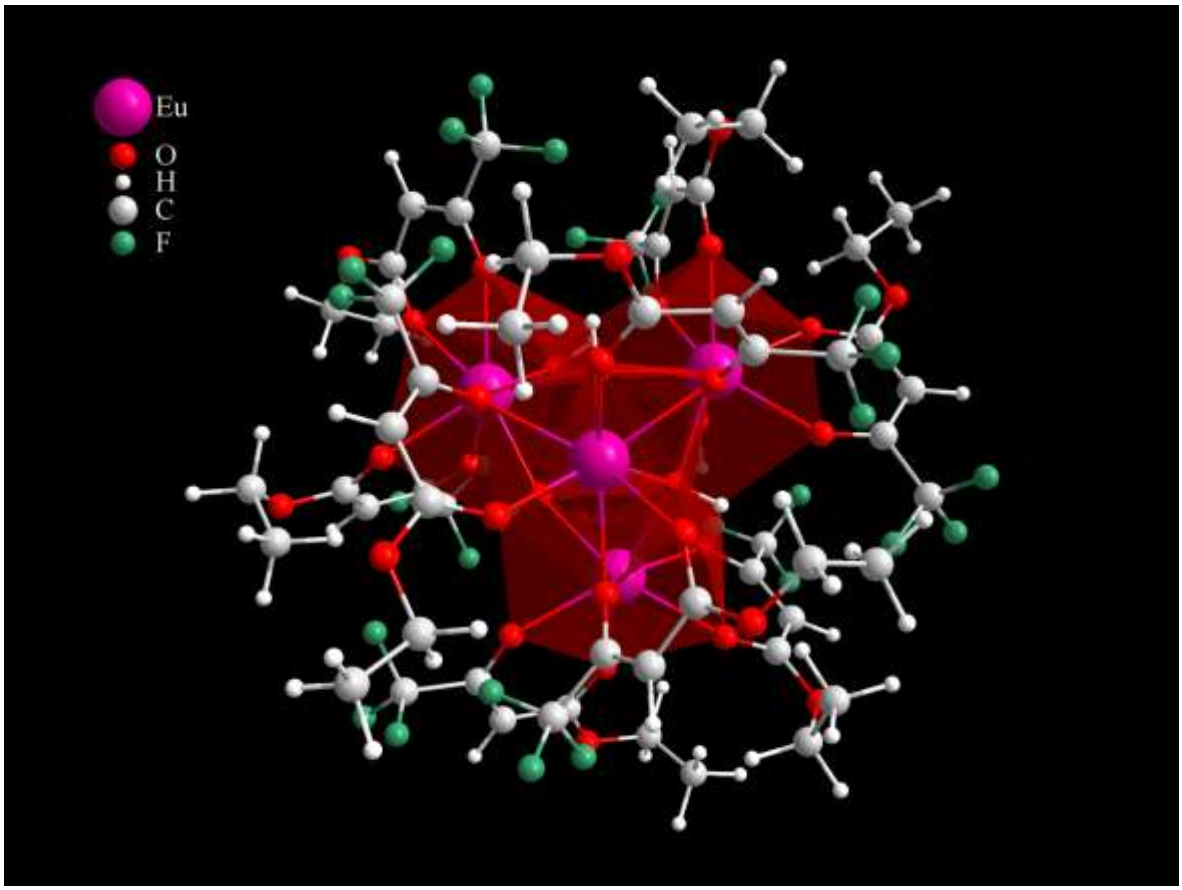
Tetramer Complex Calculation

(back to contents)



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GNORM=0.25 MMOK GEO-OK SCFCRT=1.D-10
STRUCTURE = tetramer

Eu          0.00000000  1   0.00000000  1   0.00000000  1
Eu          3.66130000  1   0.00000000  1   0.00000000  1
Eu          0.86288227  1   3.56999916  1   0.00000000  1
Eu          0.88402919  1   0.69336033  1   3.49957770  1
 O          4.42683552  1   2.15143107  1   0.64824854  1
 H          4.11544311  1   2.92139252  1   0.19285645  1
 H          4.63789335  1   2.38091999  1   1.54361608  1
 O          1.99815571  1   4.17187774  1   2.03248556  1
 H          1.70244131  1   3.79448501  1   2.85343513  1
 H          2.93646838  1   4.29752555  1   2.07170572  1
 O          3.21866378  1   1.34071834  1   3.66106633  1
 H          3.49841765  1   2.22708945  1   3.75394708  1
 H          3.90972518  1   0.82670835  1   3.26852319  1
 O          1.81004063  1   1.46342330  1  -0.58481787  1
 H          1.93345783  1   1.51998300  1  -1.51334560  1
 O          0.14517442  1   1.86384464  1   1.54728000  1
 H         -0.72871816  1   2.13782975  1   1.76945489  1
 O          1.85882685  1  -0.28106005  1   1.51059195  1
 H          2.06804424  1  -1.14372644  1   1.83120576  1
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O	-0.68971454	1	-0.36109518	1	-2.29156544	1
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O	0.54803963	1	8.15097570	1	-0.45771461	1
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H	1.02056918	1	-3.99882014	1	-2.42985334	1
C	-0.16911343	1	-3.28473493	1	-0.89503723	1
C	-1.97341504	1	-4.58593929	1	-0.06994839	1
H	-2.31503481	1	-3.69706782	1	0.19859547	1
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C	-1.58046720	1	-5.31507644	1	1.09341768	1
H	-1.23484516	1	-6.19439973	1	0.82904453	1
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C	-2.49321677	1	3.62169783	1	-1.81130001	1
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C	-1.63385738	1	-2.06196576	1	3.95347380	1
C	-1.78902162	1	-1.27894607	1	2.65861207	1
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C	-4.87544912	1	-0.21821619	1	-0.86258980	1
H	-4.33117438	1	0.57170295	1	-1.10241934	1
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C	5.06203591	1	5.15330794	1	-1.33216260	1
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C	-2.45515120	1	5.75025435	1	2.43187432	1
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H	1.44848227	1	9.05857898	1	-1.94519065	1
H	1.58631953	1	7.45936940	1	-1.97243374	1
C	2.86448901	1	8.35152047	1	-0.63712703	1
H	3.06614587	1	9.29486467	1	-0.45880924	1
H	3.58463975	1	7.96208587	1	-1.17503015	1
H	2.78877379	1	7.86689551	1	0.21024695	1
C	0.98607598	1	4.73114833	1	5.74920903	1
C	0.28004549	1	3.55074371	1	5.12586229	1
C	-0.97395316	1	3.26697104	1	5.53751804	1
H	-1.35066456	1	3.76120415	1	6.25633804	1
C	-1.74750958	1	2.23979414	1	4.91315699	1
C	-3.96353239	1	1.35935620	1	4.64890702	1
H	-4.75329952	1	1.23784098	1	5.23235734	1
H	-3.52249034	1	0.47734095	1	4.54497636	1
C	-4.41170559	1	1.86181057	1	3.29051105	1
H	-4.78897006	1	2.76253678	1	3.38391769	1
H	-5.09258853	1	1.25907832	1	2.92592313	1

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 H          -3.64378270  1   1.89252926  1   2.68324583  1
 C           2.72709434  1  -3.34433475  1   4.97677637  1
 C           2.13986254  1  -1.94505379  1   5.15957924  1
 C           2.02256035  1  -1.47782909  1   6.43001498  1
 H           2.29023146  1  -2.03102641  1   7.15393836  1
 C           1.50570742  1  -0.18260115  1   6.70068421  1
 C           1.09780200  1   1.47174359  1   8.35605045  1
 H           0.13824680  1   1.55064341  1   8.13252598  1
 H           1.59648143  1   2.17400558  1   7.87038351  1
 C           1.30152450  1   1.61567462  1   9.83384702  1
 H           0.81415995  1   0.90571918  1  10.30248677  1
 H           0.96661219  1   2.48835298  1  10.12556410  1
 H           2.25671310  1   1.54486980  1  10.04074174  1
 F           3.06167228  1  -3.53906548  1  -3.47676030  1
 F           2.79152519  1  -1.44071876  1  -3.86231275  1
 F           4.14118851  1  -2.08303580  1  -2.32603847  1
 F          -3.19566458  1   3.93591503  1  -2.89631921  1
 F          -3.34513625  1   3.61931822  1  -0.78359113  1
 F          -1.64901970  1   4.63915230  1  -1.59719208  1
 F          -0.95480912  1  -1.35494924  1   4.87144444  1
 F          -0.93664391  1  -3.17889985  1   3.75739970  1
 F          -2.78471474  1  -2.41275088  1   4.51566693  1
 F           4.82879054  1   0.81452732  1  -5.20630682  1
 F           3.54717432  1   2.18355125  1  -4.33838438  1
 F           5.56965906  1   2.66159783  1  -4.53472318  1
 F           7.49159853  1   0.18144945  1   2.99441463  1
 F           7.25269003  1  -1.59244227  1   4.17230111  1
 F           5.97681720  1   0.09530327  1   4.49818564  1
 F           5.19599200  1   5.91605294  1  -0.26839314  1
 F           5.83800560  1   4.08260565  1  -1.14007382  1
 F           5.60775492  1   5.81514146  1  -2.35052374  1
 F          -3.61226189  1   5.14443432  1   1.81466600  1
 F          -2.33670114  1   5.13904323  1   3.47512528  1
 F          -2.94735832  1   7.00381288  1   2.64571569  1
 F           1.27079702  1   5.65496588  1   4.87300293  1
 F           0.31719250  1   5.30664081  1   6.73926445  1
 F           2.14927797  1   4.36496777  1   6.28601690  1
 F           3.90522109  1  -3.30587313  1   4.44464579  1
 F           1.96505792  1  -4.07234192  1   4.15893650  1
 F           2.80845566  1  -4.05098055  1   6.08635108  1
0
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---------- End of file TETRAMER.mop----------

---------- Begin of file TETRAMER.arc----------

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                    SUMMARY OF   RM1 CALCULATION, Site No:  999

                                                  MOPAC2009 (Version: 11.03W )
                                                     Tue Oct 30 20:15:06 2012

           Empirical Formula: C54 H63 O33 Eu4 F27  =   181 atoms

RM1 SPARKLE EXTERNAL=spk_Eu.inp PRECISE XYZ BFGS T=10D GNORM=0.25 MMOK +
GEO-OK SCFCRT=1.D-10
STRUCTURE = tetramer


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

      HEAT OF FORMATION       =      -2226.17970 KCAL/MOL =   -9314.33587 KJ/MOL
      TOTAL ENERGY            =     -31420.76601 EV
      ELECTRONIC ENERGY       =    -526829.69511 EV
      CORE-CORE REPULSION     =     495408.92910 EV
      GRADIENT NORM           =          0.23092
      DIPOLE                  =          8.20321 DEBYE    POINT GROUP:       C1
          NO. OF FILLED LEVELS    =        339
          IONIZATION POTENTIAL    =          9.649153 EV
          HOMO LUMO ENERGIES (EV) =         -9.649 -1.191
          MOLECULAR WEIGHT        =       2360.885
          COSMO AREA              =        926.93 SQUARE ANGSTROMS
          COSMO VOLUME            =       1903.91 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    69    H   152    17.55288
            H    56    H   125    15.91359
            H    90    H    78    15.77338
          SCF CALCULATIONS        =        970
          COMPUTATION TIME = 39 MINUTES AND  46.675 SECONDS


          FINAL GEOMETRY OBTAINED                                  CHARGE
RM1 SPARKLE EXTERNAL=spk_Eu.inp PRECISE XYZ BFGS T=10D +
GNORM=0.25 MMOK GEO-OK SCFCRT=1.D-10
 ESTRUTURA = tetramero

 Eu    -0.26925201 +1  -0.16693142 +1  -0.09098969 +1           0.0000
 Eu     3.48290694 +1  -0.15113681 +1  -0.07998732 +1           0.0000
 Eu     0.73642074 +1   3.45294559 +1  -0.13144226 +1           0.0000
 Eu     0.73839857 +1   0.66100915 +1   3.42720327 +1           0.0000
  O     4.40062789 +1   2.07154884 +1   0.63106241 +1          -0.6123
  H     4.18584263 +1   2.97897438 +1   0.28788934 +1           0.2926
  H     5.15509892 +1   2.26659645 +1   1.21283880 +1           0.2710
  O     2.11355367 +1   4.06932971 +1   1.87137462 +1          -0.6117
  H     1.93512651 +1   3.90900757 +1   2.83538168 +1           0.2921
  H     2.89265848 +1   4.64953404 +1   1.91923073 +1           0.2708
  O     3.11805210 +1   1.44107759 +1   3.55530993 +1          -0.6109
  H     3.49370908 +1   2.16545946 +1   4.08472488 +1           0.2720
  H     3.94268613 +1   1.01843447 +1   3.19905530 +1           0.2917
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O	1.62122380 +1	1.27398474 +1	-0.66001369 +1	0.0000
H	1.98130283 +1	1.54209046 +1	-1.50190591 +1	0.2449
O	-0.00167766 +1	1.74447114 +1	1.40747010 +1	0.0000
H	-0.64422695 +1	2.29673353 +1	1.84612943 +1	0.2458
O	1.62472067 +1	-0.39067566 +1	1.43992358 +1	0.0000
H	1.99659432 +1	-1.13956254 +1	1.89947094 +1	0.2443
O	1.62992115 +1	-1.38703305 +1	-1.20489059 +1	-0.9009
O	-0.50923456 +1	-2.61525399 +1	-0.19299318 +1	-0.6898
O	-0.64334056 +1	-4.82508295 +1	-0.63626472 +1	-0.2454
O	-1.04808909 +1	2.00207322 +1	-1.10370970 +1	-0.8995
O	-0.91585789 +1	-0.30502339 +1	-2.46258136 +1	-0.6910
O	-1.66447604 +1	-0.17863523 +1	-4.58165748 +1	-0.2414
O	-0.99495390 +1	-0.70887728 +1	2.25855277 +1	-0.8996
O	-2.70682716 +1	-0.17769475 +1	0.23572923 +1	-0.6905
O	-4.88329332 +1	-0.26680072 +1	0.82241685 +1	-0.2384
O	3.99127775 +1	0.53651721 +1	-2.36115839 +1	-0.7557
O	5.79396902 +1	-0.34053681 +1	-0.88207300 +1	-0.7467
O	7.89831419 +1	-0.39234549 +1	-1.68108893 +1	-0.2519
O	4.59431452 +1	-0.17169052 +1	2.12800110 +1	-0.7572
O	4.15552147 +1	-2.34295830 +1	0.78655213 +1	-0.7331
O	5.14964445 +1	-4.22996374 +1	1.50651798 +1	-0.2409
O	3.10494438 +1	3.94972041 +1	-0.63674820 +1	-0.7586
O	1.26789002 +1	3.97946934 +1	-2.46449618 +1	-0.7342
O	1.81295725 +1	4.82916973 +1	-4.47625247 +1	-0.2388
O	-1.17262890 +1	4.48095764 +1	0.97968605 +1	-0.7558
O	0.54197276 +1	5.89815300 +1	-0.13977422 +1	-0.7463
O	0.24756145 +1	8.12942960 +1	-0.14672545 +1	-0.2523
O	0.98868445 +1	3.05442252 +1	3.99245895 +1	-0.7590
O	-1.20920523 +1	1.75382968 +1	4.43601370 +1	-0.7334
O	-2.77780150 +1	2.75989299 +1	5.69887717 +1	-0.2388
O	1.52696197 +1	-1.48994883 +1	4.26255136 +1	-0.7522
O	1.18067040 +1	0.42614449 +1	5.82736805 +1	-0.7489
O	1.62391764 +1	0.12539651 +1	8.00836311 +1	-0.2510
C	2.49676905 +1	-2.28101602 +1	-3.30878911 +1	0.5491
C	1.59509364 +1	-2.40063144 +1	-2.04162739 +1	0.3048
C	0.85616616 +1	-3.52607321 +1	-1.89718063 +1	-0.4010
H	0.94382645 +1	-4.38286225 +1	-2.57254957 +1	0.1841
C	-0.11496992 +1	-3.61884083 +1	-0.83308853 +1	0.5469
C	-1.49432775 +1	-5.05750154 +1	0.47659149 +1	0.0544
H	-2.19147727 +1	-4.21716735 +1	0.68534470 +1	0.0808
H	-2.11248808 +1	-5.91182553 +1	0.12445250 +1	0.0934
C	-0.62997299 +1	-5.41438438 +1	1.67346114 +1	-0.2376
H	-0.02212038 +1	-6.31388022 +1	1.49572506 +1	0.0845
H	-1.24655156 +1	-5.61487841 +1	2.56178458 +1	0.0944
H	0.07104658 +1	-4.61024682 +1	1.94143657 +1	0.0925
C	-2.97062217 +1	3.42404168 +1	-1.60961367 +1	0.5488
C	-2.02569039 +1	2.23103531 +1	-1.95237106 +1	0.3055
C	-2.27530152 +1	1.53264551 +1	-3.08528631 +1	-0.3985
H	-3.02973066 +1	1.83870868 +1	-3.81653971 +1	0.1841
C	-1.55734801 +1	0.30964163 +1	-3.34841876 +1	0.5434
C	-1.00174712 +1	-1.40078088 +1	-4.89691691 +1	0.0519
H	-1.33315394 +1	-2.21774793 +1	-4.21821109 +1	0.0721
H	0.09679845 +1	-1.28813505 +1	-4.76476564 +1	0.0839
C	-1.38042550 +1	-1.66971914 +1	-6.34608375 +1	-0.1996
H	-0.90609961 +1	-2.59668724 +1	-6.69973037 +1	0.0849
H	-1.05636051 +1	-0.86298047 +1	-7.01978503 +1	0.0864
H	-2.46536393 +1	-1.78406927 +1	-6.48269770 +1	0.0795
C	-1.78092387 +1	-2.39990470 +1	3.85085106 +1	0.5473
C	-2.03353580 +1	-1.39102836 +1	2.68789057 +1	0.3057
C	-3.30456874 +1	-1.29616325 +1	2.23165153 +1	-0.3997
H	-4.14345693 +1	-1.80601643 +1	2.71667990 +1	0.1844

C	-3.59793810 +1	-0.53521204 +1	1.04173385 +1	0.5462
C	-5.26798514 +1	0.37167313 +1	-0.38469698 +1	0.0531
H	-4.65712972 +1	1.27592072 +1	-0.59650309 +1	0.0860
H	-6.29579526 +1	0.71800543 +1	-0.13960065 +1	0.1023
C	-5.24382424 +1	-0.62920939 +1	-1.52714775 +1	-0.2293
H	-4.22656567 +1	-0.95588321 +1	-1.78312268 +1	0.0752
H	-5.67649909 +1	-0.18998881 +1	-2.43804697 +1	0.0872
H	-5.82564765 +1	-1.53490236 +1	-1.30177676 +1	0.0834
C	4.31727250 +1	1.18224707 +1	-4.62913771 +1	0.5471
C	4.86846358 +1	0.66810396 +1	-3.27040494 +1	0.3776
C	6.19746309 +1	0.36628105 +1	-3.11381873 +1	-0.4912
H	6.93658342 +1	0.49758763 +1	-3.90285791 +1	0.1801
C	6.59268606 +1	-0.14130524 +1	-1.84084933 +1	0.5562
C	8.35252400 +1	-0.97157775 +1	-0.47267883 +1	0.0587
H	7.96421697 +1	-0.44743841 +1	0.42785978 +1	0.0731
H	9.44535763 +1	-0.77278273 +1	-0.51931951 +1	0.0906
C	8.03506314 +1	-2.45800085 +1	-0.45801157 +1	-0.2252
H	6.95669249 +1	-2.65861522 +1	-0.38922946 +1	0.0724
H	8.50808900 +1	-2.95208603 +1	0.40293846 +1	0.0803
H	8.39800685 +1	-2.96923533 +1	-1.36157292 +1	0.0823
C	6.23140308 +1	-0.10989746 +1	3.87314856 +1	0.5397
C	5.40675078 +1	-0.89787903 +1	2.81323716 +1	0.3251
C	5.60080156 +1	-2.23801658 +1	2.67056747 +1	-0.4410
H	6.26945395 +1	-2.80899945 +1	3.31851599 +1	0.1845
C	4.90658795 +1	-2.92253489 +1	1.61686020 +1	0.5615
C	4.51435422 +1	-4.97541526 +1	0.48178501 +1	0.0562
H	5.14354676 +1	-5.89152080 +1	0.44607686 +1	0.0931
H	4.59359227 +1	-4.48444555 +1	-0.51325191 +1	0.0763
C	3.07751072 +1	-5.27383367 +1	0.87124502 +1	-0.2291
H	3.00751886 +1	-5.77214137 +1	1.84979691 +1	0.0932
H	2.60172314 +1	-5.93993368 +1	0.13703120 +1	0.0780
H	2.45939036 +1	-4.36720442 +1	0.93335032 +1	0.0787
C	5.19811178 +1	5.05932357 +1	-0.97864872 +1	0.5392
C	3.81206372 +1	4.58490350 +1	-1.50595760 +1	0.3217
C	3.44670726 +1	4.87287794 +1	-2.78477915 +1	-0.4361
H	4.11264683 +1	5.37513929 +1	-3.48974505 +1	0.1831
C	2.12755568 +1	4.50655975 +1	-3.22095508 +1	0.5662
C	0.52241865 +1	4.52066487 +1	-4.97540607 +1	0.0568
H	0.46367808 +1	5.17931057 +1	-5.86932524 +1	0.0923
H	-0.28873339 +1	4.83575242 +1	-4.28254876 +1	0.0758
C	0.44038811 +1	3.04752322 +1	-5.33432763 +1	-0.2265
H	1.23385848 +1	2.74571132 +1	-6.03401437 +1	0.0930
H	-0.51934868 +1	2.81486340 +1	-5.81785946 +1	0.0768
H	0.52644894 +1	2.39320313 +1	-4.45572365 +1	0.0781
C	-3.12294675 +1	5.32920783 +1	2.04744673 +1	0.5468
C	-1.79361668 +1	5.54951514 +1	1.27347266 +1	0.3774
C	-1.37084953 +1	6.80952727 +1	0.93337123 +1	-0.4912
H	-1.91871481 +1	7.71394068 +1	1.19397609 +1	0.1800
C	-0.14891208 +1	6.89897265 +1	0.20317171 +1	0.5563
C	1.50233888 +1	8.29963318 +1	-0.77873480 +1	0.0578
H	1.41374110 +1	9.32748556 +1	-1.19287674 +1	0.0898
H	1.64702428 +1	7.61209614 +1	-1.64079091 +1	0.0740
C	2.61807227 +1	8.18369375 +1	0.24716315 +1	-0.2257
H	2.46257946 +1	8.85120252 +1	1.10743806 +1	0.0846
H	3.58846819 +1	8.45158762 +1	-0.19505927 +1	0.0813
H	2.71864571 +1	7.16609281 +1	0.64917012 +1	0.0711
C	1.46038609 +1	5.09945435 +1	5.14161528 +1	0.5392
C	0.49314897 +1	3.92876280 +1	4.79816329 +1	0.3213
C	-0.74599054 +1	3.89433793 +1	5.35927714 +1	-0.4364
H	-1.12693476 +1	4.69389597 +1	5.99823583 +1	0.1829
C	-1.58269481 +1	2.75325940 +1	5.10724722 +1	0.5657

C	-3.64762425 +1	1.65263591 +1	5.53280630 +1	0.0559
H	-4.35918000 +1	1.79796965 +1	6.37478711 +1	0.0923
H	-3.13534061 +1	0.67950654 +1	5.70113585 +1	0.0771
C	-4.33016401 +1	1.72279530 +1	4.17835246 +1	-0.2262
H	-4.85466296 +1	2.67770126 +1	4.02620916 +1	0.0932
H	-5.08024487 +1	0.92522921 +1	4.07626816 +1	0.0766
H	-3.62474440 +1	1.61041395 +1	3.34325426 +1	0.0784
C	2.17529988 +1	-3.67524451 +1	4.99825058 +1	0.5449
C	1.84911846 +1	-2.18356734 +1	5.27577762 +1	0.3776
C	1.90532199 +1	-1.71184374 +1	6.56271889 +1	-0.4909
H	2.19946278 +1	-2.33062026 +1	7.40910546 +1	0.1792
C	1.55359456 +1	-0.34445677 +1	6.75773543 +1	0.5544
C	1.28180315 +1	1.48622125 +1	8.24054000 +1	0.0580
H	0.23408791 +1	1.69122931 +1	7.92699835 +1	0.0686
H	1.93446125 +1	2.16560036 +1	7.64859727 +1	0.0680
C	1.47531919 +1	1.67467744 +1	9.73916998 +1	-0.1985
H	0.83236348 +1	1.00699566 +1	10.33070078 +1	0.0804
H	1.23348979 +1	2.70605055 +1	10.03283097 +1	0.0763
H	2.51063251 +1	1.47959051 +1	10.05423368 +1	0.0816
F	2.08857457 +1	-3.03373989 +1	-4.34158423 +1	-0.2058
F	2.57302801 +1	-1.03859647 +1	-3.80078029 +1	-0.1917
F	3.76104293 +1	-2.66534747 +1	-3.07561722 +1	-0.2124
F	-4.18223799 +1	3.34252925 +1	-2.18014523 +1	-0.2061
F	-3.21739383 +1	3.55304245 +1	-0.30035097 +1	-0.1917
F	-2.47630699 +1	4.60469107 +1	-2.01204295 +1	-0.2122
F	-1.94620245 +1	-1.83868882 +1	5.05849621 +1	-0.2115
F	-0.55198198 +1	-2.93052741 +1	3.86179135 +1	-0.1970
F	-2.60727606 +1	-3.45649048 +1	3.83758003 +1	-0.2045
F	3.82105314 +1	0.19702830 +1	-5.39202467 +1	-0.2108
F	3.30991122 +1	2.05810954 +1	-4.48574691 +1	-0.2215
F	5.21494754 +1	1.81062661 +1	-5.40142311 +1	-0.2129
F	6.45549396 +1	1.16290808 +1	3.50117521 +1	-0.2254
F	7.44188038 +1	-0.61498183 +1	4.13661236 +1	-0.2000
F	5.60971574 +1	-0.01707679 +1	5.05811829 +1	-0.2113
F	5.18706861 +1	5.30024798 +1	0.34460011 +1	-0.2266
F	6.16556514 +1	4.14649472 +1	-1.15269265 +1	-0.2119
F	5.65893673 +1	6.18602796 +1	-1.53396927 +1	-0.2009
F	-4.15407691 +1	5.04725787 +1	1.23751319 +1	-0.2104
F	-3.05897851 +1	4.30062456 +1	2.90802753 +1	-0.2215
F	-3.52724962 +1	6.37283817 +1	2.78539929 +1	-0.2130
F	1.37048395 +1	6.12404718 +1	4.28015837 +1	-0.2129
F	1.29374887 +1	5.63263723 +1	6.35736702 +1	-0.2008
F	2.75140787 +1	4.72525515 +1	5.09672645 +1	-0.2259
F	3.38605159 +1	-4.04788512 +1	5.43937321 +1	-0.2143
F	2.16330153 +1	-3.99828360 +1	3.69627217 +1	-0.2189
F	1.31084942 +1	-4.52046781 +1	5.57819332 +1	-0.2118

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