Electronic Supplementary Material (ESI) for RSC Advances.


# RM1 Modeling of Neodymium, Promethium, and Samarium Coordination Compounds

## *Supplementary Information*

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## 1. How to run RM1 model for the lanthanides 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, Sparkle/PM7, 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.*

**To run a RM1 model for lanthanides 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 only the keyword RM1. Do not forget to set the charge n of the complex with keyword CHARGE=n

**To run a Sparkle/RM1 calculation in MOPAC 2012, proceed as follows:**

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

c. Do not forget to set the charge n of the complex with keyword CHARGE=n

d. For a Sparkle/RM1 calculation, use the keywords RM1 SPARKLE in the keyword line.

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.

## 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 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.

## Additional Tables and Figures

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**Table S1:** Unsigned mean errors, $UME_{(Nd-L)}s$ and UMEs, for Method RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 88 neodymium (III) complexes. The structures that composed the parameterization set are in red.

| Structure | Method RM1 | | Structure | Method RM1 | |
|---|---|---|---|---|---|
| | $UME_{(Nd-L)}s$ (Å) | UME (Å) | | $UME_{(Nd-L)}s$ (Å) | UME (Å) |
| ANTNND10 | 0.0357 | 0.0693 | NADQEO | 0.0590 | 0.1771 |
| BAFYUD | 0.0329 | 0.0896 | NATDET | 0.0497 | 0.1789 |
| BAWDIM10 | 0.0328 | 0.2458 | NATPAZ01 | 0.0307 | 0.0984 |
| BEXQIE | 0.0364 | 0.1692 | NIPREJ | 0.0600 | 0.0953 |
| BILSIY | 0.0492 | 0.0627 | NIRTEO | 0.0901 | 0.1469 |
| BUVWOE01 | 0.0500 | 0.0803 | NUFPUZ | 0.0743 | 0.1037 |
| CAHJAX | 0.0471 | 0.0961 | OQICEX | 0.0431 | 0.3268 |
| CANBOI | 0.0726 | 0.0586 | PAFMOZ | 0.0473 | 0.0846 |
| CUYLEO | 0.1447 | 0.1520 | PUQNUL | 0.1363 | 0.1125 |
| DICNUZ | 0.0433 | 0.3850 | QAJHEO | 0.0470 | 0.0816 |
| DUCMAP | 0.0442 | 0.1156 | QAYWOC | 0.0998 | 0.1340 |
| EGOBUX | 0.0843 | 0.2089 | QOZVIK | 0.0356 | 0.1295 |
| EGOBUX01 | 0.0822 | 0.3442 | QOZWAD | 0.0523 | 0.1060 |
| EJIPOC | 0.0407 | 0.0860 | QQQCGM01 | 0.0361 | 0.1154 |
| ELENOY | 0.0330 | 0.0521 | QUBWOZ | 0.0398 | 0.2207 |
| EXODIF | 0.0406 | 0.1577 | RAMXAE | 0.0689 | 0.5548 |
| FAHFID | 0.0393 | 0.1432 | RICNOG | 0.0528 | 0.3262 |
| FIBXET | 0.0391 | 0.1235 | RIMQIN | 0.0655 | 0.4749 |
| FIMFEM | 0.0788 | 0.1335 | RUGRAM | 0.0541 | 0.1846 |
| FUHQII | 0.0958 | 0.1767 | SAXJIL01 | 0.1167 | 0.3424 |
| GOPRIM | 0.0515 | 0.1039 | SOKBAV | 0.0623 | 0.2061 |
| GUHJAU | 0.0300 | 0.0555 | SOTXEE | 0.0508 | 0.2582 |
| HACHEZ | 0.0474 | 0.1200 | SOZGOD | 0.1282 | 0.1995 |
| HARRIB | 0.0451 | 0.1134 | SUCRIR | 0.0418 | 0.1797 |
| HEBCIA | 0.0357 | 0.2969 | SUXCAP | 0.0381 | 0.1844 |
| HERWAC | 0.0385 | 0.3092 | TAZJEJ | 0.0510 | 0.1085 |
| HODDEJ | 0.1081 | 0.1432 | TAZYOI | 0.0831 | 0.1658 |
| HOXNND01 | 0.0303 | 0.0788 | TEJDIW | 0.0351 | 0.0717 |
| IMUVER | 0.0534 | 0.1518 | TUPYOS | 0.0217 | 0.0454 |
| JALNAM | 0.0851 | 0.1928 | UHIVOW | 0.0953 | 0.1398 |
| JIRHAT | 0.0396 | 0.1425 | VEMKII | 0.1443 | 0.1962 |
| JIZDUR | 0.0554 | 0.2632 | VIVBOR | 0.0976 | 0.0759 |
| JOCDAH | 0.0828 | 0.1498 | WAGWIK | 0.0507 | 0.0827 |
| LEJSUO | 0.0264 | 0.1208 | WAGWUW | 0.0680 | 0.1153 |
| LELBUZ | 0.0744 | 0.1248 | WEFVUY | 0.0543 | 0.1053 |
| LUDQIK | 0.0345 | 0.0740 | XIFMAA | 0.0350 | 0.1399 |

| | | | | | |
|---|---|---|---|---|---|
| LULFIH | 0.0750 | 0.0953 | XIGKUT | 0.1030 | 0.2058 |
| LUSNOD | 0.0908 | 0.1198 | XIPKIQ | 0.0386 | 0.2902 |
| MINLIE | 0.0513 | 0.1067 | XONYII | 0.0339 | 0.0555 |
| MIPTIO | 0.0927 | 0.0787 | YENKOR | 0.0297 | 0.1098 |
| MOCDOX | 0.0607 | 0.1471 | YURMUT | 0.0497 | 0.0996 |
| MOCFAL | 0.0405 | 0.1216 | ZAMHIE | 0.0533 | 0.2604 |
| MOGXAI | 0.0875 | 0.1429 | ZANSIS | 0.0615 | 0.1082 |
| MUHWUI | 0.0835 | 0.1184 | ZUNBOZ | 0.0670 | 0.1200 |

**Table S2:** Unsigned mean errors, $UME_{(Pm-L)}$s and UMEs, for Method RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 20 promecium (III) complexes. The structures that composed the parameterization set are in red.

| Structure | Method RM1 | | Structure | Method RM1 | |
|---|---|---|---|---|---|
| | **$UME_{(Pm-L)}$s (Å)** | **UME (Å)** | | **$UME_{(Pm-L)}$s (Å)** | **UME (Å)** |
| Pm_BUVWUK01 | 0.0175 | 0.0593 | Pm_NOWTUO | 0.0645 | 0.4083 |
| Pm_CAZHAM | 0.0427 | 0.1578 | Pm_NUQYUT | 0.0383 | 0.1352 |
| Pm_COZLEI10 | 0.0549 | 0.1159 | Pm_QALFAK | 0.0929 | 0.3208 |
| Pm_FINDOV | 0.0272 | 0.1145 | Pm_QIPQOV | 0.0488 | 0.0551 |
| Pm_FUHQOO | 0.0395 | 0.1582 | Pm_ROCTAF | 0.0479 | 0.1894 |
| Pm_FUJYEO | 0.0287 | 0.1198 | Pm_SACNIU | 0.0362 | 0.1211 |
| Pm_GUPHUU | 0.0674 | 0.1454 | Pm_SERHED | 0.0228 | 0.1323 |
| Pm_KUYBAH | 0.0157 | 0.1499 | Pm_SOXKAR | 0.0727 | 0.2095 |
| Pm_LOFBAJ | 0.0284 | 0.0788 | Pm_VIGPAC | 0.0353 | 0.0798 |
| Pm_LUHFEZ | 0.0776 | 0.1309 | Pm_XEXJAL | 0.1152 | 0.0841 |

**Table S3:** Unsigned mean errors, $UME_{(Sm-L)}$s and UMEs, for Method RM1, as compared to the respective experimental crystallographic values, obtained from the Cambridge Structural Database,[(1)-(3)] for each of the 76 samarium (III) complexes. The structures that composed the parameterization set are in red.

| Structure | Method RM1 | | Structure | Method RM1 | |
|---|---|---|---|---|---|
| | $UME_{(Sm-L)}$s (Å) | UME (Å) | | $UME_{(Sm-L)}$s (Å) | UME (Å) |
| ABIDUK | 0.1278 | 0.1441 | LUHFEZ | 0.0245 | 0.1754 |
| ADELAW | 0.0795 | 0.0785 | MEWGOK | 0.0506 | 0.0934 |
| AGUVON | 0.0665 | 0.1045 | MIQTAH01 | 0.0423 | 0.0759 |
| AQEZIF | 0.0932 | 0.1745 | MOXJEO | 0.0277 | 0.0499 |
| AQEZIF01 | 0.0932 | 0.1737 | MUNDEF | 0.0617 | 0.0775 |
| AXUROB | 0.0483 | 0.2868 | NAFKIO | 0.0971 | 0.1507 |
| AYUKUA | 0.0737 | 0.1367 | NOWTUO | 0.0359 | 0.1546 |
| BIQVEC | 0.0372 | 0.1381 | NSMEDT01 | 0.0496 | 0.2523 |
| BITZEJ | 0.0391 | 0.0674 | OFULAC | 0.0661 | 0.4530 |
| BUVWUK01 | 0.0561 | 0.0832 | PIGYOT | 0.0410 | 0.1517 |
| CAZHAM | 0.0196 | 0.1703 | QALFAK | 0.0226 | 0.2501 |
| CORKEZ | 0.0351 | 0.1145 | QEBJAI | 0.0478 | 0.1984 |
| CUBFOU | 0.0372 | 0.1312 | QIPQOV | 0.0613 | 0.1271 |
| ECABIT | 0.0148 | 0.0464 | QOCKIC | 0.0487 | 0.0741 |
| ECOJUB | 0.0620 | 0.0981 | QQQEMA01 | 0.0248 | 0.1597 |
| FAVNUL10 | 0.0496 | 0.1158 | ROGCIZ | 0.0513 | 0.1153 |
| FIHDEG | 0.0703 | 0.1431 | RORMAM | 0.1085 | 0.2744 |
| FIMFAI | 0.0548 | 0.1053 | SMNICD | 0.0292 | 0.1030 |
| FINDOV | 0.0833 | 0.1227 | SOXKAR | 0.0436 | 0.1594 |
| FUHQOO | 0.0813 | 0.1608 | TEJDOC | 0.0290 | 0.0761 |
| FUJYEO | 0.0456 | 0.1925 | TIMPUA | 0.0594 | 0.1467 |
| GINPEY | 0.0353 | 0.0644 | UDIYAH | 0.0286 | 0.1187 |
| GUNFUR01 | 0.0767 | 0.0865 | VOFWIW | 0.0677 | 0.1218 |
| GUNGIG01 | 0.0632 | 0.0950 | WIGVOX | 0.0624 | 0.2506 |
| GUPHUU | 0.1134 | 0.2030 | WIVBUZ | 0.0579 | 0.2436 |
| HAWMUN | 0.1304 | 0.1128 | WIVCEK | 0.0417 | 0.3171 |
| IDAKAA | 0.0320 | 0.0778 | WOKHUZ | 0.0379 | 0.0822 |
| JALMIT | 0.0922 | 0.1189 | XAXYAW | 0.0610 | 0.1532 |
| JALNEQ | 0.0962 | 0.1679 | XEPLAF | 0.0321 | 0.2677 |
| JIZVOD | 0.0593 | 0.1949 | XEXJAL | 0.0525 | 0.0684 |
| KEBQEN | 0.0732 | 0.1619 | XILGOO | 0.0452 | 0.0912 |
| KEKPIZ | 0.0435 | 0.1371 | XIVFIR | 0.0994 | 0.1876 |
| KIWROX | 0.0403 | 0.1308 | XOWGAR | 0.0627 | 0.1394 |
| KIYXAR | 0.0552 | 0.1578 | XUYPUC | 0.0540 | 0.1996 |
| KUMCOK | 0.0636 | 0.1162 | YECRUT | 0.0354 | 0.1555 |
| KUYBAH | 0.0310 | 0.1094 | YENHOO | 0.0603 | 0.1122 |
| LIXDUR | 0.0735 | 0.0846 | YUBPAM | 0.0406 | 0.0689 |
| LODVUW | 0.0656 | 0.1112 | ZALDUL | 0.0857 | 0.1668 |

**Table S4**. Sparkle/AM1, Sparkle/PM3, Sparkle/PM6, Sparkle/PM7, Sparkle/RM1 and RM1 Unsigned Mean Errors of the Neodymium.

| Type of distances | N | unsigned mean errors for specific types of distances (Å) | | | | | |
|---|---|---|---|---|---|---|---|
| | | RM1 | Sparkle | | | | |
| | | | AM1 | PM3 | PM6 | PM7 | RM1 |
| Nd - Nd | 15 | **0.2592** | 0.3387 | 0.3277 | 0.4767 | 0.5853 | 0.3730 |
| Nd - O | 462 | **0.0627** | 0.0844 | 0.0796 | 0.0655 | 0.0894 | 0.0832 |
| Nd - N | 139 | 0.0422 | **0.0413** | 0.0564 | 0.1669 | 0.0689 | 0.0433 |
| Nd - C | 297 | **0.0627** | 0.2044 | 0.2232 | 0.4656 | 0.2398 | 0.2174 |
| Nd - S | 26 | **0.0630** | 0.4280 | 0.4265 | 0.5552 | 0.6476 | 0.4103 |
| Nd - Cl | 63 | **0.0588** | 0.2789 | 0.2934 | 0.3545 | 0.4005 | 0.3249 |
| Nd - Br | 6 | **0.0282** | 0.3880 | 0.3820 | 0.5103 | 1.2632 | 0.4244 |
| Nd - L | 1008 | **0.0624** | 0.1404 | 0.1465 | 0.2368 | 0.1791 | 0.1471 |
| L - L | 4633 | **0.1709** | 0.2478 | 0.2429 | 0.3526 | 0.2989 | 0.2584 |
| Nd-L, Nd-Nd and L-L’ | 5641 | **0.1515** | 0.2286 | 0.2257 | 0.3319 | 0.2775 | 0.2385 |

**Table S5**. Sparkle/AM1, Sparkle/PM3, Sparkle/PM6, Sparkle/PM7, Sparkle/RM1 and RM1 Unsigned Mean Errors of the Promecium.

| Type of distances | N | unsigned mean errors for specific types of distances (Å) | | | | | |
|---|---|---|---|---|---|---|---|
| | | RM1 | Sparkle | | | | |
| | | | AM1 | PM3 | PM6 | PM7 | RM1 |
| Pm - Pm | 2 | 0.3756 | 0.3664 | 0.3453 | **0.2590** | 0.2829 | 0.3862 |
| Pm - O | 122 | 0.0515 | 0.0555 | **0.0484** | 0.0651 | 0.0661 | 0.0557 |
| Pm - N | 30 | 0.0703 | 0.0441 | 0.0598 | 0.1923 | 0.0424 | **0.0410** |
| Pm - C | 30 | **0.0221** | 0.2549 | 0.2591 | 0.3115 | 0.1366 | 0.2435 |
| Pm - Cl | 6 | **0.0350** | 0.2381 | 0.2426 | 0.2743 | 0.0945 | 0.2583 |
| Pm - L | 190 | **0.0527** | 0.0943 | 0.0927 | 0.1327 | 0.0767 | 0.0929 |
| L - L | 733 | **0.1768** | 0.2205 | 0.1978 | 0.3201 | 0.2059 | 0.2203 |
| Pm-L, Pm-Pm and L-L’ | 923 | **0.1512** | 0.1945 | 0.1762 | 0.2815 | 0.1793 | 0.1941 |

**Table S6.** Sparkle/AM1, Sparkle/PM3, Sparkle/PM6, Sparkle/PM7, Sparkle/RM1 and RM1 Unsigned Mean Errors of the Samarium.

| Type of distances | N | unsigned mean errors for specific types of distances (Å) | | | | | |
|---|---|---|---|---|---|---|---|
| | | | Sparkle | | | | |
| | | RM1 | AM1 | PM3 | PM6 | PM7 | RM1 |
| Sm - Sm | 16 | 0.2166 | 0.2825 | **0.1852** | 0.3840 | 0.6196 | 0.2747 |
| Sm - O | 317 | **0.0625** | 0.0660 | 0.0695 | 0.0987 | 0.0765 | 0.0791 |
| Sm - N | 158 | 0.0680 | 0.0980 | 0.0887 | 0.1682 | 0.1050 | **0.0675** |
| Sm - C | 286 | **0.0489** | 0.2487 | 0.2504 | 0.4901 | 0.5426 | 0.2468 |
| Sm - S | 26 | **0.0473** | 0.4708 | 0.4580 | 0.5643 | 1.5885 | 0.4583 |
| Sm - Cl | 50 | **0.0625** | 0.2818 | 0.2921 | 0.3242 | 0.5302 | 0.3422 |
| Sm - Br | 12 | **0.0942** | 0.5142 | 0.5056 | 0.5973 | 1.1780 | 0.5524 |
| Sm - L | 865 | **0.0618** | 0.1671 | 0.1656 | 0.2800 | 0.3328 | 0.1692 |
| L - L | 3735 | **0.1548** | 0.2709 | 0.2636 | 0.3638 | 0.3985 | 0.2777 |
| Sm-L, Sm-Sm and L-L' | 4600 | **0.1373** | 0.2514 | 0.2452 | 0.3481 | 0.3862 | 0.2573 |

**Table S7.** Means and Variances of the *γ* Distribution Fits for the $UME_{(Ln-L)}$s Computed for the *N* Complexes for Each Lanthanide Trication.

| $UME_{(Ln-L)}$s | | | | |
|---|---|---|---|---|
| lanthanide ion | N | mean (Å) | variance ($Å^2$) | p-value |
| $Nd^{3+}$ | 88 | 0.0619 | 0.0030 | 0.1243 |
| $Pm^{3+}$ | 20 | 0.0527 | 0.0025 | 0.9945 |
| $Sm^{3+}$ | 76 | 0.0620 | 0.0045 | 0.9991 |

**Table S8**. Means and Variances of the *γ* Distribution Fits for the UMEs Computed for the *N* Complexes for Each Lanthanide Trication.

| UMEs | | | | |
|---|---|---|---|---|
| lanthanide ion | N | mean (Å) | variance ($Å^2$) | p-value |
| $Nd^{3+}$ | 88 | 0.1504 | 0.0394 | 0.2045 |
| $Pm^{3+}$ | 20 | 0.1512 | 0.0394 | 0.4544 |
| $Sm^{3+}$ | 76 | 0.1371 | 0.0257 | 0.7380 |

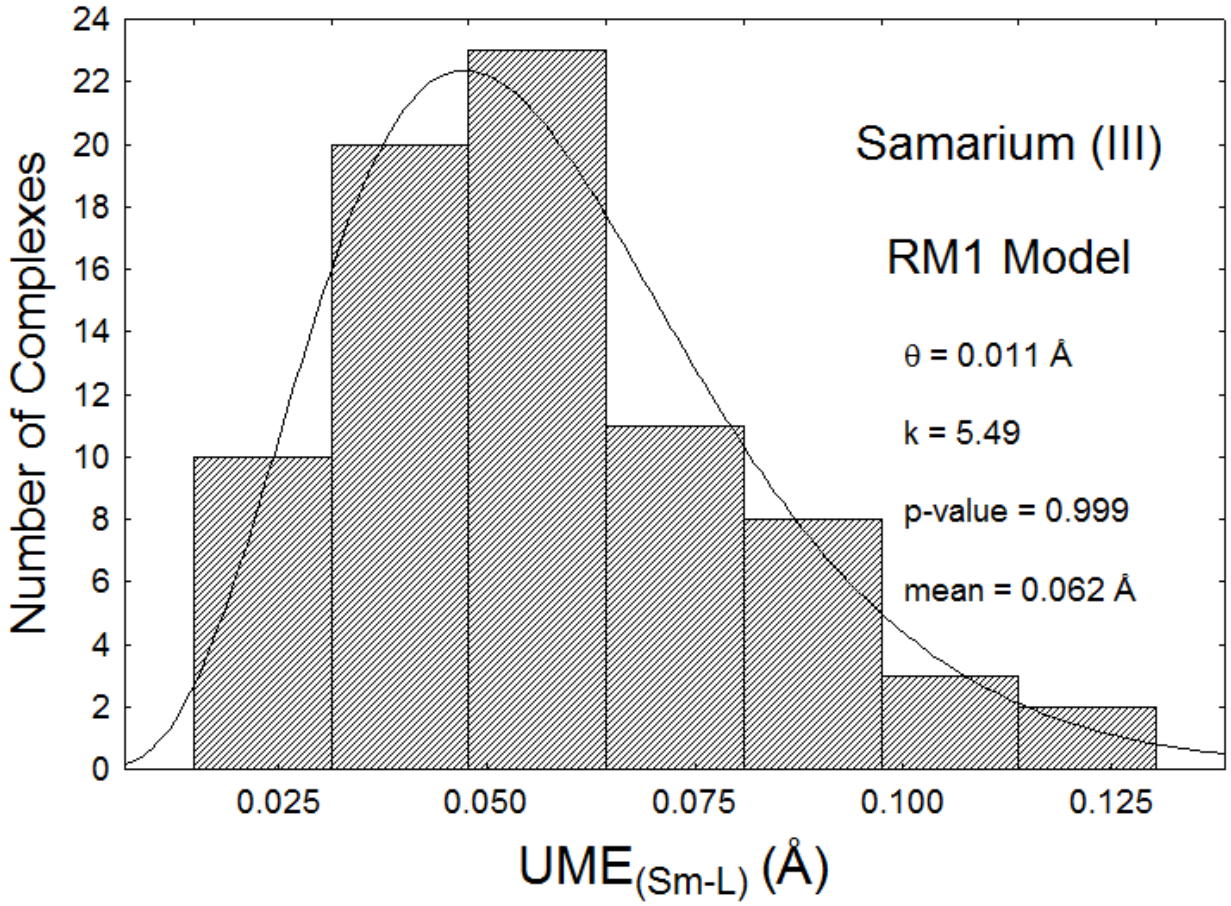


**Figure S1:** Histogram of the $UME_{(Ln-L)}$s for all 76 complexes of Sm(III) optimized via the RM1 model being advanced in this article. The shape k and scale θ are parameters of the fitted gamma distribution, and the mean is equal to kθ. The p-value of the one-sample nonparametric Kolmogorov-Smirnoff is also shown. This value is above 0.05, and therefore the data can be considered adjusted to the fitted gamma distribution within a 95% confidence interval.

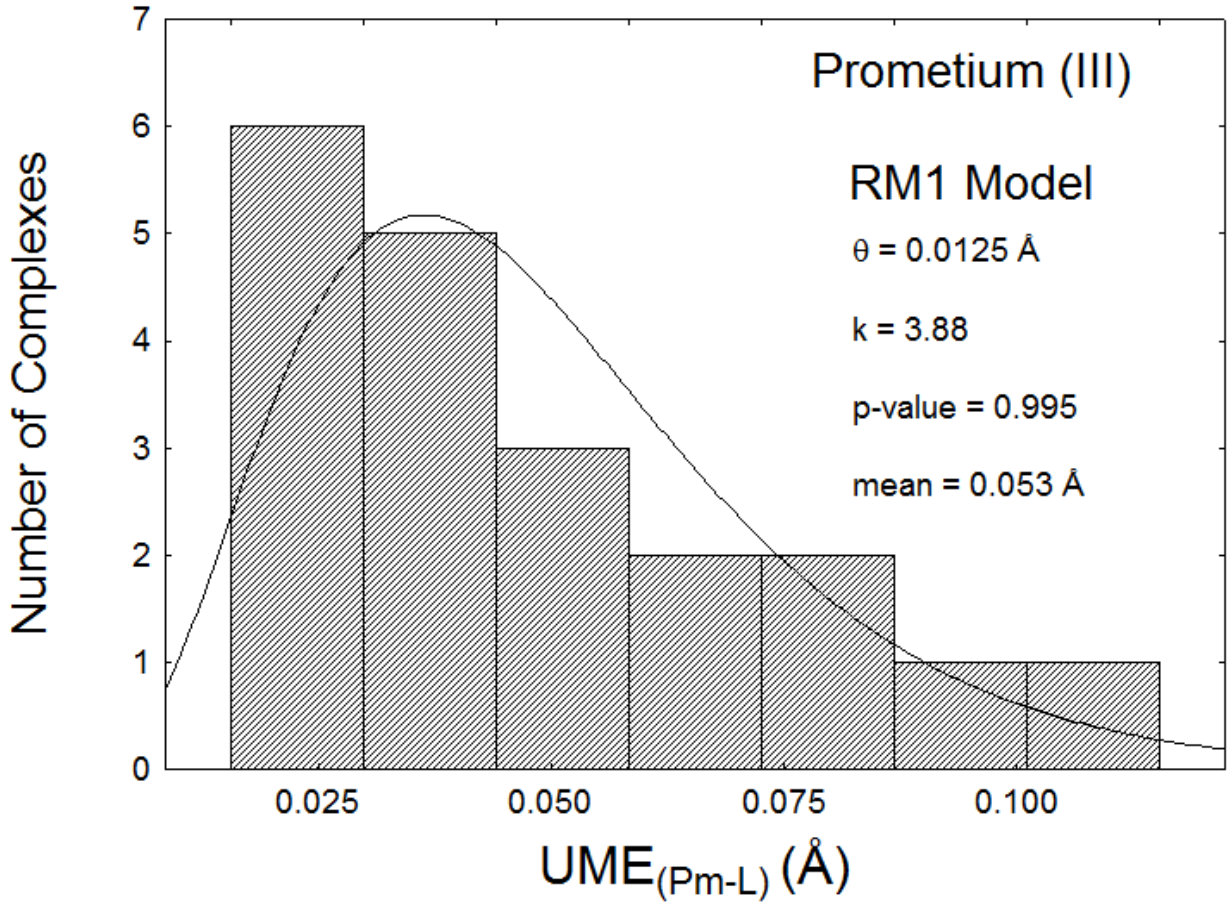


**Figure S2:** Histogram of the $UME_{(Ln-L)}$s for all 20 complexes of Pm(III) optimized via the RM1 model being advanced in this article. The shape k and scale θ are parameters of the fitted gamma distribution, and the mean is equal to kθ. The p-value of the one-sample nonparametric Kolmogorov-Smirnoff is also shown. This value is above 0.05, and therefore the data can be considered adjusted to the fitted gamma distribution within a 95% confidence interval.

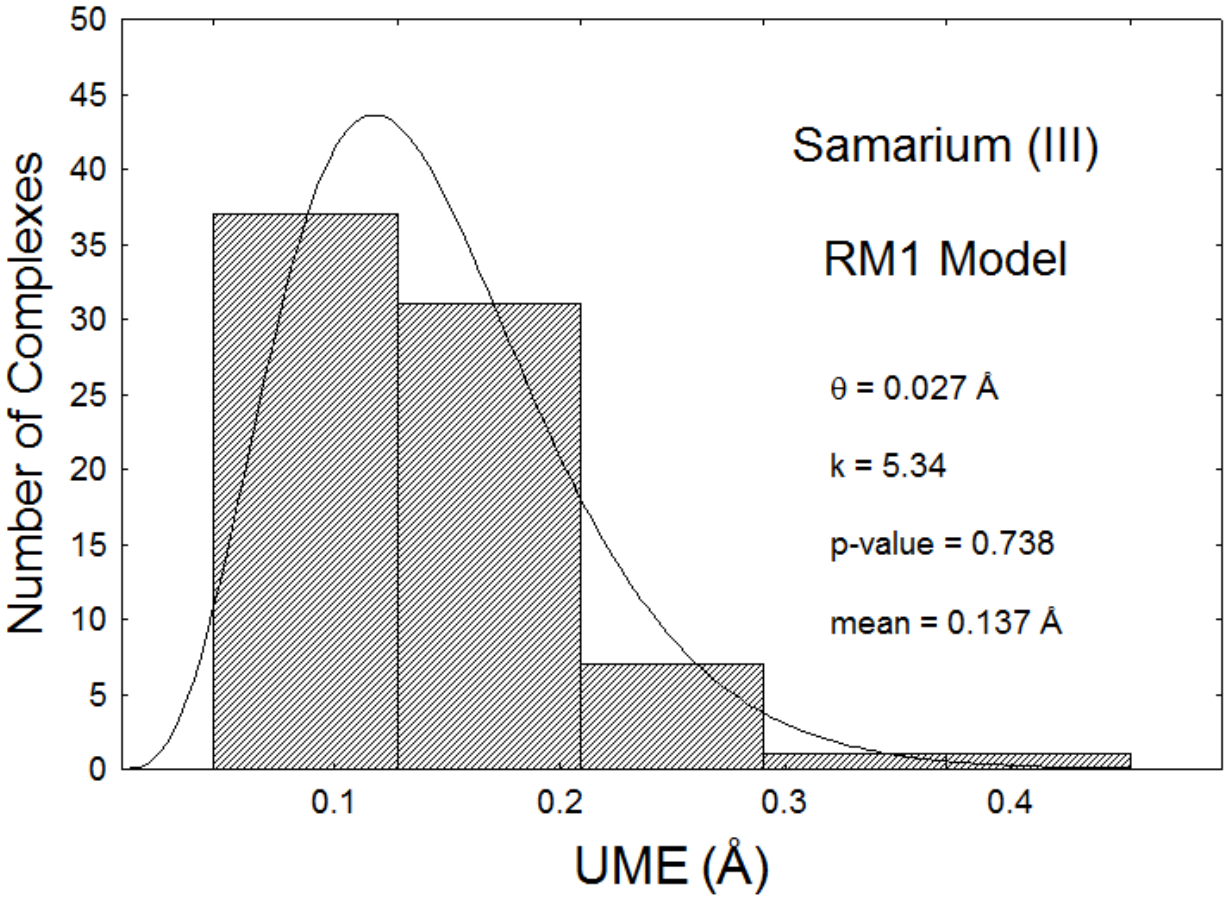


**Figure S3:** Histogram of the UMEs for all 76 complexes of Sm(III) optimized via the RM1 model being advanced in this article. The shape k and scale θ are parameters of the fitted gamma distribution, and the mean is equal to kθ. The p-value of the one-sample nonparametric Kolmogorov-Smirnoff is also shown. This value is above 0.05, and therefore the data can be considered adjusted to the fitted gamma distribution within a 95% confidence interval.

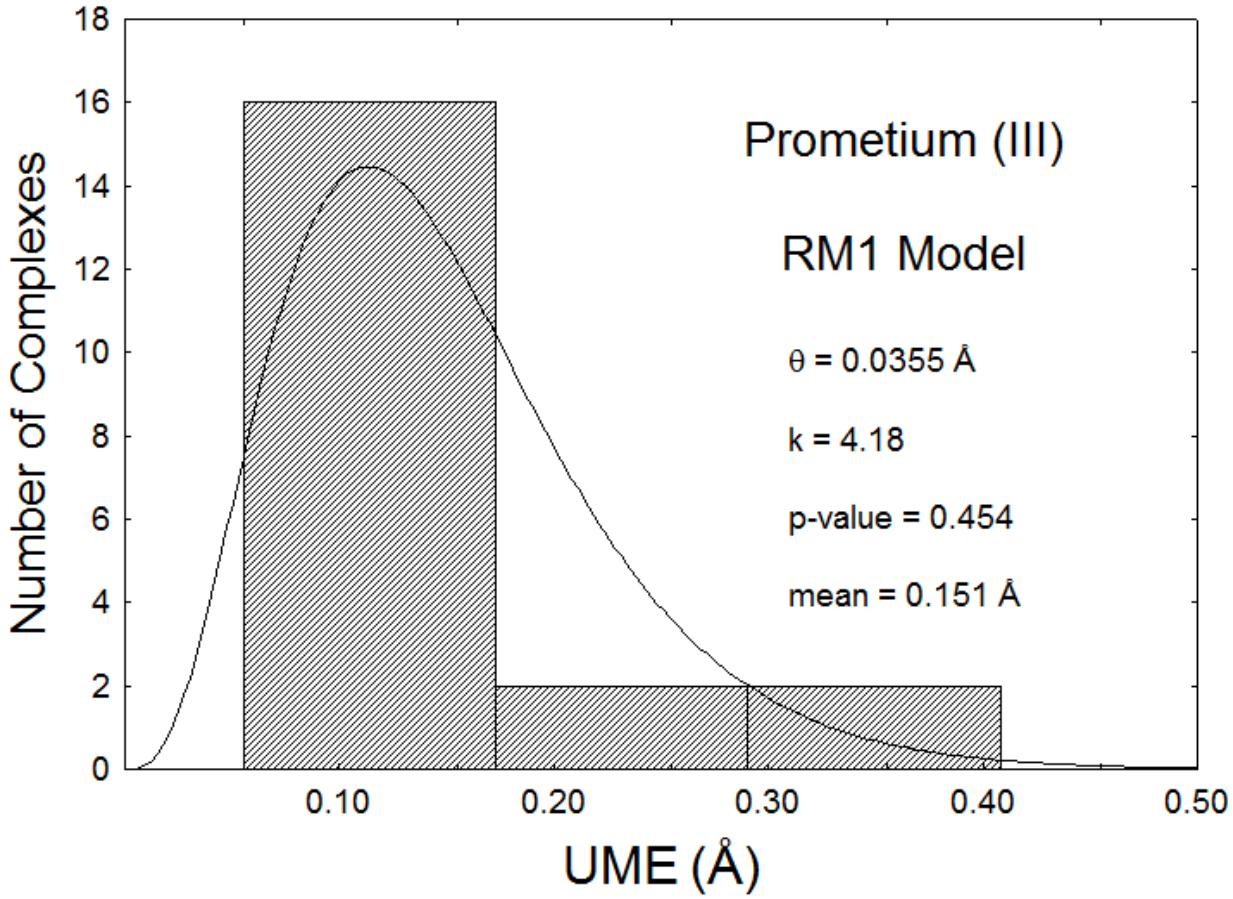


**Figure S4:** Histogram of the UMEs for all 20 complexes of Pm(III) optimized via the RM1 model being advanced in this article. The shape k and scale θ are parameters of the fitted gamma distribution, and the mean is equal to kθ. The p-value of the one-sample nonparametric Kolmogorov-Smirnoff is also shown. This value is above 0.05, and therefore the data can be considered adjusted to the fitted gamma distribution within a 95% confidence interval.

## Sample Input and Output Files

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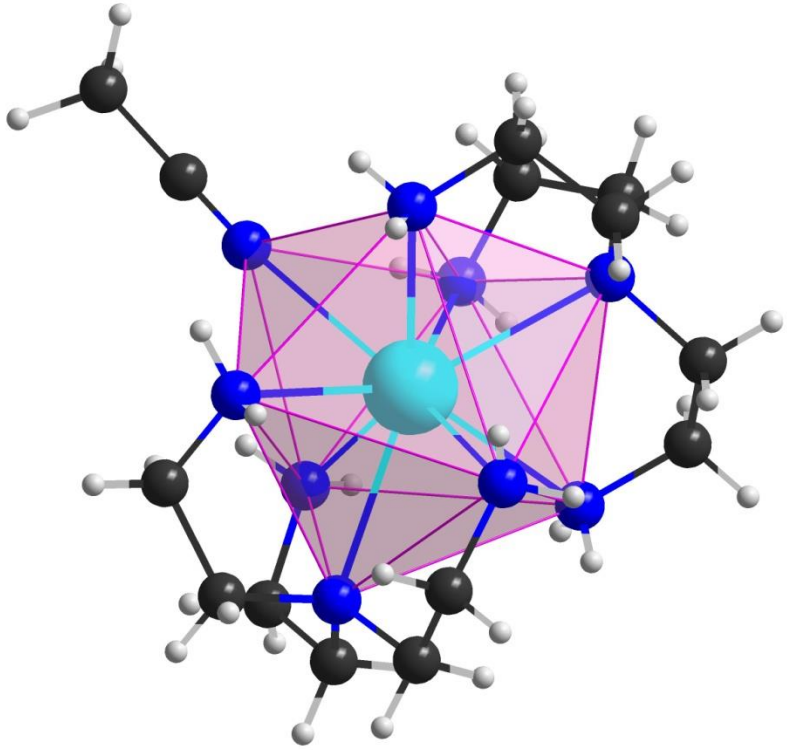
## Neodymium: BILSIY



---------- Begin of file **BILSIY.mop**----------

```
RM1 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3
COORDINATION NUMBER = 8

 Nd         0.013182  1    -0.007462  1     0.021403  1
  N         2.730082  1    -0.007462  1     0.021403  1
  N         1.112239  1     2.421343  1     0.021403  1
  N         1.058755  1     0.031612  1     2.408680  1
  N         1.135823  1    -2.279660  1    -0.621598  1
  N        -1.948946  1     1.384062  1    -1.207057  1
  N        -1.753839  1    -1.496157  1    -1.231768  1
  N        -1.699520  1     1.119766  1     1.660659  1
  N         0.495299  1     0.496202  1    -2.512422  1
  N        -1.070284  1    -1.896324  1     1.604005  1
  C         3.237819  1    -0.336197  1     1.380699  1
  C         2.184387  1    -0.922729  1     2.287602  1
  C         3.250055  1     1.314662  1    -0.427061  1
  C         2.583101  1     2.444067  1     0.266470  1
  C         3.179519  1    -1.018930  1    -0.955077  1
  C         2.615890  1    -2.342598  1    -0.709381  1
  C        -3.084197  1     0.511951  1    -1.598820  1
  C        -3.040748  1    -0.855486  1    -1.048502  1
  C        -2.405831  1     2.416113  1    -0.258072  1
```

```
 C       -2.812701  1     1.880787  1     1.059713  1
 C       -1.399316  1     2.025274  1    -2.426212  1
 C       -0.621993  1     1.100188  1    -3.271277  1
 C       -1.631604  1    -2.596158  1     2.301215  1
 C       -2.355400  1    -3.486406  1     3.185370  1
 H        3.945939  1    -0.961676  1     1.298205  1
 H        3.566345  1     0.463381  1     1.779987  1
 H        2.553563  1    -1.085520  1     3.145013  1
 H        1.864347  1    -1.736650  1     1.916904  1
 H        4.180826  1     1.349744  1    -0.250599  1
 H        3.099173  1     1.397045  1    -1.362089  1
 H        2.942846  1     3.260459  1    -0.057967  1
 H        2.745875  1     2.373504  1     1.199757  1
 H        2.913494  1    -0.737390  1    -1.825153  1
 H        4.125373  1    -1.077694  1    -0.918045  1
 H        2.959908  1    -2.678873  1     0.115717  1
 H        2.864296  1    -2.928740  1    -1.412505  1
 H       -3.887506  1     0.923578  1    -1.299708  1
 H       -3.093527  1     0.449053  1    -2.545487  1
 H       -3.703107  1    -1.377322  1    -1.482151  1
 H       -3.226073  1    -0.813474  1    -0.117906  1
 H       -3.150732  1     2.867737  1    -0.641087  1
 H       -1.697394  1     3.036631  1    -0.125162  1
 H       -3.561071  1     1.304546  1     0.951463  1
 H       -3.047470  1     2.597641  1     1.637704  1
 H       -2.122560  1     2.367722  1    -2.940070  1
 H       -0.833460  1     2.742208  1    -2.161954  1
 H       -0.267479  1     1.578053  1    -4.013399  1
 H       -1.192057  1     0.408775  1    -3.583649  1
 H        0.961697  1     2.785025  1    -0.755699  1
 H        0.726556  1     2.892260  1     0.641462  1
 H        1.348883  1     0.828738  1     2.611959  1
 H        0.488712  1    -0.230427  1     3.007799  1
 H        0.886125  1    -2.863878  1    -0.031072  1
 H        0.826842  1    -2.503576  1    -1.404118  1
 H       -1.560234  1    -1.539901  1    -2.080262  1
 H       -1.751759  1    -2.299152  1    -0.899310  1
 H       -2.046078  1     0.489580  1     2.148969  1
 H       -1.252513  1     1.667839  1     2.167143  1
 H        1.169523  1     1.045511  1    -2.550525  1
 H        0.705856  1    -0.251802  1    -2.897828  1
 H       -2.815941  1    -4.283101  1     2.601366  1
 H       -3.129418  1    -2.926806  1     3.710372  1
 H       -1.665380  1    -3.919191  1     3.909710  1
0
```

---------- End of file **BILSIY.mop**----------

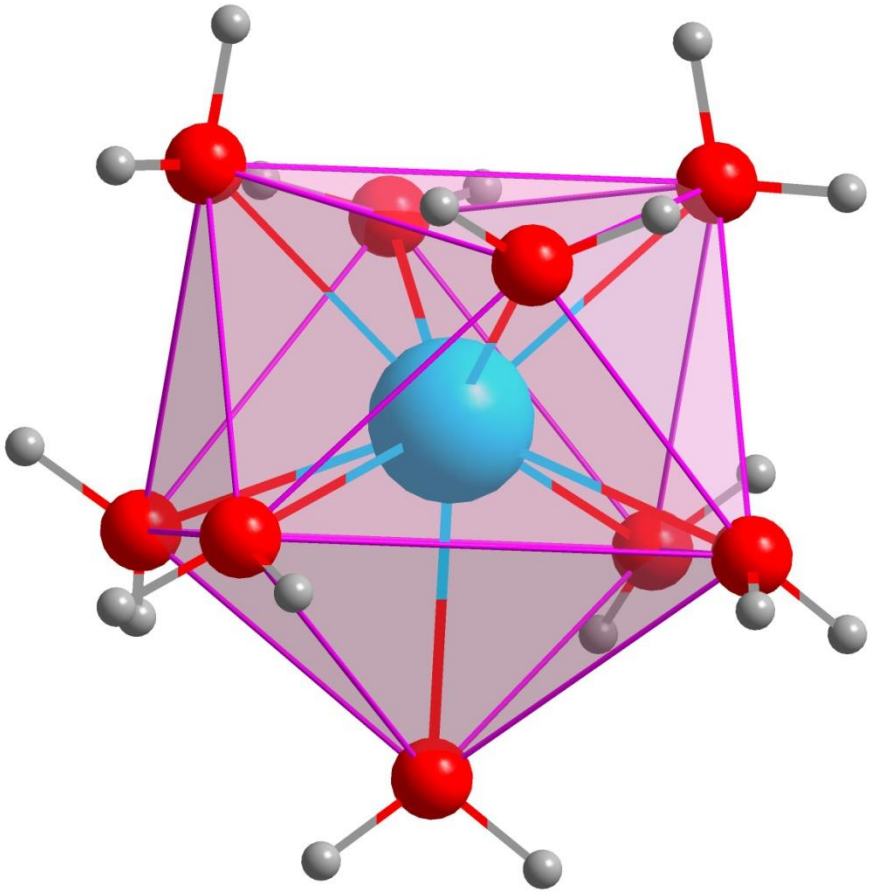
---------- Begin of file **BILSIY.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No:  999

                                                    MOPAC2012 (Version: 13.357 )
                                                    Wed Jan 07 18:28:29 2015

           Empirical Formula: C14 H39 N9 Nd  =    63 atoms

RM1 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3
 COORDINATION NUMBER = 8


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

          HEAT OF FORMATION       =        409.82737 KCAL/MOL =    1714.71771 KJ/MOL
          TOTAL ENERGY            =      -4229.81398 EV
          ELECTRONIC ENERGY       =     -39178.77493 EV
          CORE-CORE REPULSION     =      34948.96096 EV
          GRADIENT NORM           =          0.24345
          DIPOLE                  =          2.91757 DEBYE    POINT GROUP:       C1
          NO. OF FILLED LEVELS    =         70
          CHARGE ON SYSTEM        =          3
          IONIZATION POTENTIAL    =         20.535876 EV
          HOMO LUMO ENERGIES (EV) =        -20.536-10.504
          MOLECULAR WEIGHT        =        477.762
          COSMO AREA              =        354.03 SQUARE ANGSTROMS
          COSMO VOLUME            =        492.62 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    62    H    29     9.54020
            H    41    H    36     8.76622
            H    27    H    48     7.61186
          SCF CALCULATIONS        =        233
          WALL-CLOCK TIME         =  1 MINUTE AND  8.453 SECONDS
          COMPUTATION TIME        =  3 MINUTES AND 49.828 SECONDS


          FINAL GEOMETRY OBTAINED                                      CHARGE
RM1 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
NOLOG GEO-OK SCFCRT=1.D-10 CHARGE=3
 COORDINATION NUMBER = 8

 Nd    -0.06610922 +1  -0.10404005 +1   0.08355686 +1                        0.0630
  N     2.66727116 +1  -0.07776431 +1   0.01512868 +1                       -0.2477
  N     0.99389939 +1   2.27576054 +1   0.14070072 +1                       -0.3253
  N     1.07663750 +1   0.02001903 +1   2.39740319 +1                       -0.3115
  N     1.01207250 +1  -2.36721616 +1  -0.59889206 +1                       -0.3136
  N    -1.93077664 +1   1.44085867 +1  -1.18668406 +1                       -0.2478
  N    -1.86575385 +1  -1.42401898 +1  -1.21849502 +1                       -0.3113
  N    -1.73094243 +1   1.09485362 +1   1.67764878 +1                       -0.3135
  N     0.46425782 +1   0.38965949 +1  -2.41912437 +1                       -0.3253
  N    -1.03940159 +1  -1.85199190 +1   1.57198105 +1                       -0.3038
  C     3.33927165 +1  -0.26011334 +1   1.38440002 +1                       -0.0658
  C     2.35752146 +1  -0.78239086 +1   2.44483384 +1                       -0.0427
  C     3.16630253 +1   1.25283906 +1  -0.55212542 +1                       -0.0545
  C     2.50241408 +1   2.42227989 +1   0.19209802 +1                       -0.0553
  C     3.18673879 +1  -1.18508880 +1  -0.90393367 +1                       -0.0573
  C     2.52068314 +1  -2.51845983 +1  -0.54010017 +1                       -0.0514
  C    -3.13415063 +1   0.66104154 +1  -1.73763367 +1                       -0.0658
  C    -3.22125810 +1  -0.75702472 +1  -1.15229214 +1                       -0.0428
  C    -2.47192083 +1   2.51097118 +1  -0.23652044 +1                       -0.0572
  C    -2.89856482 +1   1.86326630 +1   1.08735169 +1                       -0.0513
  C    -1.29086047 +1   2.16827482 +1  -2.37112091 +1                       -0.0544
  C    -0.53420650 +1   1.16527764 +1  -3.25646437 +1                       -0.0553
  C    -1.49455247 +1  -2.66985982 +1   2.26896589 +1                        0.2975
  C    -2.05380831 +1  -3.67600530 +1   3.12701130 +1                       -0.2212
  H     4.22122620 +1  -0.95212572 +1   1.34658596 +1                        0.1415
  H     3.80817409 +1   0.68847651 +1   1.75311516 +1                        0.1258
  H     2.85336574 +1  -0.73709880 +1   3.45266116 +1                        0.1435
  H     2.12059026 +1  -1.86846448 +1   2.31707302 +1                        0.1111
```

```
H     4.28203075 +1   1.35901777 +1  -0.50544766 +1                    0.1492
H     2.94507916 +1   1.31752328 +1  -1.64959098 +1                    0.0979
H     2.84821092 +1   3.39229734 +1  -0.25688175 +1                    0.1469
H     2.85038370 +1   2.49774399 +1   1.25323650 +1                    0.1266
H     2.99862398 +1  -0.93587835 +1  -1.97776333 +1                    0.1033
H     4.30257923 +1  -1.29973504 +1  -0.86724024 +1                    0.1466
H     2.83954159 +1  -2.88625743 +1   0.46672221 +1                    0.1277
H     2.89026167 +1  -3.32107152 +1  -1.23427944 +1                    0.1462
H    -4.11062281 +1   1.18086745 +1  -1.55168126 +1                    0.1415
H    -3.11849768 +1   0.59697285 +1  -2.85616986 +1                    0.1259
H    -4.00882625 +1  -1.33288708 +1  -1.71074941 +1                    0.1435
H    -3.58873682 +1  -0.76654665 +1  -0.09542708 +1                    0.1112
H    -3.33301681 +1   3.08718824 +1  -0.66779039 +1                    0.1466
H    -1.70816533 +1   3.30683760 +1  -0.05258002 +1                    0.1034
H    -3.78533238 +1   1.19369757 +1   0.96104202 +1                    0.1276
H    -3.27578825 +1   2.65787546 +1   1.78654984 +1                    0.1462
H    -2.03365041 +1   2.73529852 +1  -2.99166304 +1                    0.1491
H    -0.59251320 +1   2.96718985 +1  -2.00829583 +1                    0.0979
H    -0.03952073 +1   1.71596528 +1  -4.10155240 +1                    0.1469
H    -1.22762849 +1   0.46358067 +1  -3.78515284 +1                    0.1265
H     0.65526674 +1   2.73348598 +1  -0.72922402 +1                    0.2087
H     0.60027268 +1   2.84854158 +1   0.90682584 +1                    0.2152
H     1.30377166 +1   1.00188561 +1   2.63321554 +1                    0.2090
H     0.46704307 +1  -0.30404207 +1   3.16719376 +1                    0.2159
H     0.60010666 +1  -3.14770659 +1  -0.05931801 +1                    0.2198
H     0.71766753 +1  -2.53919800 +1  -1.57699053 +1                    0.2042
H    -1.59856885 +1  -1.51027411 +1  -2.21457537 +1                    0.2089
H    -1.97160056 +1  -2.39749600 +1  -0.88645011 +1                    0.2157
H    -2.11432772 +1   0.43303088 +1   2.37401038 +1                    0.2196
H    -1.16499989 +1   1.76171267 +1   2.23258279 +1                    0.2042
H     1.35314180 +1   0.92847481 +1  -2.39704804 +1                    0.2088
H     0.69658813 +1  -0.47597241 +1  -2.93561356 +1                    0.2153
H    -2.46689041 +1  -4.53387158 +1   2.55783749 +1                    0.1784
H    -2.88336931 +1  -3.28399483 +1   3.75071459 +1                    0.1789
H    -1.30377609 +1  -4.09526123 +1   3.82875829 +1                    0.1787
```

---------- End of file **BILSIY.arc**----------

## Promecium: BUVWUK01



---------- Begin of file **BUVWUK01.mop**----------

```
RM1 PRECISE XYZ T=10D BFGS GNORM=0.25 +
 GEO-OK NOLOG SCFCRT=1.D-10 CYCLES=3000 CHARGE=3.0
 COORDINATION NUMBER = 9

 Pm       -0.000016  1    -0.000005  1    -0.000010  1
  O        0.000023  1     2.216623  1    -1.042645  1
  O       -1.791907  1     1.437380  1     0.871505  1
  O        0.000025  1    -0.205182  1     2.440972  1
  O        0.000031  1    -2.011304  1    -1.398265  1
  O       -1.791825  1    -1.473521  1     0.809089  1
  O       -1.791903  1     0.036087  1    -1.680580  1
  O        1.791924  1     1.437422  1     0.871448  1
  O        1.791851  1    -1.473483  1     0.809154  1
  O        1.791929  1     0.036026  1    -1.680579  1
  H       -0.776305  1     2.684470  1    -1.412084  1
  H       -1.618841  1     2.325158  1     1.248476  1
  H       -2.562491  1     1.097725  1     1.372048  1
  H        0.776524  1     2.684843  1    -1.411245  1
  H       -0.776302  1    -0.119305  1     3.030880  1
  H        0.776531  1    -0.120247  1     3.030781  1
  H       -0.776297  1    -2.565058  1    -1.618993  1
```

```
H         0.776537  1    -2.564508  1    -1.619743  1
H        -1.618701  1    -2.243909  1     1.389383  1
H        -2.562430  1    -1.737172  1     0.264695  1
H        -1.618894  1    -0.081181  1    -2.637934  1
H        -2.562604  1     0.639235  1    -1.636559  1
H         1.618618  1     2.324929  1     1.248951  1
H         2.562438  1     1.097603  1     1.371986  1
H         1.618490  1    -2.244208  1     1.388932  1
H         2.562394  1    -1.737030  1     0.264623  1
H         1.618689  1    -0.080643  1    -2.637966  1
H         2.562563  1     0.639247  1    -1.636403  1
```

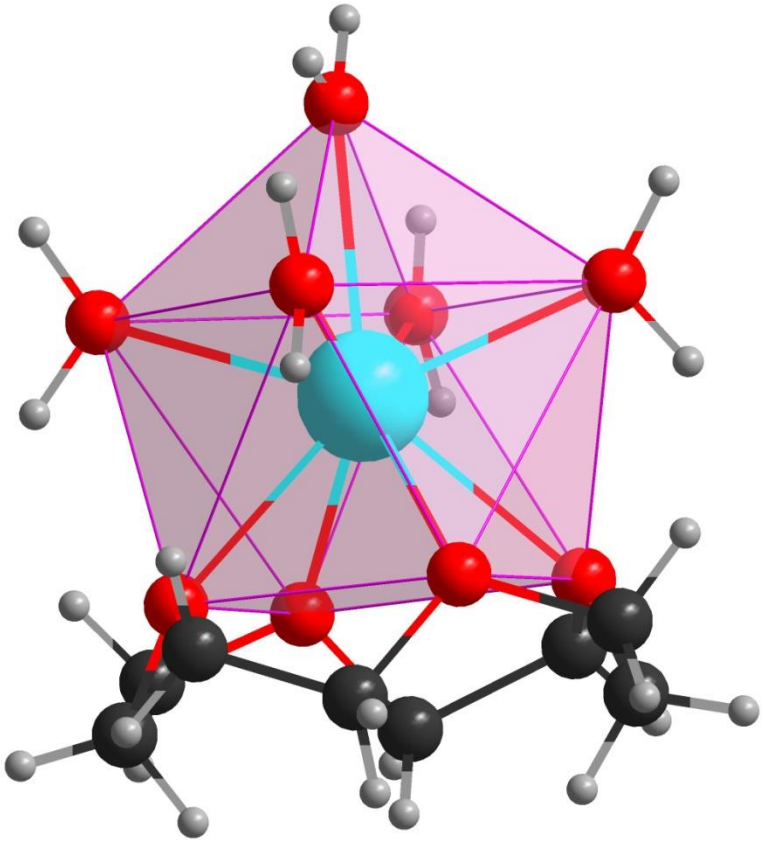
---------- End of file **BUVWUK01.mop**----------

---------- Begin of file **BUVWUK01.arc**----------

```
                    SUMMARY OF RM1 CALCULATION, Site No:  999

                                                    MOPAC2012 (Version: 13.357 )
                                                    Wed Jan 07 18:33:49 2015

           Empirical Formula: H18 O9 Pm  =    28 atoms

RM1 PRECISE XYZ T=10D BFGS GNORM=0.25 +
 GEO-OK NOLOG SCFCRT=1.D-10 CYCLES=3000 CHARGE=3.0
 COORDINATION NUMBER = 9


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

          HEAT OF FORMATION       =        -65.32532 KCAL/MOL =    -273.32114 KJ/MOL
          TOTAL ENERGY            =      -3141.57909 EV
          ELECTRONIC ENERGY       =     -14355.86194 EV
          CORE-CORE REPULSION     =      11214.28285 EV
          GRADIENT NORM           =          0.16715
          DIPOLE                  =          0.01121 DEBYE    POINT GROUP:       C3h
          NO. OF FILLED LEVELS    =         36
          CHARGE ON SYSTEM        =          3
          IONIZATION POTENTIAL    =         25.854657 EV
          HOMO LUMO ENERGIES (EV) =        -25.855-13.742
          MOLECULAR WEIGHT        =        307.137
          COSMO AREA              =        212.17 SQUARE ANGSTROMS
          COSMO VOLUME            =        245.40 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    18    H    12     7.88703
            H    25    H    11     5.44515
            H    16    H    17     0.64195
          SCF CALCULATIONS        =         69
          WALL-CLOCK TIME         =          4.859 SECONDS
          COMPUTATION TIME        =         18.078 SECONDS

          FINAL GEOMETRY OBTAINED                                      CHARGE
RM1 PRECISE XYZ T=10D BFGS GNORM=0.25 +
 GEO-OK NOLOG SCFCRT=1.D-10 CYCLES=3000 CHARGE=3.0
 COORDINATION NUMBER = 9

 Pm     0.00546672 +1   0.01376989 +1   0.00515166 +1                        0.3866
  O     0.00504725 +1   2.17574040 +1  -1.07173130 +1                       -0.3660
  O    -1.72135348 +1   1.38205947 +1   0.97745806 +1                       -0.3713
  O     0.01039826 +1  -0.15354814 +1   2.41424837 +1                       -0.3659
  O     0.00482611 +1  -1.99885057 +1  -1.32908566 +1                       -0.3659
  O    -1.72942605 +1  -1.50396610 +1   0.70454709 +1                       -0.3715
  O    -1.73673713 +1   0.17057066 +1  -1.65046316 +1                       -0.3714
  O     1.73617718 +1   1.38153839 +1   0.97155680 +1                       -0.3711
  O     1.74252344 +1  -1.50321681 +1   0.70071109 +1                       -0.3715
  O     1.74476751 +1   0.16767378 +1  -1.65370244 +1                       -0.3714
  H    -0.76329845 +1   2.69648752 +1  -1.37481299 +1                        0.3275
  H    -1.62320022 +1   2.33242455 +1   1.18099052 +1                        0.3296
  H    -2.61568610 +1   1.16492207 +1   1.30461818 +1                        0.3329
  H     0.77174631 +1   2.69407143 +1  -1.38301353 +1                        0.3275
  H    -0.75774799 +1  -0.15160981 +1   3.01684927 +1                        0.3273
  H     0.77748799 +1  -0.15103105 +1   3.01831222 +1                        0.3276
  H    -0.76368456 +1  -2.52205782 +1  -1.62736937 +1                        0.3275
  H     0.77153793 +1  -2.52543930 +1  -1.62619323 +1                        0.3277
  H    -1.62963157 +1  -2.16493630 +1   1.41690507 +1                        0.3294
  H    -2.62972283 +1  -1.66513099 +1   0.36167966 +1                        0.3329
  H    -1.64313125 +1  -0.13003411 +1  -2.57519138 +1                        0.3294
  H    -2.63147968 +1   0.56142745 +1  -1.62213472 +1                        0.3332
  H     1.64318801 +1   2.33378804 +1   1.16837476 +1                        0.3296
  H     2.62802744 +1   1.16123999 +1   1.30327152 +1                        0.3327
  H     1.64257750 +1  -2.16523383 +1   1.41203636 +1                        0.3293
  H     2.64307385 +1  -1.66341024 +1   0.35809543 +1                        0.3329
  H     1.65518592 +1  -0.13780047 +1  -2.57725916 +1                        0.3296
  H     2.63750495 +1   0.56291688 +1  -1.62462381 +1                        0.3329
```

---------- End of file **BUVWUK01.arc**----------

## Samarium: GINPEY



---------- Begin of file **GINPEY.mop**----------

```
RM1 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
GEO-OK SCFCRT=1.D-10 CHARGE=+3
 COORDINATION NUMBER = 9

 Sm       -0.437857  1    -0.262245  1     0.395383  1
  O        2.095543  1    -0.262245  1     0.395383  1
  O        0.701681  1     2.031932  1     0.395383  1
  O       -0.695487  1     1.123797  1    -1.712171  1
  O        0.710456  1    -1.151394  1    -1.734854  1
  O       -2.125069  1    -1.312903  1     1.956854  1
  O       -2.363443  1     1.196793  1     0.523206  1
  O       -1.914577  1    -1.671967  1    -0.848574  1
  O       -0.114397  1     0.536713  1     2.671836  1
  O        0.413378  1    -2.318585  1     1.329110  1
  C        2.682714  1     0.885837  1     1.037618  1
  C        2.172239  1     2.094728  1     0.407029  1
  C        0.063991  1     2.987875  1    -0.480716  1
  C        0.012374  1     2.387919  1    -1.837181  1
  C       -0.648601  1     0.351982  1    -2.955076  1
  C        0.712293  1    -0.461647  1    -2.955792  1
  C        2.005073  1    -1.704310  1    -1.478487  1
```

```
 C         2.898961  1    -0.796068  1    -0.731966  1
 H         2.446700  1     0.883753  1     1.968152  1
 H         3.627708  1     0.857295  1     0.956490  1
 H         2.465334  1     2.862751  1     0.899548  1
 H         2.501110  1     2.156553  1    -0.489772  1
 H        -0.795464  1     3.200502  1    -0.146635  1
 H         0.593771  1     3.776237  1    -0.529797  1
 H         0.869858  1     2.288763  1    -2.222758  1
 H        -0.514881  1     2.955783  1    -2.382424  1
 H        -1.374709  1    -0.245533  1    -2.992681  1
 H        -0.678364  1     0.938021  1    -3.711825  1
 H         1.447450  1     0.131523  1    -2.988899  1
 H         0.747658  1    -1.047431  1    -3.693935  1
 H         1.911460  1    -2.477177  1    -0.927791  1
 H         2.414010  1    -1.949892  1    -2.293101  1
 H         3.108320  1    -0.057724  1    -1.319615  1
 H         3.710477  1    -1.198267  1    -0.438414  1
 H        -1.960612  1    -1.013478  1     2.854015  1
 H        -2.875443  1    -1.911503  1     1.951810  1
 H        -2.219586  1     1.965909  1    -0.032827  1
 H        -3.223446  1     1.262959  1     0.944653  1
 H        -1.670239  1    -1.651599  1    -1.776633  1
 H        -2.670391  1    -2.251568  1    -0.729342  1
 H         0.619006  1     1.155664  1     2.692493  1
 H        -0.475785  1     0.439159  1     3.555850  1
 H         1.295510  1    -2.483755  1     0.988285  1
 H         0.163912  1    -3.026333  1     1.927664  1
0
```

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```
                    SUMMARY OF RM1 CALCULATION, Site No:  999

                                                    MOPAC2012 (Version: 13.357 )
                                                    Wed Jan 07 18:37:39 2015

          Empirical Formula: C8 H26 O9 Sm  =    44 atoms

RM1 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
GEO-OK SCFCRT=1.D-10 CHARGE=+3
 COORDINATION NUMBER = 9


     PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
     SCF FIELD WAS ACHIEVED

          HEAT OF FORMATION       =        235.97498 KCAL/MOL =     987.31930 KJ/MOL
          TOTAL ENERGY            =      -4244.82865 EV
          ELECTRONIC ENERGY       =     -29154.45195 EV
          CORE-CORE REPULSION     =      24909.62330 EV
          GRADIENT NORM           =          0.22742
          DIPOLE                  =          2.92825 DEBYE    POINT GROUP:       C2
          NO. OF FILLED LEVELS    =         56
          CHARGE ON SYSTEM        =          3
          IONIZATION POTENTIAL    =         21.553897 EV
          HOMO LUMO ENERGIES (EV) =        -21.554-12.366
          MOLECULAR WEIGHT        =        416.648
          COSMO AREA              =        278.63 SQUARE ANGSTROMS
          COSMO VOLUME            =        368.18 CUBIC ANGSTROMS

          MOLECULAR DIMENSIONS (Angstroms)

            Atom       Atom       Distance
            H    40    H    21     9.69565
            H    40    H    20     7.32500
            H    23    H    31     3.08753
          SCF CALCULATIONS        =        344
          WALL-CLOCK TIME         =         58.727 SECONDS
          COMPUTATION TIME        =  3 MINUTES AND 36.219 SECONDS


          FINAL GEOMETRY OBTAINED                                      CHARGE
RM1 PRECISE NOINTER XYZ BFGS T=10D GNORM=0.25 +
GEO-OK SCFCRT=1.D-10 CHARGE=+3
 COORDINATION NUMBER = 9

 Sm    -0.47238791 +1  -0.28415966 +1   0.43484663 +1                        0.6230
  O     2.11469247 +1  -0.27577713 +1   0.33124941 +1                       -0.3373
  O     0.80368203 +1   1.96652392 +1   0.34192031 +1                       -0.3368
  O    -0.56973016 +1   1.16544702 +1  -1.70871081 +1                       -0.3373
  O     0.73470393 +1  -1.08179196 +1  -1.71280586 +1                       -0.3367
  O    -2.15980324 +1  -1.26590581 +1   1.95165345 +1                       -0.3830
  O    -2.51560435 +1   1.04860440 +1   0.37497672 +1                       -0.3716
  O    -1.87817668 +1  -1.86428728 +1  -0.79379706 +1                       -0.3783
  O    -0.19827068 +1   0.63429496 +1   2.68516088 +1                       -0.3781
  O     0.43958274 +1  -2.28028223 +1   1.50188237 +1                       -0.3718
  C     2.75929198 +1   0.80008341 +1   1.02798864 +1                        0.0174
  C     2.23527649 +1   2.11800230 +1   0.43711558 +1                        0.0026
  C     0.17152972 +1   3.01198033 +1  -0.41056445 +1                        0.0158
  C    -0.03171273 +1   2.49641768 +1  -1.84376105 +1                        0.0014
  C    -0.61418498 +1   0.43979018 +1  -2.94561891 +1                        0.0175
  C     0.63479537 +1  -0.45278749 +1  -3.00736141 +1                        0.0028
  C     1.97769653 +1  -1.76951430 +1  -1.51085481 +1                        0.0158
  C     2.91130657 +1  -0.82541405 +1  -0.73764454 +1                        0.0015
  H     2.49755882 +1   0.65111054 +1   2.10575799 +1                        0.1219
  H     3.87760735 +1   0.75869741 +1   0.98517979 +1                        0.1701
  H     2.47456852 +1   2.98406427 +1   1.10314232 +1                        0.1545
  H     2.67755366 +1   2.34023569 +1  -0.56338851 +1                        0.1253
  H    -0.78123072 +1   3.23151849 +1   0.13365608 +1                        0.1214
  H     0.74126616 +1   3.97628385 +1  -0.40887293 +1                        0.1707
  H     0.91804314 +1   2.48282466 +1  -2.43008090 +1                        0.1257
  H    -0.75597395 +1   3.13722042 +1  -2.40572411 +1                        0.1543
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H    -1.57678028 +1  -0.13014401 +1  -2.91803793 +1                    0.1219
H    -0.68312885 +1   1.09585710 +1  -3.85057675 +1                    0.1700
H     1.56012740 +1   0.12707826 +1  -3.23877463 +1                    0.1252
H     0.53204925 +1  -1.23874065 +1  -3.79644190 +1                    0.1546
H     1.71050670 +1  -2.70250355 +1  -0.95386301 +1                    0.1213
H     2.45849770 +1  -2.11968526 +1  -2.45988494 +1                    0.1707
H     3.32434527 +1  -0.01325496 +1  -1.38245277 +1                    0.1256
H     3.78268517 +1  -1.37967142 +1  -0.30816559 +1                    0.1544
H    -2.48152310 +1  -0.90441401 +1   2.79247044 +1                    0.3191
H    -2.64486172 +1  -2.09795617 +1   1.83473056 +1                    0.3190
H    -2.76332520 +1   1.64672232 +1  -0.34987860 +1                    0.3262
H    -3.24692904 +1   1.10030829 +1   1.01048152 +1                    0.3251
H    -1.52461565 +1  -2.47673739 +1  -1.46079563 +1                    0.3257
H    -2.84001087 +1  -1.99043521 +1  -0.81426034 +1                    0.3265
H     0.01938484 +1   1.56703320 +1   2.85174128 +1                    0.3257
H    -0.19944477 +1   0.21182954 +1   3.55870859 +1                    0.3265
H     1.38810006 +1  -2.46702547 +1   1.60138540 +1                    0.3262
H    -0.01392125 +1  -3.02635743 +1   1.92520798 +1                    0.3253
```

---------- End of file **GINPEY.arc**----------

## 4. References

(back to contents)

(1) Allen F.H. (2002) Acta Crystallogr. B 58: 380-388.

(2) Bruno I.J., Cole J.C., Edgington P.R., Kessler M., Macrae C.F., McCabe P., Pearson J., Taylor R. (2002) Acta Crystallogr. B 58: 389-397.

(3) Allen F.H., Motherwell W.D.S. (2002) Acta Crystallogr. B 58: 407-422.