J. Braz. Chem. Soc., Vol. 20, No. 9, S1-S13, 2009.
Printed in Brazil - ©2009 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Sparkle/PM3 for the Modeling of Europium(III), Gadolinium(III), and Terbium(III) Complexes

Ricardo O. Freire,[a] Gerd B. Rocha[b] and Alfredo M. Simas*,[c]

[a]*Departamento de Química, CCET, Universidade Federal de Sergipe, 49000-100 São Cristóvão-SE, Brazil*

[b]*Departamento de Química, CCEN, Universidade Federal da Paraíba, 58059-970 João Pessoa-PB, Brazil*

[c]*Departamento de Química Fundamental, CCEN, Universidade Federal de Pernambuco, 50590-470 Recife-PE, Brazil*

1. How to run lanthanide complexes Sparkle calculations with MOPAC2007

Updated information on how to run the Sparkle Model can be found in http://www.sparkle.pro.br.

MOPAC2007 is a software released by Prof. James J. P. Stewart from Stewart Computational Chemistry of Colorado Springs, CO, and represents a recent version of the MOPAC series of molecular modeling softwares, which started in 1981.

MOPAC2007 has Sparkle/AM1 and Sparkle/PM3 fully implemented.

A MOPAC2007 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 MOPAC2007 manual at http://openmopac.net/manual/.

As the MOPAC2007 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 MOPAC2007 is 7.221.

To run a Sparkle calculation in MOPAC 2007, 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. For a Sparkle/AM1 calculation, use the keyword AM1 in the keyword line.
   c. For a Sparkle/PM3 calculation, use the keyword PM3.

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 MOPAC2007, 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. MOPAC2007 Input (.mop) and output (.arc) files

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

As an example, we are providing in the appendix of this supplementary material the content of a MOPAC2007 input and the corresponding output file for [Eu(TREN-1,2-HOIQO)$(H_2O)_2$].

In order to reproduce the calculation, please obtain MOPAC2007.exe from http://openmopac.net, which is presently free for academics, copy the contents below to a text file, name it Eu_tren.mop, and simply open it with MOPAC2007.

Warning: MOPAC2007 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. How to visualize the input (.mop) structures with RASMOL

Molecular and complex structures, as *.mop files, can be visualized with RASMOL

*e-mail: simas@ufpe.br

(http://www.umass.edu/microbio/rasmol/getras.htm). The present version is 2.6.

(1) In RASMOL, click File, then, Open;
(2) In the "Select Molecular Coordinate File", tell RASMOL to list all files of the type "MOPAC File Format";
(3) In "Look in" go to the proper folder and find your .mop file.
(2) The .mop file of interest now appears. Choose it and press OK.
(3) The molecule or complex now appears drawn on the screen.

Warning: the bond connection algorithm of RASMOL 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. Sample Input and Output Files

----------Begin of file **Eu_tren.mop**----------

```
PM3 PRECISE NOINTER XYZ T=10D BFGS GNORM=0.25 +
NOLOG GEO-OK MMOK SCFCRT=1.D-10
Eu(TREN-1,2-HOIQO)(H2O)2

Eu    -6.005800  1   -2.264900  1    0.222500  1
 O    -3.918100  1   -3.361800  1    0.580700  1
 O    -5.770500  1   -4.306300  1   -0.928800  1
 O    -4.373500  1   -1.222500  1   -1.126700  1
 O    -4.928800  1   -0.899200  1    1.827600  1
 O    -8.352800  1   -3.015400  1   -0.206100  1
 O    -6.871500  1   -0.880100  1   -1.515000  1
 O    -7.473300  1   -0.976500  1    1.561900  1
 O    -6.467700  1   -3.804500  1    2.032000  1
 C     0.000000  1    0.000000  1    0.000000  1
 H     0.969600  1    0.000000  1    0.000000  1
 H    -0.297500  1    0.924500  1    0.000000  1
 C    -0.500900  1   -0.683000  1   -1.260600  1
 H     0.030200  1   -0.380500  1   -2.013400  1
 H    -0.367100  1   -1.639900  1   -1.172000  1
 C    -2.337100  1    0.244100  1   -2.575400  1
 C    -3.799800  1    0.507000  1   -2.702500  1
 C    -4.248400  1    1.533000  1   -3.476800  1
 H    -3.630500  1    2.096200  1   -3.882200  1
 C    -5.628000  1    1.765700  1   -3.681500  1
 C    -6.107100  1    2.825200  1   -4.478700  1
 H    -5.506200  1    3.424100  1   -4.860000  1
 C    -7.439500  1    2.980700  1   -4.692900  1
 H    -7.745300  1    3.678000  1   -5.223000  1
 C    -8.330200  1    2.105600  1   -4.127200  1
 H    -9.236800  1    2.208700  1   -4.306100  1
 C    -7.922700  1    1.070000  1   -3.291100  1
 H    -8.542300  1    0.500500  1   -2.896200  1
 C    -6.564000  1    0.913800  1   -3.063600  1
 C    -6.104700  1   -0.114100  1   -2.187900  1
 C    -0.460100  1    0.298900  1    2.329000  1
 H     0.363200  1    0.810700  1    2.275500  1
 H    -0.448100  1   -0.187800  1    3.166900  1
 C    -1.605400  1    1.243700  1    2.343800  1
 H    -1.436400  1    1.923800  1    3.014000  1
```

H	-1.651300	1	1.688000	1	1.482000	1
C	-3.646500	1	0.974100	1	3.698000	1
C	-5.091400	1	0.550800	1	3.727600	1
C	-5.881900	1	1.138200	1	4.668500	1
H	-5.494900	1	1.619500	1	5.363000	1
C	-7.328700	1	1.017600	1	4.591400	1
C	-8.144000	1	1.608200	1	5.554200	1
H	-7.777000	1	2.044800	1	6.289400	1
C	-9.535400	1	1.531500	1	5.387200	1
H	-10.091900	1	1.904900	1	6.030900	1
C	-10.084300	1	0.918900	1	4.306300	1
H	-11.009000	1	0.901000	1	4.206400	1
C	-9.273300	1	0.318500	1	3.349000	1
H	-9.651500	1	-0.097100	1	2.608900	1
C	-7.856900	1	0.348200	1	3.512800	1
C	-7.024600	1	-0.299600	1	2.549100	1
C	0.324600	1	-1.855000	1	1.535000	1
H	1.097100	1	-1.584500	1	2.055800	1
H	0.644500	1	-2.252400	1	0.709800	1
C	-0.448800	1	-2.872100	1	2.301100	1
H	0.154600	1	-3.566000	1	2.609100	1
H	-0.842200	1	-2.451500	1	3.081300	1
C	-1.324300	1	-4.622400	1	0.873000	1
C	-2.440000	1	-5.166000	1	0.011800	1
C	-2.255900	1	-6.304200	1	-0.695300	1
H	-1.426400	1	-6.720600	1	-0.651500	1
C	-3.259100	1	-6.895300	1	-1.499400	1
C	-3.070800	1	-8.092900	1	-2.196700	1
H	-2.245600	1	-8.517100	1	-2.169400	1
C	-4.070700	1	-8.629800	1	-2.905700	1
H	-3.935900	1	-9.436900	1	-3.348200	1
C	-5.334100	1	-7.987100	1	-2.988900	1
H	-6.021500	1	-8.361400	1	-3.491000	1
C	-5.530900	1	-6.791700	1	-2.312300	1
H	-6.353300	1	-6.360000	1	-2.353800	1
C	-4.489400	1	-6.244000	1	-1.571800	1
C	-4.705100	1	-4.983700	1	-0.877200	1
N	-0.488100	1	-0.666700	1	1.219900	1
N	-1.899400	1	-0.429500	1	-1.539700	1
H	-2.481600	1	-0.742200	1	-0.988600	1
N	-4.763000	1	-0.263800	1	-2.012700	1
N	-2.920800	1	0.624600	1	2.624000	1
H	-3.225700	1	0.025800	1	2.087900	1
N	-5.699400	1	-0.196100	1	2.714800	1
N	-1.498600	1	-3.475100	1	1.508700	1
H	-2.259100	1	-3.075900	1	1.448900	1
N	-3.680200	1	-4.522800	1	-0.090600	1
O	-1.583900	1	0.703000	1	-3.464700	1
O	-3.230300	1	1.676300	1	4.605800	1
O	-0.298300	1	-5.280100	1	0.982100	1
H	-8.715200	1	-3.404800	1	0.593000	1
H	-7.415400	1	-3.853100	1	2.176700	1
H	-8.941000	1	-3.095500	1	-0.590800	1
H	-6.155000	1	-4.393200	1	2.638400	1

----------End of file **Eu_tren.mop**----------

----------Begin of file **Eu_tren.arc**----------

SUMMARY OF PM3 CALCULATION

MOPAC2007 (Version: 7.221W)
Fri Aug 29 01:18:10 2008
No. of days left = 197

Empirical Formula: C36 H34 N7 O11 Eu

PM3 PRECISE NOINTER XYZ T=10D BFGS GNORM=0.25 +
NOLOG GEO-OK MMOK SCFCRT=1.D-10
Eu(TREN-1,2-HOIQO)(H2O)2

PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -158.97121 KCAL = -665.13554 KJ
TOTAL ENERGY = -9191.73604 EV
ELECTRONIC ENERGY = -110505.44975 EV
CORE-CORE REPULSION = 101313.71372 EV
DIPOLE = 11.48544 DEBYE POINT GROUP: C1
NO. OF FILLED LEVELS = 141
IONIZATION POTENTIAL = 8.395586 EV
HOMO LUMO ENERGIES (EV) = -8.396 -1.376
MOLECULAR WEIGHT = 892.669

MOLECULAR DIMENSIONS (Angstroms)

Atom		Atom		Distance
H	64	H	24	14.33674
H	45	H	14	13.29931
H	35	H	68	12.59235

SCF CALCULATIONS = 607
COMPUTATION TIME = 7 MINUTES AND 16.516 SECONDS

FINAL GEOMETRY OBTAINED CHARGE
PM3 PRECISE NOINTER XYZ T=10D BFGS GNORM=0.25 +
NOLOG GEO-OK MMOK SCFCRT=1.D-10
Eu(TREN-1,2-HOIQO)(H2O)2

Eu	-5.79105160 +1	-2.1803554 +1	0.1786149 +1	3.0000
O	-3.80291633 +1	-3.6210613 +1	0.3854376 +1	-0.9267
O	-5.55156131 +1	-4.3789108 +1	-0.9268561 +1	-0.7876
O	-4.29148973 +1	-0.7735502 +1	-1.1823036 +1	-0.9220
O	-5.04919464 +1	-0.6520402 +1	1.9727506 +1	-0.9060

O	-8.24126436 +1	-2.4420556 +1	0.0053056 +1	-0.5949
O	-6.55306600 +1	-0.6241143 +1	-1.5852553 +1	-0.7908
O	-7.25553901 +1	-1.2303536 +1	1.9360606 +1	-0.8135
O	-6.48088130 +1	-3.6145731 +1	2.0679390 +1	-0.5971
C	-0.12767246 +1	0.2461158 +1	0.1817746 +1	-0.1127
H	0.94803004 +1	0.5022839 +1	0.3026277 +1	0.0432
H	-0.69115074 +1	1.1915494 +1	0.3521406 +1	0.0752
C	-0.35576350 +1	-0.2775841 +1	-1.2397881 +1	-0.0704
H	0.31018550 +1	0.2682964 +1	-1.9383722 +1	0.0823
H	-0.07245465 +1	-1.3540491 +1	-1.3054180 +1	0.0644
C	-2.20353280 +1	0.8902581 +1	-2.4939535 +1	0.2978
C	-3.67394025 +1	0.9483751 +1	-2.8130217 +1	-0.2191
C	-4.15490454 +1	1.8185968 +1	-3.7637863 +1	-0.1043
H	-3.45540481 +1	2.4680571 +1	-4.3079768 +1	0.1440
C	-5.55036127 +1	1.9085218 +1	-4.0579169 +1	-0.0112
C	-6.02618669 +1	2.8086660 +1	-5.0429642 +1	-0.0969
H	-5.30612723 +1	3.4349844 +1	-5.5825192 +1	0.1142
C	-7.37014326 +1	2.8909578 +1	-5.3124780 +1	-0.0762
H	-7.73778232 +1	3.5870809 +1	-6.0741132 +1	0.1046
C	-8.29388213 +1	2.0850033 +1	-4.6165323 +1	-0.1174
H	-9.36029191 +1	2.1690517 +1	-4.8501345 +1	0.1065
C	-7.86069994 +1	1.2033276 +1	-3.6558895 +1	-0.0421
H	-8.56370647 +1	0.5682022 +1	-3.1051666 +1	0.1186
C	-6.48304421 +1	1.1056813 +1	-3.3668466 +1	-0.0967
C	-5.96031269 +1	0.2062953 +1	-2.3770985 +1	0.2019
C	-0.56676720 +1	-0.1075521 +1	2.5997393 +1	-0.1011
H	0.45320004 +1	0.2417213 +1	2.8752759 +1	0.0426
H	-0.81939332 +1	-0.9249510 +1	3.3138916 +1	0.0744
C	-1.53230865 +1	1.0700718 +1	2.7424556 +1	-0.0736
H	-1.20079485 +1	1.7007931 +1	3.5928635 +1	0.0828
H	-1.49459952 +1	1.7193427 +1	1.8352262 +1	0.0602
C	-3.79918767 +1	1.3496427 +1	3.7886537 +1	0.2942
C	-5.24733370 +1	0.9337251 +1	3.8207179 +1	-0.2529
C	-6.11913698 +1	1.4940769 +1	4.7267842 +1	-0.0608
H	-5.74596391 +1	2.2340632 +1	5.4496933 +1	0.1482
C	-7.50478083 +1	1.1498582 +1	4.7444442 +1	-0.0285
C	-8.38993343 +1	1.7395895 +1	5.6814596 +1	-0.0835
H	-7.99419799 +1	2.4648512 +1	6.4026384 +1	0.1179
C	-9.72108914 +1	1.4051589 +1	5.6781387 +1	-0.0766
H	-10.40611343 +1	1.8613144 +1	6.4014877 +1	0.1100
C	-10.22822753 +1	0.4740675 +1	4.7466032 +1	-0.0957
H	-11.29516861 +1	0.2270070 +1	4.7644520 +1	0.1103
C	-9.39479595 +1	-0.1139890 +1	3.8279032 +1	-0.0579
H	-9.77139780 +1	-0.8365125 +1	3.0950307 +1	0.1140
C	-8.02175785 +1	0.2173742 +1	3.8182106 +1	-0.0752
C	-7.08921583 +1	-0.3506500 +1	2.8959889 +1	0.1344
C	0.29034151 +1	-1.9600737 +1	1.2134793 +1	-0.1161
H	1.32584149 +1	-1.7305667 +1	1.5488679 +1	0.0439
H	0.37304138 +1	-2.2786473 +1	0.1488741 +1	0.0781
C	-0.27214083 +1	-3.0919238 +1	2.0785880 +1	-0.0688
H	0.54441247 +1	-3.7966511 +1	2.3347561 +1	0.0805

H	-0.66128405 +1	-2.6869806 +1	3.0414897 +1	0.0619
C	-1.16368322 +1	-4.9650655 +1	0.6490765 +1	0.2997
C	-2.33681234 +1	-5.5213613 +1	-0.1134185 +1	-0.2196
C	-2.24399850 +1	-6.7277768 +1	-0.7673107 +1	-0.1044
H	-1.31215254 +1	-7.3068313 +1	-0.7082705 +1	0.1438
C	-3.32876422 +1	-7.2450512 +1	-1.5411393 +1	-0.0113
C	-3.21634082 +1	-8.4931535 +1	-2.2009983 +1	-0.0982
H	-2.28545605 +1	-9.0639959 +1	-2.1036411 +1	0.1141
C	-4.26059204 +1	-8.9741856 +1	-2.9524335 +1	-0.0749
H	-4.17317951 +1	-9.9392725 +1	-3.4631556 +1	0.1048
C	-5.45448392 +1	-8.2362454 +1	-3.0798313 +1	-0.1168
H	-6.27157714 +1	-8.6396639 +1	-3.6869601 +1	0.1075
C	-5.59153590 +1	-7.0223348 +1	-2.4502614 +1	-0.0407
H	-6.51154007 +1	-6.4332658 +1	-2.5402893 +1	0.1215
C	-4.52990310 +1	-6.5156420 +1	-1.6714123 +1	-0.0981
C	-4.60695005 +1	-5.2575332 +1	-0.9822355 +1	0.2084
N	-0.55703136 +1	-0.7250202 +1	1.2367767 +1	-0.0766
N	-1.74854979 +1	-0.1750237 +1	-1.7065181 +1	-0.0537
H	-2.45407885 +1	-0.7234838 +1	-1.2272158 +1	0.1615
N	-4.59774584 +1	0.1404652 +1	-2.1459825 +1	0.6346
N	-2.92435187 +1	0.6303773 +1	2.9716525 +1	-0.0392
H	-3.32466553 +1	-0.0488159 +1	2.3367068 +1	0.1566
N	-5.76156696 +1	-0.0021041 +1	2.9164812 +1	0.7225
N	-1.37898790 +1	-3.8348648 +1	1.4533816 +1	-0.0596
H	-2.25043926 +1	-3.3387007 +1	1.3076696 +1	0.1579
N	-3.54106413 +1	-4.8198177 +1	-0.2142965 +1	0.6288
O	-1.41404762 +1	1.7128994 +1	-2.9525342 +1	-0.4055
O	-3.39422074 +1	2.2826708 +1	4.4789702 +1	-0.4023
O	-0.06039046 +1	-5.5034025 +1	0.6132755 +1	-0.4004
H	-8.37934540 +1	-1.8067675 +1	0.7205355 +1	0.2723
H	-6.95657616 +1	-2.8715894 +1	2.4637501 +1	0.2641
H	-9.08705670 +1	-2.6663940 +1	-0.3889297 +1	0.2873
H	-6.52939585 +1	-4.3812505 +1	2.6414903 +1	0.2860

----------End of file **Eu_tren.arc**----------

----------Begin of file **Eu_9H2O.mop**----------

PM3 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3
cation nona-aqua-europium(III)

Eu	1.369000	1	-1.681000	1	1.064000	1
O	-0.594000	1	-1.511000	1	2.460000	1
O	1.716000	1	0.317000	1	2.375000	1
O	1.991000	1	-2.567000	1	-1.095000	1
O	1.397000	1	-4.078000	1	1.364000	1
O	3.707000	1	-2.249000	1	1.279000	1
O	-0.576000	1	-2.619000	1	-0.275000	1
O	1.734000	1	-2.424000	1	3.467000	1
O	0.000000	1	0.000000	1	0.000000	1
O	2.951000	1	0.000000	1	0.000000	1
H	0.156000	1	0.883000	1	0.000000	1
H	-0.274000	1	-0.199000	1	-0.664000	1
H	2.982000	1	0.809000	1	0.116000	1
H	3.708000	1	-0.126000	1	-0.283000	1
H	-1.413000	1	-1.268000	1	2.188000	1
H	-0.656000	1	-2.048000	1	2.973000	1
H	1.385000	1	0.473000	1	3.194000	1
H	2.404000	1	0.600000	1	2.332000	1
H	2.810000	1	-2.538000	1	-1.460000	1
H	1.482000	1	-2.464000	1	-1.630000	1
H	1.240000	1	-4.690000	1	0.727000	1
H	1.100000	1	-4.312000	1	2.007000	1
H	4.039000	1	-2.947000	1	1.733000	1
H	4.161000	1	-1.664000	1	1.365000	1
H	-1.285000	1	-2.255000	1	-0.461000	1
H	-0.559000	1	-3.190000	1	-0.860000	1
H	1.322000	1	-2.194000	1	4.136000	1
H	2.048000	1	-3.130000	1	3.736000	1

----------End of file **Eu_9H2O.mop**----------

----------Begin of file **Eu_9H2O.arc**----------

SUMMARY OF PM3 CALCULATION

MOPAC2007 (Version: 7.221W)
Fri Sep 5 21:31:45 2008
No. of days left = 190

Empirical Formula: H18 O9 Eu

PM3 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3
cation nona-aqua-europium(III)

PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = 323.51253 KCAL = 1353.57645 KJ
TOTAL ENERGY = -2932.93411 EV
ELECTRONIC ENERGY = -14038.14466 EV
CORE-CORE REPULSION = 11105.21054 EV
DIPOLE = 0.74707 DEBYE POINT GROUP: C1
NO. OF FILLED LEVELS = 36
CHARGE ON SYSTEM = 3
IONIZATION POTENTIAL = 25.094038 EV
HOMO LUMO ENERGIES (EV) = -25.094 -8.938
MOLECULAR WEIGHT = 314.101

MOLECULAR DIMENSIONS (Angstroms)

Atom		Atom		Distance
H	21	H	17	6.27726
H	24	H	25	6.21230
H	19	H	27	6.06404

SCF CALCULATIONS = 627
COMPUTATION TIME = 15.094 SECONDS

FINAL GEOMETRY OBTAINED CHARGE
PM3 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3
cation nona-aqua-europium(III)

Eu	1.40462264 +1	-1.5673041 +1	1.0980307 +1	3.0000
O	-0.62602985 +1	-1.6912689 +1	2.5894117 +1	-0.6346
O	1.28356344 +1	0.5437862 +1	2.4750130 +1	-0.6317
O	1.91406739 +1	-1.9374370 +1	-1.2817347 +1	-0.6249
O	1.07468252 +1	-4.0463089 +1	1.4170107 +1	-0.6357
O	3.65642145 +1	-2.7058871 +1	1.0575400 +1	-0.6315
O	-0.64859859 +1	-2.3056741 +1	-0.1895231 +1	-0.6185
O	2.23446691 +1	-2.0210425 +1	3.4355211 +1	-0.6336

O	0.13718823 +1	0.1169164 +1	-0.1659702 +1	-0.6511
O	3.21300067 +1	0.0461864 +1	0.4007516 +1	-0.6356
H	-0.08932428 +1	0.9877652 +1	-0.5352742 +1	0.3577
H	-0.54022369 +1	-0.5103638 +1	-0.4423260 +1	0.2683
H	3.32283437 +1	0.9994108 +1	0.6074852 +1	0.3202
H	4.01882657 +1	-0.0774508 +1	-0.1454768 +1	0.3161
H	-1.12646602 +1	-0.9782210 +1	3.0416101 +1	0.3187
H	-1.13852200 +1	-2.4596997 +1	2.9202422 +1	0.3165
H	0.81001136 +1	1.3875800 +1	2.3137292 +1	0.3157
H	1.70036605 +1	0.7714119 +1	3.3335148 +1	0.3164
H	2.16280332 +1	-2.4621982 +1	-2.0648355 +1	0.3582
H	1.90344393 +1	-1.0208535 +1	-1.5498264 +1	0.2641
H	0.62197075 +1	-4.7164519 +1	0.8613262 +1	0.3174
H	1.36518858 +1	-4.6375883 +1	2.1444770 +1	0.3183
H	3.89180005 +1	-3.6419587 +1	0.8812133 +1	0.3175
H	4.56190747 +1	-2.3522460 +1	1.1891585 +1	0.3144
H	-1.57684495 +1	-2.4379757 +1	0.1081006 +1	0.3216
H	-0.73760631 +1	-2.6441853 +1	-1.1092130 +1	0.3228
H	1.78275142 +1	-1.9464584 +1	4.3030049 +1	0.3161
H	3.10837346 +1	-2.3344788 +1	3.7529159 +1	0.3171

----------End of file **Eu_9H2O.arc**----------

5. Additional Tables and Figures

The directly coordinating atoms of the ligands form the coordination polyhedron of the complex, whose faces are the polygonal bases of a set of adjacent pyramids that share the same apex, where the lanthanide ion is located. Each two adjacent pyramids share one triangular face, and therefore, also one side of their polygonal bases.

The average unsigned mean error for each complex *i*, UME_i, is defined as:

$$UME_i = \frac{1}{n_i}\sum_{j=1}^{n_i}\left|R_{i,j}^{CSD} - R_{i,j}^{calc}\right|$$

where *n* is the number of ligand atoms directly coordinating the lanthanide ion. Two cases have been examined: (*i*) $UME_{(Ln\text{-}L)}$s involving only the edges of the pyramidsthat have the apex as a vertice, that is, the interatomic distances R_j between the lanthanide central ion, Ln, and the atoms of the coordination polyhedron, L, important to luminescent complex design; and (*ii*) UMEs of all the edges of the pyramids, that is, of the interatomic distances R_j between the lanthanide central ion and the atoms of the coordination polyhedron, as well as all the interatomic distances R_j between all atoms of the coordination polyhedron.

Tables S1, S2 and S3 show the Sparkle/PM3 and Sparkle/AM1 unsigned mean errors, $UME_{(Ln\text{-}L)}$s and UMEs, for the 96 structures containing Eu(III), 70 structures containing Gd(III) and the 42 structures containing Tb(III) respectively.

Figures S3 to S5 present, each, a gamma distribution fit of the respective UMEs for the present Sparkle/PM3 as well as for previously published Sparkle/AM1 models for europium, gadolinium and terbium.[1] In all cases the respective p-values were above the critical value of 0.05, ranging from 0.100 to 0.911, thus validating the usage of the sparkle model for both PM3 and AM1 for the prediction of lanthanide complexes geometries.

Table S1. Values of the coordination numbers, CNs, and unsigned mean errors, $UME_{(Eu-L)}$s, and UMEs, for Sparkle/PM3 and Sparkle/AM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database, for each of the ninety-six europium (III) complexes

Structure[a]	CN	Sparkle $UME_{(Eu-L)}$ / Å		Sparkle UME / Å	
		PM3	AM1	PM3	AM1
ACPNEU	8	0.078	0.042	0.171	0.171
BAFZEO	9	0.072	0.106	0.129	0.132
BAPXAR	9	0.068	0.005	0.140	0.093
BEKWUJ	11	0.087	0.163	0.151	0.234
BUVXAR11	9	0.078	0.049	0.200	0.242
CEXKUL	9	0.094	0.144	0.137	0.221
CEXKUL01	9	0.061	0.049	0.112	0.104
CEYRON	10	0.076	0.115	0.177	0.225
CIRKET	8	0.073	0.025	0.151	0.267
COZLEI10	8	0.095	0.084	0.166	0.212
DIWNOM	10	0.072	0.121	0.312	0.341
DOFXIF	9	0.067	0.022	0.133	0.099
DOPCEQ	9	0.086	0.123	0.134	0.224
DUCNAQ	9	0.077	0.110	0.121	0.210
ECABOZ	10	0.077	0.115	0.154	0.205
EGOBEH	9	0.071	0.090	0.101	0.124
FETGUG	8	0.082	0.063	0.250	0.248
FOCQOD	9	0.084	0.062	0.160	0.189
FOCQUJ	9	0.067	0.056	0.121	0.129
FOCREU	9	0.110	0.103	0.198	0.304
FUXPOD	9	0.027	0.075	0.294	0.255
FUZZOP	8	0.060	0.059	0.275	0.212
GACJOJ	10	0.106	0.172	0.089	0.188
GAPRUK	8	0.021	0.049	0.052	0.087
GEBYAN	9	0.085	0.110	0.097	0.175
GINPIC	9	0.053	0.061	0.149	0.198
HANBIH	9	0.058	0.031	0.147	0.204
HAZGAQ	8	0.030	0.052	0.051	0.077
JAXXOV	8	0.094	0.052	0.150	0.135
JUCZIQ	9	0.054	0.063	0.177	0.218
JUDBOZ	9	0.098	0.080	0.218	0.265
JUGBUI	10	0.071	0.128	0.123	0.175
KAFDOK	9	0.046	0.043	0.132	0.166
KAKPAN	8	0.077	0.037	0.362	0.345
KELNOE	8	0.063	0.041	0.350	0.197
KIFKOZ02	9	0.051	0.071	0.105	0.115
KIHSEZ	10	0.076	0.107	0.119	0.164
LAPJAN	10	0.062	0.092	0.110	0.168
LEJTAV	8	0.067	0.042	0.154	0.234
LELRUP	8	0.100	0.056	0.187	0.134
LOWBEE	10	0.100	0.088	0.136	0.151
LUHFUP	9	0.092	0.105	0.137	0.153
LUHGAW	9	0.093	0.101	0.122	0.142
MASKAS	8	0.072	0.026	0.228	0.194
MEBDUS	9	0.095	0.110	0.141	0.195
MIHNOG	8	0.073	0.027	0.134	0.132
MIHPOI	9	0.066	0.054	0.109	0.157
MOYJUF	9	0.078	0.101	0.110	0.140
MUHROW	9	0.097	0.102	0.138	0.141
MUHRUC	9	0.095	0.101	0.168	0.240
NIGWUV	9	0.065	0.077	0.097	0.156
NOHLUR	9	0.047	0.037	0.109	0.145
NUXHIX	7	0.103	0.143	0.159	0.225
PHASEU	10	0.079	0.144	0.123	0.199
PUHYEW01	10	0.087	0.128	0.129	0.245
PIEUAC01	8	0.061	0.023	0.208	0.144
PITCUQ	8	0.074	0.042	0.358	0.174
QAKWUU	8	0.065	0.032	0.133	0.145
QALFEO	9	0.089	0.100	0.230	0.276
QALFOY	8	0.047	0.040	0.182	0.208
QECGOU	6	0.124	0.066	0.256	0.211
QHDOEU	7	0.101	0.045	0.186	0.152
QIGJAR	9	0.201	0.188	0.228	0.215
QIMREJ	10	0.082	0.129	0.303	0.202
QIQHAZ	9	0.131	0.128	0.291	0.350
QUBWUF	10	0.053	0.138	0.154	0.205
SOPFUY	9	0.037	0.020	0.113	0.102
SUXXIS	12	0.076	0.230	0.117	0.313
TMHPEU10	8	0.100	0.059	0.132	0.127
TOKMUB	8	0.080	0.121	0.099	0.142
TUQTOO	9	0.100	0.065	0.239	0.274
VUSGOF	9	0.090	0.124	0.116	0.307
WAVNUC	9	0.056	0.077	0.105	0.094
WELBUK	11	0.065	0.173	0.294	0.274
WOMCIK	9	0.060	0.092	0.095	0.133
XECLEW	9	0.085	0.094	0.155	0.226
XECLIA	8	0.204	0.071	0.318	0.209
XICHIA	8	0.072	0.068	0.188	0.098
XICHOG	8	0.082	0.068	0.083	0.085
XICHUM	8	0.094	0.078	0.078	0.077
XIHQIO	9	0.192	0.205	0.142	0.171
XILGII	9	0.070	0.076	0.118	0.123
XIWTAY	9	0.095	0.103	0.145	0.199
XIWTUS	8	0.085	0.050	0.145	0.120
YEZFAK	8	0.069	0.031	0.153	0.186
YICSEI	8	0.107	0.103	0.136	0.122
YODYIZ	8	0.057	0.041	0.107	0.149
YOJDIK	8	0.073	0.031	0.161	0.131
YUXREO	9	0.080	0.103	0.173	0.245
ZAMHOK	9	0.042	0.055	0.262	0.291
ZACXAC	9	0.061	0.033	0.132	0.132
ZESSUL	8	0.123	0.095	0.136	0.159
ZEXJUH	8	0.068	0.055	0.119	0.161
ZIDCUK	8	0.107	0.121	0.177	0.184
ZUCCIJ	8	0.071	0.070	0.129	0.133

[a]The structures are identified by their respective codes of reference from the Cambridge Structural Database.

Table S2. Values of the coordination numbers, CNs, and unsigned mean errors, $UME_{(Gd\text{-}L)}$s, and UMEs, for Sparkle/PM3 and Sparkle/AM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database, for each of the seventy gadolinium (III) complexes

Structure[a]	CN	Sparkle $UME_{(Eu\text{-}L)}$ / Å		Sparkle UME / Å	
		PM3	AM1	PM3	AM1
ACAQGD	9	0.081	0.085	0.113	0.156
ADUPEU	7	0.153	0.116	0.092	0.088
BIFZEV	9	0.043	0.034	0.302	0.290
BUVVOD	9	0.068	0.061	0.169	0.283
BUVVOD01	9	0.065	0.058	0.081	0.277
COSTAF	9	0.130	0.136	0.288	0.462
CULNIG10	7	0.100	0.097	0.196	0.236
DIQBIO	10	0.104	0.093	0.182	0.186
DIYNEE	8	0.030	0.024	0.219	0.230
DUFBEL	8	0.030	0.026	0.110	0.156
EHAXEQ	8	0.073	0.062	0.103	0.099
FONMEA	8	0.062	0.057	0.124	0.154
FUHQUU	9	0.035	0.029	0.090	0.096
FUXPUJ	9	0.024	0.026	0.131	0.258
GAKYAS	8	0.033	0.026	0.194	0.227
GAWBEL	8	0.024	0.030	0.083	0.097
GEGCIE	9	0.046	0.038	0.069	0.066
GIDQUF	8	0.072	0.037	0.103	0.066
GINPOI	9	0.051	0.057	0.096	0.285
GIRKUN	9	0.089	0.101	0.103	0.352
GODMER	10	0.095	0.101	0.148	0.236
HEDMIM	9	0.061	0.067	0.120	0.198
JARBUZ	9	0.068	0.078	0.138	0.153
JOPJIH	9	0.061	0.063	0.100	0.142
JOPJIH01	9	0.042	0.040	0.066	0.090
LANITB	9	0.056	0.071	0.256	0.310
LASZOU	9	0.028	0.027	0.110	0.094
LASZIO	9	0.191	0.246	0.283	0.463
LEJVEB	8	0.035	0.025	0.156	0.254
LOKNEE	9	0.057	0.056	0.127	0.135
LOQKEH	9	0.055	0.039	0.077	0.092
MIPTOU	7	0.140	0.103	0.068	0.063
NAVWIQ	9	0.090	0.104	0.135	0.185
NIGHEQ	10	0.055	0.039	0.100	0.061
NIGXAC	9	0.070	0.056	0.099	0.105
NIVQEO	8	0.053	0.048	0.123	0.141
PADEGA10	10	0.054	0.077	0.099	0.120
PALHAL	8	0.131	0.109	0.140	0.126
PEBDOP	9	0.050	0.042	0.246	0.229
PROPGD	8	0.060	0.062	0.137	0.197
PUZHUN	10	0.074	0.094	0.106	0.134
SERYOD	8	0.053	0.068	0.101	0.301
TUFLUB	9	0.051	0.048	0.168	0.241
UDOMIJ	9	0.049	0.040	0.179	0.097
UDOMOP	9	0.043	0.043	0.118	0.096
VEDSEC	10	0.077	0.060	0.112	0.089
VETDON	9	0.047	0.039	0.096	0.094
VIGBOC	9	0.053	0.046	0.073	0.086
WALQAB	9	0.038	0.032	0.081	0.093
WAVPAK	9	0.052	0.068	0.218	0.140
WAXCIH	9	0.084	0.067	0.125	0.155
WEWNOB	6	0.050	0.017	0.084	0.051
WIRTUM	5	0.086	0.094	0.111	0.127
WUCCOM	9	0.084	0.069	0.180	0.158
XIVFOX	8	0.069	0.031	0.135	0.018
XUBGUW	10	0.057	0.073	0.094	0.096
YAVSUJ	9	0.079	0.087	0.149	0.344
YEGTOT	8	0.007	0.005	0.081	0.093
YEWGEM	8	0.089	0.082	0.110	0.136
YIYLAT	9	0.038	0.053	0.093	0.122
YOVFIY01	9	0.034	0.027	0.102	0.109
YUWZOF	6	0.028	0.044	0.177	0.185
ZAXQAQ	8	0.033	0.034	0.136	0.224
ZAZQEW	8	0.007	0.006	0.065	0.086
ZENGUU	6	0.101	0.119	0.136	0.157
ZIPJIR	9	0.043	0.036	0.122	0.146
ZIZNUR	8	0.055	0.051	0.147	0.150
ZUNCAM	8	0.112	0.097	0.103	0.110
ZZZARA01	9	0.063	0.055	0.174	0.265

[a]The structures are identified by their respective codes of reference from the Cambridge Structural Database.

Table S3. Values of the coordination numbers, CNs, and unsigned mean errors, $UME_{(Tb-L)}$s and UMEs, for Sparkle/PM3 and Sparkle/AM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database, for each of the forty-two terbium (III) complexes

Structure[a]	CN	Sparkle $UME_{(Eu-L)}$ / Å		Sparkle UME / Å	
		PM3	AM1	PM3	AM1
BACBUC	9	0.130	0.156	0.187	0.234
BAFWUB	9	0.040	0.035	0.110	0.138
BAFZOY	9	0.079	0.096	0.132	0.127
BUVXEV01	9	0.070	0.051	0.171	0.206
COSVOV	9	0.130	0.134	0.140	0.370
CULSEH	8	0.052	0.053	0.129	0.118
DIFHEF	8	0.062	0.034	0.100	0.092
DUCQEX	9	0.070	0.085	0.129	0.166
FAGZAP	8	0.044	0.029	0.196	0.250
FOPPUV	9	0.053	0.046	0.146	0.155
HANBUT	9	0.027	0.030	0.130	0.180
IDOZEG	9	0.088	0.100	0.128	0.139
JAXWOU01	8	0.093	0.116	0.186	0.241
JAXWOU	9	0.077	0.097	0.199	0.246
JEXWOY	9	0.031	0.034	0.112	0.117
KITGAV	9	0.032	0.021	0.140	0.219
KUYBEL	9	0.025	0.050	0.230	0.245
LEJTEZ	8	0.031	0.038	0.178	0.180
LEYHOM	9	0.028	0.074	0.177	0.244
LIFJEP	10	0.070	0.092	0.125	0.147
MIHNUM	8	0.060	0.027	0.121	0.137
MIHPIC	8	0.056	0.028	0.121	0.137
MIWTAN	10	0.078	0.083	0.115	0.150
NASTUW	10	0.076	0.097	0.108	0.135
NAXRAF	10	0.099	0.102	0.141	0.143
NIGYUX	9	0.065	0.063	0.105	0.136
PAGBOO	4	0.059	0.043	0.071	0.055
PEJZAF	8	0.027	0.023	0.189	0.163
QALFUE	8	0.029	0.029	0.194	0.162
QAWHIF	8	0.065	0.049	0.081	0.079
SEGVEF	8	0.020	0.018	0.089	0.058
TOKVIY	9	0.095	0.123	0.117	0.173
VAPTEL01	6	0.154	0.120	0.212	0.181
VAPTEL	6	0.165	0.131	0.227	0.166
XARXET	8	0.055	0.059	0.270	0.228
XAXXUP	7	0.092	0.064	0.167	0.176
XEXJIT	7	0.118	0.084	0.111	0.103
XOCDIC	8	0.070	0.084	0.152	0.202
XORGAM	8	0.061	0.052	0.434	0.292
XUGBUW	7	0.092	0.074	0.161	0.183
ZUNCEQ	8	0.107	0.096	0.115	0.124
ZZZARD01	9	0.068	0.051	0.173	0.244

[a]The structures are identified by their respective codes of reference from the Cambridge Structural Database.

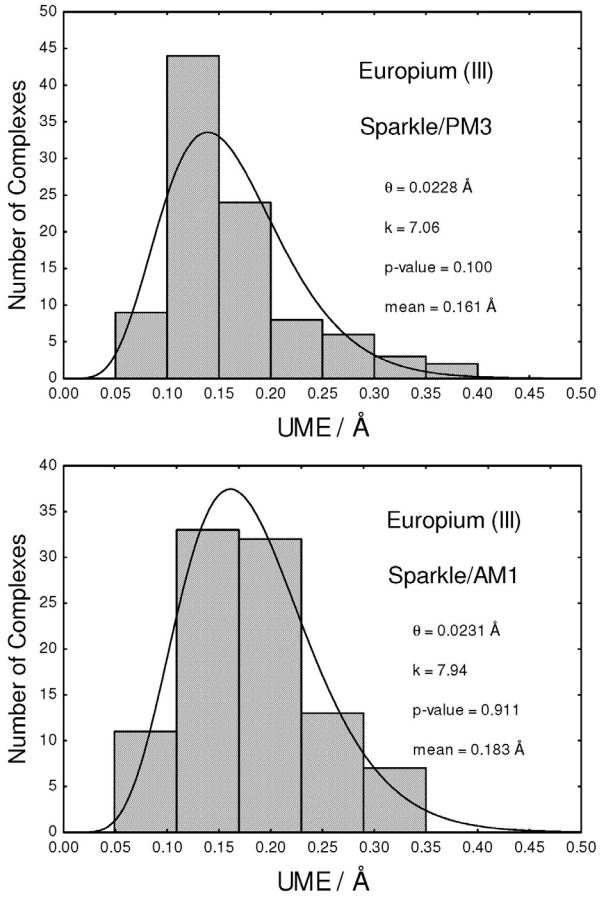
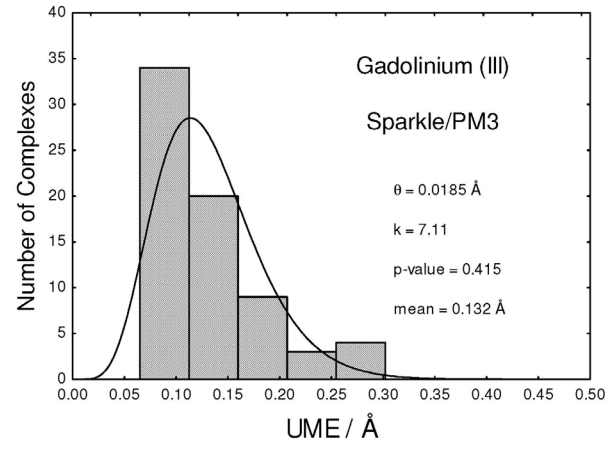


Figure S1. Probability densities of the Gamma distribution fits of the UMEs for the Eu(III) Sparkle/PM3 and Sparkle/AM1 models, superimposed to histograms of the same data for all 96 Eu(III) complexes considered; where k is the shape parameter and θ is the scale parameter of the gamma distribution; p-value is a measure of the significance of the gamma distribution fit; and mean is the expected value of the fitted gamma distribution, which is set to be equal to the arithmetic mean value of the 96 UMEs.



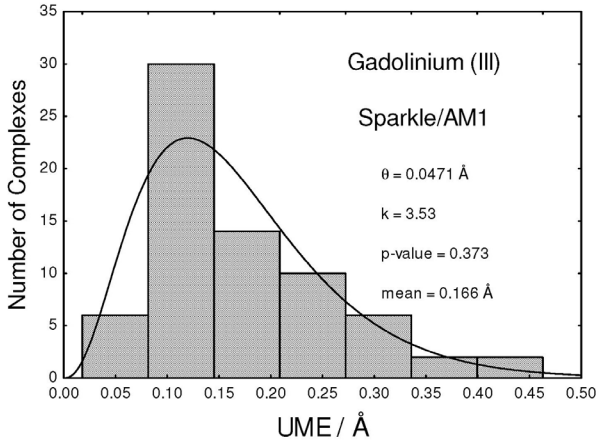
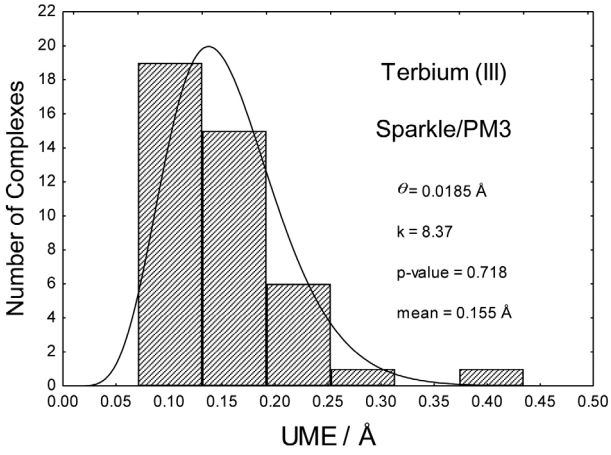


Figure S2. Probability densities of the Gamma distribution fits of the UMEs for the Gd(III) Sparkle/PM3 and Sparkle/AM1 models, superimposed to histograms of the same data for all 70 Gd(III) complexes considered; where k is the shape parameter and θ is the scale parameter of the gamma distribution; p-value is a measure of the significance of the gamma distribution fit; and mean is the expected value of the fitted gamma distribution, which is set to be equal to the arithmetic mean value of the 70 UMEs.



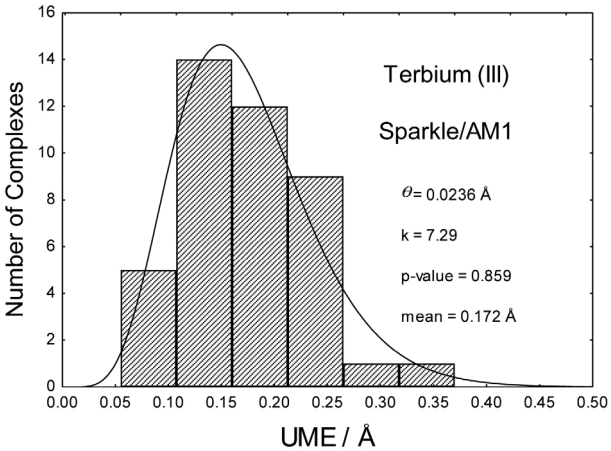


Figure S3. Probability densities of the Gamma distribution fits of the UMEs for the Tb(III) Sparkle/PM3 and Sparkle/AM1 models, uperimposed to histograms of the same data for all 42 Tb(III) complexes considered; where k is the shape parameter and θ is the scale parameter of the gamma distribution; p-value is a measure of the significance of the gamma distribution fit; and mean is the expected value of the fitted gamma distribution, which is set to be equal to the arithmetic mean value of the 42 UMEs.

References

1. Freire, R.O.; Rocha, G.B.; Simas, A.M.; *Inorg. Chem.* **2005**, *44*, 3299.