Supporting Information

Implementing f-Block Metal Ions in Medicine: Tuning the Size Selectivity of Expanded Macrocycles

Nikki A. Thiele,[§] Joshua J. Woods,[§#] and Justin J. Wilson[§*]

[§]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853, United States
[#]Robert F. Smith School for Chemical and Biomolecular Engineering, Cornell University, Ithaca, New York, 14853, United States

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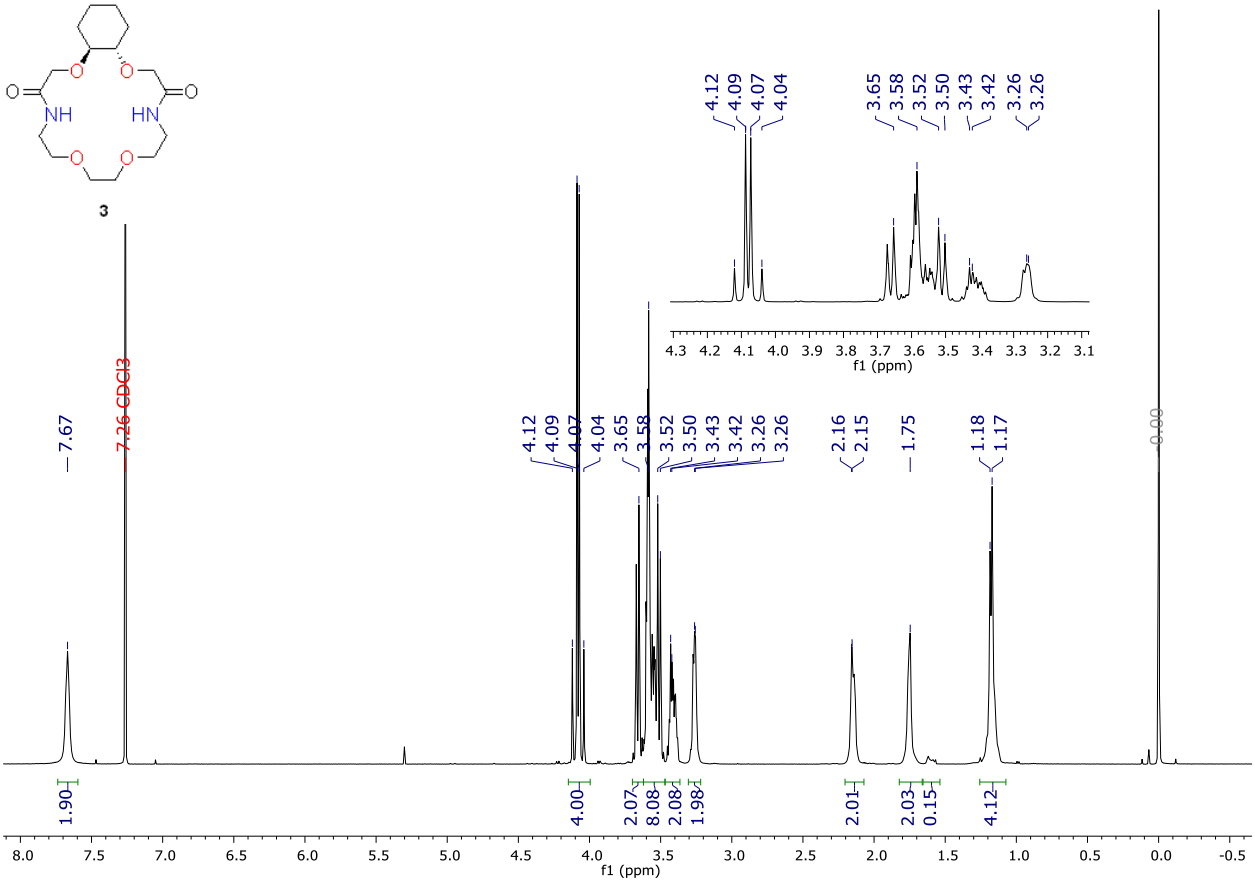

Figure S1. ^{1}H NMR spectrum of (16a*S*,20a*S*)-dodecahydro-2*H*,11*H*-benzo[*b*][1,4,10,13]tetraoxa[7,16]diazacyclooctadecine-3,14(4*H*,15*H*)-dione (3). 500 MHz, $CDCl_3$.

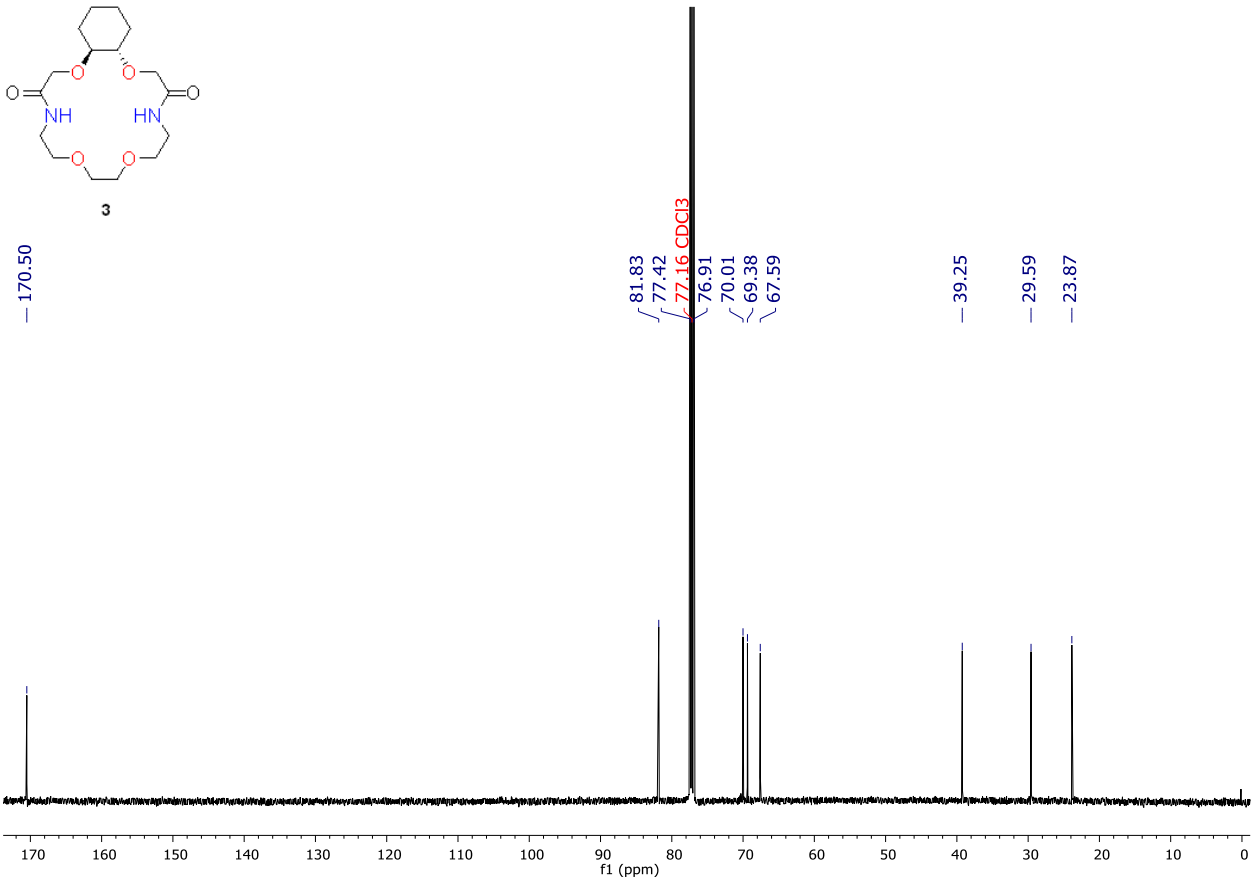

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of (16a*S*,20a*S*)-dodecahydro-2*H*,11*H*-benzo[*b*][1,4,10,13]tetraoxa[7,16]diazacyclooctadecine-3,14(4*H*,15*H*)-dione (3). 126 MHz, $CDCl_3$.

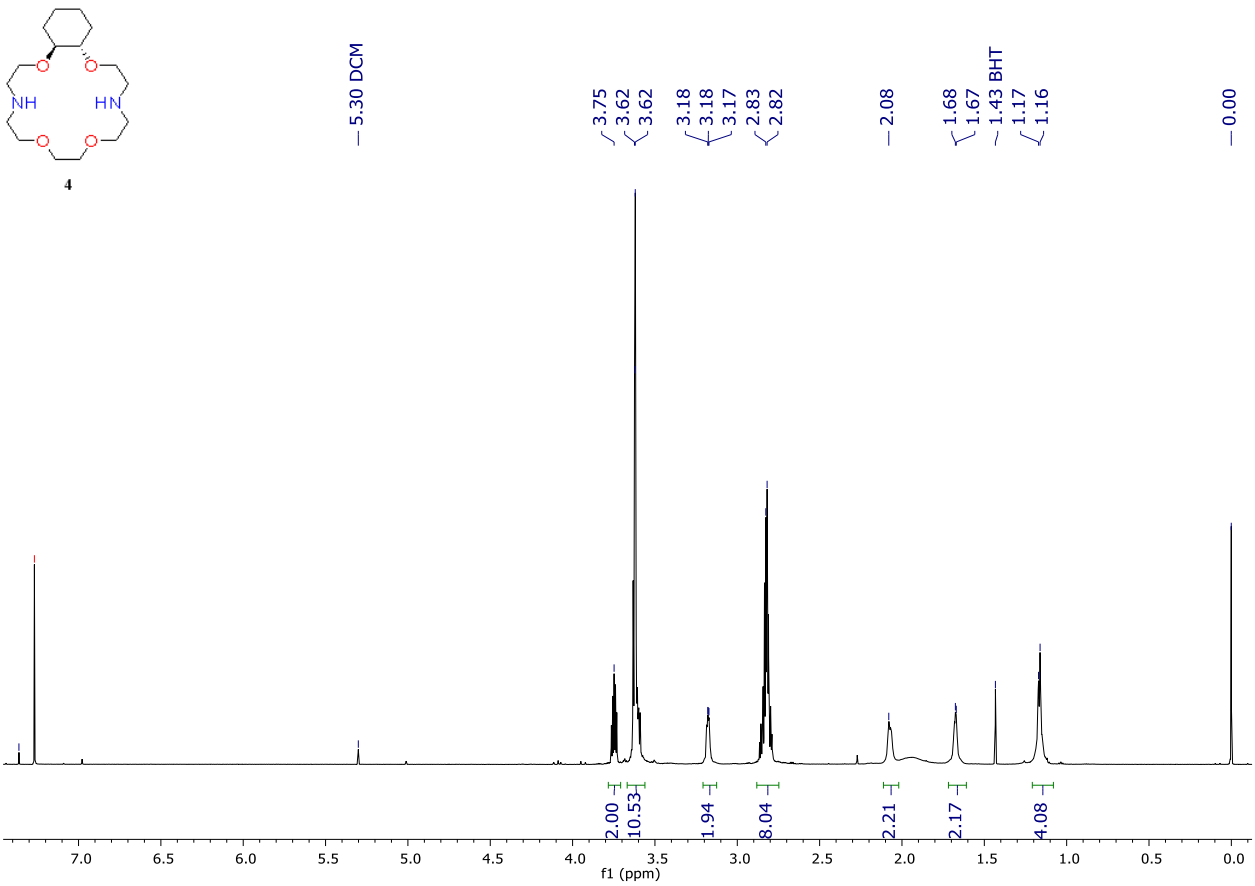

Figure S3. ^{1}H NMR spectrum of (16a*S*,20a*S*)-hexadecahydro-2*H*,11*H*-benzo[*b*][1,4,10,13]tetraoxa[7,16]diazacyclooctadecine (4). 600 MHz, $CDCl_3$.

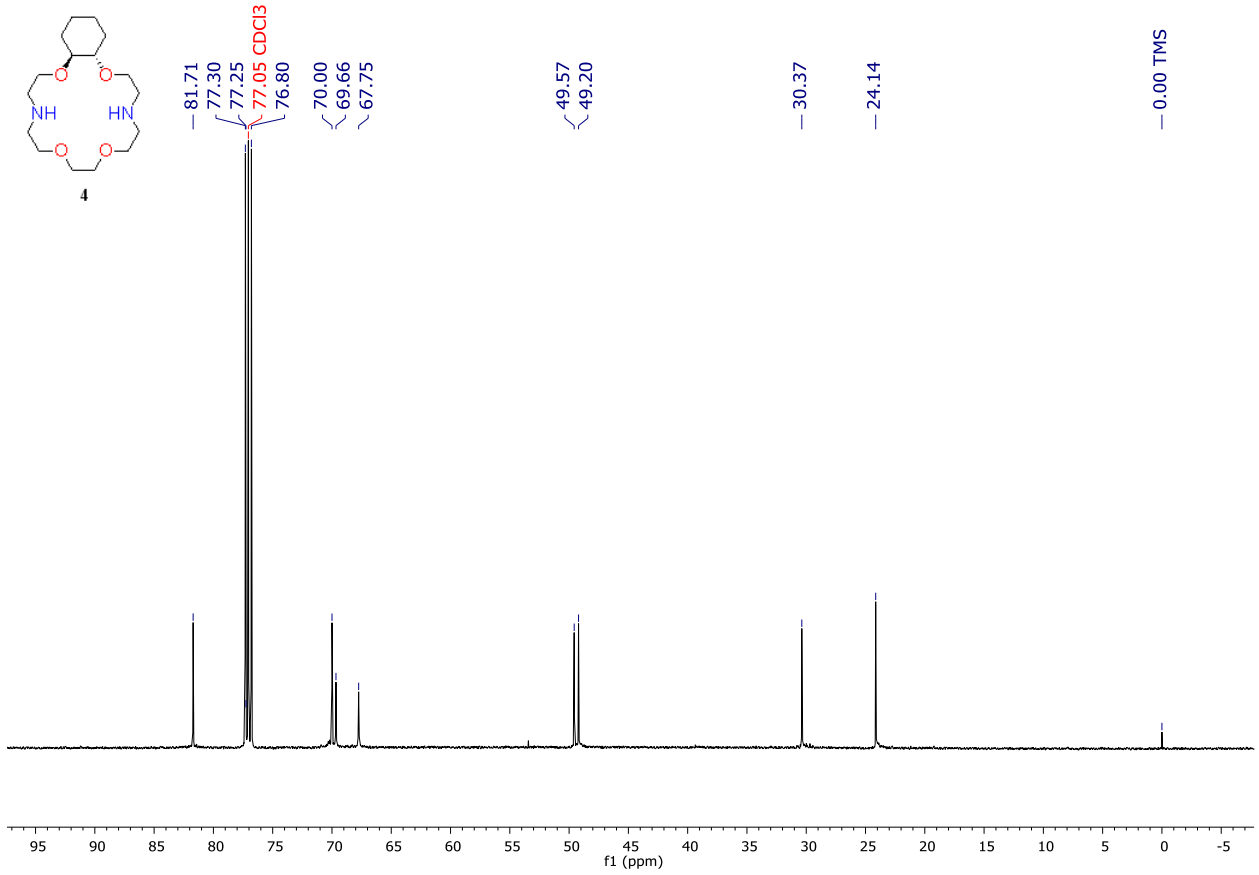

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of (16a*S*,20a*S*)-hexadecahydro-2*H*,11*H*-benzo[*b*][1,4,10,13]tetraoxa[7,16]diazacyclooctadecine (4). 126 MHz, $CDCl_3$.

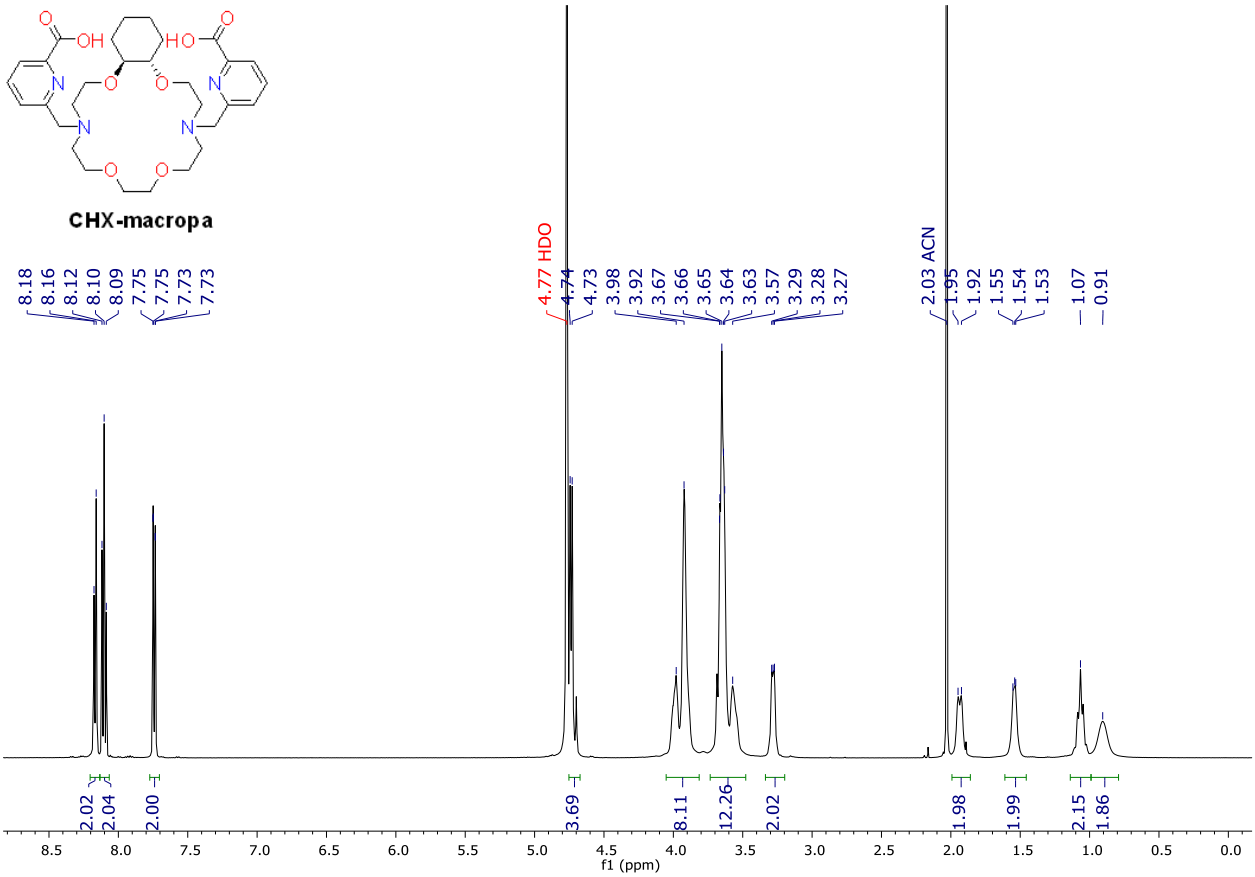

Figure S5. ^{1}H NMR spectrum of CHX-macropa. 500 MHz, D_2O, pD ≈ 1–2.

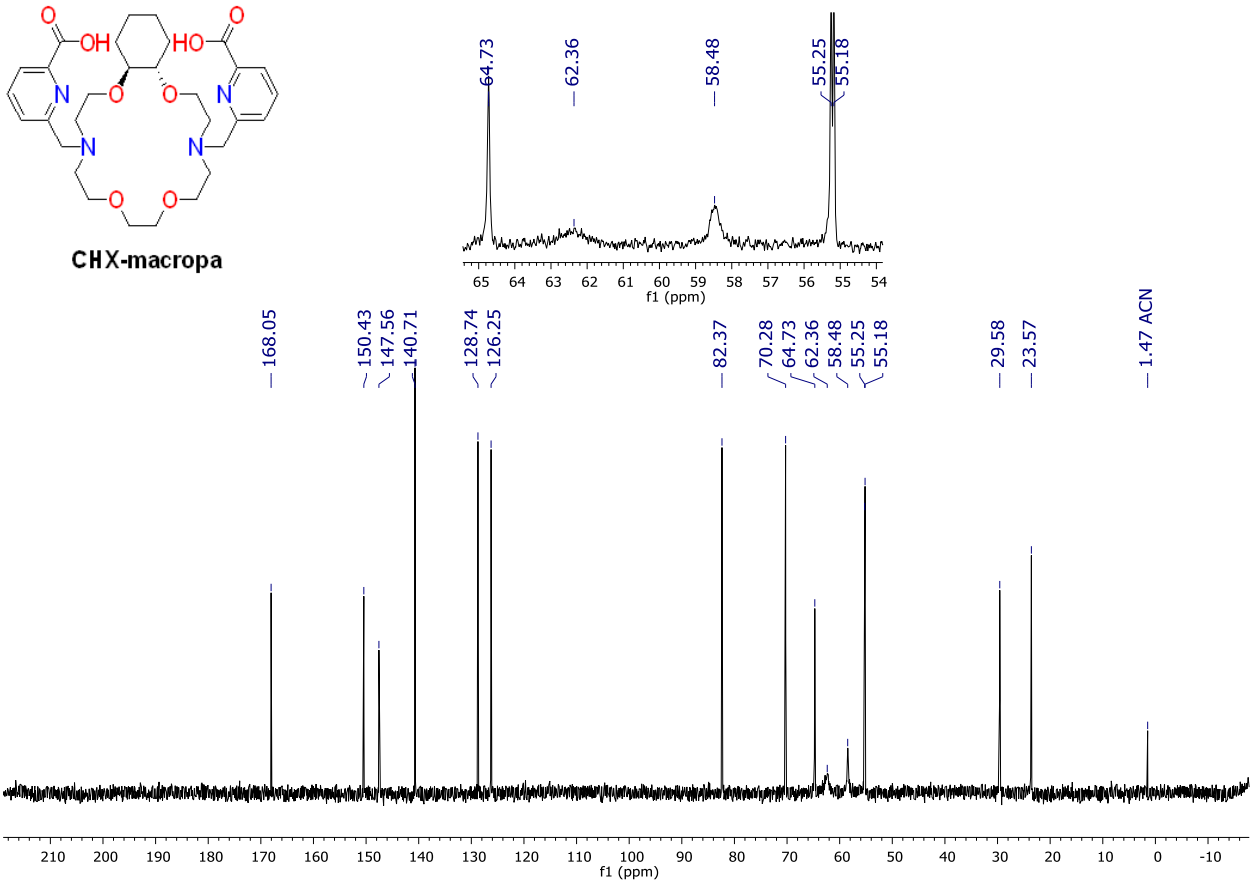

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of CHX-macropa. 126 MHz, D_2O, pD ≈ 1–2.

2. HIGH RESOLUTION MASS SPECTRA

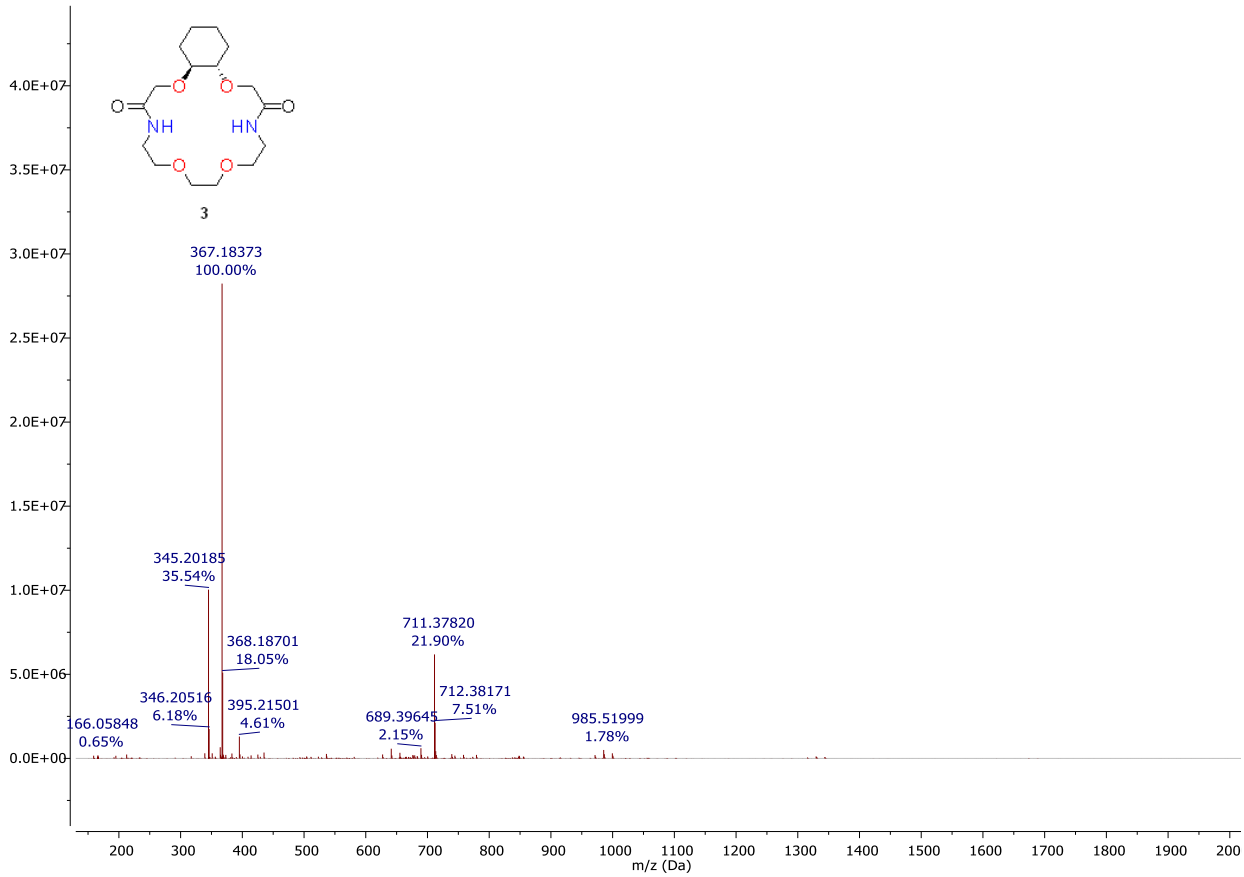

Figure S7. ESI HRMS of (16a*S*,20a*S*)-dodecahydro-2*H*,11*H*-benzo[*b*][1,4,10,13]tetraoxa[7,16]diazacyclooctadecine-3,14(4*H*,15*H*)-dione (3). The sample was analyzed using a mobile phase of CH_3CN:H_2O (50:50) containing 1% formic acid. Three ions were observed, corresponding to $[M+H]^+$ (*m/z* 345.20185), $[M+Na]^+$ (*m/z* 367.18373), and $[2M+Na]^+$ (*m/z* 711.37820) species.

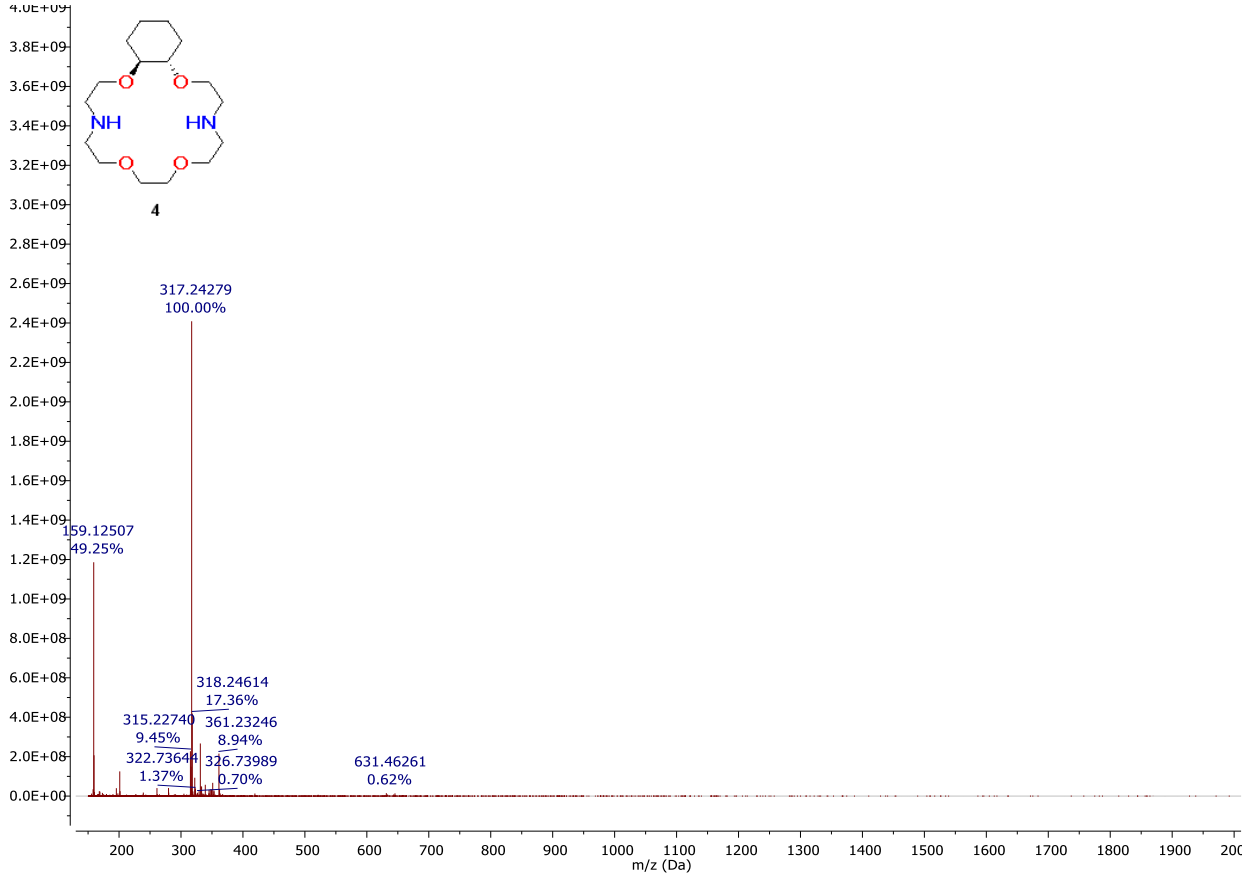

Figure S8. ESI HRMS of (16a*S*,20a*S*)-hexadecahydro-2*H*,11*H*-benzo[*b*][1,4,10,13]tetraoxa[7,16]diazacyclooctadecine (4). The sample was analyzed using a mobile phase of CH_3CN:H_2O (70:30) containing 0.1% formic acid. Two ions were observed, corresponding to $[M+H]^+$ (*m/z* 317.24279) and $[M+2H]^{2+}$ (*m/z* 159.12507).

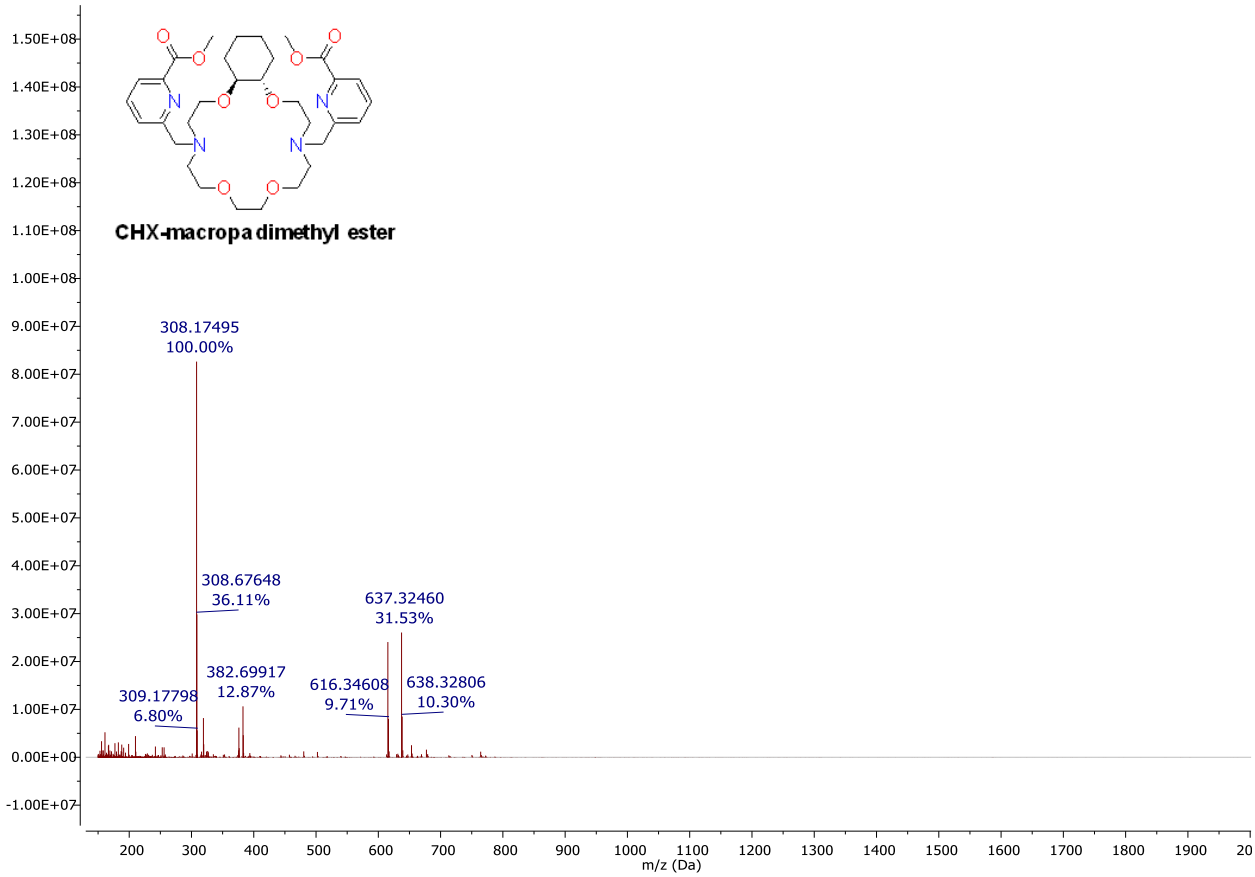

Figure S9. ESI HRMS of CHX-macropa dimethyl ester. The sample was analyzed using a mobile phase of CH_3CN:H_2O (70:30) containing 0.1% formic acid. Three ions were observed, corresponding to $[M+Na]^+$ (*m/z* 637.32460), $[M+H]^+$ (*m/z* 615.34266), and $[M+2H]^{2+}$ (*m/z* 308.17495).

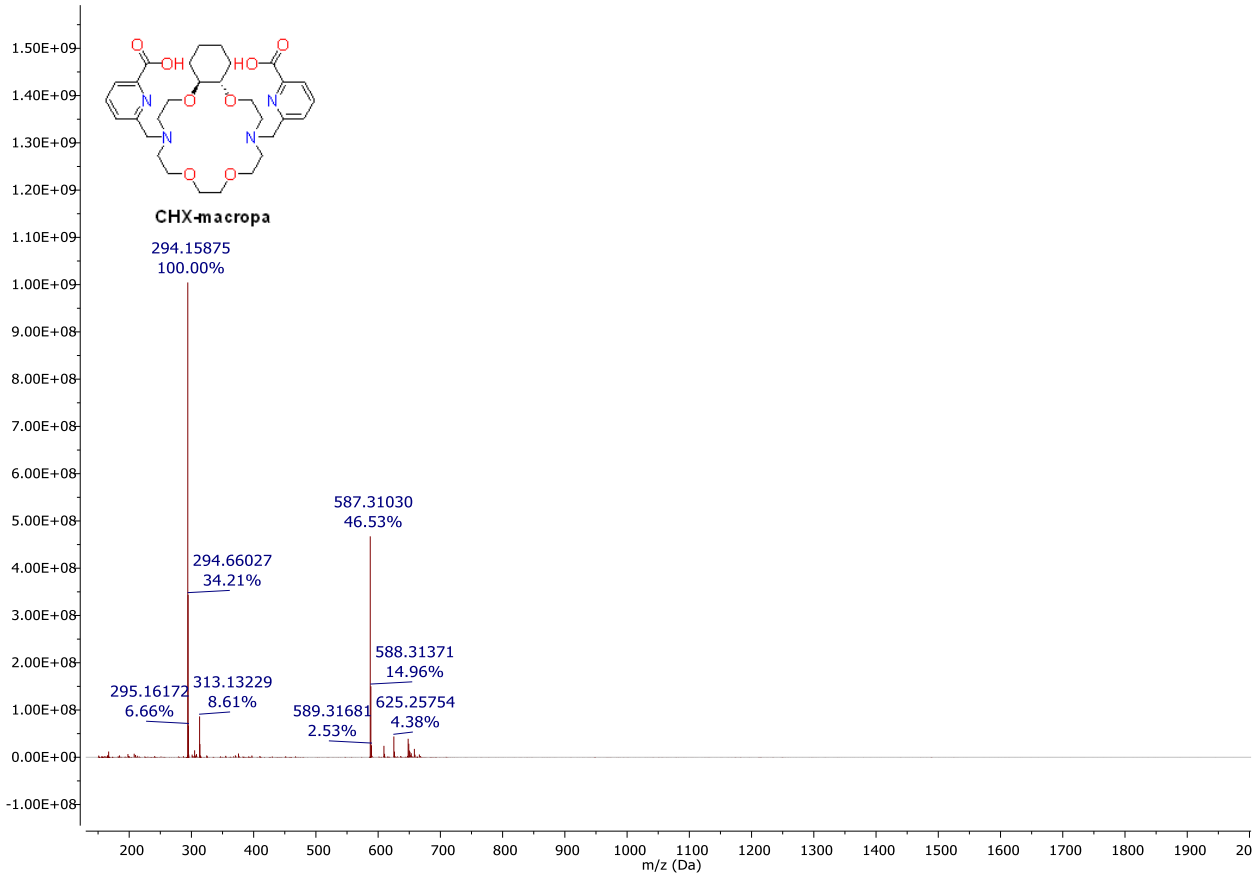

Figure S10. ESI HRMS of CHX-macropa. The sample was analyzed using a mobile phase of CH_3CN:H_2O (70:30) containing 0.1% formic acid. Two ions were observed, corresponding to $[M+H]^+$ (*m/z* 587.31030), and $[M+2H]^{2+}$ (*m/z* 294.15875).

3. HPLC CHROMATOGRAMS

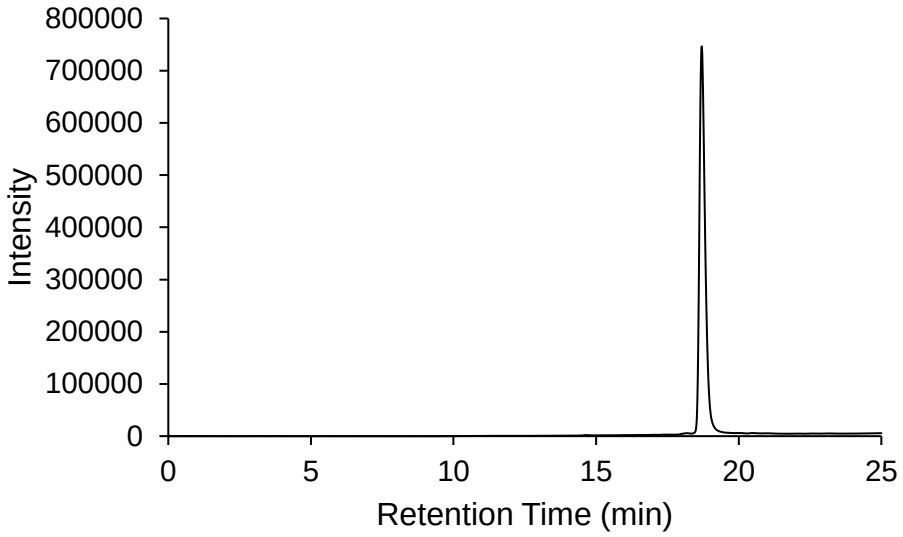

Figure S11. HPLC chromatogram of CHX-macropa. Retention time (t_R) = 18.70 min using a binary MeOH/H_2O mobile phase containing 0.1% TFA (program: 10% MeOH for 5 min, followed by a linear gradient to 100% MeOH over 20 min).

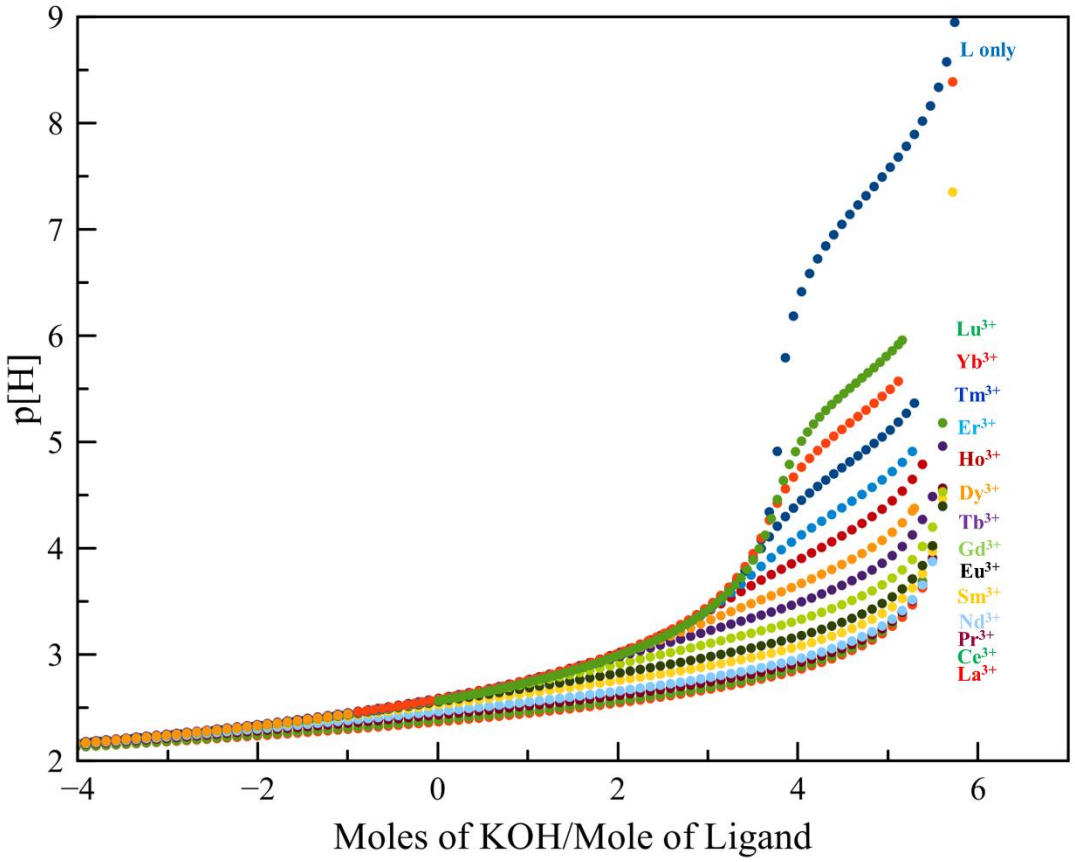

Figure S12. Potentiometric titration curves for CHX-macropa (1.1 mM) in the absence and presence of 1 equiv of Ln^{3+}. *I* = 0.1 M KCl, 25 °C.

5. X-RAY DIFFRACTION

Table S1. X-ray crystal data and structure refinement details for $[H_2CHX\text{-macropa}]Cl_2$ and $[La(CHX\text{-macropa})(OH_2)]PF_6 \cdot 2H_2O$

Compound	$[H_2CHX\text{-macropa}]Cl_2$	$[La(CHX\text{-macropa})(OH_2)]PF_6 \cdot 2H_2O$
Empirical Formula	$C_{30}H_{44}Cl_2N_4O_8$	$C_{30}H_{40}F_6LaN_4O_{11}P$
Formula Weight	659.59	916.54
a (Å)	19.58465(8)	10.41560(10)
b (Å)	7.96797(3)	17.16140(10)
c (Å)	21.32022(9)	20.93460(10)
α(∘)	90	90
β (∘)	90.7846(4)	93.4570(10)
γ(∘)	90	90
V (Å^3)	3326.71(2)	3735.17(5)
Z	4	4
Crystal System	Monoclinic	Monoclinic
Space Group	$P2_1/c$	$P2_1/c$
ρ_{calc} (Mg/m^3)	1.317	1.630
μ (mm^{-1})	2.204	10.059
T (K)	100.00(10)	100.01(10)
2θ range (º)	2.256 – 70.067	3.332 – 78.052
Independent Reflections	6315	7962
R_{int}	0.0438	0.064
Number of Parameters	419	860
Largest diff. peak and hole	0.499/-0.238	0.624/-0.939
GoF	1.030	1.097
R1/wR2 (all data)	0.0412/0.1108	0.0377/0.0901
R1/wR2 (>2θ)	0.0398/0.1096	0.0355/0.0884

Mo Kα λ=0.7107; $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma_w[(F_o^2)^2]\}^{1/2}$

GoF = $\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$, where *n* is the number of data and *p* is the number of refined parameters.

Table S2. Selected interatomic distances for $[H_2CHX\text{-macropa}]Cl_2$

Selected Interatomic Distances (Å)			
O(1)-C(2)	1.4229(18)	N(4)-C(29)	1.348(2)
O(1)-C(3)	1.4384(17)	C(1)-C(2)	1.512(2)
O(2)-C(8)	1.4377(17)	C(3)-C(4)	1.530(2)
O(2)-C(9)	1.4165(19)	C(3)-C(8)	1.516(2)
O(3)-C(12)	1.417(2)	C(4)-C(5)	1.528(2)
O(3)-C(13)	1.4300(19)	C(5)-C(6)	1.523(2)
O(4)-C(14)	1.418(2)	C(6)-C(7)	1.528(2)
O(4)-C(15)	1.423(2)	C(7)-C(8)	1.525(2)
O(5)-H(5)	0.865(17)	C(9)-C(10)	1.508(2)
O(5)-C(23)	1.313(3)	C(11)-C(12)	1.509(2)
O(6)-C(23)	1.205(2)	C(13)-C(14)	1.503(2)
O(7)-H(7)	0.884(17)	C(15)-C(16)	1.500(3)
O(7)-C(30)	1.321(3)	C(17)-C(18)	1.505(2)
O(8)-C(30)	1.208(2)	C(18)-C(19)	1.385(3)
N(1)-H(1)	0.865(15)	C(19)-C(20)	1.388(3)
N(1)-C(1)	1.512(2)	C(20)-C(21)	1.384(3)
N(1)-C(16)	1.5131(19)	C(21)-C(22)	1.395(3)
N(1)-C(17)	1.497(2)	C(22)-C(23)	1.510(3)
N(2)-H(2)	0.850(15)	C(24)-C(25)	1.513(2)
N(2)-C(10)	1.5159(18)	C(25)-C(26)	1.389(2)
N(2)-C(11)	1.5048(19)	C(26)-C(27)	1.389(2)
N(2)-C(24)	1.5020(19)	C(27)-C(28)	1.387(3)
N(3)-C(18)	1.342(2)	C(28)-C(29)	1.375(3)
N(3)-C(22)	1.334(2)	C(29)-C(30)	1.508(3)
N(4)-C(25)	1.330(2)		

Table S3. Selected interatomic angles for $[H_2CHX\text{-macropa}]Cl_2$

Selected Interatomic Angles (°)			
C(2)-O(1)-C(3)	112.91(12)	O(4)-C(14)-C(13)	107.04(15)
C(9)-O(2)-C(8)	114.04(11)	O(4)-C(15)-C(16)	107.59(14)
C(12)-O(3)-C(13)	113.21(14)	C(15)-C(16)-N(1)	115.24(13)
C(14)-O(4)-C(15)	114.31(14)	N(1)-C(17)-C(18)	110.72(13)
C(1)-N(1)-C(16)	112.87(12)	N(3)-C(18)-C(17)	115.24(15)
C(17)-N(1)-C(1)	112.17(12)	N(3)-C(18)-C(19)	123.40(17)
C(17)-N(1)-C(16)	112.48(13)	C(19)-C(18)-C(17)	121.36(17)
C(11)-N(2)-C(10)	110.85(12)	C(18)-C(19)-C(20)	118.1(2)
C(24)-N(2)-C(10)	113.14(11)	C(21)-C(20)-C(19)	119.5(2)
C(24)-N(2)-C(11)	113.74(11)	C(20)-C(21)-C(22)	118.12(19)
C(22)-N(3)-C(18)	117.69(16)	N(3)-C(22)-C(21)	123.20(19)
C(25)-N(4)-C(29)	117.42(14)	N(3)-C(22)-C(23)	115.26(17)
N(1)-C(1)-C(2)	113.35(13)	C(21)-C(22)-C(23)	121.54(17)
O(1)-C(2)-C(1)	109.69(13)	O(5)-C(23)-C(22)	116.61(16)
O(1)-C(3)-C(4)	111.18(12)	O(6)-C(23)-O(5)	121.0(2)
O(1)-C(3)-C(8)	106.20(12)	O(6)-C(23)-C(22)	122.3(2)
C(8)-C(3)-C(4)	109.96(13)	N(2)-C(24)-C(25)	112.32(12)
C(5)-C(4)-C(3)	111.78(13)	N(4)-C(25)-C(24)	116.94(14)
C(6)-C(5)-C(4)	110.48(14)	N(4)-C(25)-C(26)	123.28(14)
C(5)-C(6)-C(7)	109.31(13)	C(26)-C(25)-C(24)	119.73(14)
C(8)-C(7)-C(6)	111.76(13)	C(27)-C(26)-C(25)	118.36(16)
O(2)-C(8)-C(3)	107.17(11)	C(28)-C(27)-C(26)	118.96(17)
O(2)-C(8)-C(7)	110.22(12)	C(29)-C(28)-C(27)	118.41(16)
C(3)-C(8)-C(7)	111.65(13)	N(4)-C(29)-C(28)	123.49(16)
O(2)-C(9)-C(10)	108.35(12)	N(4)-C(29)-C(30)	116.23(16)
C(9)-C(10)-N(2)	114.34(12)	C(28)-C(29)-C(30)	120.26(15)
N(2)-C(11)-C(12)	114.13(13)	O(7)-C(30)-C(29)	118.48(15)
O(3)-C(12)-C(11)	109.02(13)	O(8)-C(30)-O(7)	120.79(19)
O(3)-C(13)-C(14)	111.11(14)	O(8)-C(30)-C(29)	120.7(2)

Table S4. Selected interatomic distances for the major and minor components of [La(CHX-macropa)(OH_2)]PF_6•2H_2O

Selected Interatomic Distances (Å)			
Component 1	Occ. = 0.849	Component 2	Occ. = 0.151
La(1A)-O(1A)	2.779(3)	La(1B)-O(1B)	2.680(18)
La(1A)-O(2A)	2.988(10)	La(1B)-O(2B)	2.927(16)
La(1A)-O(3A)	2.817(3)	La(1B)-O(3B)	2.81(2)
La(1A)-O(4A)	2.884(3)	La(1B)-O(4B)	2.78(6)
La(1A)-O(5A)	2.482(3)	La(1B)-O(5B)	2.486(17)
La(1A)-O(7A)	2.456(6)	La(1B)-O(7B)	2.44(4)
La(1A)-O(9A)	2.520(4)	La(1B)-O(9B)	2.61(3)
La(1A)-N(1A)	2.943(3)	La(1B)-N(2B)	2.92(2)
La(1A)-N(2)	2.878(3)	La(1B)-N(2)	3.044(4)
La(1A)-N(3)	2.705(3)	La(1B)-N(3)	3.033(5)
La(1A)-N(4A)	2.735(5)	La(1B)-N(4B)	2.63(1)

Table S5. Selected interatomic angles for the major and minor components of [La(CHX-macropa)(OH_2)]PF_6•2H_2O

Selected Interatomic Angles (°)			
Component 1	Occ. = 0.849	Component 2	Occ. = 0.151
N(2)-La(1A)-O(2A)	61.03(14)	N(3)-La(1B)-N(2)	53.24(9)
N(2)-La(1A)-O(4A)	118.18(9)	O(1B)-La(1B)-N(2)	64.5(4)
N(2)-La(1A)-N(1A)	175.59(9)	O(1B)-La(1B)-N(3)	70.9(4)
N(3)-La(1A)-N(2)	58.30(8)	O(1B)-La(1B)-O(2B)	58.3(6)
N(3)-La(1A)-O(1A)	143.20(9)	O(1B)-La(1B)-O(3B)	140.7(6)
N(3)-La(1A)-O(2A)	109.72(19)	O(1B)-La(1B)-O(4B)	103.0(13)
N(3)-La(1A)-O(3A)	74.59(9)	O(1B)-La(1B)-N(2B)	116.5(6)
N(3)-La(1A)-O(4A)	110.77(9)	O(2B)-La(1B)-N(2)	121.8(4)
N(3)-La(1A)-N(1A)	125.37(8)	O(2B)-La(1B)-N(3)	112.4(4)
N(3)-La(1A)-N(4A)	82.60(11)	O(3B)-La(1B)-N(2)	117.0(5)
O(1A)-La(1A)-N(2)	117.29(8)	O(3B)-La(1B)-N(3)	144.6(5)
O(1A)-La(1A)-O(2A)	56.46(14)	O(3B)-La(1B)-O(2B)	101.2(6)
O(1A)-La(1A)-O(3A)	138.70(9)	O(3B)-La(1B)-N(2B)	59.7(7)
O(1A)-La(1A)-O(4A)	102.85(10)	O(4B)-La(1B)-N(2)	58.4(10)
O(1A)-La(1A)-N(1A)	61.68(9)	O(4B)-La(1B)-N(3)	106.0(12)
O(3A)-La(1A)-N(2)	60.54(9)	O(4B)-La(1B)-O(2B)	125.4(15)
O(3A)-La(1A)-O(2A)	103.27(18)	O(4B)-La(1B)-O(3B)	59.4(11)
O(3A)-La(1A)-O(4A)	58.24(10)	O(4B)-La(1B)-N(2B)	117.9(11)
O(3A)-La(1A)-N(1A)	117.02(10)	O(5B)-La(1B)-N(2)	108.5(5)
O(4A)-La(1A)-O(2A)	127.2(2)	O(5B)-La(1B)-N(3)	59.4(4)
O(4A)-La(1A)-N(1A)	58.96(10)	O(5B)-La(1B)-O(1B)	74.0(6)
O(5A)-La(1A)-N(2)	111.85(9)	O(5B)-La(1B)-O(2B)	65.7(5)
O(5A)-La(1A)-N(3)	60.13(9)	O(5B)-La(1B)-O(3B)	131.5(7)

O(5A)-La(1A)-O(1A)	129.10(10)	O(5B)-La(1B)-O(4B)	165.4(13)
O(5A)-La(1A)-O(2A)	169.4(2)	O(5B)-La(1B)-O(9B)	128.9(7)
O(5A)-La(1A)-O(3A)	77.87(9)	O(5B)-La(1B)-N(2B)	75.3(6)
O(5A)-La(1A)-O(4A)	62.56(9)	O(5B)-La(1B)-N(4B)	63.0(7)
O(5A)-La(1A)-O(9A)	126.64(11)	O(7B)-La(1B)-N(2)	70.1(9)
O(5A)-La(1A)-N(1A)	70.29(10)	O(7B)-La(1B)-N(3)	68.1(9)
O(5A)-La(1A)-N(4A)	67.93(11)	O(7B)-La(1B)-O(1B)	131.1(10)
O(7A)-La(1A)-N(2)	70.95(16)	O(7B)-La(1B)-O(2B)	166.4(8)
O(7A)-La(1A)-N(3)	67.61(16)	O(7B)-La(1B)-O(3B)	76.6(10)
O(7A)-La(1A)-O(1A)	76.49(17)	O(7B)-La(1B)-O(4B)	65.3(16)
O(7A)-La(1A)-O(2A)	61.9(2)	O(7B)-La(1B)-O(5B)	105.4(7)
O(7A)-La(1A)-O(3A)	129.20(18)	O(7B)-La(1B)-O(9B)	125.6(8)
O(7A)-La(1A)-O(4A)	168.88(13)	O(7B)-La(1B)-N(2B)	110.1(10)
O(7A)-La(1A)-O(5A)	109.00(12)	O(7B)-La(1B)-N(4B)	62.7(9)
O(7A)-La(1A)-O(9A)	124.35(13)	O(9B)-La(1B)-N(2)	89.3(8)
O(7A)-La(1A)-N(1A)	112.32(17)	O(9B)-La(1B)-N(3)	135.7(8)
O(7A)-La(1A)-N(4A)	60.64(15)	O(9B)-La(1B)-O(1B)	71.7(7)
O(9A)-La(1A)-N(2)	87.55(11)	O(9B)-La(1B)-O(2B)	64.3(7)
O(9A)-La(1A)-N(3)	139.64(11)	O(9B)-La(1B)-O(3B)	69.1(8)
O(9A)-La(1A)-O(1A)	69.08(11)	O(9B)-La(1B)-O(4B)	61.1(16)
O(9A)-La(1A)-O(2A)	62.7(2)	O(9B)-La(1B)-N(2B)	87.5(9)
O(9A)-La(1A)-O(3A)	69.61(11)	N(2B)-La(1B)-N(2)	176.1(5)
O(9A)-La(1A)-O(4A)	64.47(10)	N(2B)-La(1B)-N(3)	130.6(4)
O(9A)-La(1A)-N(1A)	88.11(11)	N(2B)-La(1B)-O(2B)	58.6(5)
O(9A)-La(1A)-N(4A)	137.75(14)	N(4B)-La(1B)-N(2)	125.7(5)
N(1A)-La(1A)-O(2A)	117.41(15)	N(4B)-La(1B)-N(3)	84.3(5)
N(4A)-La(1A)-N(2)	126.67(11)	N(4B)-La(1B)-O(1B)	136.9(6)
N(4A)-La(1A)-O(1A)	72.77(11)	N(4B)-La(1B)-O(2B)	103.7(6)
N(4A)-La(1A)-O(2A)	109.1(2)	N(4B)-La(1B)-O(3B)	77.0(7)
N(4A)-La(1A)-O(3A)	145.16(11)	N(4B)-La(1B)-O(4B)	117.7(14)
N(4A)-La(1A)-O(4A)	108.40(10)	N(4B)-La(1B)-O(9B)	140.0(9)
N(4A)-La(1A)-N(1A)	57.57(11)	N(4B)-La(1B)-N(2B)	56.5(7)

Note: ***The description and justification provided below for the refinement of [La(CHX-macropa)(OH$_2$)]PF$_6$•2H$_2$O using whole-molecule disorder closely follows that of K. Suntharalingam, T. C. Johnstone, P. M. Bruno, W. Lin, M. T. Hemann, and S. J. Lippard (J. Am. Chem. Soc. 2013, 135, 14060–14063, Supporting Information), who describe the refinement of whole-molecule disorder in an osmium nitrido complex.***

Initial solution and refinement of [La(CHX-macropa)(OH$_2$)]PF$_6$•2H$_2$O. Colorless crystals of La(CHX-macropa)]PF_6 were grown upon standing at room temperature in an aqueous solution of KPF_6. A full data set was acquired at 100 K using Cu Kα radiation and the observed intensities fit well into a P-centered monoclinic lattice. Integration, absorption correction and data reduction were performed without issue. The experimental intensities showed no evidence for twinning. The value of $|E^2-1| = 0.936$ is significantly closer to 0.968 than 0.736, suggesting that the structure is centrosymmetric, and the initial solution was attempted in the space group $P2_1/c$. Using the intrinsic phasing method of SHELXT, a solution was obtained in which the general framework of the molecule was unequivocally established. Following anisotropic refinement, the model had a large residual electron density of approximately 6.5 electrons, a hole of approximately 3 electrons within 1Å of the lanthanum center, and large R_1 and wR_2 values. Refinement of this peak as positional disorder of the metal atom gave physically unrealistic interatomic distances between the metal center and some of the donating atoms in the macrocycle. Furthermore, the crystallographic occupancies for the two disordered components refined as 50.5% and 49.5% respectively, which did not make physical sense in regard to the size of the original residual electron density in the model where the lanthanum center was not treated as disordered. To determine if the large residual electron density was the result of pseudosymmetry, where the two lanthanum centers belong to pseudocrystallographically related molecules that almost, but don't exactly, overlap, attempts were made to solve the structure in a lower symmetry space group. These attempts were unsuccessful. For example, two independent molecules were observed in the asymmetric unit when solved in the $P1$ or $P\bar{1}$ space groups; however, some of the atoms in the macrocycle could not be found in the difference map and both La centers showed high residual electron density. Following initial refinement, it was decided to treat the molecule with whole-molecule disorder following similar procedures employed for the refinement of whole-molecule disorder in an osmium nitrido complex (K. Suntharalingam, T. C. Johnstone, P. M. Bruno, W. Lin, M. T. Hemann, and S. J. Lippard *J. Am. Chem. Soc.* **2013**, *135*, 14060–14063, Supporting Information).

Refinement with whole-molecule disorder. The high residual electron density near the La center was assigned as a second La atom and the occupancies of these two atoms was constrained to sum to unity. After this assignment, the remainder of the second component of the whole molecule disorder could be found. These steps are shown schematically in Figure S12. A few atoms could not be found in the second component of the disorder and were therefore excluded from the disorder and left in PART 0 with full occupancy. These atoms include: N2, N3, C13, C14, C21, C20, and C23.

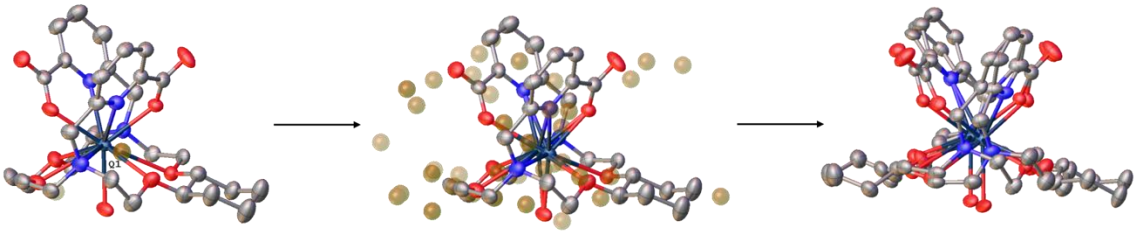

Figure S13. Schematic depiction of the initial steps of the refinement of the whole-molecule disorder.

Several restraints were employed in order to achieve a stable full-matrix least-squares refinement. The extensive use of restraints is justified by the high degree of disorder present in the molecule. Most of the restraints were used to restrain the interatomic distances and angles of the disordered components of the ligand to be similar. Note that the metal-ligand interatomic distances and angles were not treated with similar restraints. The size and directionality of the ellipsoids of the disordered atoms were restrained to be similar with a standard deviation of 0.02. In the second component of the disorder, the pyridine rings had to be restrained to be approximately coplanar using the FLAT command due to the low occupancy of the disordered component. Only one atom (O8B) had to be treated with the EADP command and was constrained to have a thermal ellipsoid identical to that of the analogous oxygen atom in the first component of the disorder (O8A). Without this constraint, the refinement was not stable. The resulting structure is shown in Figure S13.

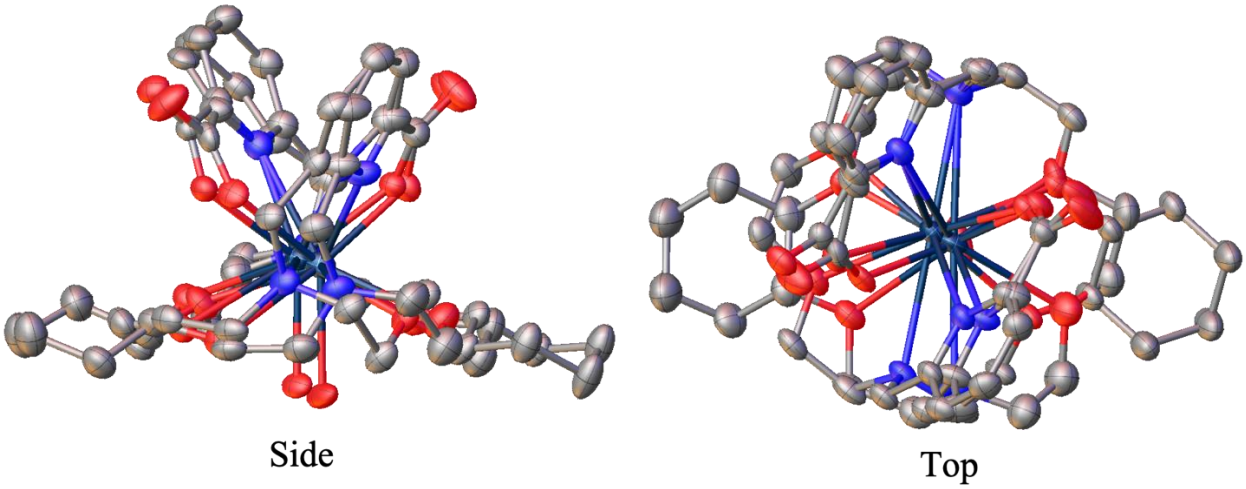

Figure S14. ORTEP plot of the disordered molecule from two different angles. Ellipsoids are shown at the 50% probability level. Hydrogen atoms, outer sphere counterions and outer sphere water molecules are removed for clarity.

Following treatment of the whole molecule disorder, the disorder in the PF_6^- counterion and the solvent water molecules could be resolved. The disorder in the PF_6^- counterion and one water molecule was easily solved. The disordered component of the second water molecule (O11B) gave an unrealistic thermal ellipsoid and an unstable refinement, which generated an A level alert upon CheckCIF validation. This was remedied by constraining the thermal ellipsoids of O11A and O11B to be identical using the EADP command. No attempt was made to locate the

hydrogen atoms on the coordinated or solvent water molecules on the Fourier difference map due to the extreme disorder of the entire structure.

Validation. The initial and final structures were checked for twinning and missed symmetry using PLATON. The most significant CheckCIF alerts arise from the poor data to parameter ratio (9.26), which is a result of the extensive use of restraints, which are required for stable refinement. Additionally, a C level alert arises from the large average U_{eq} of O10B, which was not treated with the EADP constraints. The remaining two C level alerts are due to short halogen donor/acceptor distances between F1 and O10A/B. This alert is most likely the result of not assigning the hydrogen atoms in those water molecules.

Justification. The lack of twinning and missed symmetry, in addition to the relative occupancies of the two disordered components (85:15), all contributed to the decision to describe the structure using whole-molecule disorder. If the structure was a simple case of belonging to a lower symmetry space group, the relative occupancies would be expected to be closer to 50:50 or 75:25, etc. Due to the significant disorder, a detailed analysis of the interatomic distances and angles was not carried out. A few gross structural trends pertaining to the ligand conformation and metal chelation environment are discussed in the main text. Selected interatomic distances and angles are reported in Tables S4 and S5 for both the major and minor components of the structure.

6. DFT CALCULATIONS

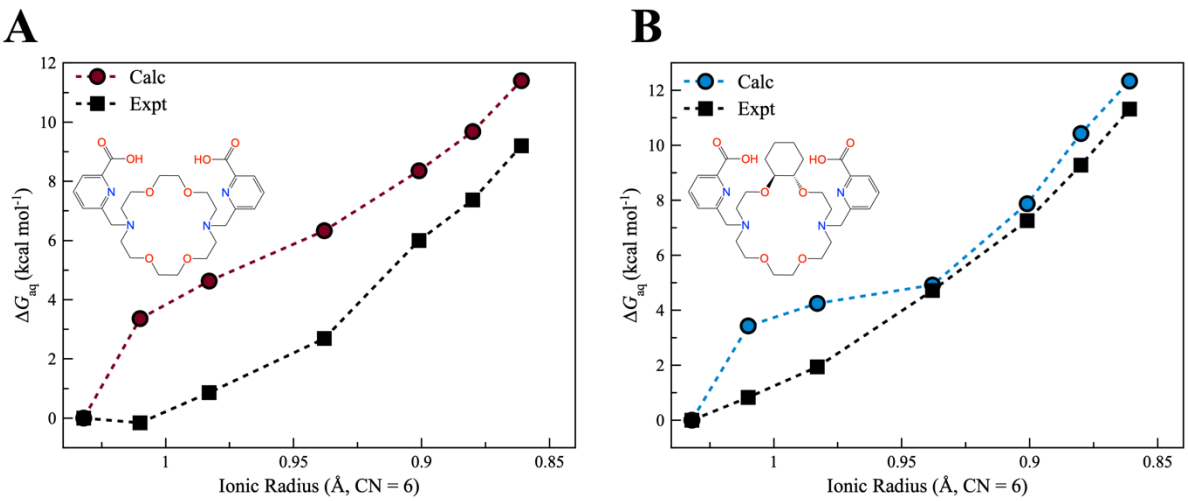

Figure S15. Calculated and experimental Gibbs free energies (kcal mol^{-1}) for the exchange reaction shown in Equation (4) for (A) macropa and (B) CHX-macropa.

Table S6. Calculated and experimental Gibbs free energies of the exchange reaction shown in Equation (4) for macropa and CHX-macropa.

		ΔG_{aq}^{calc}	ΔG_{aq}^{expt} [a]
macropa			
	La	0.0	–
	Ce	3.36	-0.16
	Nd	4.63	0.86
	Gd	6.33	2.69
	Ho	8.36	6.0
	Tm	9.68	7.37
	Lu	11.4	9.2
CHX-macropa			
	La	0.0	–
	Ce	3.43	0.74
	Nd	4.25	1.78
	Gd	4.92	4.63
	Ho	7.88	7.29
	Tm	10.43	9.31
	Lu	12.34	11.39

[a] Calculated using $\Delta G = -RT \ln K$

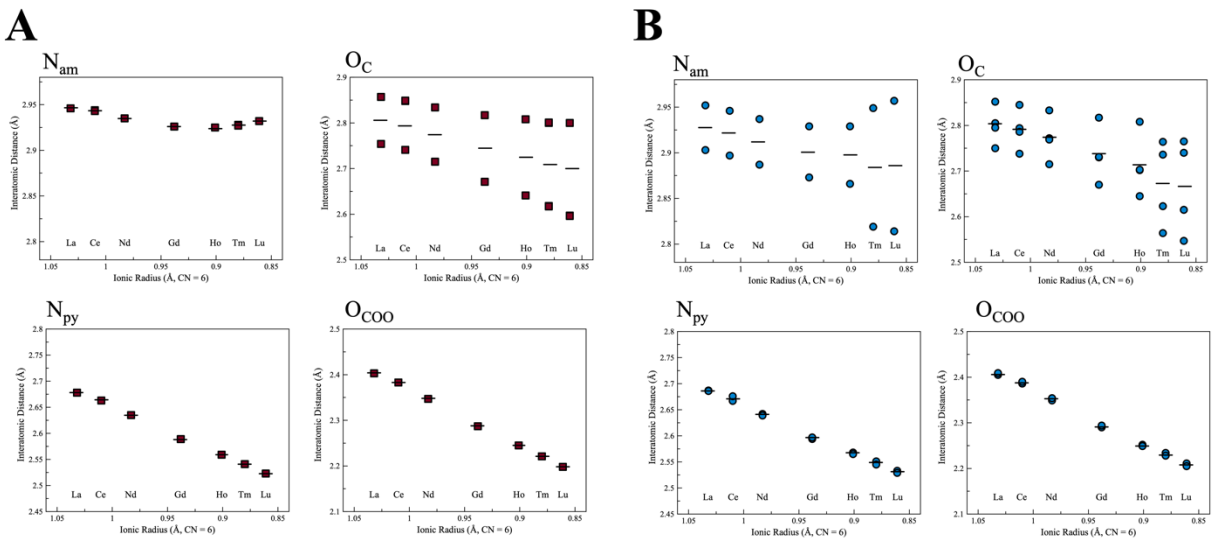

Figure S16. Variation of calculated bond distances of the metal coordination environment for (A) macropa and (B) CHX-macropa at the TPPSh/LC RECP/6-31G(d,p) level. All structures were calculated in the Δ(δλδ)(δλδ) conformation. N_{am} = amine nitrogen atoms, O_C = crown oxygen atoms, N_{py} = pyridine nitrogen atoms, O_{COO} = carboxylate oxygen atoms.

7. COMPLEX STABILITY: TRANSCHELATION CHALLENGES

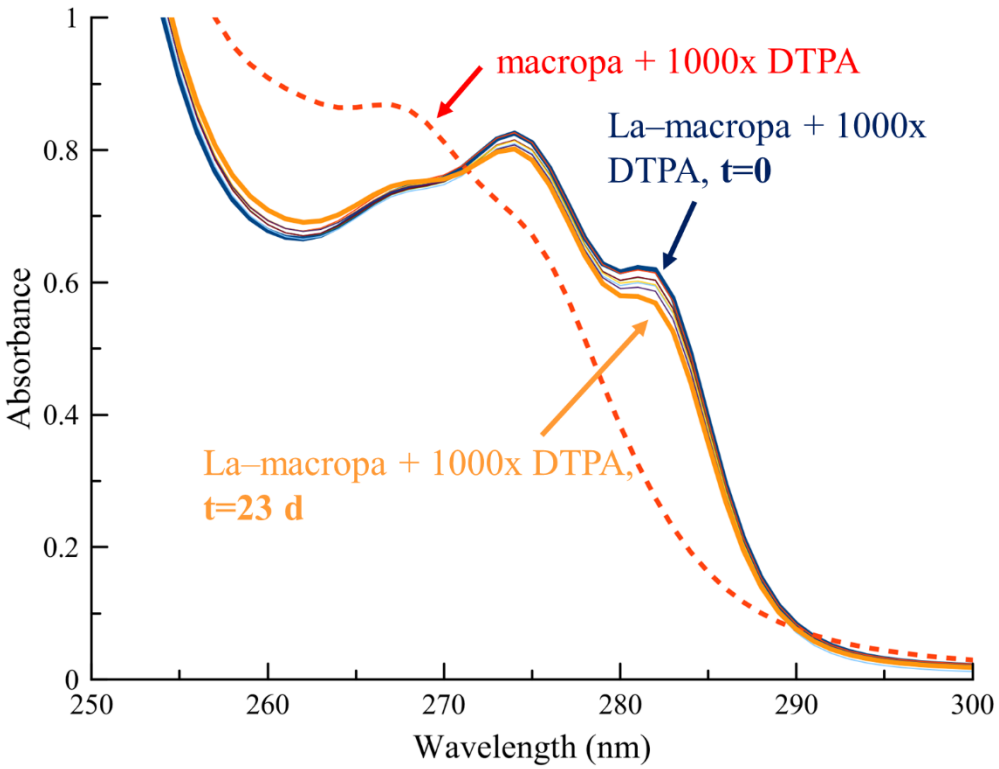

Figure S17. Stability of La–macropa in the presence of a competing ligand. Challenges were carried out in triplicate in pH 7.4 MOPS buffer by adding 1000 equiv of DTPA to a solution of La–macropa. UV-vis spectra of the samples were acquired at various time points over the course of several weeks. Shown in the representative traces above, approximately 87% of the La–macropa complex remained intact after 23 days at room temperature.

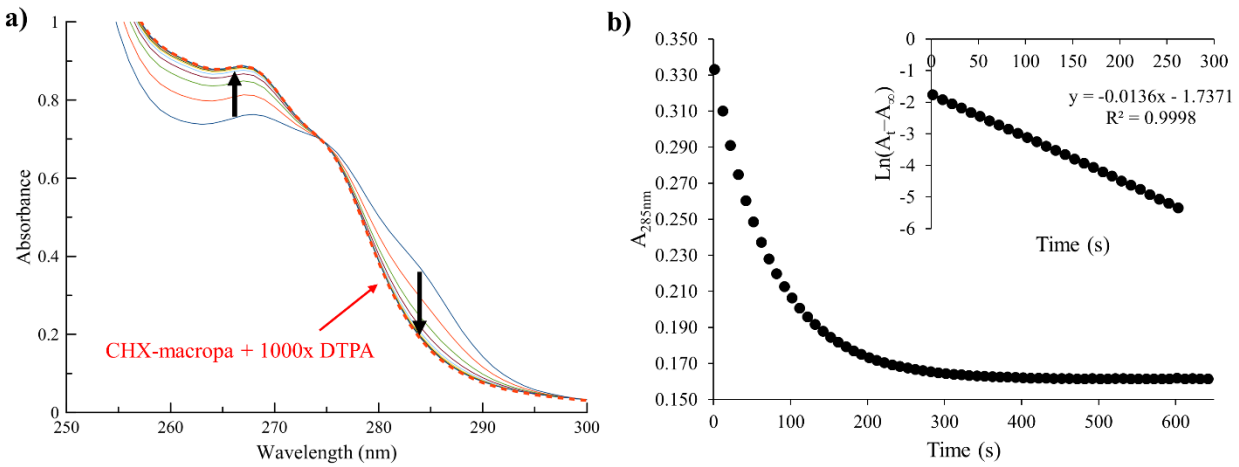

Figure S18. Stability of Gd–CHX-macropa in the presence of a competing ligand. (a) Time course of the UV spectra of Gd–CHX-macropa in pH 7.4 MOPS buffer at RT with 1000 equiv of DTPA. The final spectrum matches that of a solution of CHX-macropa with 1000 equiv of DTPA (red dotted line), confirming the lack of intact Gd–CHX-macropa complex at the end of the experiment. (b) Plot of the change in absorbance at 285 nm versus time; the inset shows the linear fit of the data to the first-order integrated rate law.

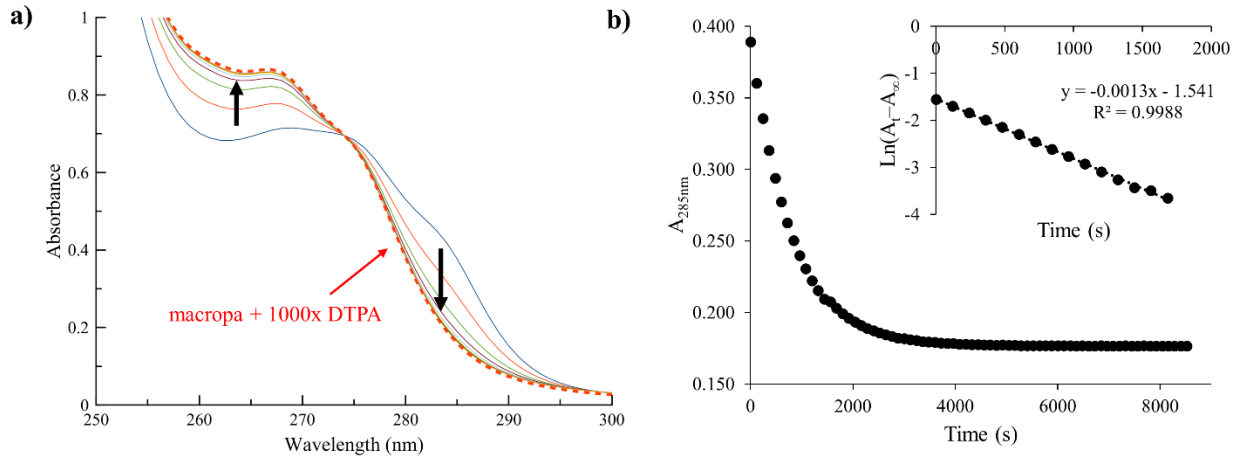

Figure S19. Stability of Gd–macropa in the presence of a competing ligand. (a) Time course of the UV spectra of Gd–macropa in pH 7.4 MOPS buffer at RT with 1000 equiv of DTPA. The final spectrum matches that of a solution of macropa with 1000 equiv of DTPA (red dotted line), confirming the lack of intact Gd–macropa complex at the end of the experiment. (b) Plot of the change in absorbance at 285 nm versus time; the inset shows the linear fit of the data to the first-order integrated rate law.

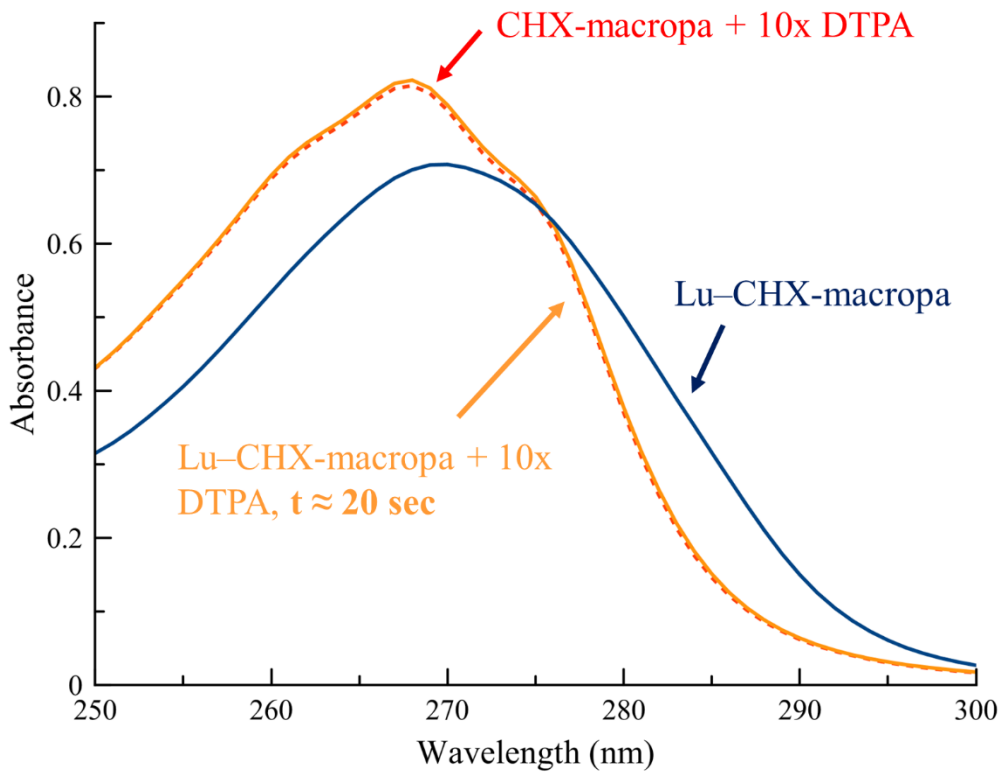

Figure S20. Stability of Lu–CHX-macropa in the presence of a competing ligand. Challenges were carried out in triplicate in pH 7.4 MOPS buffer by adding 10 equiv of DTPA to a solution of Lu–CHX-macropa. Shown in the representative UV traces above, Lu^{3+} was stripped from CHX-macropa by DTPA during the course of mixing and spectral acquisition (~20 sec).

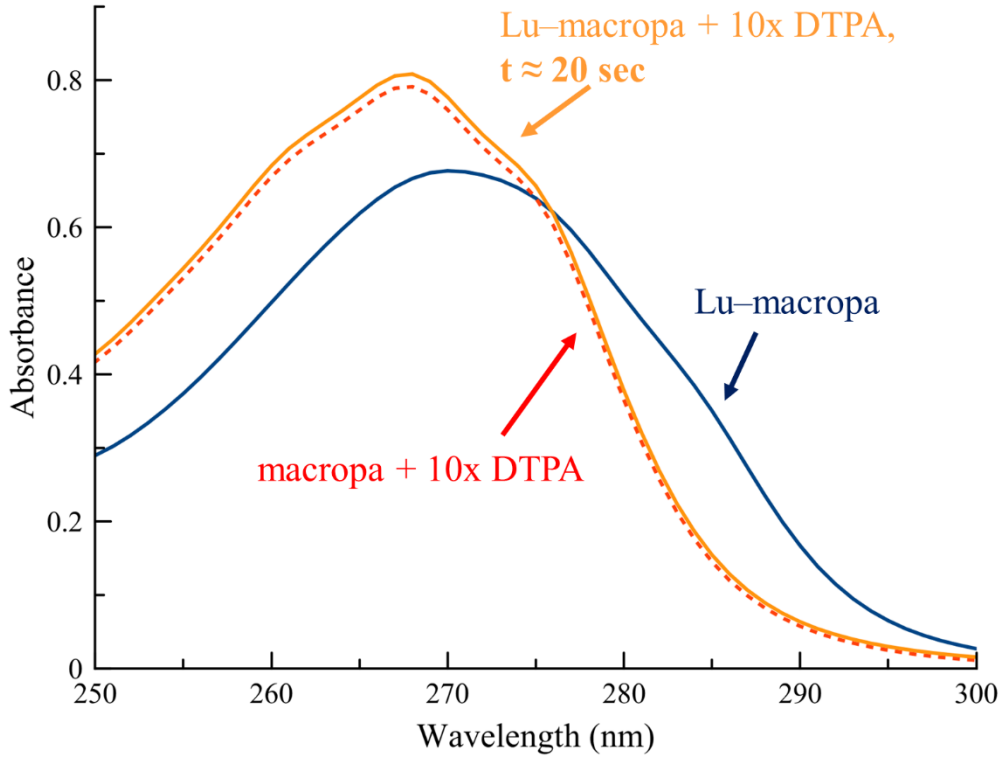

Figure S21. Stability of Lu–macropa in the presence of a competing ligand. Challenges were carried out in triplicate in pH 7.4 MOPS buffer by adding 10 equiv of DTPA to a solution of Lu–macropa. Shown in the representative UV traces above, Lu^{3+} was stripped from macropa by DTPA during the course of mixing and spectral acquisition (~20 sec).

8. OPTIMIZED COORDINATES FROM DFT CALCULATIONS

[macropa]$^{2-}$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	8	-1.23203	2.699716	3.186994
2	8	0.479952	2.535567	1.691333
3	8	-0.794995	6.537722	5.904991
4	8	-0.146078	3.310896	7.311443
5	7	-1.61575	5.352197	2.396456
6	7	-3.063711	7.410738	4.025787
7	6	-0.431826	3.139944	2.315959
8	6	-0.554158	4.648636	1.96741
9	6	0.472767	5.238219	1.205251
10	1	1.279276	4.589342	0.880731
11	6	0.406007	6.594158	0.909042
12	1	1.193343	7.082809	0.335006
13	6	-0.693942	7.327189	1.367754
14	1	-0.788505	8.392505	1.165423
15	6	-1.685659	6.663818	2.101295
16	6	-2.930623	7.404087	2.572044
17	1	-2.927798	8.426067	2.12801
18	1	-3.79296	6.862334	2.175448
19	6	-2.020529	8.180453	4.699055
20	1	-2.304129	9.254551	4.777852
21	1	-1.107659	8.129102	4.095593
22	6	-1.668693	7.643744	6.086872
23	1	-1.151976	8.44249	6.655407
24	1	-2.564436	7.351682	6.649037
25	6	-0.949841	5.4921	6.862012
26	1	-2.005491	5.323305	7.105233
27	1	-0.410732	5.733107	7.797246
28	6	-0.330054	4.248843	6.239425
29	1	-0.970205	3.84937	5.447768
30	1	0.647958	4.49995	5.796992
31	6	0.013145	1.96556	6.907842
32	1	0.213678	1.42334	7.841925
33	1	0.900004	1.843754	6.260885
34	6	-4.382737	7.776932	4.540703
35	1	-4.551474	8.880199	4.491707
36	1	-4.420852	7.497794	5.601433
37	8	-4.328917	6.410392	7.522414
38	8	-6.041743	6.573988	9.017181
39	8	-4.766411	2.571186	4.802409
40	8	-5.414546	5.798653	3.397378
41	7	-3.945442	3.757684	8.312276
42	7	-2.497291	1.699391	6.68276
43	6	-5.129476	5.969892	8.392958
44	6	-5.007085	4.461151	8.741367
45	6	-6.033975	3.871445	9.503469
46	1	-6.840554	4.520242	9.827978
47	6	-5.967108	2.515498	9.799619
48	1	-6.7544	2.02677	10.373651
49	6	-4.86711	1.782568	9.340872
50	1	-4.772473	0.717248	9.543143
51	6	-3.875447	2.446048	8.607354
52	6	-2.630448	1.705909	8.136541
53	1	-2.633195	0.68385	8.580404
54	1	-1.768142	2.247663	8.533219
55	6	-3.54043	0.92948	6.009595
56	1	-3.256871	-0.144687	5.931387
57	1	-4.453419	0.981167	6.612841

58	6	-3.892048	1.465486	4.621433
59	1	-4.40826	0.66625	4.053156
60	1	-2.996297	1.7577	4.059371
61	6	-4.610432	3.617459	3.846244
62	1	-3.554565	3.785898	3.603771
63	1	-5.149081	3.37741	2.910508
64	6	-5.230144	4.860591	4.469226
65	1	-4.589845	5.260092	5.260749
66	1	-6.207979	4.60924	4.911889
67	6	-5.574046	7.143928	3.801074
68	1	-5.774817	7.686137	2.867035
69	1	-6.460847	7.265517	4.448145
70	6	-1.178233	1.332806	6.168087
71	1	-1.009805	0.229507	6.217259
72	1	-1.139906	1.611842	5.107333

Zero-point correction =	0.590037 (Hartree/Particle)
Thermal correction to Energy =	0.626113
Thermal correction to Enthalpy =	0.627058
Thermal correction to Gibbs Free Energy =	0.521165
Sum of electronic and zero-point Energies =	-1831.5345
Sum of electronic and thermal Energies =	-1831.4985
Sum of electronic and thermal Enthalpies =	-1831.4975
Sum of electronic and thermal Free Energies =	-1831.6034
E(SCF) in SMD solvation model =	-1832.4013

$[CHX\text{-}macropa]^{2-}$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-0.696423	-0.131317	-0.239815
2	7	-1.806169	0.476716	-0.981081
3	6	-1.499185	0.523265	-2.406803
4	1	-1.321414	-0.498146	-2.82122
5	1	-0.560706	1.079212	-2.519919
6	6	-2.555448	1.180456	-3.291858
7	8	-2.693028	2.542712	-2.910746
8	6	-3.949322	3.116322	-3.263117
9	1	-4.76959	2.400581	-3.118445
10	1	-3.948593	3.45645	-4.31542
11	6	-4.118345	4.314752	-2.340988
12	8	-5.257284	5.051836	-2.808492
13	6	-5.570859	6.195003	-2.050211
14	1	-6.490316	6.589092	-2.50024
15	1	-4.794307	6.976127	-2.161441
16	6	-5.773853	5.980014	-0.536306
17	7	-6.418255	4.72642	-0.160823
18	6	-7.634501	4.426666	-0.929132
19	6	-8.02439	2.959252	-0.864375
20	7	-7.271472	2.126185	-1.606303
21	6	-7.591458	0.821106	-1.634844
22	6	-6.757714	-0.161928	-2.503619
23	8	-5.684555	0.285901	-2.988195
24	8	-7.271987	-1.307013	-2.612862
25	6	-8.686149	0.3092	-0.911108
26	1	-8.88317	-0.752866	-1.009906
27	6	-9.453305	1.168142	-0.134218

28	1	-10.299832	0.798035	0.44313
29	6	-9.122007	2.528088	-0.111256
30	1	-9.700557	3.242008	0.472029
31	1	-8.491088	5.057158	-0.605572
32	1	-7.415249	4.640485	-1.975978
33	6	-6.664465	4.677544	1.279721
34	1	-7.227042	5.58138	1.607503
35	1	-7.295126	3.807767	1.487212
36	6	-5.418228	4.533719	2.160801
37	8	-5.10854	3.163104	2.29481
38	1	-5.643362	4.988606	3.14244
39	1	-4.559441	5.084614	1.746191
40	1	-6.329765	6.872711	-0.162956
41	1	-4.796597	6.003577	-0.042857
42	1	-4.278636	3.96606	-1.316203
43	1	-3.216616	4.948876	-2.377592
44	1	-2.196558	1.108383	-4.337551
45	1	-3.522046	0.662855	-3.242362
46	6	-3.11275	-0.12426	-0.697303
47	6	-3.517897	-0.062632	0.774654
48	8	-3.386503	1.264052	1.241477
49	1	-2.910938	-0.754776	1.381848
50	1	-4.564623	-0.405043	0.850446
51	1	-3.172012	-1.189952	-1.008784
52	1	-3.869825	0.408481	-1.276598
53	6	0.465977	0.817417	0.016848
54	7	0.392536	1.53355	1.154987
55	6	1.388468	2.38411	1.460161
56	6	1.324379	3.201489	2.784094
57	8	0.323624	3.000751	3.51989
58	8	2.309396	3.971435	2.958065
59	6	2.505879	2.54453	0.620344
60	1	3.262099	3.252834	0.942132
61	6	2.594018	1.792429	-0.545947
62	1	3.454243	1.885231	-1.208763
63	6	1.558853	0.903485	-0.855193
64	1	1.596316	0.283349	-1.74829
65	1	-0.324041	-1.047934	-0.750453
66	1	-1.061918	-0.424861	0.744667
67	6	-3.825901	2.898519	2.889238
68	6	-3.532251	1.41624	2.651277
69	6	-2.264276	0.972814	3.401791
70	6	-2.329821	1.29542	4.900307
71	6	-2.537208	2.801921	5.093268
72	6	-3.825699	3.248765	4.387061

Zero-point correction =	0.682300 (Hartree/Particle)
Thermal correction to Energy =	0.722132
Thermal correction to Enthalpy =	0.723076
Thermal correction to Gibbs Free Energy =	0.60656
Sum of electronic and zero-point Energies =	-1987.5182
Sum of electronic and thermal Energies =	-1987.4784
Sum of electronic and thermal Enthalpies =	-1987.4774
Sum of electronic and thermal Free Energies =	-1987.594
E(SCF) in SMD solvation model =	-1988.484

[La(macropa)]$^{+}$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.625179	-0.94578	-0.706342
2	7	2.896656	-0.623162	0.542306
3	8	1.705915	-2.083882	-1.580218
4	6	3.119761	-2.219402	-1.36051
5	6	3.292094	-1.573152	1.610865
6	6	2.235058	-1.726431	2.681354
7	8	1.049192	-2.280538	2.064905
8	6	0.082604	-2.5837	3.080871
9	6	-1.163977	-3.120279	2.424714
10	8	-1.701949	-2.085358	1.581998
11	8	-1.045019	-2.284712	-2.062823
12	6	-0.077834	-2.58704	-3.078488
13	6	1.169788	-3.12064	-2.421858
14	7	-2.895481	-0.629008	-0.541985
15	6	-3.289196	-1.580825	-1.609535
16	6	-2.231888	-1.733406	-2.679856
17	6	-3.115521	-2.223795	1.362352
18	6	-3.623376	-0.951773	0.706983
19	6	3.220063	0.764885	0.969112
20	6	-3.221409	0.758051	-0.970073
21	6	-2.704424	1.780705	0.015575
22	6	2.701142	1.785747	-0.017363
23	6	-1.064544	2.298436	1.586122
24	6	-1.639956	3.538691	1.858222
25	6	-2.801543	3.892214	1.170107
26	6	-3.352476	2.997164	0.24965
27	6	3.346899	3.003246	-0.252403
28	6	2.794224	3.896559	-1.173505
29	6	1.633246	3.540342	-1.86127
30	6	1.060185	2.299214	-1.588189
31	57	0.000572	-0.606964	0.000165
32	1	4.307526	0.8884	1.095823
33	1	2.735065	0.939217	1.935677
34	1	-4.309088	0.879467	-1.096976
35	1	-2.736663	0.932418	-1.936756
36	1	-1.173281	4.179099	2.597682
37	1	-3.285144	4.845818	1.357811
38	1	-4.268437	3.236572	-0.280601
39	1	4.262434	3.244799	0.277611
40	1	3.276015	4.85093	-1.361967
41	1	1.165329	4.17933	-2.601174
42	7	1.571806	1.455939	-0.669795
43	7	-1.5745	1.453505	0.668319
44	6	0.169958	1.799247	2.314879
45	8	0.45954	0.551506	2.055397
46	8	0.793381	2.555433	3.055602
47	6	-0.173485	1.797115	-2.316354
48	8	-0.460484	0.548958	-2.055988
49	8	-0.798148	2.551342	-3.058026
50	1	4.708714	-1.044517	-0.527765
51	1	3.624284	-2.346793	-2.326778
52	1	3.311773	-3.116856	-0.758436
53	1	-4.706719	-1.052787	0.528515
54	1	-3.474336	-0.125063	1.4048
55	1	-3.619846	-2.351253	2.328714
56	1	-3.305789	-3.122174	0.761097
57	1	-1.967812	-0.779064	-3.145942

58	1	-2.591819	-2.436193	-3.442835
59	1	-3.456174	-2.561381	-1.157384
60	1	-4.237245	-1.273004	-2.077509
61	1	2.59623	-2.427731	3.445112
62	1	1.969272	-0.772038	3.146368
63	1	4.239584	-1.2631	2.078492
64	1	3.460837	-2.553895	1.159784
65	1	0.963299	-4.017359	-1.823346
66	1	1.899188	-3.37563	-3.200102
67	1	0.153215	-1.674523	-3.641733
68	1	-0.484774	-3.344519	-3.762255
69	1	3.474523	-0.120052	-1.404974
70	1	-1.892955	-3.37583	3.20317
71	1	-0.955788	-4.017218	1.82712
72	1	0.490971	-3.339756	3.76536
73	1	-0.150173	-1.671092	3.643256

Zero-point correction =	0.600781 (Hartree/particle)
Thermal correction to Energy =	0.636349
Thermal correction to Enthalpy =	0.637293
Thermal correction to Gibbs Free Energy =	0.535744
Sum of electronic and zero-point Energies =	-1863.240111
Sum of electronic and thermal Energies =	-1863.204543
Sum of electronic and thermal Enthalpies =	-1863.203599
Sum of electronic and thermal Free Energies =	-1863.305148
E(SCF) in SMD solvation model =	-1863.943541

$[Ce(macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.566801	-0.901548	-0.921199
2	7	2.920827	-0.580483	0.372137
3	8	1.600634	-2.059138	-1.653783
4	6	3.027467	-2.1814	-1.533133
5	6	3.386299	-1.527821	1.414387
6	6	2.386289	-1.700848	2.534959
7	8	1.175337	-2.257113	1.971105
8	6	0.274453	-2.605033	3.031028
9	6	-1.005222	-3.125418	2.428867
10	8	-1.592852	-2.064504	1.654366
11	8	-1.167039	-2.262722	-1.970476
12	6	-0.264641	-2.607764	-3.030065
13	6	1.016967	-3.122864	-2.427445
14	7	-2.918613	-0.591895	-0.372428
15	6	-3.380667	-1.541037	-1.414561
16	6	-2.379825	-1.710965	-2.534837
17	6	-3.019135	-2.192654	1.533248
18	6	-3.563476	-0.915133	0.920929
19	6	3.265018	0.808049	0.77775
20	6	-3.267603	0.795331	-0.778299
21	6	-2.684988	1.815841	0.171845
22	6	2.678319	1.826262	-0.172339
23	6	-0.953335	2.323083	1.643214
24	6	-1.504307	3.56609	1.949914
25	6	-2.701902	3.92753	1.330696
26	6	-3.310999	3.036223	0.443943
27	6	3.299493	3.049034	-0.444827

28	6	2.686632	3.937769	-1.33159
29	6	1.490294	3.5715	-1.950439
30	6	0.944309	2.326395	-1.643372
31	58	0.001474	-0.568827	0.000307
32	1	4.357915	0.936713	0.832515
33	1	2.844977	0.979471	1.774637
34	1	-4.360936	0.920058	-0.833455
35	1	-2.847878	0.96809	-1.775088
36	1	-0.992202	4.20256	2.662219
37	1	-3.16802	4.883764	1.547015
38	1	-4.255446	3.280839	-0.031068
39	1	4.243122	3.297418	0.02985
40	1	3.14895	4.895768	-1.548255
41	1	0.975571	4.205821	-2.662775
42	7	1.51469	1.487812	-0.755784
43	7	-1.520181	1.482031	0.755672
44	6	0.316655	1.812697	2.29731
45	8	0.580123	0.564	2.01557
46	8	0.988778	2.559361	3.004291
47	6	-0.323666	1.810655	-2.297163
48	8	-0.581674	0.560808	-2.015415
49	8	-0.999079	2.554425	-3.004058
50	1	4.660667	-0.992195	-0.816521
51	1	3.463897	-2.309807	-2.531861
52	1	3.268387	-3.074014	-0.941785
53	1	-4.656971	-1.010107	0.816189
54	1	-3.362916	-0.092308	1.610696
55	1	-3.455382	-2.322661	2.531847
56	1	-3.256174	-3.086353	0.941968
57	1	-2.133776	-0.763089	-3.022995
58	1	-2.780922	-2.419911	-3.271127
59	1	-3.538921	-2.517976	-0.951846
60	1	-4.346475	-1.220711	-1.835162
61	1	2.790052	-2.408105	3.271415
62	1	2.137025	-0.753663	3.022834
63	1	4.351123	-1.204134	1.834688
64	1	3.547702	-2.504342	0.95188
65	1	0.843228	-3.997071	-1.78676
66	1	1.700821	-3.408327	-3.235816
67	1	-0.063403	-1.718838	-3.640522
68	1	-0.714515	-3.387499	-3.659815
69	1	3.362942	-0.079676	-1.611144
70	1	-1.687987	-3.412756	3.2375
71	1	-0.828247	-3.999509	1.788907
72	1	0.72741	-3.382687	3.66114
73	1	0.069903	-1.716555	3.641036

Zero-point correction =	0.600809 (Hartree/particle)
Thermal correction to Energy =	0.636422
Thermal correction to Enthalpy =	0.637367
Thermal correction to Gibbs Free Energy =	0.535578
Sum of electronic and zero-point Energies =	-1863.889429
Sum of electronic and thermal Energies =	-1863.853816
Sum of electronic and thermal Enthalpies =	-1863.852872
Sum of electronic and thermal Free Energies =	-1863.95466
E(SCF) in SMD solvation model =	-1864.597076

[Nd(macropa)]$^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	0.864407	-3.524978	1.009768
2	7	0.558314	-2.919465	-0.305668
3	8	2.057416	-1.546649	1.650695
4	6	2.149766	-2.980206	1.60397
5	6	1.511765	-3.419704	-1.325038
6	6	1.715113	-2.439658	-2.457429
7	8	2.265792	-1.223431	-1.899862
8	6	2.655218	-0.3498	-2.967121
9	6	3.151115	0.943173	-2.374632
10	8	2.060727	1.542212	-1.650689
11	8	2.268578	1.218644	1.899826
12	6	2.656233	0.344103	2.966981
13	6	3.149252	-0.949911	2.374357
14	7	0.564635	2.918322	0.305795
15	6	1.51903	3.416511	1.325283
16	6	1.720327	2.4359	2.457539
17	6	2.156325	2.975556	-1.603739
18	6	0.872146	3.52317	-1.009616
19	6	-0.827693	-3.266945	-0.713549
20	6	-0.820664	3.268646	0.713581
21	6	-1.840583	2.645263	-0.21002
22	6	-1.846357	-2.641326	0.209932
23	6	-2.321758	0.876866	-1.64475
24	6	-3.574151	1.39978	-1.960267
25	6	-3.955882	2.602091	-1.362134
26	6	-3.072696	3.244268	-0.490911
27	6	-3.079765	-3.237649	0.490854
28	6	-3.961578	-2.59347	1.361997
29	6	-3.577253	-1.391936	1.96004
30	6	-2.323728	-0.871768	1.644512
31	60	0.555342	-0.000705	-0.000039
32	1	-0.965008	-4.360058	-0.732433
33	1	-0.988143	-2.88067	-1.725735
34	1	-0.955705	4.362041	0.732543
35	1	-0.981973	2.882634	1.725732
36	1	-4.20198	0.864843	-2.663433
37	1	-4.920565	3.047225	-1.585015
38	1	-3.331168	4.194573	-0.035384
39	1	-3.340261	-4.187447	0.035425
40	1	-4.927218	-3.036506	1.584912
41	1	-4.203933	-0.855613	2.663176
42	7	-1.492923	-1.470028	0.768026
43	7	-1.48965	1.473259	-0.76822
44	6	-1.782752	-0.390385	-2.277156
45	8	-0.528702	-0.618672	-1.987707
46	8	-2.509654	-1.093189	-2.974936
47	6	-1.781898	0.394266	2.276937
48	8	-0.527282	0.619638	1.987646
49	8	-2.507265	1.098754	2.974617
50	1	0.941612	-4.623009	0.944954
51	1	2.263287	-3.367209	2.624579
52	1	3.041033	-3.268289	1.032265
53	1	0.951767	4.62103	-0.944806
54	1	0.050131	3.285997	-1.688773
55	1	2.270828	3.362444	-2.624282
56	1	3.048186	3.26152	-1.031899

57	1	0.784709	2.190905	2.968954
58	1	2.441938	2.853123	3.172276
59	1	2.486761	3.58416	0.84726
60	1	1.18742	4.383332	1.734377
61	1	2.435927	-2.85844	-3.172057
62	1	0.780027	-2.19285	-2.968946
63	1	1.178234	-4.385911	-1.734028
64	1	2.479131	-3.589225	-0.846934
65	1	3.999723	-0.792015	1.698899
66	1	3.462557	-1.617412	3.185778
67	1	1.791623	0.154702	3.615083
68	1	3.457605	0.810757	3.556119
69	1	0.042856	-3.286004	1.688854
70	1	3.465595	1.610011	-3.186143
71	1	4.001446	0.783498	-1.699416
72	1	3.455514	-0.818222	-3.556317
73	1	1.790945	-0.158587	-3.615142

Zero-point correction =	0.601092 (Hartree/particle)
Thermal correction to Energy =	0.63661
Thermal correction to Enthalpy =	0.637554
Thermal correction to Gibbs Free Energy =	0.536286
Sum of electronic and zero-point Energies =	-1865.142549
Sum of electronic and thermal Energies =	-1865.107031
Sum of electronic and thermal Enthalpies =	-1865.106087
Sum of electronic and thermal Free Energies =	-1865.207355
E(SCF) in SMD solvation model =	-1865.849657

$[Gd(macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	0.81777	3.463319	-1.123821
2	7	0.527664	2.917321	0.219202
3	8	2.045317	1.465169	-1.637213
4	6	2.106705	2.90093	-1.691187
5	6	1.487897	3.462841	1.206945
6	6	1.735163	2.507314	2.350619
7	8	2.274324	1.28439	1.797605
8	6	2.719142	0.445277	2.869099
9	6	3.171679	-0.867429	2.288916
10	8	2.037837	-1.472785	1.639105
11	8	2.271162	-1.292591	-1.796004
12	6	2.721235	-0.455151	-2.866639
13	6	3.17785	0.855746	-2.285539
14	7	0.517037	-2.919158	-0.219754
15	6	1.475594	-3.468267	-1.207187
16	6	1.72781	-2.513188	-2.350159
17	6	2.094923	-2.908763	1.691617
18	6	0.804491	-3.466642	1.12324
19	6	-0.854668	3.269895	0.627841
20	6	-0.866485	-3.266371	-0.629033
21	6	-1.880325	-2.585917	0.258797
22	6	-1.870754	2.592916	-0.260071
23	6	-2.314049	-0.772993	1.650199
24	6	-3.57793	-1.255232	1.981551
25	6	-3.993906	-2.458869	1.40888
26	6	-3.128192	-3.144633	0.553823

27	6	-3.116607	3.156001	-0.555319
28	6	-3.984592	2.47323	-1.410473
29	6	-3.572761	1.268094	-1.983002
30	6	-2.310637	0.781426	-1.651399
31	64	0.527561	-0.000945	-0.000003
32	1	-1.004937	4.36118	0.597831
33	1	-1.001433	2.930635	1.658679
34	1	-1.020854	-4.357096	-0.599476
35	1	-1.011622	-2.926181	-1.6598
36	1	-4.187751	-0.690993	2.677659
37	1	-4.969721	-2.873097	1.642575
38	1	-3.409855	-4.099888	0.123132
39	1	-3.395004	4.112262	-0.124735
40	1	-4.958914	2.890857	-1.644346
41	1	-4.184465	0.705958	-2.679159
42	7	-1.494879	1.413134	-0.784207
43	7	-1.500374	-1.407501	0.783089
44	6	-1.730544	0.484541	2.25657
45	8	-0.474935	0.669451	1.942954
46	8	-2.421924	1.220294	2.956503
47	6	-1.73147	-0.478277	-2.257428
48	8	-0.476646	-0.667703	-1.943346
49	8	-2.425293	-1.211686	-2.957403
50	1	0.885104	4.563984	-1.115119
51	1	2.206629	3.216654	-2.737356
52	1	2.996159	3.243892	-1.147909
53	1	0.868132	-4.56752	1.114137
54	1	-0.016588	-3.183983	1.785612
55	1	2.193533	-3.225865	2.737494
56	1	2.983525	-3.253838	1.14828
57	1	0.81323	-2.26718	-2.897438
58	1	2.468401	-2.951785	-3.032006
59	1	2.427638	-3.656989	-0.706624
60	1	1.123064	-4.431857	-1.605805
61	1	2.476721	2.943337	3.033076
62	1	0.819038	2.265163	2.897034
63	1	1.139308	4.428215	1.604727
64	1	2.441108	3.647043	0.706928
65	1	3.990408	0.722765	-1.560302
66	1	3.530963	1.503403	-3.096163
67	1	1.895748	-0.28493	-3.568953
68	1	3.553752	-0.94046	-3.394575
69	1	-0.003848	3.18314	-1.786587
70	1	3.521235	-1.516224	3.100187
71	1	3.985771	-0.737592	1.564818
72	1	3.552637	0.927327	3.398479
73	1	1.891736	0.278334	3.569937

Zero-point correction =	0.601435 (Hartree/particle)
Thermal correction to Energy =	0.636899
Thermal correction to Enthalpy =	0.637843
Thermal correction to Gibbs Free Energy =	0.536705
Sum of electronic and zero-point Energies =	-1867.542965
Sum of electronic and thermal Energies =	-1867.5075
Sum of electronic and thermal Enthalpies =	-1867.506556
Sum of electronic and thermal Free Energies =	-1867.607694
E(SCF) in SMD solvation model =	-1868.249385

$[Ho(macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-0.775236	3.431873	1.182463
2	7	-0.495216	2.920088	-0.174713
3	8	-2.020093	1.424987	1.628705
4	6	-2.065776	2.859281	1.734026
5	6	-1.456363	3.493289	-1.144896
6	6	-1.741391	2.547113	-2.287439
7	8	-2.277672	1.325759	-1.728675
8	6	-2.77011	0.507232	-2.7939
9	6	-3.187568	-0.817756	-2.217308
10	8	-2.021876	-1.424939	-1.62681
11	8	-2.276123	-1.326066	1.730286
12	6	-2.76547	-0.507561	2.796949
13	6	-3.184319	0.817576	2.22177
14	7	-0.494856	-2.919806	0.173784
15	6	-1.45614	-3.493248	1.143653
16	6	-1.739862	-2.548133	2.287381
17	6	-2.065658	-2.859083	-1.734887
18	6	-0.774681	-3.431113	-1.183637
19	6	0.886884	3.267052	-0.583207
20	6	0.887208	-3.266974	0.582304
21	6	1.896258	-2.556543	-0.286617
22	6	1.895936	2.556866	0.285912
23	6	2.301763	-0.722956	-1.658011
24	6	3.569842	-1.184648	-2.000881
25	6	4.005075	-2.387542	-1.440956
26	6	3.150951	-3.094375	-0.591593
27	6	3.15051	3.095043	0.590793
28	6	4.004888	2.388521	1.440147
29	6	3.570024	1.18552	2.000114
30	6	2.302044	0.723463	1.657369
31	67	-0.506516	-0.00014	0.000088
32	1	1.051795	4.355305	-0.52677
33	1	1.024813	2.953071	-1.623302
34	1	1.052065	-4.355215	0.52557
35	1	1.025102	-2.953243	1.622473
36	1	4.167701	-0.606671	-2.696097
37	1	4.985538	-2.786112	-1.682244
38	1	3.445421	-4.051633	-0.174121
39	1	3.444688	4.052343	0.17321
40	1	4.985252	2.78738	1.681361
41	1	4.168089	0.60769	2.695277
42	7	1.500397	1.375477	0.79193
43	7	1.500423	-1.375216	-0.792499
44	6	1.693642	0.528018	-2.25011
45	8	0.441346	0.694789	-1.912868
46	8	2.361044	1.275805	-2.960324
47	6	1.694552	-0.527786	2.249555
48	8	0.442296	-0.695164	1.912481
49	8	2.362435	-1.275343	2.959553
50	1	-0.837256	4.532698	1.206326
51	1	-2.161991	3.137089	2.791216
52	1	-2.953022	3.22852	1.204595
53	1	-0.836033	-4.531964	-1.208024
54	1	0.046601	-3.127317	-1.835967
55	1	-2.160997	-3.135066	-2.792633

56	1	-2.952697	-3.230433	-1.206599
57	1	-0.839438	-2.30238	2.857675
58	1	-2.493898	-2.995408	2.94869
59	1	-2.397548	-3.697358	0.62936
60	1	-1.091999	-4.452401	1.542171
61	1	-2.495818	2.994007	-2.948554
62	1	-0.841524	2.30042	-2.85819
63	1	-1.09144	4.451599	-1.544698
64	1	-2.397359	3.699015	-0.63047
65	1	-3.968251	0.707457	1.462156
66	1	-3.562077	1.45603	3.028277
67	1	-1.970441	-0.357144	3.538
68	1	-3.623507	-0.995791	3.279785
69	1	0.04623	3.128884	1.834954
70	1	-3.567376	-1.456488	-3.022606
71	1	-3.969542	-0.707363	-1.455739
72	1	-3.629352	0.99558	-3.274476
73	1	-1.977169	0.356578	-3.537148

Zero-point correction =	0.601552 (Hartree/particle)
Thermal correction to Energy =	0.637056
Thermal correction to Enthalpy =	0.638
Thermal correction to Gibbs Free Energy =	0.536423
Sum of electronic and zero-point Energies =	-1869.297072
Sum of electronic and thermal Energies =	-1869.261568
Sum of electronic and thermal Enthalpies =	-1869.260624
Sum of electronic and thermal Free Energies =	-1869.362201
E(SCF) in SMD solvation model =	-1870.003304

$[Tm(macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-0.752033	3.411265	1.215548
2	7	-0.474737	2.923448	-0.149915
3	8	-2.007916	1.3976	1.611442
4	6	-2.044465	2.82989	1.752597
5	6	-1.435362	3.511963	-1.110966
6	6	-1.750686	2.565617	-2.245433
7	8	-2.285568	1.348975	-1.674368
8	6	-2.814874	0.539945	-2.728636
9	6	-3.200796	-0.793225	-2.149847
10	8	-2.009182	-1.39799	-1.609641
11	8	-2.284074	-1.349938	1.675408
12	6	-2.809704	-0.541198	2.731749
13	6	-3.197649	0.79225	2.155028
14	7	-0.47369	-2.923347	0.148097
15	6	-1.434899	-3.512408	1.108203
16	6	-1.749215	-2.567596	2.244228
17	6	-2.042904	-2.829921	-1.754922
18	6	-0.750011	-3.410389	-1.217864
19	6	0.907703	3.266473	-0.556358
20	6	0.908554	-3.266492	0.555237
21	6	1.912379	-2.536689	-0.303403
22	6	1.911155	2.537371	0.303295
23	6	2.296697	-0.691027	-1.664023
24	6	3.567617	-1.138498	-2.014534
25	6	4.016814	-2.339639	-1.461878

26	6	3.171637	-3.059907	-0.614945
27	6	3.169997	3.061326	0.615323
28	6	4.01515	2.341776	1.462867
29	6	3.566349	1.140491	2.015507
30	6	2.295836	0.692248	1.6645
31	69	-0.491326	-0.000342	-0.000086
32	1	1.081988	4.352496	-0.485288
33	1	1.041354	2.966511	-1.601246
34	1	1.082995	-4.352457	0.483661
35	1	1.041497	-2.967061	1.600359
36	1	4.156562	-0.551825	-2.710065
37	1	5.000401	-2.727262	-1.708205
38	1	3.475767	-4.017461	-0.205125
39	1	3.473814	4.018915	0.20535
40	1	4.998406	2.729995	1.709578
41	1	4.155312	0.554199	2.711346
42	7	1.503716	1.355396	0.798679
43	7	1.50465	-1.354759	-0.798614
44	6	1.671649	0.554542	-2.248135
45	8	0.421858	0.70956	-1.895929
46	8	2.323363	1.309344	-2.965418
47	6	1.671591	-0.553834	2.248363
48	8	0.422044	-0.709848	1.89577
49	8	2.323526	-1.307867	2.966246
50	1	-0.812527	4.51153	1.261629
51	1	-2.14179	3.080679	2.816373
52	1	-2.928891	3.216004	1.23064
53	1	-0.809407	-4.510673	-1.264859
54	1	0.070161	-3.092112	-1.864424
55	1	-2.138599	-3.078006	-2.819478
56	1	-2.927167	-3.219111	-1.235001
57	1	-0.861984	-2.313861	2.83139
58	1	-2.512523	-3.019674	2.891495
59	1	-2.365726	-3.738873	0.584039
60	1	-1.05696	-4.46223	1.515696
61	1	-2.514283	3.017019	-2.89282
62	1	-0.863913	2.310689	-2.832755
63	1	-1.056382	4.460672	-1.52004
64	1	-2.365909	3.740392	-0.587121
65	1	-3.952537	0.695913	1.364836
66	1	-3.601359	1.425774	2.952565
67	1	-2.043105	-0.40301	3.504554
68	1	-3.687891	-1.029768	3.176708
69	1	0.068181	3.094321	1.862739
70	1	-3.607133	-1.427362	-2.945521
71	1	-3.95295	-0.696411	-1.357142
72	1	-3.694528	1.028446	-3.17077
73	1	-2.05098	0.401413	-3.504067

Zero-point correction =	0.601644 (Hartree/particle)
Thermal correction to Energy =	0.637147
Thermal correction to Enthalpy =	0.638091
Thermal correction to Gibbs Free Energy =	0.536296
Sum of electronic and zero-point Energies =	-1870.456187
Sum of electronic and thermal Energies =	-1870.420683
Sum of electronic and thermal Enthalpies =	-1870.419739
Sum of electronic and thermal Free Energies =	-1870.521535
E(SCF) in SMD solvation model =	-1871.163476

[Lu(macropa)]$^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-0.734487	3.394862	1.24557
2	7	-0.460055	2.929174	-0.127079
3	8	-1.995562	1.373015	1.598338
4	6	-2.026541	2.802854	1.771253
5	6	-1.420881	3.530987	-1.079015
6	6	-1.757182	2.587891	-2.21006
7	8	-2.289786	1.372879	-1.633817
8	6	-2.836733	0.569775	-2.68309
9	6	-3.203106	-0.769094	-2.105708
10	8	-1.996991	-1.373177	-1.596276
11	8	-2.288445	-1.373508	1.635183
12	6	-2.832229	-0.570642	2.686295
13	6	-3.200194	0.768533	2.110698
14	7	-0.459392	-2.928985	0.125849
15	6	-1.420495	-3.531255	1.077197
16	6	-1.755772	-2.589367	2.209537
17	6	-2.025865	-2.802651	-1.772496
18	6	-0.733341	-3.394012	-1.247133
19	6	0.92216	3.268464	-0.532844
20	6	0.922763	-3.268343	0.531852
21	6	1.921722	-2.52178	-0.317672
22	6	1.921073	2.522265	0.31705
23	6	2.289337	-0.665669	-1.66789
24	6	3.561909	-1.102078	-2.025851
25	6	4.022002	-2.302371	-1.480391
26	6	3.184075	-3.033527	-0.635749
27	6	3.183231	3.034486	0.635162
28	6	4.0214	2.303728	1.479899
29	6	3.561752	1.103258	2.025324
30	6	2.289364	0.666346	1.667327
31	71	-0.477851	-0.000218	-0.000036
32	1	1.105388	4.352203	-0.449056
33	1	1.050982	2.980815	-1.581857
34	1	1.10606	-4.352045	0.447789
35	1	1.051345	-2.980932	1.580956
36	1	4.143421	-0.508173	-2.72149
37	1	5.007589	-2.68158	-1.73175
38	1	3.495451	-3.991917	-0.23337
39	1	3.494261	3.992953	0.232698
40	1	5.006822	2.683334	1.731299
41	1	4.14347	0.509545	2.720955
42	7	1.504427	1.339045	0.80224
43	7	1.504722	-1.338663	-0.80277
44	6	1.650952	0.575932	-2.244332
45	8	0.403382	0.721219	-1.879924
46	8	2.289639	1.336358	-2.967248
47	6	1.651736	-0.57569	2.243667
48	8	0.404199	-0.721625	1.879418
49	8	2.290882	-1.335767	2.966537
50	1	-0.796331	4.494141	1.311357
51	1	-2.123489	3.029357	2.840435
52	1	-2.910182	3.201934	1.257977
53	1	-0.794373	-4.493293	-1.313649
54	1	0.087115	-3.065868	-1.888198
55	1	-2.121805	-3.026964	-2.842227

56	1	-2.909249	-3.204105	-1.260649
57	1	-0.877699	-2.332393	2.808907
58	1	-2.525532	-3.045725	2.846104
59	1	-2.343417	-3.772117	0.545404
60	1	-1.033186	-4.475343	1.488932
61	1	-2.527277	3.043739	-2.846583
62	1	-0.879608	2.329918	-2.809715
63	1	-1.032893	4.474209	-1.492066
64	1	-2.343472	3.773337	-0.547304
65	1	-3.936898	0.682346	1.302635
66	1	-3.619095	1.398497	2.902992
67	1	-2.081578	-0.441666	3.476198
68	1	-3.721957	-1.057787	3.109479
69	1	0.086123	3.067757	1.886989
70	1	-3.624328	-1.399598	-2.896309
71	1	-3.93736	-0.682348	-1.295507
72	1	-3.727602	1.056909	-3.103884
73	1	-2.088427	0.440394	-3.475158

Zero-point correction =	0.601747 (Hartree/particle)
Thermal correction to Energy =	0.637238
Thermal correction to Enthalpy =	0.638182
Thermal correction to Gibbs Free Energy =	0.536231
Sum of electronic and zero-point Energies =	-1871.589643
Sum of electronic and thermal Energies =	-1871.554152
Sum of electronic and thermal Enthalpies =	-1871.553207
Sum of electronic and thermal Free Energies =	-1871.655159
E(SCF) in SMD solvation model =	-1872.297659

$[La(CHX\text{-}macropa)]^+$		$(\Delta(\delta\lambda\delta)(\delta\lambda\delta))$		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.58812	-0.930931	-0.509061
2	7	2.856094	-0.452598	0.685838
3	8	1.652718	-2.06864	-1.343281
4	6	3.043134	-2.24897	-1.027787
5	6	3.210391	-1.277783	1.869385
6	6	2.043892	-1.456476	2.817255
7	8	0.986752	-2.150612	2.09354
8	6	0.128985	-2.888368	2.99624
9	6	-1.196513	-3.19033	2.303501
10	8	-1.731402	-1.927364	1.808786
11	8	-1.106936	-2.29126	-1.799231
12	6	-0.140666	-2.671443	-2.790117
13	6	1.10463	-3.162808	-2.096381
14	7	-2.894039	-0.467106	-0.41975
15	6	-3.33036	-1.498877	-1.393585
16	6	-2.288441	-1.774192	-2.455392
17	6	-3.155703	-1.933297	1.595344
18	6	-3.572748	-0.658963	0.882955
19	6	3.199657	0.967539	0.959645
20	6	-3.220836	0.877642	-0.968133
21	6	-2.678643	1.986007	-0.09739
22	6	2.697947	1.8859	-0.129737
23	6	-1.023248	2.615608	1.413189
24	6	-1.562655	3.89284	1.555344
25	6	-2.714609	4.206434	0.832034

26	6	-3.292324	3.237669	0.007511
27	6	3.36231	3.064641	-0.482948
28	6	2.825803	3.868905	-1.4912
29	6	1.662035	3.460777	-2.144779
30	6	1.070955	2.261086	-1.751522
31	57	-0.040275	-0.464998	0.1144
32	1	4.288858	1.0875	1.074203
33	1	2.719106	1.249093	1.90281
34	1	-4.310705	0.992252	-1.083061
35	1	-2.756615	0.955177	-1.95733
36	1	-4.201574	3.446817	-0.546528
37	1	1.205441	4.027816	-2.947728
38	7	1.566597	1.506884	-0.750478
39	7	-1.558322	1.696262	0.586323
40	6	0.19584	2.153604	2.188668
41	8	0.444272	0.878463	2.049865
42	8	0.845114	2.958979	2.851342
43	6	-0.166003	1.706764	-2.434211
44	8	-0.474804	0.49694	-2.051552
45	8	-0.773519	2.392315	-3.253576
46	1	4.665356	-1.046706	-0.304764
47	1	3.58619	-2.525708	-1.940518
48	1	3.149579	-3.068142	-0.305031
49	1	-4.669346	-0.681715	0.765279
50	1	-3.325014	0.194732	1.518255
51	1	-3.676032	-1.969069	2.557943
52	1	-3.436427	-2.828266	1.026372
53	1	-2.008076	-0.872479	-3.008325
54	1	-2.67074	-2.536372	-3.147408
55	1	-3.52307	-2.431649	-0.860108
56	1	-4.273256	-1.203887	-1.879307
57	1	2.367094	-2.069196	3.66426
58	1	1.645804	-0.501272	3.169266
59	1	4.057445	-0.833902	2.413006
60	1	3.52975	-2.265752	1.528301
61	1	0.890487	-4.007979	-1.428632
62	1	1.829226	-3.487026	-2.853737
63	1	0.094181	-1.802135	-3.416365
64	1	-0.551283	-3.474556	-3.417235
65	1	3.474939	-0.181489	-1.296132
66	1	-1.019545	-3.837182	1.429122
67	6	-2.118314	-3.920905	3.295523
68	6	0.795513	-4.199516	3.441429
69	1	-0.081099	-2.246747	3.86388
70	1	-3.17063	5.18772	0.919502
71	1	-1.077694	4.592578	2.226074
72	1	3.321619	4.792762	-1.772539
73	1	4.279388	3.344827	0.024988
74	6	-0.10278	-4.973597	4.416379
75	1	1.763364	-3.988128	3.906578
76	1	0.994897	-4.805889	2.548078
77	6	-1.47403	-5.229897	3.783932
78	1	-0.224395	-4.395586	5.341668
79	1	0.376055	-5.917874	4.693434
80	1	-3.078744	-4.151311	2.826498
81	1	-2.318064	-3.260973	4.149811
82	1	-2.14667	-5.715352	4.49779
83	1	-1.364049	-5.91792	2.935084

Zero-point correction = 0.694220 (Hartree/particle)
Thermal correction to Energy = 0.733138

Thermal correction to Enthalpy =	0.734082
Thermal correction to Gibbs Free Energy =	0.625695
Sum of electronic and zero-point Energies =	-2019.222824
Sum of electronic and thermal Energies =	-2019.183906
Sum of electronic and thermal Enthalpies =	-2019.182961
Sum of electronic and thermal Free Energies =	-2019.291349
E(SCF) in SMD solvation model =	-2020.019989

$[La(CHX\text{-}macropa)]^+$		(Δ(λδλ)(λδλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.708494	0.805986	-0.0937
2	7	2.664553	0.402171	-1.079258
3	8	2.01525	1.888916	1.206546
4	6	3.150725	0.997446	1.311057
5	6	2.609415	1.336136	-2.230872
6	6	2.008901	2.68501	-1.863492
7	8	0.639165	2.499616	-1.443862
8	6	-0.36795	3.226633	-2.166892
9	6	-1.583034	2.336314	-2.324686
10	8	-1.97652	1.904566	-1.005831
11	8	-0.489695	2.183958	2.132057
12	6	0.398026	3.328699	2.237363
13	6	1.808895	2.75097	2.35449
14	7	-2.641513	0.344648	1.281779
15	6	-2.507799	0.986687	2.614465
16	6	-1.851226	2.355964	2.567543
17	6	-3.25251	1.231734	-0.999071
18	6	-3.664064	1.041934	0.454048
19	6	2.907033	-0.972495	-1.589413
20	6	-2.992645	-1.086804	1.487525
21	6	-2.77057	-1.91311	0.242851
22	6	2.630321	-2.016878	-0.533344
23	6	-1.459426	-2.217306	-1.659534
24	6	-2.160783	-3.365177	-2.025252
25	6	-3.222216	-3.775063	-1.216371
26	6	-3.543978	-3.033614	-0.076629
27	6	3.324256	-3.229126	-0.464711
28	6	2.954447	-4.16781	0.502301
29	6	1.922584	-3.865436	1.392297
30	6	1.302011	-2.6219	1.284206
31	57	0.005989	0.398199	0.125205
32	1	4.167523	1.745718	-0.418918
33	1	4.507103	0.054811	-0.054977
34	1	3.919138	1.437256	1.954465
35	1	2.818762	0.05348	1.756585
36	1	1.972617	0.869811	-2.986074
37	1	3.611488	1.498388	-2.661968
38	1	2.037944	3.343007	-2.738318
39	1	2.545895	3.172525	-1.044226
40	1	0.001726	3.50032	-3.161209
41	1	-0.619265	4.141344	-1.61621
42	1	-1.34326	1.457571	-2.933544
43	1	-2.400177	2.907593	-2.783793
44	6	0.115066	4.255128	3.429085
45	1	0.320031	3.904806	1.30264
46	6	2.851928	3.873538	2.402718
47	1	1.853407	2.134423	3.263152

48	1	-1.875308	0.330764	3.217537
49	1	-3.488095	1.089167	3.107734
50	1	-2.36849	3.059151	1.90107
51	1	-1.869876	2.764505	3.581492
52	1	-3.166582	0.284123	-1.539437
53	1	-3.993995	1.86408	-1.504786
54	1	-3.842802	2.032483	0.880869
55	1	-4.621656	0.5035	0.482426
56	1	3.936148	-1.080002	-1.965463
57	1	2.217751	-1.140502	-2.424907
58	1	-4.034013	-1.188943	1.82953
59	1	-2.334378	-1.476482	2.27273
60	1	-1.869462	-3.890562	-2.927406
61	1	-3.803918	-4.654486	-1.47498
62	1	-4.375381	-3.320702	0.558926
63	1	4.131105	-3.433784	-1.16096
64	1	3.474534	-5.118784	0.564045
65	1	1.591961	-4.548122	2.166458
66	7	1.638112	-1.730681	0.329488
67	7	-1.74566	-1.527167	-0.537366
68	6	-0.339468	-1.639652	-2.508602
69	8	0.007392	-0.428897	-2.163519
70	8	0.149631	-2.31452	-3.412774
71	6	0.204142	-2.176133	2.236072
72	8	-0.072706	-0.903079	2.155739
73	8	-0.337888	-3.002629	2.967353
74	1	2.805862	4.433146	1.459275
75	1	3.859196	3.451121	2.478468
76	6	2.583422	4.817855	3.584579
77	6	1.160581	5.381308	3.503547
78	1	0.13418	3.66846	4.356937
79	1	-0.882709	4.694951	3.336162
80	1	3.318573	5.628435	3.584731
81	1	2.711926	4.272231	4.528492
82	1	0.945224	6.013307	4.370529
83	1	1.069768	6.021132	2.615571

Zero-point correction =	0.693494 (Hartree/Particle)
Thermal correction to Energy =	0.732626
Thermal correction to Enthalpy =	0.73357
Thermal correction to Gibbs Free Energy =	0.624687
Sum of electronic and zero-point Energies =	-2019.220335
Sum of electronic and thermal Energies =	-2019.181203
Sum of electronic and thermal Enthalpies =	-2019.180259
Sum of electronic and thermal Free Energies =	-2019.289142
E(SCF) in SMD solvation model =	-2020.013167

$[La(CHX\text{-}macropa)]^+$		(Δ(λλλ)(λλλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-3.751525	1.302856	0.367123
2	7	-2.666955	0.714832	1.194582
3	8	-2.206438	1.593172	-1.440276
4	6	-3.538604	1.141141	-1.129725
5	6	-2.461468	1.55346	2.404415
6	6	-1.699091	2.834438	2.063524
7	8	-0.302098	2.596117	1.789522

8	6	0.521593	2.26544	2.95349
9	6	1.979534	2.33816	2.502606
10	8	2.099767	1.589093	1.261488
11	8	0.215081	2.479181	-2.162237
12	6	-0.701388	2.127306	-3.2202
13	6	-2.103399	2.306408	-2.685698
14	7	2.525537	0.717733	-1.443033
15	6	2.328637	1.379765	-2.761033
16	6	1.558706	2.689091	-2.636855
17	6	3.449682	1.318348	0.839796
18	6	3.547053	1.465205	-0.671358
19	6	-2.986578	-0.683245	1.582317
20	6	2.941784	-0.689873	-1.6896
21	6	2.829882	-1.566195	-0.464657
22	6	-2.820144	-1.650523	0.431375
23	6	1.626319	-2.065376	1.463664
24	6	2.463383	-3.137945	1.771654
25	6	3.525712	-3.418051	0.912007
26	6	3.723329	-2.612585	-0.212491
27	6	-3.63622	-2.775575	0.278002
28	6	-3.386079	-3.659195	-0.775686
29	6	-2.347429	-3.383186	-1.664914
30	6	-1.590398	-2.229087	-1.460566
31	57	-0.034884	0.578917	-0.097276
32	1	-3.799107	2.374539	0.576831
33	1	-4.728146	0.878334	0.644878
34	1	-4.270991	1.764392	-1.655507
35	1	-3.650125	0.107657	-1.468416
36	1	3.743142	0.324373	1.188725
37	1	4.132207	2.053926	1.278811
38	1	3.42883	2.526688	-0.899776
39	1	4.562817	1.178719	-0.988753
40	1	-4.006075	-0.756898	1.991007
41	1	-2.271905	-0.969071	2.360328
42	1	3.967476	-0.727231	-2.087883
43	1	2.257825	-1.089531	-2.445734
44	1	2.26473	-3.707022	2.672501
45	1	4.202641	-4.241078	1.119286
46	1	4.554171	-2.790849	-0.887552
47	1	-4.448921	-2.955174	0.974513
48	1	-4.003918	-4.542469	-0.904872
49	1	-2.107624	-4.016926	-2.510863
50	7	-1.811605	-1.395708	-0.424725
51	7	1.793686	-1.314451	0.356918
52	6	0.49805	-1.654068	2.394843
53	8	-0.124989	-0.566783	2.026642
54	8	0.267277	-2.325629	3.396953
55	6	-0.480616	-1.8302	-2.420738
56	8	0.038058	-0.656131	-2.174974
57	8	-0.161995	-2.595899	-3.326303
58	6	2.867229	1.808578	3.638959
59	1	2.243521	3.382532	2.276373
60	1	-0.53116	1.087934	-3.519056
61	1	-0.550929	2.800551	-4.073528
62	1	-2.333521	3.363751	-2.507214
63	1	-2.811937	1.900351	-3.416472
64	1	2.012736	3.378629	-1.921092
65	1	1.52702	3.19378	-3.610027
66	1	3.29447	1.572555	-3.256532
67	1	1.758136	0.686722	-3.38391
68	1	-1.803913	3.56933	2.865612
69	1	-2.078074	3.294758	1.147104

70	1	-3.422336	1.812549	2.877555
71	1	-1.88436	0.961795	3.119458
72	1	0.298213	1.226781	3.225421
73	6	0.316286	3.188374	4.161237
74	1	0.527388	4.226945	3.874206
75	6	1.230289	2.750763	5.321052
76	1	-0.721311	3.146499	4.505815
77	6	2.698478	2.68914	4.888294
78	1	0.911978	1.761374	5.673595
79	1	1.104851	3.441638	6.160595
80	1	3.918947	1.802853	3.338297
81	1	2.584123	0.772181	3.861464
82	1	3.319989	2.296774	5.699059
83	1	3.06353	3.701664	4.669974

Zero-point correction =	0.694604 (Hartree/Particle)
Thermal correction to Energy =	0.73347
Thermal correction to Enthalpy =	0.734414
Thermal correction to Gibbs Free Energy =	0.625881
Sum of electronic and zero-point Energies =	-2019.214789
Sum of electronic and thermal Energies =	-2019.175924
Sum of electronic and thermal Enthalpies =	-2019.17498
Sum of electronic and thermal Free Energies =	-2019.283513
E(SCF) in SMD solvation model =	-2020.010223

$[La(CHX\text{-}macropa)]^+$		(Δ(δλλ)(δλλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-3.632231	-1.051693	-0.013703
2	7	-2.701373	-0.519224	-1.041005
3	8	-1.857353	-1.785406	1.453699
4	6	-3.092841	-2.192116	0.840994
5	6	-2.776249	-1.242846	-2.334344
6	6	-2.147458	-2.628002	-2.303609
7	8	-0.754405	-2.579036	-1.925382
8	6	0.13205	-2.469625	-3.059769
9	6	1.519825	-2.844522	-2.599128
10	8	1.923124	-1.921698	-1.574516
11	8	0.710051	-2.596907	1.615154
12	6	-0.001865	-2.402852	2.881384
13	6	-1.475999	-2.646433	2.564273
14	7	2.788551	-0.550681	0.735126
15	6	2.913907	-1.491968	1.873183
16	6	2.135794	-2.794795	1.680019
17	6	3.316707	-2.037581	-1.255338
18	6	3.715231	-0.857531	-0.382215
19	6	-3.052682	0.904656	-1.312367
20	6	3.089209	0.836007	1.195063
21	6	2.671106	1.850163	0.151858
22	6	-2.706967	1.797702	-0.144721
23	6	1.196871	2.333135	-1.587755
24	6	1.78104	3.580085	-1.808008
25	6	2.860015	3.953982	-1.005513
26	6	3.324408	3.073657	-0.024333
27	6	-3.449997	2.938893	0.173565
28	6	-3.044281	3.7343	1.247509
29	6	-1.928431	3.354916	1.994155

30	6	-1.252569	2.191116	1.629021
31	57	0.016816	-0.563173	-0.095685
32	1	-4.121552	1.004173	-1.556695
33	1	-2.47264	1.226288	-2.183968
34	1	4.159756	0.953602	1.424096
35	1	2.513328	1.012187	2.1083
36	1	1.386004	4.209784	-2.596747
37	1	3.348586	4.912524	-1.150707
38	1	4.177994	3.328976	0.595269
39	1	-4.32631	3.197054	-0.412209
40	1	-3.6028	4.628924	1.504902
41	1	-1.569795	3.916594	2.848922
42	7	-1.62279	1.444374	0.569564
43	7	1.61946	1.504979	-0.61306
44	6	0.049371	1.814397	-2.439284
45	8	-0.247829	0.560558	-2.221637
46	8	-0.512325	2.572109	-3.227731
47	6	-0.062989	1.677412	2.420854
48	8	0.353637	0.497986	2.044635
49	8	0.41353	2.36669	3.319601
50	1	-4.580361	-1.376944	-0.471922
51	1	-3.841607	-2.401056	1.612748
52	1	-2.925417	-3.121475	0.285221
53	1	4.738962	-1.027221	-0.009694
54	1	3.738494	0.02766	-1.021544
55	1	3.905002	-1.997427	-2.181581
56	1	3.512672	-3.009808	-0.785449
57	1	-1.595366	-3.688674	2.23092
58	6	-2.331205	-2.37548	3.808244
59	1	-3.864191	-0.229106	0.667973
60	1	2.21122	-2.775021	-3.448857
61	1	1.539517	-3.868	-2.202523
62	1	-0.183239	-3.174998	-3.838454
63	1	0.11137	-1.445071	-3.448999
64	1	-3.822223	-1.337842	-2.672289
65	1	-2.23383	-0.630771	-3.059312
66	1	-2.237712	-3.085056	-3.296024
67	1	-2.631974	-3.298054	-1.592775
68	1	2.379666	-3.289831	0.74113
69	1	2.386195	-3.489091	2.48624
70	1	2.516981	-0.981509	2.754775
71	1	3.970932	-1.735252	2.073827
72	6	0.443055	-3.347538	4.00461
73	1	0.13528	-1.356578	3.179942
74	1	0.36141	-4.388554	3.663917
75	6	-0.414948	-3.129261	5.264402
76	1	1.490902	-3.165971	4.263646
77	6	-1.907904	-3.296389	4.963067
78	1	-0.231376	-2.119443	5.652963
79	1	-0.09682	-3.830903	6.041755
80	1	-3.391805	-2.526434	3.583188
81	1	-2.205287	-1.323872	4.093165
82	1	-2.505513	-3.070847	5.851648
83	1	-2.117857	-4.340818	4.696125

Zero-point correction =	0.694487 (Hartree/Particle)
Thermal correction to Energy =	0.733323
Thermal correction to Enthalpy =	0.734267
Thermal correction to Gibbs Free Energy =	0.626189
Sum of electronic and zero-point Energies =	-2019.2198

Sum of electronic and thermal Energies =	-2019.180964
Sum of electronic and thermal Enthalpies =	-2019.18002
Sum of electronic and thermal Free Energies =	-2019.288099
E(SCF) in SMD solvation model =	-2020.015131

[La(CHX-macropa)]$^+$		(Δ(λλδ)(λλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-3.567393	-0.67034	0.748947
2	7	-2.826474	-0.503411	-0.538882
3	8	-1.752991	-2.109548	1.355357
4	6	-2.64382	-1.099124	1.889152
5	6	-3.168613	-1.620275	-1.455857
6	6	-2.144628	-1.839457	-2.551031
7	8	-0.925006	-2.302143	-1.929661
8	6	0.069289	-2.626376	-2.91387
9	6	1.262767	-3.183406	-2.165163
10	8	1.799179	-2.222872	-1.235991
11	8	0.912256	-2.174795	2.099786
12	6	-0.059937	-2.658895	3.064454
13	7	2.844287	-0.470127	0.570972
14	6	3.153919	-1.470772	1.624018
15	6	2.093004	-1.587758	2.701796
16	6	2.741613	-1.282261	-1.801871
17	6	3.629159	-0.783768	-0.663386
18	6	-3.130558	0.811145	-1.160534
19	6	3.144281	0.906102	1.046145
20	6	2.649297	1.915693	0.034718
21	6	-2.613901	1.925558	-0.277497
22	6	1.083358	2.322096	-1.644484
23	6	1.619947	3.57964	-1.916165
24	6	2.721147	4.000358	-1.166485
25	6	3.257181	3.154336	-0.191616
26	6	-3.209543	3.187644	-0.191013
27	6	-2.660905	4.134601	0.6783
28	6	-1.560157	3.790691	1.466366
29	6	-1.035789	2.505901	1.336458
30	57	0.00937	-0.549423	0.017174
31	1	-4.369033	-1.406448	0.619684
32	1	-4.039138	0.275177	1.033393
33	1	-3.2376	-1.498108	2.714052
34	1	-2.047629	-0.255411	2.25747
35	1	2.191931	-0.45872	-2.27301
36	1	3.350028	-1.787009	-2.561776
37	1	4.390389	-1.536461	-0.431298
38	1	4.154884	0.110877	-1.011305
39	1	-4.212183	0.932139	-1.328926
40	1	-2.62143	0.863496	-2.128959
41	1	4.223618	1.039238	1.219186
42	1	2.619401	1.068128	1.993456
43	1	1.178015	4.181452	-2.701889
44	1	3.173644	4.969704	-1.351487
45	1	4.129837	3.447813	0.382629
46	1	-4.08371	3.420648	-0.790116
47	1	-3.104136	5.122756	0.753653
48	1	-1.108857	4.472451	2.177983
49	7	-1.535954	1.612509	0.461954
50	7	1.573594	1.529777	-0.672587
51	6	-0.069363	1.723823	-2.433306

52	8	-0.280588	0.459439	-2.168585
53	8	-0.703125	2.422366	-3.220545
54	6	0.11264	1.992796	2.187682
55	8	0.31646	0.705904	2.064627
56	8	0.749477	2.770585	2.893967
57	1	2.481077	-2.256735	3.474953
58	1	1.819108	-0.6251	3.144189
59	1	4.121713	-1.245608	2.100973
60	1	3.239239	-2.444732	1.135956
61	1	-2.511001	-2.619051	-3.231805
62	1	-1.923761	-0.928468	-3.116765
63	1	-3.218678	-2.530857	-0.853973
64	1	-4.15747	-1.462067	-1.91587
65	1	0.322909	-1.72388	-3.484453
66	1	-0.323952	-3.38785	-3.601411
67	1	2.044838	-3.503131	-2.863536
68	1	0.957565	-4.039111	-1.557418
69	6	-2.332118	-3.815203	3.087279
70	6	0.502898	-3.816088	3.909903
71	1	0.952253	-4.54704	3.224465
72	6	-0.583071	-4.497516	4.757987
73	1	1.298846	-3.454801	4.567465
74	6	-1.247079	-3.152032	2.235077
75	1	-3.145413	-4.146384	2.432496
76	1	-2.752435	-3.099438	3.804096
77	6	-1.740091	-4.989818	3.88241
78	1	-0.361451	-1.818818	3.707308
79	1	-0.860695	-3.891207	1.523067
80	1	-1.382091	-5.76532	3.192515
81	1	-2.522401	-5.44647	4.496428
82	1	-0.965184	-3.790538	5.506466
83	1	-0.136575	-5.329326	5.311642

Zero-point correction =	0.694022 (Hartree/Particle)
Thermal correction to Energy =	0.732938
Thermal correction to Enthalpy =	0.733882
Thermal correction to Gibbs Free Energy =	0.626254
Sum of electronic and zero-point Energies =	-2019.213017
Sum of electronic and thermal Energies =	-2019.174101
Sum of electronic and thermal Enthalpies =	-2019.173157
Sum of electronic and thermal Free Energies =	-2019.280785
E(SCF) in SMD solvation model =	-2020.005243

$[La(CHX\text{-}macropa)]^+$		(Δ(λδδ)(λδδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.664528	0.623852	0.623204
2	7	2.822882	0.532019	-0.612121
3	8	1.82581	1.747902	1.693548
4	6	2.845014	0.743929	1.905498
5	6	3.109779	1.674731	-1.519279
6	6	1.94948	2.027026	-2.431446
7	8	0.879801	2.5183	-1.581793
8	6	-0.149228	3.240369	-2.287015
9	6	-1.295067	2.329215	-2.6766
10	8	-1.854936	1.836288	-1.443221
11	8	-0.874961	2.287631	1.934909

12	6	0.115879	3.186465	2.507143
13	6	1.388509	2.432788	2.897285
14	7	-2.858107	0.489842	0.824917
15	6	-3.074501	1.387085	1.994256
16	6	-1.819757	1.619668	2.817571
17	6	-3.028997	1.026433	-1.650577
18	6	-3.746607	0.88119	-0.311825
19	6	3.058326	-0.75856	-1.315446
20	6	-3.095305	-0.92231	1.230341
21	6	-2.672467	-1.883759	0.143085
22	6	2.587967	-1.914146	-0.459982
23	6	-1.184538	-2.265255	-1.612722
24	6	-1.768871	-3.495167	-1.911536
25	6	-2.853821	-3.914319	-1.138123
26	6	-3.327079	-3.09287	-0.111613
27	6	3.191466	-3.175663	-0.456814
28	6	2.682367	-4.164762	0.389667
29	6	1.615737	-3.86363	1.240023
30	6	1.083351	-2.576377	1.19419
31	57	-0.008647	0.532252	0.075311
32	1	4.325261	1.492285	0.541646
33	1	4.306183	-0.26052	0.709925
34	1	3.507003	1.044972	2.723352
35	1	2.350366	-0.194105	2.174739
36	1	0.275693	3.725755	-3.172566
37	1	-0.505731	4.011287	-1.598048
38	1	-0.951239	1.484937	-3.28541
39	1	-2.058902	2.898876	-3.222179
40	1	-2.728862	0.068553	-2.083432
41	1	-3.699467	1.538473	-2.353198
42	1	-4.205021	1.844397	-0.074816
43	1	-4.563531	0.157749	-0.435453
44	1	4.12464	-0.881361	-1.561964
45	1	2.484095	-0.753839	-2.248034
46	1	-4.156289	-1.081645	1.479062
47	1	-2.496557	-1.124287	2.12542
48	1	-1.375003	-4.075816	-2.737695
49	1	-3.342128	-4.861848	-1.343833
50	1	-4.186632	-3.383536	0.483436
51	1	4.040111	-3.376708	-1.102349
52	1	3.131127	-5.153232	0.399732
53	1	1.198875	-4.580175	1.938364
54	7	1.541996	-1.643328	0.338378
55	7	-1.611614	-1.501074	-0.588525
56	6	-0.05742	-1.667011	-2.440944
57	8	0.191853	-0.414299	-2.157152
58	8	0.517139	-2.357805	-3.278789
59	6	-0.01709	-2.1019	2.128916
60	8	-0.20652	-0.807238	2.091115
61	8	-0.628065	-2.913363	2.819681
62	1	-2.079845	2.273396	3.652506
63	1	-1.377351	0.689791	3.186036
64	1	-3.868833	0.99851	2.649983
65	1	-3.398571	2.360278	1.618779
66	1	2.259637	2.835472	-3.104626
67	1	1.590164	1.170526	-3.010633
68	1	3.313641	2.550112	-0.898132
69	1	4.003536	1.479255	-2.132654
70	6	-0.404662	4.056217	3.655868
71	1	0.370666	3.83904	1.662721
72	6	2.460833	3.42192	3.38015
73	1	1.160897	1.681718	3.666875

74	1	2.748926	4.044846	2.523314
75	1	3.357416	2.882628	3.703253
76	6	1.947163	4.31612	4.519851
77	6	0.674836	5.059566	4.095066
78	1	-0.661772	3.433577	4.521308
79	1	-1.315844	4.57166	3.333054
80	1	2.730369	5.025325	4.805025
81	1	1.736539	3.704341	5.406968
82	1	0.291102	5.669469	4.918635
83	1	0.904361	5.745959	3.269319

Zero-point correction =	0.693980 (Hartree/Particle)
Thermal correction to Energy =	0.73289
Thermal correction to Enthalpy =	0.733834
Thermal correction to Gibbs Free Energy =	0.625916
Sum of electronic and zero-point Energies =	-2019.213648
Sum of electronic and thermal Energies =	-2019.174739
Sum of electronic and thermal Enthalpies =	-2019.173795
Sum of electronic and thermal Free Energies =	-2019.281713
E(SCF) in SMD solvation model =	-2020.00448

$[La(CHX\text{-}macropa)]^+$		(Δ(δδλ)(δδλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	57	0.122759	-0.038387	-0.242011
2	8	2.561635	-0.724889	-1.461748
3	6	3.803545	-0.02467	-1.278979
4	6	3.549732	1.239957	-0.470749
5	7	2.617917	1.069904	0.667711
6	6	3.171137	0.230315	1.758876
7	6	2.985007	-1.2763	1.572264
8	8	1.5786	-1.568563	1.486545
9	6	1.002767	-2.627756	2.307056
10	6	-0.482072	-2.262626	2.4286
11	8	-1.059415	-1.987735	1.119919
12	6	-1.718675	-3.02148	0.37279
13	6	-2.772006	-2.334649	-0.496294
14	7	-2.233775	-1.263832	-1.371249
15	6	-1.870782	-1.741973	-2.725324
16	6	-0.729606	-2.742836	-2.728018
17	8	0.352439	-2.189333	-1.954411
18	6	1.631256	-2.813601	-2.149163
19	6	2.641293	-1.734353	-2.483378
20	1	3.647963	-2.171067	-2.502384
21	1	2.428248	-1.277036	-3.456565
22	1	1.582697	-3.541376	-2.966109
23	1	1.91212	-3.336785	-1.228086
24	1	-1.01597	-3.717753	-2.311741
25	1	-0.400536	-2.897399	-3.762499
26	1	-1.562457	-0.856122	-3.285959
27	1	-2.734177	-2.206975	-3.230515
28	6	-3.241416	-0.179555	-1.54132
29	6	-3.41351	0.635392	-0.281032
30	6	-4.644767	1.178283	0.099846
31	6	-4.711238	1.968619	1.250308
32	6	-3.556745	2.169809	2.006655
33	6	-2.371712	1.57136	1.578413

34	7	-2.300919	0.842206	0.447286
35	6	-1.08756	1.684578	2.385395
36	8	-0.125895	0.908097	1.96234
37	8	-1.043019	2.451479	3.344098
38	1	-3.540095	2.759509	2.915938
39	1	-4.21122	-0.588986	-1.863132
40	1	-2.868962	0.482882	-2.330891
41	1	-3.312343	-3.094394	-1.083273
42	1	-3.490765	-1.871577	0.185224
43	1	-2.234217	-3.713651	1.043698
44	1	-0.982825	-3.586426	-0.209053
45	1	1.126389	-3.582434	1.773088
46	1	3.43285	-1.771417	2.435713
47	1	3.471199	-1.66231	0.673145
48	1	2.638309	0.506573	2.671782
49	1	4.24307	0.439693	1.912824
50	6	2.291976	2.422224	1.209224
51	6	1.503956	3.240226	0.20954
52	6	1.584623	4.632981	0.127734
53	6	0.791608	5.301091	-0.810233
54	6	-0.033745	4.56538	-1.662113
55	6	-0.039358	3.176369	-1.537202
56	7	0.695953	2.539394	-0.605881
57	6	-0.865361	2.276923	-2.444233
58	8	-0.604424	1.005359	-2.29798
59	8	-1.692269	2.776614	-3.203367
60	1	2.251367	5.180945	0.785638
61	1	3.2054	2.962288	1.502944
62	1	1.667297	2.267057	2.095082
63	1	3.107039	1.986597	-1.133379
64	1	4.523389	1.631131	-0.130285
65	1	4.217564	0.260043	-2.254115
66	1	4.52306	-0.696141	-0.790756
67	1	-5.530082	0.988005	-0.49833
68	1	-5.655847	2.407822	1.556041
69	1	-0.659943	5.023799	-2.418701
70	1	0.832122	6.383567	-0.882519
71	6	1.60971	-2.734627	3.714638
72	6	-1.262321	-3.278802	3.261515
73	1	-0.523999	-1.279011	2.907106
74	1	-1.215576	-4.276306	2.804792
75	1	-2.31518	-2.978768	3.303759
76	6	-0.658999	-3.359298	4.672688
77	6	0.825797	-3.729694	4.589841
78	1	-1.205517	-4.099412	5.265183
79	1	-0.774832	-2.392982	5.179363
80	1	1.592946	-1.739833	4.178392
81	1	2.653002	-3.062009	3.66442
82	1	0.928853	-4.741485	4.175073
83	1	1.274073	-3.752884	5.587924

Zero-point correction =	0.693182 (Hartree/Particle)
Thermal correction to Energy =	0.732644
Thermal correction to Enthalpy =	0.733588
Thermal correction to Gibbs Free Energy =	0.622834
Sum of electronic and zero-point Energies =	-2019.212173
Sum of electronic and thermal Energies =	-2019.172711
Sum of electronic and thermal Enthalpies =	-2019.171767

Sum of electronic and thermal Free Energies =	-2019.282521
E(SCF) in SMD solvation model =	-2020.008389

[La(CHX-macropa)]$^{+}$		(Δ(δδδ)(δδδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.600363	-0.549956	-0.687345
2	7	2.855846	-0.432568	0.59009
3	8	1.850887	-2.005921	-1.553555
4	6	3.27435	-1.79751	-1.499284
5	6	3.24323	-1.504506	1.542542
6	6	2.113599	-1.897783	2.479087
7	8	1.060433	-2.459717	1.65573
8	6	0.058991	-3.186335	2.392812
9	6	-1.105592	-2.278197	2.748226
10	8	-1.644054	-1.731663	1.525678
11	8	-0.857663	-2.374882	-1.753659
12	6	0.034873	-3.437166	-2.181825
13	6	1.401391	-2.897072	-2.617866
14	7	-2.790805	-0.536038	-0.77255
15	6	-3.043987	-1.455232	-1.91312
16	6	-1.78302	-1.768878	-2.70263
17	6	-2.977861	-2.113226	1.148495
18	6	-3.595693	-0.936883	0.406478
19	6	3.120368	0.90449	1.192676
20	6	-3.10545	0.8646	-1.162723
21	6	-2.676487	1.83655	-0.085311
22	6	2.59711	2.016483	0.308585
23	6	-1.170454	2.261263	1.641539
24	6	-1.798686	3.463781	1.964669
25	6	-2.911595	3.84922	1.215817
26	6	-3.370915	3.018112	0.190856
27	6	3.161613	3.294131	0.261409
28	6	2.612168	4.241542	-0.607741
29	6	1.544417	3.884107	-1.433757
30	6	1.048814	2.584356	-1.341517
31	57	0.073526	-0.488328	-0.079709
32	1	0.501686	-3.626183	3.294713
33	1	-0.274133	-3.995552	1.735949
34	1	-0.769937	-1.427536	3.347038
35	1	-1.880569	-2.831263	3.289798
36	1	4.199267	1.042627	1.367529
37	1	2.600265	0.944673	2.155549
38	1	-4.18154	0.984858	-1.365348
39	1	-2.55266	1.085399	-2.082438
40	1	-1.410019	4.049937	2.789352
41	1	1.095383	4.56705	-2.145612
42	7	1.549242	1.691424	-0.467468
43	7	-1.585975	1.486849	0.620789
44	6	0.008343	1.724351	2.438182
45	8	0.352881	0.50552	2.116525
46	8	0.539373	2.433627	3.290157
47	6	-0.070358	2.062324	-2.228327
48	8	-0.268633	0.774386	-2.114626
49	8	-0.692648	2.840745	-2.946529
50	1	4.690588	-0.539724	-0.519186
51	1	3.672072	-1.64113	-2.50927
52	1	3.751235	-2.691801	-1.083253
53	1	-4.630743	-1.18685	0.122663
54	1	-3.632286	-0.089409	1.094412
55	1	-3.569539	-2.322727	2.046753

56	1	-2.941689	-3.022473	0.534757
57	1	-1.326108	-0.868211	-3.121837
58	1	-2.028869	-2.475909	-3.496486
59	1	-3.438125	-2.396571	-1.518696
60	1	-3.805759	-1.04033	-2.589049
61	1	2.472949	-2.67094	3.16965
62	1	1.72486	-1.040596	3.037309
63	1	4.119236	-1.203944	2.136893
64	1	3.524461	-2.391766	0.9704
65	1	3.350813	0.327955	-1.285162
66	6	2.347036	-4.087247	-2.8599
67	1	1.305348	-2.295715	-3.533382
68	1	2.496758	-4.616164	-1.908735
69	1	3.326572	-3.736729	-3.197069
70	6	1.768246	-5.059105	-3.901208
71	6	-0.559092	-4.379575	-3.233295
72	1	0.199131	-4.006608	-1.258352
73	6	0.386756	-5.566827	-3.475342
74	1	-0.698102	-3.852108	-4.184698
75	1	-1.542822	-4.724364	-2.895776
76	1	2.462127	-5.894405	-4.036692
77	1	1.69031	-4.552599	-4.872194
78	1	-0.03716	-6.221491	-4.242878
79	1	0.476263	-6.165053	-2.559003
80	1	3.030285	5.242429	-0.652213
81	1	4.011522	3.540343	0.889413
82	1	-4.252955	3.278518	-0.385132
83	1	-3.431981	4.775507	1.438948

Zero-point correction =	0.695693 (Hartree/Particle)
Thermal correction to Energy =	0.734072
Thermal correction to Enthalpy =	0.735016
Thermal correction to Gibbs Free Energy =	0.629018
Sum of electronic and zero-point Energies =	-2027.574059
Sum of electronic and thermal Energies =	-2027.53568
Sum of electronic and thermal Enthalpies =	-2027.534736
Sum of electronic and thermal Free Energies =	-2027.640734
E(SCF) in SMD solvation model =	-2028.361864

$[Ce(CHX\text{-}macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.581054	-0.913583	-0.500258
2	7	2.849384	-0.438322	0.695736
3	8	1.647822	-2.066671	-1.317939
4	6	3.04191	-2.235897	-1.012975
5	6	3.208296	-1.262958	1.878118
6	6	2.039326	-1.456912	2.819297
7	8	0.987314	-2.146041	2.083851
8	6	0.131727	-2.895767	2.978062
9	6	-1.196792	-3.185257	2.286955
10	8	-1.725914	-1.915186	1.804986
11	8	-1.109358	-2.302323	-1.766123
12	6	-0.144711	-2.698464	-2.75199
13	6	1.102542	-3.174774	-2.052439
14	7	-2.887374	-0.459005	-0.414342
15	6	-3.330991	-1.497071	-1.377788

16	6	-2.287842	-1.791815	-2.432508
17	6	-3.152449	-1.908639	1.608543
18	6	-3.564296	-0.635852	0.891316
19	6	3.188019	0.982511	0.969436
20	6	-3.208972	0.881727	-0.974713
21	6	-2.657336	1.992775	-0.114165
22	6	2.677333	1.896871	-0.118715
23	6	-1.002352	2.614528	1.399448
24	6	-1.531556	3.89642	1.535897
25	6	-2.677738	4.217242	0.80637
26	6	-3.260892	3.24998	-0.015989
27	6	3.331636	3.080629	-0.474375
28	6	2.789984	3.877101	-1.48594
29	6	1.631861	3.455783	-2.141445
30	6	1.050996	2.252427	-1.744999
31	58	-0.039863	-0.459801	0.118745
32	1	4.277226	1.107604	1.078405
33	1	2.711673	1.262307	1.915212
34	1	-4.298599	1.001747	-1.086171
35	1	-2.748822	0.947791	-1.96655
36	1	-4.167219	3.463977	-0.57293
37	1	1.172972	4.015211	-2.948426
38	7	1.549772	1.506576	-0.739236
39	7	-1.54048	1.697241	0.572458
40	6	0.205868	2.139733	2.182595
41	8	0.438097	0.861142	2.046905
42	8	0.862898	2.936871	2.847745
43	6	-0.175844	1.680284	-2.429403
44	8	-0.470129	0.468527	-2.041219
45	8	-0.790261	2.352968	-3.254338
46	1	4.659677	-1.02233	-0.29947
47	1	3.579625	-2.510335	-1.929563
48	1	3.159847	-3.053177	-0.289903
49	1	-4.661359	-0.651754	0.777323
50	1	-3.308286	0.220117	1.520054
51	1	-3.661706	-1.934051	2.577464
52	1	-3.448512	-2.803934	1.048229
53	1	-2.003453	-0.899385	-2.998212
54	1	-2.670613	-2.563112	-3.114113
55	1	-3.534107	-2.422348	-0.835451
56	1	-4.269603	-1.198721	-1.869578
57	1	2.361426	-2.078711	3.66022
58	1	1.636558	-0.507465	3.180674
59	1	4.047731	-0.811405	2.427018
60	1	3.540674	-2.246107	1.535699
61	1	0.89277	-4.009782	-1.37076
62	1	1.827166	-3.508627	-2.805543
63	1	0.087699	-1.839643	-3.39341
64	1	-0.555419	-3.512788	-3.364431
65	1	3.460402	-0.166692	-1.288601
66	1	-1.026871	-3.825363	1.406361
67	6	-2.116759	-3.920941	3.277076
68	6	0.796997	-4.214291	3.402482
69	1	-0.074305	-2.266316	3.855526
70	1	-3.125964	5.202548	0.888707
71	1	-1.044545	4.593965	2.207436
72	1	3.278082	4.804472	-1.769196
73	1	4.245546	3.369947	0.034123
74	6	-0.099002	-4.997768	4.372167
75	1	1.768139	-4.011859	3.864855
76	1	0.989346	-4.809627	2.500182
77	6	-1.475782	-5.238957	3.745424

78	1	-0.211643	-4.432261	5.306296
79	1	0.376912	-5.94814	4.633005
80	1	-3.082017	-4.14067	2.812967
81	1	-2.306115	-3.26997	4.140512
82	1	-2.146228	-5.729817	4.457641
83	1	-1.374887	-5.916995	2.887458

Zero-point correction =	0.694421 (Hartree/particle)
Thermal correction to Energy =	0.733289
Thermal correction to Enthalpy =	0.734233
Thermal correction to Gibbs Free Energy =	0.626093
Sum of electronic and zero-point Energies =	-2019.87228
Sum of electronic and thermal Energies =	-2019.833412
Sum of electronic and thermal Enthalpies =	-2019.832468
Sum of electronic and thermal Free Energies =	-2019.940608
E(SCF) in SMD solvation model =	-2020.670909

$[Nd(CHX\text{-}macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.56855	-0.885513	-0.484804
2	7	2.838678	-0.413782	0.712845
3	8	1.636962	-2.062242	-1.272804
4	6	3.036865	-2.214393	-0.986064
5	6	3.205002	-1.236554	1.893834
6	6	2.031911	-1.45612	2.823159
7	8	0.988857	-2.136505	2.067789
8	6	0.13625	-2.90627	2.946791
9	6	-1.195034	-3.17736	2.255457
10	8	-1.715382	-1.895786	1.794917
11	8	-1.114998	-2.319003	-1.709861
12	6	-0.152794	-2.743486	-2.68541
13	6	1.09634	-3.193959	-1.97418
14	7	-2.876357	-0.44391	-0.405035
15	6	-3.332486	-1.491635	-1.351326
16	6	-2.287685	-1.819253	-2.393584
17	6	-3.145306	-1.867178	1.629573
18	6	-3.54955	-0.596661	0.905307
19	6	3.169669	1.008186	0.9848
20	6	-3.189122	0.889956	-0.984727
21	6	-2.621679	2.00477	-0.140744
22	6	2.643886	1.914667	-0.102132
23	6	-0.968301	2.611774	1.379332
24	6	-1.480447	3.901058	1.507611
25	6	-2.616157	4.234743	0.767158
26	6	-3.20804	3.270979	-0.052923
27	6	3.28061	3.106531	-0.463291
28	6	2.730291	3.888194	-1.48154
29	6	1.582343	3.443393	-2.139855
30	6	1.019132	2.234445	-1.736346
31	60	-0.039277	-0.449955	0.126953
32	1	4.258893	1.141747	1.083939
33	1	2.700876	1.286352	1.934778
34	1	-4.278242	1.019453	-1.09056
35	1	-2.736054	0.937263	-1.98079
36	1	-4.109224	3.493617	-0.614777
37	1	1.119774	3.988616	-2.954435

38	7	1.523158	1.504305	-0.721725
39	7	-1.510861	1.69902	0.550615
40	6	0.220387	2.11492	2.175638
41	8	0.428523	0.832073	2.039109
42	8	0.88617	2.895962	2.85122
43	6	-0.189943	1.631368	-2.42233
44	8	-0.461894	0.418911	-2.019625
45	8	-0.813658	2.279082	-3.260195
46	1	4.649367	-0.984193	-0.290453
47	1	3.564475	-2.486915	-1.909058
48	1	3.173035	-3.027708	-0.261769
49	1	-4.647371	-0.601787	0.79785
50	1	-3.280368	0.262703	1.523392
51	1	-3.633844	-1.875651	2.60955
52	1	-3.468362	-2.761924	1.084165
53	1	-1.995942	-0.943082	-2.980484
54	1	-2.671766	-2.605419	-3.057301
55	1	-3.553172	-2.403971	-0.794518
56	1	-4.263787	-1.187696	-1.853277
57	1	2.352286	-2.093091	3.653518
58	1	1.621226	-0.516726	3.200392
59	1	4.031043	-0.771941	2.451746
60	1	3.559572	-2.211368	1.549973
61	1	0.891616	-4.009369	-1.267796
62	1	1.821948	-3.546308	-2.717728
63	1	0.076783	-1.903997	-3.352896
64	1	-0.563396	-3.576693	-3.272069
65	1	3.436406	-0.14337	-1.275717
66	1	-1.032859	-3.804293	1.364266
67	6	-2.113435	-3.92446	3.238498
68	6	0.800574	-4.234755	3.339605
69	1	-0.066193	-2.296496	3.838864
70	1	-3.051178	5.226562	0.841586
71	1	-0.9907	4.593971	2.181965
72	1	3.205002	4.821176	-1.769072
73	1	4.188908	3.412152	0.045704
74	6	-0.093598	-5.035388	4.297117
75	1	1.774706	-4.044782	3.801124
76	1	0.986422	-4.811463	2.423904
77	6	-1.476297	-5.255358	3.67511
78	1	-0.196514	-4.490708	5.244695
79	1	0.378589	-5.994077	4.533222
80	1	-3.08422	-4.129068	2.779224
81	1	-2.290514	-3.289735	4.116457
82	1	-2.144359	-5.757382	4.381771
83	1	-1.385378	-5.915868	2.802449

Zero-point correction =	0.694694 (Hartree/Particle)
Thermal correction to Energy =	0.733509
Thermal correction to Enthalpy =	0.734453
Thermal correction to Gibbs Free Energy =	0.626468
Sum of electronic and zero-point Energies =	-2021.125552
Sum of electronic and thermal Energies =	-2021.086738
Sum of electronic and thermal Enthalpies =	-2021.085793
Sum of electronic and thermal Free Energies =	-2021.193778
E(SCF) in SMD solvation model =	-2021.923685

[Gd(CHX-macropa)]$^{+}$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.547989	-0.84865	-0.430875
2	7	2.824441	-0.360189	0.761725
3	8	1.609807	-2.051271	-1.166807
4	6	3.014605	-2.18904	-0.89388
5	6	3.195924	-1.164542	1.953082
6	6	2.005655	-1.439926	2.843913
7	8	0.992093	-2.107875	2.038698
8	6	0.14675	-2.929824	2.876013
9	6	-1.187483	-3.162826	2.17955
10	8	-1.696589	-1.854768	1.784905
11	8	-1.133717	-2.346021	-1.586969
12	6	-0.174081	-2.819511	-2.540565
13	6	1.076777	-3.222347	-1.807433
14	7	-2.864629	-0.409952	-0.372586
15	6	-3.342495	-1.478544	-1.28287
16	6	-2.296752	-1.868392	-2.301065
17	6	-3.131033	-1.782092	1.68585
18	6	-3.525305	-0.516765	0.948154
19	6	3.145447	1.066325	1.009236
20	6	-3.163387	0.908201	-0.9906
21	6	-2.568931	2.032856	-0.180713
22	6	2.598251	1.944265	-0.089867
23	6	-0.918996	2.624589	1.346751
24	6	-1.404751	3.925223	1.456365
25	6	-2.522961	4.275049	0.69641
26	6	-3.128163	3.312844	-0.115548
27	6	3.209878	3.141432	-0.476996
28	6	2.64964	3.885208	-1.517716
29	6	1.518366	3.396208	-2.173878
30	6	0.979285	2.187106	-1.740955
31	64	-0.040614	-0.421078	0.155314
32	1	4.234386	1.213846	1.092247
33	1	2.687555	1.356572	1.960819
34	1	-4.251289	1.054005	-1.087702
35	1	-2.723173	0.918246	-1.99333
36	1	-4.02131	3.545668	-0.686026
37	1	1.05229	3.90721	-3.008407
38	7	1.488269	1.495488	-0.701917
39	7	-1.467425	1.71483	0.519101
40	6	0.236893	2.09888	2.168137
41	8	0.413236	0.811033	2.031425
42	8	0.908566	2.858123	2.862568
43	6	-0.203437	1.532071	-2.419991
44	8	-0.451064	0.329649	-1.973459
45	8	-0.831711	2.12893	-3.291584
46	1	4.631072	-0.939997	-0.245106
47	1	3.530065	-2.483647	-1.816814
48	1	3.161248	-2.982944	-0.150471
49	1	-4.624518	-0.503378	0.856836
50	1	-3.230848	0.349622	1.543488
51	1	-3.573143	-1.758887	2.687692
52	1	-3.507915	-2.673344	1.172303
53	1	-1.992635	-1.025176	-2.92837
54	1	-2.685131	-2.682047	-2.928265
55	1	-3.591947	-2.363983	-0.696281
56	1	-4.261411	-1.169659	-1.803894

57	1	2.316455	-2.104455	3.656528
58	1	1.570204	-0.523282	3.246441
59	1	3.979375	-0.660988	2.536942
60	1	3.610996	-2.119779	1.621725
61	1	0.878648	-4.000058	-1.05802
62	1	1.805663	-3.608465	-2.530506
63	1	0.050708	-2.017246	-3.253836
64	1	-0.582355	-3.685368	-3.079916
65	1	3.405738	-0.124472	-1.236455
66	1	-1.035986	-3.744218	1.256902
67	6	-2.100078	-3.95429	3.132533
68	6	0.817373	-4.273957	3.194132
69	1	-0.054677	-2.370469	3.800661
70	1	-2.937193	5.276839	0.753625
71	1	-0.911758	4.613775	2.13284
72	1	3.105659	4.821022	-1.825591
73	1	4.108943	3.477979	0.028865
74	6	-0.072148	-5.12544	4.111693
75	1	1.793039	-4.104956	3.660974
76	1	1.001037	-4.800921	2.248426
77	6	-1.461004	-5.307927	3.490479
78	1	-0.166092	-4.634392	5.089106
79	1	0.398875	-6.097057	4.290407
80	1	-3.077417	-4.132021	2.676353
81	1	-2.263403	-3.366353	4.045009
82	1	-2.123471	-5.847085	4.174694
83	1	-1.379434	-5.919884	2.582117

Zero-point correction =	0.695151 (Hartree/Particle)
Thermal correction to Energy =	0.733873
Thermal correction to Enthalpy =	0.734818
Thermal correction to Gibbs Free Energy =	0.627159
Sum of electronic and zero-point Energies =	-2023.526029
Sum of electronic and thermal Energies =	-2023.487307
Sum of electronic and thermal Enthalpies =	-2023.486362
Sum of electronic and thermal Free Energies =	-2023.594021
E(SCF) in SMD solvation model =	-2024.325013

$[Gd(CHX\text{-}macropa)]^+$		(Δ(λδλ)(λδλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-3.641596	-0.718733	0.386776
2	7	-2.730551	-0.386385	-0.74551
3	8	-1.775172	-1.737238	1.45991
4	6	-2.896159	-0.858299	1.707945
5	6	-2.827263	-1.379012	-1.838929
6	6	-2.181709	-2.701763	-1.46044
7	8	-0.773031	-2.491459	-1.21217
8	6	0.143493	-3.249701	-2.019328
9	6	1.277251	-2.337793	-2.430605
10	8	1.825678	-1.782326	-1.21927
11	8	0.814606	-2.180054	1.838698
12	6	-0.091352	-3.272762	2.15289
13	6	-1.406908	-2.608972	2.557869
14	7	2.767697	-0.238796	0.907495
15	6	2.84659	-0.979353	2.186938
16	6	2.220335	-2.358025	2.096342

17	6	3.045601	-1.050238	-1.454967
18	6	3.698914	-0.815551	-0.101079
19	6	-3.021102	0.965503	-1.281162
20	6	3.066709	1.193584	1.155663
21	6	2.610553	2.043265	-0.004976
22	6	-2.561315	2.027562	-0.311467
23	6	1.086511	2.244754	-1.752531
24	6	1.642539	3.450262	-2.175008
25	6	2.735399	3.954913	-1.466354
26	6	3.240069	3.234713	-0.381
27	6	-3.1867	3.27258	-0.186152
28	6	-2.683694	4.195625	0.733593
29	6	-1.594377	3.84148	1.532238
30	6	-1.042847	2.573161	1.3655
31	64	0.026677	-0.381428	0.107122
32	1	-4.1559	-1.661871	0.171803
33	1	-4.416299	0.05062	0.494023
34	1	-3.559386	-1.290423	2.462491
35	1	-2.514954	0.097055	2.078452
36	1	-2.290036	-0.962954	-2.69417
37	1	-3.87535	-1.561739	-2.130022
38	1	-2.304192	-3.417757	-2.279332
39	1	-2.617554	-3.131499	-0.553848
40	1	-0.360173	-3.62617	-2.915874
41	1	0.515248	-4.100823	-1.43609
42	1	0.913037	-1.524343	-3.066689
43	1	2.050476	-2.916466	-2.952069
44	6	0.387361	-4.216856	3.262618
45	1	-0.251697	-3.847716	1.229288
46	1	2.28692	-0.400731	2.925108
47	1	3.889143	-1.08503	2.528946
48	1	2.66391	-2.979345	1.30786
49	1	2.367712	-2.855901	3.056955
50	1	2.811345	-0.120215	-1.980723
51	1	3.711833	-1.656477	-2.08209
52	1	4.067924	-1.776759	0.268654
53	1	4.575434	-0.168329	-0.236695
54	1	-4.094815	1.089534	-1.491121
55	1	-2.475957	1.086164	-2.223497
56	1	4.141636	1.348361	1.336646
57	1	2.523895	1.505307	2.054941
58	1	1.222936	3.945143	-3.043216
59	1	3.205256	4.886035	-1.767736
60	1	4.107674	3.586715	0.167579
61	1	-4.050421	3.509131	-0.799068
62	1	-3.150987	5.169938	0.838435
63	1	-1.172255	4.501248	2.281467
64	7	-1.495954	1.702185	0.441679
65	7	1.539908	1.578971	-0.671971
66	6	-0.039302	1.554943	-2.496076
67	8	-0.26287	0.335489	-2.08481
68	8	-0.645991	2.149934	-3.385504
69	6	0.087953	2.050337	2.228591
70	8	0.300151	0.769996	2.084335
71	8	0.711614	2.819246	2.958367
72	1	1.315809	-4.712842	2.962901
73	6	-0.682429	-5.280886	3.566427
74	1	0.596231	-3.637753	4.171644
75	6	-2.479474	-3.670869	2.832963
76	1	-1.228299	-1.99096	3.448595
77	1	-2.665039	-4.229561	1.906155
78	1	-3.423902	-3.198321	3.120447

79	6	-2.019195	-4.631831	3.940043
80	1	-2.784617	-5.396191	4.105996
81	1	-1.911987	-4.080659	4.883429
82	1	-0.326678	-5.926342	4.375348
83	1	-0.818981	-5.922815	2.685923

Zero-point correction =	0.694387 (Hartree/Particle)
Thermal correction to Energy =	0.733237
Thermal correction to Enthalpy =	0.734181
Thermal correction to Gibbs Free Energy =	0.626287
Sum of electronic and zero-point Energies =	-2023.528873
Sum of electronic and thermal Energies =	-2023.490022
Sum of electronic and thermal Enthalpies =	-2023.489078
Sum of electronic and thermal Free Energies =	-2023.596972
E(SCF) in SMD solvation model =	-2024.318646

$[Gd(CHX\text{-}macropa)]^+$		(Δ(λλλ)(λλλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.66146	0.829639	0.202225
2	7	2.73974	0.413994	-0.890482
3	8	1.795229	1.796801	1.344836
4	6	2.967205	0.97611	1.55063
5	6	2.849445	1.320042	-2.05606
6	6	2.205802	2.665703	-1.753795
7	8	0.78287	2.536423	-1.548869
8	6	0.024337	2.558397	-2.776511
9	6	-1.417462	2.789882	-2.383374
10	8	-1.794838	1.8086	-1.395068
11	8	-0.772833	2.502794	1.532649
12	6	-0.001314	2.541883	2.779635
13	6	1.427435	2.831066	2.317286
14	7	-2.786818	0.417569	0.775569
15	6	-2.875399	1.310435	1.95236
16	6	-2.2054	2.642516	1.648086
17	6	-3.011373	1.071415	-1.64448
18	6	-3.709535	0.870527	-0.302851
19	6	3.006709	-0.98153	-1.31118
20	6	-3.065188	-0.983422	1.164701
21	6	-2.591093	-1.928769	0.086371
22	6	2.524851	-1.955765	-0.262443
23	6	-1.081306	-2.259609	-1.653138
24	6	-1.624471	-3.504545	-1.964397
25	6	-2.700046	-3.963049	-1.200486
26	6	-3.203928	-3.158614	-0.176235
27	6	3.123587	-3.201717	-0.046792
28	6	2.612117	-4.037988	0.947621
29	6	1.54321	-3.596166	1.730651
30	6	1.014633	-2.334114	1.46821
31	64	-0.005996	0.523525	-0.029663
32	1	4.112566	1.792441	-0.059104
33	1	4.485255	0.110825	0.305685
34	1	3.658285	1.449539	2.248525
35	1	2.654041	0.014799	1.963351
36	1	-2.754264	0.126103	-2.128331
37	1	-3.660953	1.650123	-2.309975
38	1	-4.165617	1.819697	-0.003942

39	1	-4.529496	0.15306	-0.435208
40	1	4.079408	-1.141572	-1.501878
41	1	2.466826	-1.169612	-2.245351
42	1	-4.138307	-1.141711	1.354424
43	1	-2.52364	-1.197267	2.092193
44	1	-1.207674	-4.065389	-2.79295
45	1	-3.15786	-4.924017	-1.413934
46	1	-4.060476	-3.473984	0.410838
47	1	3.975079	-3.505035	-0.647354
48	1	3.058947	-5.011637	1.123604
49	1	1.121071	-4.182987	2.538244
50	7	1.473316	-1.550774	0.471546
51	7	-1.532954	-1.508236	-0.629418
52	6	0.030748	-1.626646	-2.465719
53	8	0.26553	-0.381646	-2.147916
54	8	0.620909	-2.285488	-3.320565
55	6	-0.086057	-1.717517	2.309274
56	8	-0.302484	-0.456801	2.041853
57	8	-0.68262	-2.400764	3.139506
58	1	0.141899	1.603701	-3.298484
59	1	0.37165	3.387412	-3.40596
60	1	-2.058274	2.706278	-3.266135
61	1	-1.54397	3.780968	-1.935024
62	1	-0.047742	1.544073	3.233541
63	6	-0.487698	3.618335	3.758484
64	1	1.406597	3.764651	1.740956
65	6	2.391842	2.990903	3.495206
66	1	-2.520727	3.032182	0.678267
67	1	-2.453649	3.388377	2.404842
68	1	-3.921856	1.480069	2.255677
69	1	-2.352457	0.817223	2.775728
70	1	2.388128	3.373598	-2.570786
71	1	2.58817	3.098776	-0.827004
72	1	3.899459	1.475815	-2.354078
73	1	2.323984	0.842115	-2.886265
74	1	3.390973	3.249642	3.128558
75	1	2.470942	2.047274	4.049662
76	6	1.896066	4.092098	4.446105
77	1	-0.58042	4.574161	3.224946
78	6	0.482979	3.776296	4.939657
79	1	-1.476515	3.35905	4.148571
80	1	0.497563	2.850819	5.529955
81	1	0.118209	4.567886	5.601465
82	1	1.902488	5.060091	3.927963
83	1	2.590168	4.178082	5.28776

Zero-point correction =	0.695633 (Hartree/Particle)
Thermal correction to Energy =	0.734069
Thermal correction to Enthalpy =	0.735013
Thermal correction to Gibbs Free Energy =	0.628664
Sum of electronic and zero-point Energies =	-2023.522648
Sum of electronic and thermal Energies =	-2023.484212
Sum of electronic and thermal Enthalpies =	-2023.483268
Sum of electronic and thermal Free Energies =	-2023.589617
E(SCF) in SMD solvation model =	-2024.310884

[Gd(CHX-macropa)]$^{+}$		(Δ(δλλ)(δλλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-0.515351	-3.681797	-0.580718
2	7	-0.357036	-2.797393	0.598039
3	8	-1.707014	-1.91246	-1.671479
4	6	-1.687079	-3.333142	-1.481882
5	6	-1.364171	-3.057919	1.649264
6	6	-2.675523	-2.319183	1.388546
7	8	-2.511759	-0.889404	1.438197
8	6	-2.443701	-0.281885	2.770773
9	6	-2.743357	1.196999	2.554091
10	8	-1.841679	1.690886	1.52387
11	8	-2.569677	0.674023	-1.765053
12	6	-2.450635	-0.077847	-2.991625
13	6	-2.681546	-1.527316	-2.651927
14	7	-0.626188	2.701828	-0.884313
15	6	-1.460767	2.831855	-2.10046
16	6	-2.780359	2.081202	-1.999189
17	6	-2.192947	3.014723	1.09215
18	6	-1.07573	3.574447	0.227043
19	6	1.019445	-3.004163	1.124331
20	6	0.767493	3.093706	-1.236148
21	6	1.725748	2.679038	-0.145947
22	6	2.024692	-2.430222	0.149892
23	6	2.144718	1.179096	1.58213
24	6	3.334768	1.818122	1.924131
25	6	3.720161	2.935385	1.181293
26	6	2.897538	3.384615	0.146088
27	6	3.312125	-2.947762	-0.02146
28	6	4.149687	-2.376898	-0.983436
29	6	3.670046	-1.335118	-1.780056
30	6	2.370308	-0.883528	-1.55706
31	64	-0.533903	-0.019889	-0.086038
32	1	1.228034	-4.073199	1.28651
33	1	1.101669	-2.48475	2.083107
34	1	0.839966	4.179668	-1.403108
35	1	1.039681	2.587709	-2.167685
36	1	3.911182	1.435337	2.758384
37	1	4.637392	3.465721	1.41776
38	1	3.154278	4.269806	-0.426718
39	1	3.645646	-3.78574	0.582016
40	1	5.154921	-2.761278	-1.125955
41	1	4.257228	-0.875506	-2.566617
42	7	1.586173	-1.396116	-0.59057
43	7	1.37671	1.583082	0.551332
44	6	1.602323	-0.001194	2.360543
45	8	0.405528	-0.365751	1.984195
46	8	2.278313	-0.52514	3.243197
47	6	1.717918	0.194795	-2.399654
48	8	0.447975	0.364436	-2.1399
49	8	2.383474	0.823587	-3.220238
50	1	-0.605086	-4.736973	-0.274318
51	1	-1.546617	-3.826938	-2.452302
52	1	-2.652393	-3.669972	-1.079981
53	1	-1.38475	4.564042	-0.14746
54	1	-0.213897	3.727505	0.880901
55	1	-2.291706	3.678265	1.956961
56	1	-3.167899	2.986438	0.591675
57	1	-3.690693	-1.683577	-2.247795
58	1	-2.558682	-2.136954	-3.556412
59	1	-1.453145	0.068726	-3.418377
60	1	-3.222128	0.252596	-3.697585

61	1	0.396258	-3.585887	-1.173678
62	6	-2.595577	1.95755	3.879371
63	1	-3.769478	1.297141	2.166892
64	6	-3.430052	-0.869766	3.787182
65	1	-1.413236	-0.39174	3.126396
66	1	-1.5668	-4.13675	1.755995
67	1	-0.947274	-2.702252	2.59552
68	1	-3.436105	-2.63971	2.104468
69	1	-3.066712	-2.508216	0.391567
70	1	-3.408199	2.431284	-1.180912
71	1	-3.347138	2.21304	-2.928381
72	1	-0.882492	2.404101	-2.922913
73	1	-1.663636	3.890411	-2.334906
74	1	-4.452605	-0.811342	3.390248
75	6	-3.334813	-0.111144	5.123618
76	1	-3.205742	-1.924775	3.972139
77	1	-2.797983	3.023618	3.740449
78	1	-1.558552	1.8624	4.223738
79	6	-3.562429	1.390524	4.930531
80	1	-4.597548	1.57009	4.610176
81	1	-3.428344	1.923299	5.877042
82	1	-2.342632	-0.277766	5.56224
83	1	-4.065385	-0.525814	5.825193

Zero-point correction =	0.695372 (Hartree/Particle)
Thermal correction to Energy =	0.733908
Thermal correction to Enthalpy =	0.734852
Thermal correction to Gibbs Free Energy =	0.627813
Sum of electronic and zero-point Energies =	-2023.526582
Sum of electronic and thermal Energies =	-2023.488047
Sum of electronic and thermal Enthalpies =	-2023.487103
Sum of electronic and thermal Free Energies =	-2023.594141
E(SCF) in SMD solvation model =	-2024.322375

$[Gd(CHX\text{-}macropa)]^+$		(Δ(λλδ)(λλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	0.670794	3.457289	-0.991999
2	7	0.525927	2.816983	0.348521
3	8	2.051646	1.545194	-1.364153
4	6	1.131905	2.439615	-2.038487
5	6	1.670869	3.206962	1.204319
6	6	1.931537	2.225502	2.324993
7	8	2.32782	0.972815	1.725443
8	6	2.720171	0.032341	2.734589
9	6	3.149741	-1.220414	2.00493
10	8	2.067386	-1.742653	1.214124
11	8	2.148809	-1.120225	-1.907058
12	6	2.783777	-0.244069	-2.870383
13	6	3.188489	0.998896	-2.083263
14	7	0.308456	-2.867055	-0.41086
15	6	1.315096	-3.302122	-1.409399
16	6	1.545372	-2.290286	-2.511603
17	6	1.151636	-2.613111	1.921683
18	6	0.555508	-3.56552	0.885627
19	6	-0.765317	3.181467	0.977603
20	6	-1.069305	-3.132748	-0.891205

21	6	-2.052055	-2.501491	0.069114
22	6	-1.890958	2.605817	0.149045
23	6	-2.333438	-0.834114	1.672012
24	6	-3.619894	-1.268887	1.982712
25	6	-4.126939	-2.367971	1.284351
26	6	-3.329519	-3.00737	0.331218
27	6	-3.154797	3.192096	0.027601
28	6	-4.094443	2.602859	-0.822509
29	6	-3.739928	1.47208	-1.562653
30	6	-2.457342	0.955494	-1.392756
31	64	0.48792	-0.027971	-0.024687
32	1	1.381625	4.2896	-0.929159
33	1	-0.286832	3.875275	-1.315195
34	1	1.622809	2.94691	-2.870736
35	1	0.292147	1.849983	-2.421476
36	1	0.378827	-2.001651	2.400267
37	1	1.698012	-3.170743	2.690866
38	1	1.226224	-4.416981	0.724952
39	1	-0.382112	-3.964328	1.283717
40	1	-0.880139	4.273645	1.062898
41	1	-0.798828	2.752285	1.984718
42	1	-1.26378	-4.213756	-0.973642
43	1	-1.189535	-2.685244	-1.88345
44	1	-4.176957	-0.756029	2.758301
45	1	-5.123513	-2.742292	1.497171
46	1	-3.686233	-3.885813	-0.196466
47	1	-3.391922	4.094617	0.581319
48	1	-5.082604	3.040426	-0.92573
49	1	-4.411393	0.99448	-2.266863
50	7	-1.573564	1.490569	-0.530152
51	7	-1.58857	-1.417836	0.714582
52	6	-1.634138	0.29492	2.40176
53	8	-0.371527	0.416045	2.073717
54	8	-2.24772	0.992407	3.205151
55	6	-1.917393	-0.216546	-2.186129
56	8	-0.636193	-0.415673	-1.999284
57	8	-2.659084	-0.875821	-2.909739
58	1	2.239388	-2.729523	-3.234175
59	1	0.623416	-1.987084	-3.015644
60	1	1.031375	-4.268456	-1.856627
61	1	2.262253	-3.439979	-0.882789
62	1	2.758679	2.596832	2.944373
63	1	1.050528	2.050477	2.950656
64	1	2.558975	3.235068	0.569413
65	1	1.524434	4.213534	1.628411
66	1	1.873604	-0.156667	3.407108
67	1	3.559183	0.43803	3.316508
68	1	3.506283	-1.98505	2.704292
69	1	3.947084	-0.988347	1.29421
70	1	2.048047	0.018778	-3.644829
71	6	4.033848	-0.884663	-3.498792
72	1	3.847105	0.672248	-1.269402
73	6	3.943723	2.015793	-2.942264
74	6	4.823062	0.122338	-4.351122
75	1	3.757303	-1.744656	-4.115674
76	1	4.665922	-1.259746	-2.683078
77	6	5.203901	1.362716	-3.534223
78	1	4.197837	2.888094	-2.330305
79	1	3.317191	2.362237	-3.773146
80	1	4.219143	0.425397	-5.216698
81	1	5.718453	-0.364886	-4.749545
82	1	5.890734	1.080013	-2.725676

83	1	5.73145	2.089104	-4.159996

Zero-point correction =	0.695086 (Hartree/Particle)
Thermal correction to Energy =	0.733681
Thermal correction to Enthalpy =	0.734625
Thermal correction to Gibbs Free Energy =	0.62815
Sum of electronic and zero-point Energies =	-2023.518951
Sum of electronic and thermal Energies =	-2023.480355
Sum of electronic and thermal Enthalpies =	-2023.479411
Sum of electronic and thermal Free Energies =	-2023.585886
E(SCF) in SMD solvation model =	-2024.310769

$[Gd(CHX\text{-}macropa)]^+$		($\Delta(\lambda\delta\delta)(\lambda\delta\delta)$)		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-3.722226	0.756937	-0.520285
2	7	-2.886556	0.446644	0.677207
3	8	-1.767684	1.741036	-1.489638
4	6	-2.913185	0.926945	-1.802716
5	6	-3.166997	1.399683	1.78298
6	6	-1.93141	1.746619	2.591773
7	8	-0.984476	2.326339	1.649632
8	6	-0.025777	3.298856	2.149864
9	6	1.210075	2.596963	2.707152
10	8	1.679508	1.747892	1.631053
11	8	0.91723	2.480561	-1.430612
12	6	-0.080039	3.242725	-2.13783
13	6	-1.175831	2.33848	-2.656878
14	7	2.816415	0.501665	-0.482149
15	6	3.151181	1.659149	-1.34696
16	6	2.017204	2.04581	-2.273447
17	6	2.68977	0.787429	2.009741
18	6	3.590641	0.566729	0.79597
19	6	-3.108325	-0.948713	1.130725
20	6	3.073952	-0.781413	-1.183878
21	6	2.530729	-1.916383	-0.344938
22	6	-2.588332	-1.922636	0.098793
23	6	0.967826	-2.487487	1.286147
24	6	1.466403	-3.783968	1.392714
25	6	2.541253	-4.142162	0.574826
26	6	3.097357	-3.193756	-0.288202
27	6	-3.180583	-3.162907	-0.161258
28	6	-2.639966	-3.9759	-1.160387
29	6	-1.551873	-3.516914	-1.907169
30	6	-1.028199	-2.262969	-1.599667
31	64	-0.023252	0.498952	0.051362
32	1	-4.260512	1.689961	-0.33683
33	1	-4.478192	-0.0222	-0.683254
34	1	-3.530366	1.446174	-2.547073
35	1	-2.572479	-0.020721	-2.227187
36	6	-0.599103	4.319322	3.136874
37	1	0.283196	3.828398	1.240473
38	1	0.388082	3.803377	-2.954211
39	1	-0.495328	3.948939	-1.413497
40	1	-1.933101	2.926294	-3.19198
41	1	-0.780034	1.553904	-3.311706
42	1	2.184806	-0.128369	2.328793

43	1	3.285545	1.172823	2.842574
44	1	4.323294	1.37762	0.732489
45	1	4.153106	-0.36098	0.945773
46	1	-4.177719	-1.137813	1.31503
47	1	-2.566225	-1.098912	2.069811
48	1	4.150463	-0.927899	-1.36474
49	1	2.558781	-0.763976	-2.149651
50	1	1.020008	-4.463032	2.110032
51	1	2.963093	-5.141079	0.627364
52	1	3.95875	-3.435394	-0.902167
53	1	-4.049076	-3.480183	0.40662
54	1	-3.081636	-4.945111	-1.370481
55	1	-1.113305	-4.084645	-2.719694
56	7	-1.515236	-1.507062	-0.596177
57	7	1.466208	-1.595975	0.409532
58	6	-0.133546	-1.939462	2.173077
59	8	-0.306834	-0.647848	2.036814
60	8	-0.761484	-2.68615	2.918784
61	6	0.087469	-1.613631	-2.397888
62	8	0.292394	-0.360955	-2.076231
63	8	0.695365	-2.257745	-3.248635
64	1	2.333449	2.891704	-2.895694
65	1	1.684559	1.215432	-2.902959
66	1	4.058073	1.467287	-1.942048
67	1	3.350322	2.514409	-0.697158
68	1	-2.212276	2.488197	3.342042
69	1	-1.479622	0.873495	3.068745
70	1	-3.538644	2.328497	1.344691
71	1	-3.945696	1.013263	2.458046
72	1	-1.484726	4.791102	2.697288
73	6	0.470705	5.365586	3.494733
74	1	-0.910544	3.825228	4.064851
75	6	2.272332	3.634153	3.103548
76	1	0.93355	1.964757	3.56297
77	1	0.752005	5.934659	2.598762
78	6	1.709233	4.677084	4.082325
79	1	0.05357	6.082598	4.208484
80	1	1.443088	4.190806	5.030174
81	1	2.485212	5.413229	4.314177
82	1	2.612056	4.133092	2.186487
83	1	3.144049	3.139768	3.544546

Zero-point correction =	0.694971 (Hartree/Particle)
Thermal correction to Energy =	0.733553
Thermal correction to Enthalpy =	0.734497
Thermal correction to Gibbs Free Energy =	0.62782
Sum of electronic and zero-point Energies =	-2023.521934
Sum of electronic and thermal Energies =	-2023.483353
Sum of electronic and thermal Enthalpies =	-2023.482409
Sum of electronic and thermal Free Energies =	-2023.589086
E(SCF) in SMD solvation model =	-2024.312748

$[Gd(CHX\text{-}macropa)]^+$		(Δ(δδλ)(δδλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	1.572158	3.302982	-0.635257
2	7	1.129809	2.562419	0.569513

3	8	2.428464	1.204685	-1.436276
4	6	2.679658	2.617257	-1.421284
5	6	2.142651	2.538091	1.649132
6	6	3.183074	1.430169	1.505722
7	8	2.520339	0.151094	1.48018
8	6	2.889635	-0.88101	2.449659
9	6	1.597765	-1.662401	2.706456
10	8	0.98481	-2.054724	1.443683
11	8	2.261602	-1.472612	-1.445472
12	6	3.551378	-0.868263	-1.641973
13	6	3.34315	0.487525	-2.283061
14	7	-0.175996	-2.688807	-1.056485
15	6	0.526482	-2.866954	-2.345419
16	6	2.025676	-2.65774	-2.233122
17	6	1.340445	-3.316448	0.854625
18	6	0.181723	-3.718128	-0.051141
19	6	-0.113765	3.214567	1.0715
20	6	-1.636269	-2.734247	-1.332612
21	6	-2.42926	-2.147374	-0.189821
22	6	-1.24384	3.002377	0.09027
23	6	-2.47627	-0.581257	1.529415
24	6	-3.767607	-0.947749	1.90344
25	6	-4.396742	-1.969608	1.191209
26	6	-3.713397	-2.591192	0.143813
27	6	-2.297456	3.903278	-0.088261
28	6	-3.275012	3.61754	-1.045988
29	6	-3.155328	2.468632	-1.831179
30	6	-2.063424	1.632168	-1.605975
31	64	0.420257	-0.088793	-0.114583
32	1	1.604654	2.359787	2.58299
33	1	2.661539	3.508022	1.733397
34	1	3.864057	1.496935	2.354617
35	1	3.777276	1.518374	0.594181
36	6	3.436966	-0.345772	3.781247
37	1	3.642777	-1.527216	1.974324
38	1	0.867981	-0.951649	3.104143
39	6	1.797563	-2.809618	3.696748
40	1	4.184835	-1.505806	-2.266942
41	1	4.017372	-0.755467	-0.658753
42	1	4.299053	1.023226	-2.342189
43	1	2.915379	0.402157	-3.288378
44	1	0.115049	-2.113238	-3.019185
45	1	0.347183	-3.869816	-2.768218
46	1	2.542287	-3.504794	-1.762409
47	1	2.439244	-2.522448	-3.239087
48	1	0.042738	4.291609	1.238729
49	1	-0.374648	2.7422	2.0232
50	1	-1.969481	-3.763849	-1.534213
51	1	-1.82494	-2.136471	-2.23156
52	1	-4.231401	-0.437316	2.739615
53	1	-5.398644	-2.292671	1.456441
54	1	-4.165724	-3.405726	-0.412646
55	1	-2.347247	4.809601	0.506424
56	1	-4.106207	4.300136	-1.193453
57	1	-3.862286	2.211702	-2.611461
58	7	-1.157358	1.879615	-0.642516
59	7	-1.835589	-1.148821	0.487823
60	6	-1.681751	0.458632	2.294503
61	8	-0.423492	0.513554	1.947073
62	8	-2.232123	1.145987	3.151852
63	6	-1.769138	0.397838	-2.435979
64	8	-0.593221	-0.116844	-2.191761

65	8	-2.606264	-0.029032	-3.229079
66	1	0.700505	3.39797	-1.285121
67	1	1.908504	4.320378	-0.374751
68	1	2.686336	3.007425	-2.446501
69	1	3.672473	2.79924	-0.986216
70	1	0.408561	-4.684028	-0.53014
71	1	-0.689255	-3.867099	0.592797
72	1	1.44428	-4.081385	1.628448
73	1	2.292628	-3.225786	0.32245
74	1	4.402757	0.148512	3.634779
75	6	3.617983	-1.479871	4.80666
76	1	2.735369	0.39861	4.179476
77	1	2.533182	-3.532145	3.31976
78	1	0.847965	-3.33888	3.832253
79	6	2.311978	-2.249189	5.032087
80	1	2.4683	-3.069072	5.739817
81	1	1.557089	-1.585043	5.471266
82	1	3.982517	-1.051918	5.745576
83	1	4.394191	-2.172245	4.453772

Zero-point correction =	0.694760 (Hartree/Particle)
Thermal correction to Energy =	0.733625
Thermal correction to Enthalpy =	0.734569
Thermal correction to Gibbs Free Energy =	0.626645
Sum of electronic and zero-point Energies =	-2023.520738
Sum of electronic and thermal Energies =	-2023.481874
Sum of electronic and thermal Enthalpies =	-2023.480929
Sum of electronic and thermal Free Energies =	-2023.588853
E(SCF) in SMD solvation model =	-2024.314927

$[Gd(CHX\text{-}macropa)]^+$		(Δ(δδδ)(δδδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	1.264026	3.458123	-0.662161
2	7	0.839715	2.749658	0.567485
3	8	1.884183	1.386616	-1.649392
4	6	2.370487	2.711388	-1.382124
5	6	1.842725	2.952903	1.640673
6	6	2.067766	1.706715	2.47178
7	8	2.513299	0.661783	1.556403
8	6	3.264009	-0.441617	2.151016
9	6	2.291709	-1.418272	2.819448
10	8	1.369854	-1.871053	1.769335
11	8	2.295697	-1.381762	-1.47741
12	6	3.257359	-0.517556	-2.110341
13	6	2.560662	0.687409	-2.712581
14	7	0.029248	-2.829157	-0.602754
15	6	0.995437	-3.376546	-1.590498
16	6	1.654339	-2.289369	-2.414153
17	6	1.375874	-3.273006	1.446989
18	6	0.119586	-3.592631	0.663019
19	6	-0.493153	3.243624	0.999656
20	6	-1.353267	-2.918556	-1.142011
21	6	-2.325101	-2.2171	-0.22073
22	6	-1.54698	2.845565	-0.009356
23	6	-2.572395	-0.580116	1.418007
24	6	-3.91233	-0.904546	1.619749

25	6	-4.464555	-1.928472	0.847352
26	6	-3.658666	-2.609489	-0.068794
27	6	-2.679406	3.61865	-0.28365
28	6	-3.566864	3.193215	-1.275521
29	6	-3.280327	2.035567	-2.001264
30	6	-2.125793	1.326158	-1.676332
31	64	0.436743	-0.058538	0.005488
32	6	4.40616	0.019921	3.066157
33	1	3.695227	-0.946954	1.278965
34	1	1.661396	-0.871894	3.529941
35	6	3.024255	-2.553204	3.553219
36	1	3.817856	-1.076361	-2.870128
37	1	3.947304	-0.20342	-1.322269
38	1	3.283192	1.348715	-3.202207
39	1	1.797155	0.389221	-3.436116
40	1	-0.487281	4.338794	1.119238
41	1	-0.724572	2.790626	1.968672
42	1	-1.655673	-3.970897	-1.264825
43	1	-1.366835	-2.437281	-2.125088
44	1	-4.474546	-0.364215	2.372539
45	1	-5.504243	-2.21418	0.973745
46	1	-4.052398	-3.435323	-0.652253
47	1	-2.855144	4.538002	0.265318
48	1	-4.455342	3.776637	-1.496374
49	1	-3.90627	1.675154	-2.809417
50	7	-1.304521	1.704229	-0.678606
51	7	-1.813499	-1.200004	0.494231
52	6	-1.846495	0.466732	2.238681
53	8	-0.563214	0.517957	1.99285
54	8	-2.465971	1.17093	3.032033
55	6	-1.673712	0.099489	-2.443091
56	8	-0.490427	-0.327812	-2.087767
57	8	-2.401242	-0.398427	-3.299279
58	1	1.595109	4.486329	-0.443895
59	1	2.588916	3.219499	-2.32851
60	1	3.296434	2.655376	-0.795064
61	1	0.088872	-4.679208	0.477342
62	1	-0.742742	-3.335846	1.281165
63	1	1.356475	-3.874403	2.358938
64	1	2.284387	-3.526485	0.886051
65	1	0.9226	-1.740586	-3.012049
66	1	2.425357	-2.731899	-3.056867
67	1	1.776459	-3.920064	-1.052479
68	1	0.506249	-4.095452	-2.26241
69	1	2.849433	1.921914	3.201442
70	1	1.151818	1.384262	2.971929
71	1	1.548459	3.779445	2.303341
72	1	2.79463	3.233569	1.181092
73	1	0.405973	3.516302	-1.335073
74	1	3.50609	-3.21688	2.825249
75	1	2.305199	-3.151976	4.121581
76	6	4.119738	-2.017723	4.487882
77	6	5.128929	-1.179735	3.695736
78	1	4.018497	0.625238	3.892146
79	1	5.090623	0.652103	2.489945
80	1	4.612457	-2.864318	4.975838
81	1	3.676167	-1.40617	5.284498
82	1	5.931009	-0.81861	4.34665
83	1	5.600532	-1.798395	2.920555

Zero-point correction = 0.695076 (Hartree/Particle)

Thermal correction to Energy =	0.733862
Thermal correction to Enthalpy =	0.734806
Thermal correction to Gibbs Free Energy =	0.62609
Sum of electronic and zero-point Energies =	-2023.520944
Sum of electronic and thermal Energies =	-2023.482159
Sum of electronic and thermal Enthalpies =	-2023.481214
Sum of electronic and thermal Free Energies =	-2023.589931
E(SCF) in SMD solvation model =	-2024.316075

$[Ho(CHX\text{-}macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.540028	-0.829093	-0.383112
2	7	2.817395	-0.325321	0.801937
3	8	1.595286	-2.035375	-1.100742
4	6	2.999948	-2.172963	-0.824588
5	6	3.184399	-1.115254	2.003412
6	6	1.980313	-1.422298	2.865096
7	8	0.987969	-2.080419	2.026175
8	6	0.149709	-2.942365	2.829086
9	6	-1.182932	-3.151978	2.123843
10	8	-1.685735	-1.827295	1.77824
11	8	-1.143846	-2.358851	-1.505281
12	6	-0.186484	-2.854989	-2.447984
13	6	1.067579	-3.22742	-1.706236
14	7	-2.860965	-0.389528	-0.342727
15	6	-3.348786	-1.477949	-1.222215
16	6	-2.306779	-1.900853	-2.230575
17	6	-3.120618	-1.71775	1.738536
18	6	-3.510797	-0.459957	0.985389
19	6	3.131327	1.104431	1.029048
20	6	-3.152041	0.914221	-0.991387
21	6	-2.54023	2.047805	-0.207982
22	6	2.574351	1.958448	-0.083849
23	6	-0.893745	2.635634	1.323159
24	6	-1.363637	3.942972	1.417262
25	6	-2.470026	4.299704	0.643103
26	6	-3.082796	3.335821	-0.161197
27	6	3.174517	3.153763	-0.494336
28	6	2.612899	3.86826	-1.554543
29	6	1.492001	3.351171	-2.206794
30	6	0.962929	2.147575	-1.748007
31	67	-0.042919	-0.398902	0.177918
32	1	4.219609	1.261509	1.104776
33	1	2.676948	1.406757	1.978525
34	1	-4.238992	1.070201	-1.083704
35	1	-2.720197	0.896682	-1.997549
36	1	-3.97087	3.572622	-0.737918
37	1	1.026932	3.836281	-3.05719
38	7	1.470776	1.48519	-0.689408
39	7	-1.444336	1.725258	0.498126
40	6	0.239753	2.095195	2.163346
41	8	0.401026	0.805086	2.024802
42	8	0.908168	2.841618	2.87433
43	6	-0.205808	1.462375	-2.418346
44	8	-0.449209	0.274068	-1.932793
45	8	-0.829029	2.022148	-3.317474
46	1	4.623079	-0.922329	-0.197411

47	1	3.513364	-2.486403	-1.742427
48	1	3.14181	-2.954471	-0.06723
49	1	-4.610803	-0.435841	0.906309
50	1	-3.199992	0.414285	1.559872
51	1	-3.518826	-1.663915	2.757633
52	1	-3.543354	-2.606221	1.259051
53	1	-2.00308	-1.078112	-2.884718
54	1	-2.698256	-2.732383	-2.832097
55	1	-3.600878	-2.346122	-0.611751
56	1	-4.267502	-1.178497	-1.749136
57	1	2.281219	-2.103525	3.667748
58	1	1.529207	-0.519555	3.280404
59	1	3.93781	-0.588341	2.605282
60	1	3.636247	-2.058339	1.684951
61	1	0.875576	-3.983701	-0.933438
62	1	1.798138	-3.630459	-2.418237
63	1	0.031984	-2.073808	-3.186177
64	1	-0.5914	-3.739059	-2.960003
65	1	3.400281	-0.116053	-1.198966
66	1	-1.031799	-3.695557	1.17892
67	6	-2.092763	-3.982218	3.045598
68	6	0.829702	-4.292388	3.094166
69	1	-0.056639	-2.422384	3.775391
70	1	-2.871578	5.307327	0.686266
71	1	-0.869922	4.631015	2.093736
72	1	3.060942	4.801694	-1.880798
73	1	4.067777	3.509962	0.008336
74	6	-0.057579	-5.184476	3.974786
75	1	1.803142	-4.135088	3.569984
76	1	1.019268	-4.780157	2.128766
77	6	-1.446182	-5.346517	3.346798
78	1	-0.153876	-4.734272	4.971456
79	1	0.416428	-6.161092	4.113949
80	1	-3.070322	-4.146388	2.585085
81	1	-2.256715	-3.43286	3.981593
82	1	-2.105419	-5.916998	4.008363
83	1	-1.362836	-5.919649	2.413544

Zero-point correction =	0.695371 (Hartree/Particle)
Thermal correction to Energy =	0.734049
Thermal correction to Enthalpy =	0.734993
Thermal correction to Gibbs Free Energy =	0.627288
Sum of electronic and zero-point Energies =	-2025.280109
Sum of electronic and thermal Energies =	-2025.241431
Sum of electronic and thermal Enthalpies =	-2025.240487
Sum of electronic and thermal Free Energies =	-2025.348191
E(SCF) in SMD solvation model =	-2026.078449

$[Tm(CHX\text{-}macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.527058	-0.86874	-0.263867
2	7	2.792657	-0.307138	0.88591
3	8	1.564021	-2.012968	-1.038048
4	6	2.947157	-2.202555	-0.683369
5	6	3.142293	-1.042211	2.128633
6	6	1.92137	-1.34603	2.972418

7	8	0.97193	-2.027305	2.112296
8	6	0.111322	-2.928418	2.841711
9	6	-1.081197	-3.193439	1.933423
10	8	-1.630676	-1.893914	1.557186
11	8	-1.161765	-2.358296	-1.394279
12	6	-0.23433	-2.772882	-2.404442
13	6	1.05109	-3.164368	-1.728948
14	7	-2.864573	-0.36282	-0.197757
15	6	-3.364542	-1.534781	-0.949742
16	6	-2.397333	-1.964932	-2.028596
17	6	-2.964498	-1.558749	1.97794
18	6	-3.422255	-0.340383	1.172283
19	6	3.106296	1.129993	1.045113
20	6	-3.197462	0.886178	-0.926253
21	6	-2.545246	2.065348	-0.246653
22	6	2.561982	1.93248	-0.112807
23	6	-0.867672	2.694163	1.234255
24	6	-1.31286	4.012958	1.274165
25	6	-2.419145	4.353316	0.491515
26	6	-3.064121	3.363565	-0.255414
27	6	3.176745	3.10368	-0.569403
28	6	2.629828	3.780535	-1.661162
29	6	1.504625	3.251376	-2.295298
30	6	0.958685	2.074145	-1.790383
31	69	-0.0736	-0.377211	0.196894
32	1	4.194015	1.291611	1.123017
33	1	2.645829	1.479819	1.975378
34	1	-4.287374	1.039139	-0.977173
35	1	-2.811448	0.7972	-1.946841
36	1	-3.959766	3.58897	-0.824954
37	1	1.046077	3.707969	-3.164809
38	7	1.456377	1.445163	-0.705724
39	7	-1.43953	1.762746	0.451015
40	6	0.23744	2.147362	2.107313
41	8	0.355391	0.847057	2.016232
42	8	0.919104	2.894276	2.805257
43	6	-0.226372	1.3916	-2.43542
44	8	-0.502579	0.229911	-1.903527
45	8	-0.831206	1.929992	-3.358975
46	1	4.600839	-0.996249	-0.046768
47	1	3.489076	-2.573336	-1.562381
48	1	3.013313	-2.958905	0.108953
49	1	-4.524364	-0.31618	1.170699
50	1	-3.070795	0.57088	1.657221
51	1	-2.985421	-1.322319	3.04789
52	1	-3.626054	-2.410601	1.803223
53	1	-2.181589	-1.158647	-2.736793
54	1	-2.808654	-2.829247	-2.5674
55	1	-3.491491	-2.368338	-0.256701
56	1	-4.348572	-1.33005	-1.399477
57	1	2.209851	-2.007682	3.795795
58	1	1.451497	-0.439712	3.357674
59	1	3.871052	-0.477618	2.726146
60	1	3.619354	-1.987943	1.855822
61	1	0.900885	-3.987776	-1.017458
62	1	1.774246	-3.485617	-2.488941
63	1	-0.06363	-1.942453	-3.099496
64	1	-0.639258	-3.635498	-2.951628
65	1	3.43751	-0.175543	-1.103716
66	1	-0.712513	-3.616278	0.989811
67	6	-2.06658	-4.18489	2.559868
68	6	0.827688	-4.239456	3.191339

69	1	-0.239004	-2.421988	3.753271
70	1	-2.801347	5.369347	0.490911
71	1	-0.806551	4.721846	1.919065
72	1	3.09058	4.694504	-2.022911
73	1	4.070574	3.470504	-0.075424
74	6	-0.143987	-5.238719	3.83664
75	1	1.673512	-4.045186	3.858727
76	1	1.238389	-4.662916	2.265163
77	6	-1.341774	-5.496821	2.914494
78	1	-0.497192	-4.843269	4.79819
79	1	0.378359	-6.175445	4.054299
80	1	-2.884702	-4.394919	1.863047
81	1	-2.505655	-3.758427	3.470222
82	1	-2.053277	-6.181715	3.385877
83	1	-0.996719	-5.98341	1.992406

Zero-point correction =	0.695073 (Hartree/Particle)
Thermal correction to Energy =	0.733808
Thermal correction to Enthalpy =	0.734752
Thermal correction to Gibbs Free Energy =	0.627265
Sum of electronic and zero-point Energies =	-2026.440025
Sum of electronic and thermal Energies =	-2026.40129
Sum of electronic and thermal Enthalpies =	-2026.400346
Sum of electronic and thermal Free Energies =	-2026.507833
E(SCF) in SMD solvation model =	-2027.235764

$[Lu(CHX\text{-}macropa)]^+$		(Δ(δλδ)(δλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.525957	-0.862861	-0.249975
2	7	2.794192	-0.298456	0.898803
3	8	1.557051	-2.002192	-1.022115
4	6	2.939706	-2.194885	-0.664996
5	6	3.143243	-1.029739	2.143112
6	6	1.9194	-1.34394	2.978863
7	8	0.977635	-2.022921	2.109659
8	6	0.11545	-2.928561	2.830145
9	6	-1.073517	-3.185201	1.915673
10	8	-1.619926	-1.882686	1.544645
11	8	-1.166169	-2.361986	-1.377382
12	6	-0.238439	-2.773635	-2.387744
13	6	1.04863	-3.156775	-1.711653
14	7	-2.864833	-0.359607	-0.191916
15	6	-3.367825	-1.53698	-0.932818
16	6	-2.403507	-1.974913	-2.010859
17	6	-2.94251	-1.536921	1.992083
18	6	-3.416193	-0.327985	1.179921
19	6	3.101502	1.139145	1.053147
20	6	-3.196896	0.884219	-0.928428
21	6	-2.537714	2.064159	-0.257093
22	6	2.551856	1.933616	-0.107656
23	6	-0.862035	2.687265	1.227957
24	6	-1.302452	4.007556	1.267328
25	6	-2.404006	4.352311	0.47978
26	6	-3.051	3.364612	-0.268124
27	6	3.162939	3.1041	-0.571272
28	6	2.615804	3.772359	-1.668005

29	6	1.493677	3.2349	-2.300444
30	6	0.950687	2.059858	-1.787689
31	71	-0.078174	-0.367286	0.198706
32	1	4.188465	1.307712	1.128557
33	1	2.641218	1.490209	1.98304
34	1	-4.286343	1.041612	-0.976062
35	1	-2.815595	0.786756	-1.949972
36	1	-3.94498	3.592933	-0.839117
37	1	1.035327	3.683268	-3.17433
38	7	1.447699	1.439067	-0.697774
39	7	-1.433586	1.758415	0.441659
40	6	0.23299	2.131526	2.107102
41	8	0.346374	0.8311	2.008199
42	8	0.910685	2.870396	2.817164
43	6	-0.230324	1.368724	-2.429144
44	8	-0.505251	0.212288	-1.885117
45	8	-0.834093	1.894581	-3.36046
46	1	4.599638	-0.994536	-0.0343
47	1	3.480217	-2.57183	-1.542197
48	1	3.001809	-2.94799	0.130657
49	1	-4.518391	-0.312635	1.18394
50	1	-3.069675	0.590026	1.655225
51	1	-2.937735	-1.2879	3.059347
52	1	-3.609811	-2.388848	1.84252
53	1	-2.191077	-1.173701	-2.725817
54	1	-2.815461	-2.843422	-2.542439
55	1	-3.492741	-2.364827	-0.232484
56	1	-4.353249	-1.335451	-1.380948
57	1	2.206425	-2.009868	3.799445
58	1	1.444149	-0.442206	3.368037
59	1	3.863576	-0.459053	2.744986
60	1	3.630307	-1.971329	1.873328
61	1	0.902676	-3.979785	-0.998813
62	1	1.773507	-3.475753	-2.470926
63	1	-0.072598	-1.943898	-3.084722
64	1	-0.639035	-3.639725	-2.93272
65	1	3.438493	-0.171067	-1.091219
66	1	-0.702198	-3.600208	0.969969
67	6	-2.062588	-4.180528	2.529527
68	6	0.829496	-4.24299	3.171718
69	1	-0.237215	-2.429238	3.744809
70	1	-2.782187	5.369837	0.477579
71	1	-0.797178	4.714032	1.915676
72	1	3.074262	4.685341	-2.035103
73	1	4.055327	3.47631	-0.078705
74	6	-0.145591	-5.247662	3.803361
75	1	1.67237	-4.054902	3.844616
76	1	1.244354	-4.658342	2.243715
77	6	-1.340013	-5.496506	2.874075
78	1	-0.502637	-4.861058	4.767101
79	1	0.375213	-6.186747	4.014494
80	1	-2.879186	-4.382381	1.828267
81	1	-2.503435	-3.762972	3.44317
82	1	-2.05372	-6.185263	3.33642
83	1	-0.991876	-5.974746	1.948785

Zero-point correction =	0.695197 (Hartree/Particle)
Thermal correction to Energy =	0.733896
Thermal correction to Enthalpy =	0.73484
Thermal correction to Gibbs Free Energy =	0.627457

Sum of electronic and zero-point Energies =	-2027.573571
Sum of electronic and thermal Energies =	-2027.534873
Sum of electronic and thermal Enthalpies =	-2027.533929
Sum of electronic and thermal Free Energies =	-2027.641312
E(SCF) in SMD solvation model =	-2028.369889

$[Lu(CHX\text{-}macropa)]^+$		(Δ(λδλ)(λδλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-0.639702	-3.618177	0.544658
2	7	-0.605859	-2.714662	-0.637216
3	8	0.947313	-2.141967	1.521081
4	6	-0.254483	-2.886641	1.825171
5	6	0.310027	-3.203212	-1.68559
6	6	1.760891	-3.020702	-1.275498
7	8	2.031723	-1.612231	-1.085843
8	6	3.06702	-1.049984	-1.909741
9	6	2.596691	0.297216	-2.405607
10	8	2.225834	1.054757	-1.238397
11	8	2.3675	0.060211	1.689788
12	6	3.043653	-1.174106	2.05547
13	6	1.945335	-2.100743	2.570543
14	7	1.192412	2.542395	0.83456
15	6	1.964933	2.378863	2.082445
16	6	3.033484	1.312522	1.942139
17	6	1.976523	2.442017	-1.541603
18	6	2.007175	3.198913	-0.221793
19	6	-1.959721	-2.508521	-1.193388
20	6	-0.047345	3.304869	1.107692
21	6	-1.03041	3.111746	-0.021029
22	6	-2.768136	-1.636709	-0.262562
23	6	-1.727369	1.696818	-1.730071
24	6	-2.686514	2.604785	-2.171825
25	6	-2.809148	3.816074	-1.487176
26	6	-1.957165	4.083686	-0.413425
27	6	-4.157294	-1.739113	-0.13088
28	6	-4.818056	-0.909791	0.777576
29	6	-4.072723	-0.029558	1.56534
30	6	-2.691833	0.000117	1.387103
31	71	0.369028	-0.088919	0.118086
32	1	0.059723	-4.446992	0.387284
33	1	-1.636507	-4.060768	0.664514
34	1	-0.064076	-3.606542	2.625035
35	1	-1.0206	-2.183522	2.158271
36	1	0.123286	-2.605675	-2.580291
37	1	0.134714	-4.265884	-1.924811
38	1	2.420292	-3.414562	-2.055079
39	1	1.990207	-3.529529	-0.33513
40	1	3.269229	-1.702216	-2.765461
41	1	3.982589	-0.950298	-1.31395
42	1	1.726334	0.193666	-3.060707
43	1	3.414413	0.808035	-2.929842
44	1	1.262213	2.059051	2.854824
45	1	2.440963	3.322617	2.396113
46	1	3.739571	1.521379	1.128748
47	1	3.587599	1.263285	2.880899
48	1	1.019385	2.532131	-2.062634
49	1	2.77405	2.813013	-2.197695
50	1	3.046108	3.256342	0.116326

51	1	1.671128	4.230096	-0.392116
52	1	-2.482269	-3.465212	-1.351114
53	1	-1.86634	-2.011517	-2.164883
54	1	0.16309	4.377304	1.24239
55	1	-0.487641	2.928128	2.037453
56	1	-3.289173	2.351754	-3.036502
57	1	-3.539003	4.555892	-1.801123
58	1	-2.002008	5.031938	0.112315
59	1	-4.704693	-2.461616	-0.727571
60	1	-5.896343	-0.971171	0.887666
61	1	-4.518017	0.61356	2.315618
62	7	-2.060676	-0.755997	0.467022
63	7	-0.947276	1.929693	-0.656062
64	6	-1.429416	0.399199	-2.447708
65	8	-0.365215	-0.208126	-1.99443
66	8	-2.159584	0.011438	-3.358324
67	6	-1.768486	0.84153	2.241213
68	8	-0.5039	0.573671	2.050628
69	8	-2.229797	1.682908	3.01037
70	6	4.159365	-1.041151	3.098156
71	1	3.460547	-1.601725	1.132788
72	6	2.522661	-3.488239	2.881599
73	1	1.491953	-1.65199	3.464861
74	1	2.905571	-3.925668	1.949955
75	1	1.743135	-4.158155	3.256971
76	6	3.655729	-3.386276	3.914522
77	1	3.760648	-0.587905	4.014998
78	1	4.954605	-0.389716	2.722237
79	6	4.745696	-2.425782	3.427552
80	1	4.073996	-4.380417	4.099784
81	1	3.249879	-3.030299	4.870379
82	1	5.528306	-2.313284	4.184111
83	1	5.227961	-2.83994	2.532094

Zero-point correction =	0.695369 (Hartree/Particle)
Thermal correction to Energy =	0.733862
Thermal correction to Enthalpy =	0.734806
Thermal correction to Gibbs Free Energy =	0.62819
Sum of electronic and zero-point Energies =	-2027.579304
Sum of electronic and thermal Energies =	-2027.540811
Sum of electronic and thermal Enthalpies =	-2027.539867
Sum of electronic and thermal Free Energies =	-2027.646483
E(SCF) in SMD solvation model =	-2028.368598

$[Lu(CHX\text{-}macropa)]^+$		(Δ(λλλ)(λλλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.633531	-0.836277	-0.270566
2	7	2.765172	-0.396871	0.852044
3	8	1.681648	-1.831852	-1.232433
4	6	2.852482	-1.050436	-1.561871
5	6	2.909849	-1.278642	2.026832
6	6	2.23355	-2.615063	1.761972
7	8	0.807954	-2.455118	1.595497
8	6	0.094847	-2.475927	2.849413
9	6	-1.362122	-2.668027	2.502996
10	8	-1.740119	-1.658784	1.545873

11	8	-0.871885	-2.564866	-1.236498
12	6	-0.146221	-2.763639	-2.494551
13	6	1.298465	-2.984679	-2.050744
14	7	-2.840426	-0.42379	-0.622394
15	6	-2.984861	-1.414745	-1.705482
16	6	-2.307784	-2.713315	-1.296261
17	6	-2.936993	-0.903778	1.835754
18	6	-3.716403	-0.759184	0.530917
19	6	3.031707	1.010199	1.21633
20	6	-3.085796	0.948594	-1.105985
21	6	-2.528905	1.939795	-0.110983
22	6	2.481078	1.930707	0.152092
23	6	-0.967108	2.297824	1.57388
24	6	-1.454967	3.575927	1.836792
25	6	-2.525413	4.041569	1.069949
26	6	-3.083914	3.206639	0.100179
27	6	3.041071	3.178573	-0.143882
28	6	2.48553	3.9486	-1.167692
29	6	1.413977	3.436804	-1.903194
30	6	0.921926	2.180964	-1.556457
31	71	-0.019905	-0.528852	0.096884
32	1	4.124814	-1.776672	0.001981
33	1	4.431398	-0.104142	-0.452566
34	1	3.484191	-1.574831	-2.278183
35	1	2.522377	-0.111382	-2.008513
36	1	-2.64347	0.059756	2.257583
37	1	-3.541391	-1.446196	2.570061
38	1	-4.23445	-1.701709	0.324578
39	1	-4.493469	0.004439	0.66372
40	1	4.109904	1.197031	1.342736
41	1	2.540229	1.22449	2.171202
42	1	-4.15941	1.141552	-1.258821
43	1	-2.581354	1.075144	-2.069641
44	1	-1.002023	4.155985	2.632507
45	1	-2.939711	5.029999	1.243098
46	1	-3.942766	3.524236	-0.482362
47	1	3.900865	3.53174	0.416302
48	1	2.903597	4.921726	-1.406082
49	1	0.964204	3.964024	-2.736573
50	7	1.417991	1.465174	-0.527299
51	7	-1.466548	1.515296	0.596767
52	6	0.128126	1.654892	2.396913
53	8	0.334364	0.400309	2.096925
54	8	0.731007	2.309367	3.246034
55	6	-0.171197	1.484703	-2.338599
56	8	-0.377446	0.251877	-1.957043
57	8	-0.771179	2.081833	-3.230494
58	1	0.252193	-1.531101	3.378072
59	1	0.445814	-3.320873	3.454855
60	1	-1.973221	-2.583686	3.406224
61	1	-1.526225	-3.64849	2.042623
62	1	1.307143	-3.839793	-1.362389
63	6	2.223995	-3.28386	-3.232444
64	1	-2.598687	-3.005871	-0.285634
65	1	-2.57524	-3.527737	-1.970285
66	1	-4.043267	-1.607488	-1.949037
67	1	-2.494913	-1.007301	-2.59317
68	1	2.4205	-3.316986	2.582657
69	1	2.583607	-3.06683	0.831895
70	1	3.96741	-1.448434	2.289501
71	1	2.421975	-0.781654	2.868511
72	6	-0.654219	-3.962198	-3.307905

73	1	-0.215832	-1.833904	-3.072254
74	1	-0.717363	-4.841511	-2.652712
75	6	0.277094	-4.265764	-4.493093
76	1	-1.657894	-3.764649	-3.695572
77	6	1.710453	-4.503354	-4.014789
78	1	3.239102	-3.483992	-2.87322
79	1	2.26843	-2.418512	-3.905422
80	1	0.25889	-3.425725	-5.199474
81	1	-0.10163	-5.13994	-5.03158
82	1	1.746807	-5.395455	-3.37587
83	1	2.376312	-4.692065	-4.862401

Zero-point correction =	0.695962 (Hartree/Particle)
Thermal correction to Energy =	0.734254
Thermal correction to Enthalpy =	0.735198
Thermal correction to Gibbs Free Energy =	0.629297
Sum of electronic and zero-point Energies =	-2027.573719
Sum of electronic and thermal Energies =	-2027.535426
Sum of electronic and thermal Enthalpies =	-2027.534482
Sum of electronic and thermal Free Energies =	-2027.640383
E(SCF) in SMD solvation model =	-2028.361864

$[Lu(CHX\text{-}macropa)]^+$		(Δ(δλλ)(δλλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	3.307188	-1.200573	-0.702609
2	7	2.754364	-0.523476	0.487396
3	8	1.165179	-1.995763	-1.433709
4	6	2.494068	-2.424524	-1.052617
5	6	3.347123	-1.171112	1.696057
6	6	2.727116	-0.841723	3.067255
7	8	1.844674	-1.867392	3.544664
8	6	0.440725	-1.614503	3.417901
9	6	-0.002082	-2.302628	2.10302
10	8	-1.109076	-1.58584	1.446048
11	8	-1.519808	-2.000848	-1.736206
12	6	-0.706824	-2.361073	-2.858504
13	6	0.549847	-2.967954	-2.299428
14	7	-3.020392	-0.324588	-0.07254
15	6	-3.632826	-1.398096	-0.895193
16	6	-2.840131	-1.616067	-2.162004
17	6	-2.464696	-1.749928	1.89814
18	6	-3.280419	-0.570081	1.368809
19	6	3.164041	0.896758	0.478125
20	6	-3.569745	0.98416	-0.521702
21	6	-2.848076	2.128665	0.143556
22	6	2.626321	1.688196	-0.694901
23	6	-0.889392	2.742635	1.239183
24	6	-1.374404	4.018002	1.515911
25	6	-2.658413	4.341601	1.068847
26	6	-3.420104	3.377554	0.401372
27	6	3.393683	2.726117	-1.238785
28	6	2.889001	3.485412	-2.293986
29	6	1.62956	3.174442	-2.804744
30	6	0.925752	2.120823	-2.227301
31	71	-0.317828	-0.131319	-0.234407
32	1	4.264964	0.976999	0.466857

33	1	2.806469	1.367789	1.399917
34	1	-4.650791	1.047578	-0.324554
35	1	-3.410995	1.044397	-1.603605
36	1	-0.759464	4.705657	2.084918
37	1	4.377299	2.930928	-0.828936
38	7	1.401708	1.396656	-1.186585
39	7	-1.59504	1.845247	0.526226
40	6	0.409292	2.183198	1.774111
41	8	0.531782	0.904847	1.533868
42	8	1.210895	2.893118	2.376808
43	6	-0.441069	1.728	-2.751354
44	8	-0.96778	0.696479	-2.128902
45	8	-0.950411	2.350332	-3.673156
46	1	4.36291	-1.486575	-0.559414
47	1	2.95233	-2.939664	-1.904625
48	1	2.418281	-3.136259	-0.220594
49	1	-4.347939	-0.760138	1.561921
50	1	-2.993324	0.328352	1.918262
51	1	-2.503461	-1.741915	2.990533
52	1	-2.843526	-2.716228	1.547419
53	1	-2.765194	-0.715336	-2.780388
54	1	-3.282567	-2.431973	-2.74786
55	1	-3.621522	-2.328554	-0.323371
56	1	-4.681727	-1.166361	-1.12945
57	1	3.541171	-0.808336	3.797635
58	1	2.221681	0.128821	3.057241
59	1	4.421869	-0.918412	1.723026
60	1	3.285247	-2.256814	1.571819
61	1	0.326033	-3.878948	-1.729898
62	1	1.237835	-3.215924	-3.116848
63	1	-0.495326	-1.468565	-3.459441
64	1	-1.228066	-3.103046	-3.47734
65	1	3.263992	-0.517142	-1.554814
66	6	-0.217917	-3.817879	2.215221
67	1	0.811323	-2.120676	1.390641
68	6	-0.237002	-2.158628	4.680207
69	6	-0.222564	-3.691319	4.740299
70	1	-1.274933	-1.798125	4.716664
71	1	0.277116	-1.726064	5.54393
72	6	-0.914712	-4.285064	3.505433
73	1	0.786125	-4.259825	2.202755
74	1	-0.732442	-4.181102	1.317284
75	1	-0.891258	-5.379489	3.539885
76	1	-1.975166	-4.000802	3.506012
77	1	-0.716549	-4.035771	5.654441
78	1	0.816626	-4.038326	4.784263
79	1	-4.43964	3.586557	0.094319
80	1	-3.078988	5.322159	1.26843
81	1	1.174107	3.708427	-3.630567
82	1	3.474877	4.296335	-2.71513
83	1	0.265304	-0.539089	3.31103

Zero-point correction =	0.69413 (Hartree/particle)
Thermal correction to Energy =	0.733069
Thermal correction to Enthalpy =	0.734014
Thermal correction to Gibbs Free Energy =	0.625498
Sum of electronic and zero-point Energies =	-2027.556421
Sum of electronic and thermal Energies =	-2027.517482
Sum of electronic and thermal Enthalpies =	-2027.516538

Sum of electronic and thermal Free Energies =	-2027.625054
E(SCF) in SMD solvation model =	-2028.357091

[Lu(CHX-macropa)]$^{+}$		(Δ(λλδ)(λλδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	0.872413	3.506724	-1.153292
2	7	0.650771	2.927587	0.201511
3	8	2.113045	1.478502	-1.402827
4	6	1.298196	2.420079	-2.143454
5	6	1.751816	3.321014	1.108875
6	6	1.981323	2.323667	2.222941
7	8	2.415825	1.087219	1.608837
8	6	3.076187	0.200466	2.539789
9	6	3.22454	-1.123639	1.800191
10	8	1.94032	-1.547203	1.270171
11	8	2.189987	-1.247463	-1.738073
12	6	2.654769	-0.411176	-2.804213
13	6	3.16803	0.84949	-2.150391
14	7	0.265645	-2.821473	-0.228967
15	6	1.324354	-3.377405	-1.098793
16	6	1.651403	-2.477425	-2.268027
17	6	1.041277	-2.340587	2.083221
18	6	0.406959	-3.376273	1.146438
19	6	-0.66479	3.330042	0.743526
20	6	-1.083882	-3.073107	-0.776555
21	6	-2.08595	-2.307903	0.057363
22	6	-1.746667	2.716816	-0.115769
23	6	-2.35513	-0.525654	1.528674
24	6	-3.6742	-0.874673	1.806577
25	6	-4.208202	-1.987928	1.152121
26	6	-3.400007	-2.729316	0.286387
27	6	-2.994469	3.306195	-0.34517
28	6	-3.885438	2.686562	-1.225238
29	6	-3.496658	1.520519	-1.89014
30	6	-2.235386	1.000333	-1.61049
31	71	0.523214	0.041614	-0.029978
32	1	1.635359	4.291448	-1.101216
33	1	-0.044865	3.97519	-1.522349
34	1	1.888805	2.845749	-2.961946
35	1	0.437991	1.885949	-2.557831
36	1	0.292129	-1.669687	2.512625
37	1	1.58497	-2.833587	2.889945
38	1	1.012434	-4.290265	1.118454
39	1	-0.572892	-3.65364	1.544825
40	1	-0.778717	4.425805	0.762678
41	1	-0.754271	2.959706	1.770323
42	1	-1.335323	-4.145814	-0.772264
43	1	-1.118198	-2.718657	-1.812104
44	1	-3.774093	-3.626388	-0.196043
45	1	-4.125565	1.019283	-2.616836
46	7	-1.402122	1.565053	-0.716483
47	7	-1.598625	-1.201323	0.643792
48	6	-1.620893	0.598816	2.223872
49	8	-0.347553	0.641594	1.91618
50	8	-2.209696	1.359819	2.986544
51	6	-1.65304	-0.209827	-2.307771
52	8	-0.397295	-0.421922	-1.996522
53	8	-2.335308	-0.884055	-3.073984
54	1	2.417697	-2.957813	-2.890859

55	1	0.774231	-2.240759	-2.878768
56	1	1.05196	-4.377989	-1.472173
57	1	2.22754	-3.481051	-0.49335
58	1	2.773987	2.70978	2.871203
59	1	1.081335	2.12457	2.811228
60	1	2.667976	3.370358	0.515927
61	1	1.573916	4.319255	1.540819
62	1	1.826333	-0.199479	-3.492191
63	1	3.461117	-0.916768	-3.35344
64	1	3.94659	0.609558	-1.421299
65	1	3.574338	1.549313	-2.888443
66	6	3.960442	-2.176216	2.631918
67	1	3.805245	-0.93307	0.889411
68	6	4.465057	0.719757	2.948589
69	1	2.431948	0.069597	3.422061
70	6	5.358226	-1.652069	3.005334
71	6	5.241764	-0.325348	3.766956
72	1	4.376888	1.645365	3.525343
73	1	5.017638	0.961345	2.031056
74	1	4.731398	-0.497599	4.723809
75	1	6.234789	0.066939	4.007507
76	1	5.877519	-2.400181	3.612091
77	1	5.956308	-1.507858	2.095888
78	1	4.026149	-3.1112	2.064769
79	1	3.417146	-2.386089	3.561245
80	1	-4.859788	3.12752	-1.411752
81	1	-3.254769	4.236565	0.148871
82	1	-5.232055	-2.297222	1.338112
83	1	-4.234782	-0.28931	2.526261

Zero-point correction =	0.694866 (Hartree/Particle)
Thermal correction to Energy =	0.733579
Thermal correction to Enthalpy =	0.734523
Thermal correction to Gibbs Free Energy =	0.627388
Sum of electronic and zero-point Energies =	-2027.568105
Sum of electronic and thermal Energies =	-2027.529392
Sum of electronic and thermal Enthalpies =	-2027.528447
Sum of electronic and thermal Free Energies =	-2027.635583
E(SCF) in SMD solvation model =	-2028.358228

[Lu(CHX-macropa)]$^+$		(Δ(λδδ)(λδδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	-3.695385	0.781216	-0.490416
2	7	-2.867114	0.461493	0.704521
3	8	-1.696701	1.691556	-1.42916
4	6	-2.872689	0.934168	-1.767113
5	6	-3.109145	1.421601	1.808926
6	6	-1.835027	1.792179	2.544182
7	8	-0.916905	2.305108	1.534895
8	6	0.061894	3.2924	1.9587
9	6	1.26304	2.60339	2.596183
10	8	1.691953	1.645533	1.599858
11	8	0.963289	2.431676	-1.313576
12	6	-0.026261	3.233025	-1.988296
13	6	-1.113693	2.354687	-2.562549
14	7	2.865703	0.444892	-0.456193

15	6	3.206726	1.61902	-1.288166
16	6	2.062442	2.043939	-2.182861
17	6	2.70511	0.710315	2.025194
18	6	3.626427	0.470674	0.828031
19	6	-3.088521	-0.931708	1.149705
20	6	3.094179	-0.826899	-1.179453
21	6	2.507748	-1.952083	-0.356763
22	6	-2.556057	-1.892204	0.111252
23	6	0.932611	-2.481007	1.274113
24	6	1.398816	-3.7886	1.38668
25	6	2.460641	-4.177457	0.565792
26	6	3.039454	-3.244383	-0.298725
27	6	-3.148676	-3.127987	-0.169826
28	6	-2.611751	-3.925774	-1.18267
29	6	-1.52549	-3.454038	-1.923898
30	6	-0.998442	-2.208321	-1.592012
31	71	0.011985	0.457654	0.059299
32	1	-4.216002	1.725229	-0.312223
33	1	-4.465933	0.016067	-0.653538
34	1	-3.458743	1.493999	-2.506767
35	1	-2.573809	-0.019731	-2.208298
36	6	-0.489705	4.424841	2.829367
37	1	0.406097	3.719058	1.009406
38	1	0.451158	3.837755	-2.766644
39	1	-0.452744	3.897183	-1.231472
40	1	-1.875271	2.968151	-3.061345
41	1	-0.71387	1.613202	-3.263226
42	1	2.204873	-0.202234	2.357535
43	1	3.276514	1.124966	2.860424
44	1	4.38598	1.258071	0.7837
45	1	4.157257	-0.475715	0.975384
46	1	-4.158585	-1.130756	1.321597
47	1	-2.555879	-1.088735	2.092845
48	1	4.167043	-1.007674	-1.352315
49	1	2.590399	-0.779653	-2.150113
50	1	0.939667	-4.452061	2.110498
51	1	2.856861	-5.186723	0.619548
52	1	3.895541	-3.507545	-0.911326
53	1	-4.01854	-3.451362	0.39253
54	1	-3.055752	-4.890261	-1.408878
55	1	-1.09118	-4.005012	-2.75013
56	7	-1.479354	-1.467208	-0.57386
57	7	1.4484	-1.603693	0.393438
58	6	-0.146692	-1.894995	2.159714
59	8	-0.303485	-0.605263	1.984669
60	8	-0.773286	-2.605513	2.940387
61	6	0.113274	-1.54443	-2.378861
62	8	0.339989	-0.309629	-2.004973
63	8	0.699357	-2.154687	-3.26833
64	1	2.366841	2.921585	-2.765559
65	1	1.729149	1.243665	-2.848904
66	1	4.101566	1.43628	-1.904541
67	1	3.427901	2.451829	-0.616674
68	1	-2.066816	2.577899	3.265622
69	1	-1.376775	0.936713	3.043604
70	1	-3.520597	2.338442	1.380935
71	1	-3.843525	1.033401	2.530537
72	6	2.360715	3.632522	2.905015
73	1	0.958304	2.064506	3.504547
74	6	1.823106	4.789851	3.764809
75	1	2.730803	4.024924	1.948771
76	1	3.206755	3.153916	3.408993

77	6	0.617905	5.459921	3.092372
78	1	2.623194	5.517355	3.933633
79	1	1.527886	4.412097	4.752697
80	1	0.930018	5.921346	2.146007
81	1	0.224002	6.262982	3.722768
82	1	-0.830185	4.041273	3.798193
83	1	-1.351676	4.880799	2.330288

Zero-point correction =	0.695632 (Hartree/Particle)
Thermal correction to Energy =	0.73404
Thermal correction to Enthalpy =	0.734984
Thermal correction to Gibbs Free Energy =	0.62883
Sum of electronic and zero-point Energies =	-2027.572326
Sum of electronic and thermal Energies =	-2027.533918
Sum of electronic and thermal Enthalpies =	-2027.532974
Sum of electronic and thermal Free Energies =	-2027.639128
E(SCF) in SMD solvation model =	-2028.362565

$[Lu(CHX\text{-}macropa)]^+$		(Δ(δδλ)(δδλ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	1.484456	3.302859	-0.672298
2	7	1.070943	2.572106	0.547173
3	8	2.302369	1.185921	-1.457028
4	6	2.558423	2.596305	-1.485221
5	6	2.098696	2.568389	1.608049
6	6	3.142886	1.470252	1.4375
7	8	2.492796	0.182977	1.425196
8	6	2.870375	-0.825112	2.42055
9	6	1.574845	-1.572215	2.740016
10	8	0.930689	-1.99255	1.501164
11	8	2.241821	-1.493914	-1.278964
12	6	3.502532	-0.844916	-1.52323
13	6	3.225916	0.441366	-2.270441
14	7	-0.198093	-2.693746	-0.979506
15	6	0.542924	-2.910249	-2.237511
16	6	2.034253	-2.675548	-2.082768
17	6	1.26273	-3.287727	0.971127
18	6	0.11263	-3.697433	0.06247
19	6	-0.178025	3.207024	1.051421
20	6	-1.647769	-2.723678	-1.293626
21	6	-2.446976	-2.076247	-0.189355
22	6	-1.303175	2.929314	0.08087
23	6	-2.466651	-0.489963	1.508881
24	6	-3.774522	-0.805763	1.868554
25	6	-4.431195	-1.8091	1.15438
26	6	-3.752918	-2.466781	0.126583
27	6	-2.380874	3.792711	-0.137455
28	6	-3.321944	3.465483	-1.118295
29	6	-3.136994	2.317695	-1.89299
30	6	-2.028871	1.518261	-1.621096
31	71	0.3921	-0.097299	-0.069979
32	1	1.580627	2.386255	2.552465
33	1	2.610434	3.543252	1.680481
34	1	3.84912	1.53871	2.264536
35	1	3.709498	1.564467	0.50947
36	6	3.474577	-0.263371	3.716074

37	1	3.593906	-1.500622	1.940726
38	1	4.17071	-1.50277	-2.088103
39	1	3.950147	-0.629332	-0.549669
40	1	4.154966	1.009761	-2.401921
41	1	2.77478	0.255407	-3.25135
42	1	0.146085	-2.185817	-2.949352
43	1	0.38921	-3.929509	-2.630213
44	1	2.553424	-3.516788	-1.60487
45	1	2.470869	-2.528155	-3.076984
46	1	-0.051747	4.293945	1.175936
47	1	-0.415121	2.76739	2.024259
48	1	-1.999861	-3.75388	-1.457394
49	1	-1.806713	-2.165252	-2.223137
50	1	-4.229708	-0.273607	2.695873
51	1	-5.448571	-2.092151	1.406021
52	1	-4.223705	-3.272606	-0.42723
53	1	-2.472258	4.706175	0.441142
54	1	-4.169627	4.119673	-1.297187
55	1	-3.803698	2.038352	-2.700581
56	7	-1.166915	1.795707	-0.626913
57	7	-1.829323	-1.088036	0.481958
58	6	-1.639455	0.520153	2.272723
59	8	-0.382637	0.534648	1.915515
60	8	-2.158041	1.224774	3.135783
61	6	-1.644277	0.305468	-2.439716
62	8	-0.470333	-0.172108	-2.121336
63	8	-2.407632	-0.139113	-3.295414
64	1	0.596015	3.403283	-1.297612
65	1	1.838645	4.318318	-0.428865
66	1	2.529034	2.961656	-2.519107
67	1	3.567285	2.785518	-1.091318
68	1	0.32457	-4.684916	-0.378061
69	1	-0.773166	-3.802304	0.694974
70	1	1.330055	-4.020193	1.778959
71	1	2.226997	-3.244905	0.455921
72	6	1.780843	-2.691449	3.761224
73	1	0.867385	-0.838506	3.133676
74	1	2.490555	-3.441383	3.388798
75	1	0.825049	-3.195616	3.941783
76	6	2.347452	-2.0994	5.061506
77	6	3.663182	-1.370909	4.76903
78	1	2.805419	0.508878	4.116786
79	1	4.446806	0.20157	3.523591
80	1	2.506431	-2.898952	5.791531
81	1	1.622691	-1.402321	5.50043
82	1	4.070588	-0.923873	5.681064
83	1	4.409752	-2.092774	4.411396

Zero-point correction =	0.695901 (Hartree/Particle)
Thermal correction to Energy =	0.734413
Thermal correction to Enthalpy =	0.735357
Thermal correction to Gibbs Free Energy =	0.628723
Sum of electronic and zero-point Energies =	-2027.570898
Sum of electronic and thermal Energies =	-2027.532387
Sum of electronic and thermal Enthalpies =	-2027.531442
Sum of electronic and thermal Free Energies =	-2027.638076
E(SCF) in SMD solvation model =	-2028.364898

[Lu(CHX-macropa)]$^{+}$		(Δ(δδδ)(δδδ))		0 imaginary frequencies
Center Number	Atomic Number	X	Y	Z
1	6	1.809387	2.927524	-1.079848
2	7	1.549864	2.341343	0.257513
3	8	2.345305	0.670979	-1.720245
4	6	2.693813	2.04212	-1.948669
5	6	2.80052	2.233871	1.043204
6	6	2.757205	1.084074	2.030051
7	8	2.597774	-0.136258	1.261533
8	6	2.833738	-1.322669	2.045829
9	6	1.518946	-1.82934	2.602921
10	8	0.626575	-2.072666	1.497235
11	8	1.549968	-1.875044	-1.471649
12	6	2.94195	-1.603389	-1.779696
13	6	3.077106	-0.283702	-2.533333
14	7	-0.958049	-2.686755	-0.742749
15	6	-0.28946	-3.3183	-1.907532
16	6	0.713717	-2.380562	-2.556683
17	6	0.471102	-3.452319	1.114369
18	6	-0.883917	-3.565986	0.443009
19	6	0.557272	3.187972	0.973541
20	6	-2.36331	-2.334475	-1.040571
21	6	-2.914321	-1.447235	0.05412
22	6	-0.761944	3.133578	0.236912
23	6	-2.424023	0.097479	1.723632
24	6	-3.744793	0.128123	2.165375
25	6	-4.680497	-0.664302	1.498433
26	6	-4.257167	-1.477703	0.445337
27	6	-1.688177	4.178868	0.186652
28	6	-2.818169	4.040055	-0.625825
29	6	-2.967756	2.894114	-1.411721
30	6	-1.994285	1.902793	-1.308521
31	71	0.29845	-0.133607	-0.097723
32	1	3.553954	-1.108166	2.843988
33	1	3.275113	-2.059453	1.36733
34	1	1.036238	-1.068956	3.219208
35	1	1.657001	-2.747006	3.184765
36	6	3.678934	-2.760041	-2.462026
37	1	3.383883	-1.44111	-0.790791
38	1	0.906207	4.230785	1.039481
39	1	0.434472	2.793377	1.98646
40	1	-2.994341	-3.232942	-1.13485
41	1	-2.390298	-1.798286	-1.994523
42	1	-3.996547	0.753403	3.014165
43	1	-5.720584	-0.671677	1.809353
44	1	-4.952589	-2.135619	-0.065609
45	1	-1.520789	5.085463	0.758845
46	1	-3.552962	4.83781	-0.672391
47	1	-3.791502	2.758152	-2.102924
48	7	-0.953885	2.005278	-0.464692
49	7	-2.026311	-0.644751	0.670804
50	6	-1.320777	0.865777	2.419269
51	8	-0.127997	0.602459	1.948817
52	8	-1.583347	1.644014	3.331987
53	6	-1.951893	0.656355	-2.164525
54	8	-0.853259	-0.036947	-1.995108
55	8	-2.882132	0.377193	-2.916098
56	1	2.282425	3.920237	-1.00086

57	1	2.542825	2.307243	-3.003326
58	1	3.752031	2.193765	-1.711661
59	1	-1.088169	-4.618113	0.187749
60	1	-1.64158	-3.243454	1.161074
61	1	0.494448	-4.080204	2.012258
62	1	1.288665	-3.751521	0.447059
63	1	0.220821	-1.538894	-3.044268
64	1	1.325308	-2.936591	-3.26912
65	1	0.238547	-4.214647	-1.565512
66	1	-1.023128	-3.642345	-2.65661
67	1	3.710994	1.034745	2.569585
68	1	1.927931	1.178066	2.736673
69	1	3.017238	3.169218	1.581202
70	1	3.628878	2.053055	0.355116
71	1	0.845084	3.059926	-1.569859
72	6	4.566841	0.053733	-2.709087
73	1	2.587119	-0.341317	-3.516778
74	1	5.004586	0.239959	-1.718767
75	1	4.68722	0.966836	-3.299917
76	6	5.323661	-1.098976	-3.391294
77	6	5.168405	-2.409034	-2.609554
78	1	3.27445	-2.948301	-3.463057
79	1	3.539292	-3.67314	-1.872935
80	1	5.689547	-3.225172	-3.119164
81	1	5.628527	-2.306253	-1.617674
82	1	6.379925	-0.827911	-3.483801
83	1	4.943195	-1.234686	-4.412376

Zero-point correction =	0.695693 (Hartree/Particle)
Thermal correction to Energy =	0.734072
Thermal correction to Enthalpy =	0.735016
Thermal correction to Gibbs Free Energy =	0.629018
Sum of electronic and zero-point Energies =	-2027.574059
Sum of electronic and thermal Energies =	-2027.53568
Sum of electronic and thermal Enthalpies =	-2027.534736
Sum of electronic and thermal Free Energies =	-2027.640734
E(SCF) in SMD solvation model =	-2028.361864