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ELECTRONIC SUPPLEMENTARY INFORMATION

On the contribution of f electrons to the quadratic hyperpolarizability: the case of Lanthanide Terpyridyl Complexes

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Supplementary text. Effect of basis sets/pseudopotentials and spin-orbit coupling

We investigated the effect of the basis set extension on the computed properties of the **L***Gd*$(NO_3)_3$ complex. The results obtained for the UV-visible spectra (Table S1) illustrate the small influence of the basis set extension with diffuse orbitals. Moreover, the polarizability changes by less then 1% and the first hyperpolarizability undergoes a small increase of *ca.* 4% when adding diffuse orbitals to the basis set, leading to an increase from 239 to 250 10^{-30} esu. Noteworthy, the latter value is slightly closer to the experimental one, i.e. 246 10^{-30} esu, but we stress that experimental error amount to about 15%. These results were expected. Indeed, regarding the usual requirements to include diffuse orbitals when computing electrical and optical properties, it is known that their influence is important and can even become dramatic when considering small molecules[25] but remains limited for large sized species[26]. The possible inclusion of core polarization[27] in the case of the 4f-in core calculations was not further considered as we also carried out all electron calculations which take into account all electronic interactions.

Besides, it has been shown that spin-orbit coupling may affect computed electrical properties like polarizabilities for systems containing heavy atoms,[28] although its influence was found small in the case of the Yb atom.[29] To check the importance of spin-orbit coupling (SOC) effects in the present series of complexes, we carried out computations in the gas phase for the Lu complex using the ADF package,[30] since the gaussian09 program does not allow such calculations. The calculations were carried out with Kramers' symmetry and the non-collinear approximation. Using the ZORA Hamiltonian and the PBE GGA functional[31] along with a TZP STO basis set, we found that the mean polarizability of the Lu complex undergoes little variation when taking SOC into account, its value changing from 655 to 653 au. We further checked the influence of SOC on the computed UV-visible spectra at the same level of theory and using the Tamm-Dancoff approximation.[32] In the case of the lutetium complex SOC does not modify the UV-visible data and for the Gd complex modification are tiny, the first absorption band being red-shifted from 1.976 eV to 1.973 eV upon inclusion of SOC, whereas the oscillator strength remains unchanged (0.100).

Table S1: TD-DFT wavelengths (λ, nm) and oscillator strengths (*f*) computed using the PBE0 functional and different basis sets for the **L***Gd*$(NO_3)_3$ complex. Basis set 1: LANL2DZ basis set augmented with polarization functions for C, N, O whereas the Stuttgart RSC 1997 basis set has been used for Gd. Basis set 2: basis set 1 augmented with diffuse functions on C, N and O atoms. Basis set 3: 4f-in-core basis set.

	λ nm (*f*)		
	Basis set 1	Basis set 2	Basis set 3
1st band	476 (0.19)	488 (0.18)	487 (0.18)
2nd band	367 (0.56)	374 (0.55)	374 (0.56)

Table S2: computed UV-visible absorption wavelengths using different functionals

Ln^{3+}/M^{3+}ion ($4f^n$) *spin multiplicity*	λ_{max} nm calc.				
	λ_{max}[7] nm exp	B3LYP	CAM-B3LYP	M062X	PBE0
Y^{3+} *2S+1=1*	454 ; 392		300 ; 250	336 ; 233	480, 372, 326
La^{3+} ($4f^0$) *2S+1=1*	453 ; 391	515 ; 384	332 ; 255	338 ; 230	475, 370, 323
Gd^{3+} ($4f^7$) *2S+1= 8*	452 ; 393	524 ; 384	303	334	476, 367, 325
Dy^{3+} ($4f^9$) *2S+1= 6*	450 ; 394	521 ; 383	-	336 ; 295	482, 370, 326
Yb^{3+} ($4f^{13}$) *2S+1=2*	452 ; 394	-	327 ; 288	335	472, 376
Lu^{3+} ($4f^{14}$) *2S+1=1*	-	528 ; 389; 288	335 ; 234	339 ; 230	482, 373, 327

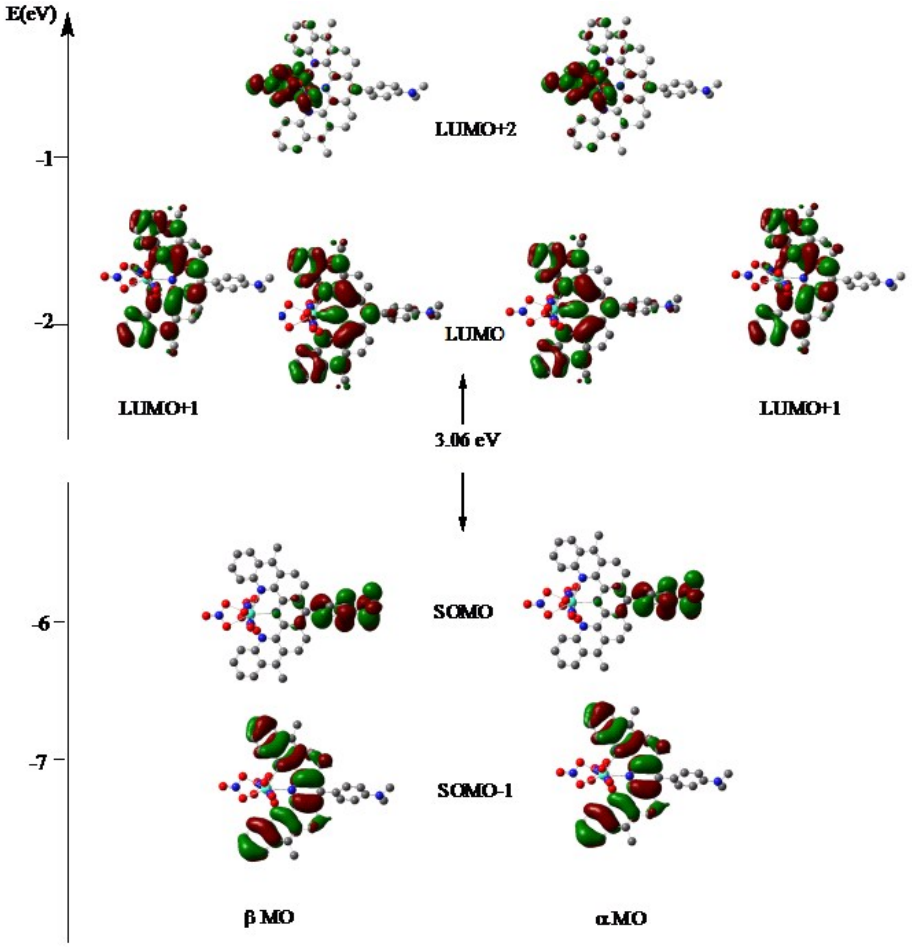

Figure S1: Frontier MO diagram of **L***Gd*$(NO_3)_3$

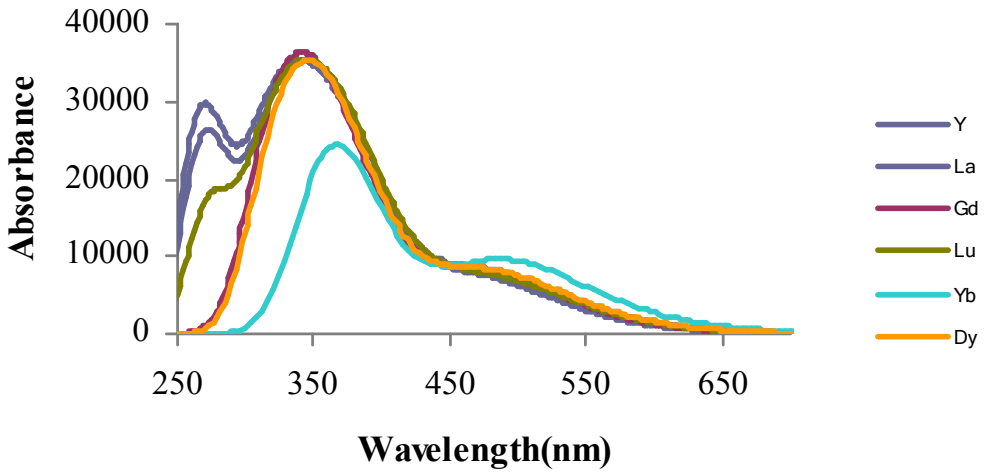

Figure S2: simulated absorption spectra of investigated complexes.

Optimized Cartesian coordinates in Å

Y Complex

C	-2.07021000	5.95673000	0.20513000
C	-1.29144000	4.77337000	0.08336000
C	-1.83858000	3.53360000	0.53654000
C	-3.13203000	3.53437000	1.12390000
C	-3.86029000	4.70014000	1.24053000
C	-3.32843000	5.92574000	0.77202000
C	0.02775000	4.79219000	-0.46474000
C	0.75872000	3.61344000	-0.44127000
C	0.11789000	2.41814000	0.00320000
N	-1.14147000	2.35517000	0.43181000
C	2.18391000	3.50804000	-0.91712000
C	2.97611000	2.51506000	-0.07519000
C	2.29256000	1.17905000	-0.03425000
C	0.88782000	1.15000000	-0.03151000
C	2.99377000	-0.04201000	-0.00814000
C	2.25441000	-1.24080000	0.01202000
C	0.85162000	-1.16824000	-0.00907000
N	0.19130000	0.00146000	-0.02532000
C	0.04512000	-2.41352000	-0.05124000
C	0.64441000	-3.62354000	0.40914000
C	2.06428000	-3.55875000	0.90677000
C	2.89702000	-2.59655000	0.06829000
N	-1.20615000	-2.31796000	-0.50009000
C	-1.92663000	-3.48139000	-0.62867000
C	-1.42268000	-4.73253000	-0.15616000
C	-0.12086000	-4.78016000	0.42976000
C	-3.19514000	-3.45802000	-1.26868000
C	-3.94095000	-4.60947000	-1.41285000
C	-3.45560000	-5.84413000	-0.91858000
C	-2.22182000	-5.89968000	-0.30220000

C	4.47729000	-0.06737000	-0.00295000
C	5.21523000	0.52204000	1.03635000
C	6.60775000	0.49468000	1.05327000
C	7.34078000	-0.12726000	0.00903000
C	6.59175000	-0.69687000	-1.05363000
C	5.19913000	-0.67568000	-1.04280000
N	8.71771000	-0.18602000	0.03162000
C	9.42513000	-0.60169000	-1.16655000
Y	-2.23190000	0.02116000	0.01167000
O	-4.34819000	-1.12495000	0.37002000
N	-5.10242000	-0.11627000	0.19703000
O	-6.31785000	-0.19603000	0.28130000
C	0.37572000	-6.06623000	1.02969000
C	0.57237000	6.07282000	-1.03500000
O	-4.51271000	0.97430000	-0.06954000
O	-2.88510000	0.48742000	2.34773000
N	-2.19426000	-0.43185000	2.88339000
O	-2.17764000	-0.61359000	4.09104000
N	-2.59940000	0.62527000	-2.82053000
O	-2.76532000	0.87351000	-4.00500000
O	-3.16216000	-0.35933000	-2.25251000
C	9.44251000	0.62383000	0.99489000
O	-1.52094000	-1.14915000	2.08186000
O	-1.85511000	1.33645000	-2.07834000
H	9.25654000	1.70776000	0.86215000
H	9.14018000	-1.62478000	-1.46079000
H	-3.57072000	-2.51439000	-1.65725000
H	-4.91131000	-4.56414000	-1.91470000
H	-4.05393000	-6.75208000	-1.03278000
H	-1.84550000	-6.85743000	0.06106000
H	2.53772000	-4.55211000	0.87774000
H	2.06752000	-3.22458000	1.96515000
H	3.00176000	-2.99670000	-0.96122000
H	3.91335000	-2.51765000	0.48670000
H	3.08056000	2.90521000	0.95820000
H	3.99443000	2.40859000	-0.48226000
H	2.19289000	3.18232000	-1.97806000
H	2.68710000	4.48608000	-0.87355000
H	-1.66113000	6.90718000	-0.14161000
H	-3.91137000	6.84596000	0.86554000
H	-4.85191000	4.67341000	1.70039000
H	-3.54382000	2.59700000	1.49321000
H	-0.38240000	-6.49076000	1.70387000
H	1.29550000	-5.92793000	1.60563000
H	0.56989000	-6.81673000	0.24607000
H	1.51772000	5.92396000	-1.56489000
H	0.73705000	6.81808000	-0.23996000
H	-0.14563000	6.50986000	-1.74452000
H	4.66157000	-1.13004000	-1.88036000
H	7.09772000	-1.16483000	-1.89835000
H	7.12658000	0.96333000	1.88985000

H	4.69060000	1.00852000	1.86394000
H	10.50370000	-0.60465000	-0.96141000
H	9.23447000	0.07056000	-2.02616000
H	10.51857000	0.43981000	0.87827000
H	9.16897000	0.35228000	2.02735000

La Complex

C	1.87126000	5.98428000	-0.32461000
C	1.10169000	4.79912000	-0.16849000
C	1.64726000	3.55979000	-0.61900000
C	2.93133000	3.55303000	-1.22586000
C	3.65402000	4.71928000	-1.36989000
C	3.12002000	5.94897000	-0.91340000
C	-0.20247000	4.80734000	0.41728000
C	-0.91480000	3.61619000	0.44335000
C	-0.28093000	2.42305000	-0.02242000
N	0.96211000	2.37899000	-0.49510000
C	-2.31483000	3.48706000	0.98217000
C	-3.13338000	2.51699000	0.13917000
C	-2.44954000	1.18378000	0.03925000
C	-1.04343000	1.14653000	0.01749000
C	-3.15876000	-0.03041000	-0.02403000
C	-2.42784000	-1.23188000	-0.08356000
C	-1.02305000	-1.17004000	-0.04980000
N	-0.35091000	-0.00584000	-0.01366000
C	-0.23986000	-2.43336000	0.00443000
C	-0.84934000	-3.63954000	-0.46003000
C	-2.24157000	-3.53251000	-1.02287000
C	-3.08812000	-2.57641000	-0.19161000
N	0.99595000	-2.36619000	0.49283000
C	1.69558000	-3.53619000	0.63961000
C	1.17274000	-4.78815000	0.19685000
C	-0.12232000	-4.82076000	-0.40814000
C	2.97038000	-3.50556000	1.26531000
C	3.70568000	-4.66059000	1.43403000
C	3.19448000	-5.90261000	0.98502000
C	1.95502000	-5.96139000	0.37867000
C	-4.64271000	-0.04637000	-0.02541000
C	-5.38029000	0.57756000	-1.04441000
C	-6.77320000	0.55876000	-1.05737000
C	-7.50656000	-0.08995000	-0.02995000
C	-6.75757000	-0.69461000	1.01302000
C	-5.36481000	-0.68098000	0.99828000
N	-8.88446000	-0.14133000	-0.05024000
C	-9.58975000	-0.57940000	1.14142000
La	2.28662000	0.01601000	-0.00581000
O	4.73979000	-1.04687000	-0.19750000
N	5.40184000	0.01752000	-0.00524000
O	6.62861000	0.01795000	-0.00588000
C	-0.63971000	-6.12297000	-0.95442000
C	-0.74461000	6.09534000	0.97372000

O	4.73926000	1.08143000	0.18782000
O	2.94936000	0.38513000	-2.57509000
N	2.40707000	-0.66126000	-3.04147000
O	2.44783000	-0.92781000	-4.23743000
N	2.40133000	0.69668000	3.03242000
O	2.44253000	0.96356000	4.22838000
O	2.94354000	-0.34990000	2.56635000
C	-9.60690000	0.70365000	-0.98479000
O	1.81811000	-1.41810000	-2.21159000
O	1.81220000	1.45295000	2.20255000
H	-9.41640000	1.78187000	-0.81610000
H	-9.31014000	-1.61051000	1.41144000
H	3.36223000	-2.55244000	1.62295000
H	4.68382000	-4.61403000	1.92028000
H	3.78131000	-6.81485000	1.12225000
H	1.56722000	-6.92495000	0.04370000
H	-2.73896000	-4.51344000	-1.05208000
H	-2.18619000	-3.16188000	-2.06742000
H	-3.23683000	-2.99886000	0.82344000
H	-4.08790000	-2.46970000	-0.64314000
H	-3.27477000	2.93722000	-0.87787000
H	-4.13722000	2.39410000	0.57705000
H	-2.27164000	3.11980000	2.02851000
H	-2.82761000	4.46042000	1.00048000
H	1.46615000	6.93863000	0.01626000
H	3.69667000	6.87039000	-1.03105000
H	4.63966000	4.69136000	-1.84219000
H	3.34032000	2.60915000	-1.58980000
H	0.09523000	-6.56600000	-1.64305000
H	-1.58022000	-6.00542000	-1.49994000
H	-0.80142000	-6.85024000	-0.14257000
H	-1.68918000	5.95698000	1.50737000
H	-0.90830000	6.83039000	0.16926000
H	-0.02369000	6.54002000	1.67591000
H	-4.82736000	-1.16256000	1.82050000
H	-7.26361000	-1.18447000	1.84521000
H	-7.29192000	1.05534000	-1.87776000
H	-4.85555000	1.08562000	-1.85882000
H	-10.66913000	-0.57131000	0.94057000
H	-9.39156000	0.07225000	2.01513000
H	-10.68360000	0.52004000	-0.87314000
H	-9.33572000	0.46556000	-2.02597000

Gd Complex

C	1.94420000	6.01078000	-0.28186000
C	1.17011000	4.82025000	-0.13143000
C	1.74631000	3.56269000	-0.51324000
C	3.07339000	3.55130000	-1.03866000
C	3.79696000	4.72323000	-1.18088000
C	3.22902000	5.96890000	-0.79860000

C	-0.16603000	4.84269000	0.38860000
C	-0.88502000	3.65042000	0.40200000
C	-0.23520000	2.44082000	-0.01369000
N	1.04410000	2.37863000	-0.40394000
C	-2.31682000	3.54501000	0.88533000
C	-3.11579000	2.54751000	0.04097000
C	-2.42865000	1.20361000	-0.01075000
C	-1.01757000	1.16697000	-0.00764000
C	-3.14293000	-0.01645000	-0.04759000
C	-2.40993000	-1.22456000	-0.08644000
C	-0.99993000	-1.16604000	-0.06948000
N	-0.32806000	0.00515000	-0.03139000
C	-0.20364000	-2.43055000	-0.05140000
C	-0.82330000	-3.63980000	-0.51006000
C	-2.24864000	-3.55001000	-1.01454000
C	-3.07362000	-2.57947000	-0.16236000
N	1.05781000	-2.36005000	0.38949000
C	1.76824000	-3.53756000	0.50695000
C	1.22986000	-4.79219000	0.06431000
C	-0.08380000	-4.81927000	-0.50950000
C	3.06457000	-3.52190000	1.10281000
C	3.79806000	-4.68729000	1.24908000
C	3.27138000	-5.92909000	0.80045000
C	2.01501000	-5.97516000	0.21787000
C	-4.63462000	-0.03408000	-0.03669000
C	-5.38995000	0.57456000	-1.06001000
C	-6.78811000	0.54945000	-1.05876000
C	-7.51269000	-0.08725000	-0.00831000
C	-6.74515000	-0.67988000	1.03739000
C	-5.34774000	-0.66182000	1.00579000
N	-8.89579000	-0.13784000	-0.00898000
C	-9.59914000	-0.60588000	1.18510000
Gd	2.15926000	0.02243000	0.00701000
O	4.45247000	-0.99057000	-0.24055000
N	5.10610000	0.04065000	0.15347000
O	6.33605000	0.04924000	0.20966000
C	-0.61994000	-6.11736000	-1.07544000
C	-0.74007000	6.15178000	0.88911000
O	4.40545000	1.06202000	0.48734000
O	2.89478000	0.61586000	-2.34755000
N	2.39531000	-0.41513000	-2.92320000
O	2.49857000	-0.59760000	-4.13663000
N	2.13190000	0.35713000	2.94813000
O	2.11140000	0.50853000	4.16980000
O	2.79490000	-0.58428000	2.38926000
C	-9.64499000	0.66013000	-0.97929000
O	1.78085000	-1.24349000	-2.16144000
O	1.48675000	1.13527000	2.15666000
H	-9.45993000	1.74582000	-0.86706000
H	-9.31495000	-1.64234000	1.43148000
H	3.47307000	-2.57728000	1.45192000

H	4.78649000	-4.64897000	1.71469000
H	3.85649000	-6.84487000	0.91953000
H	1.61429000	-6.93339000	-0.11467000
H	-2.73761000	-4.53526000	-0.99567000
H	-2.24624000	-3.20540000	-2.06874000
H	-3.19085000	-2.99121000	0.86031000
H	-4.08542000	-2.48156000	-0.58532000
H	-3.23177000	2.94081000	-0.98915000
H	-4.12920000	2.43827000	0.45715000
H	-2.32077000	3.21665000	1.94476000
H	-2.82237000	4.52097000	0.84627000
H	1.51342000	6.97119000	0.00308000
H	3.80548000	6.89043000	-0.91540000
H	4.80917000	4.68684000	-1.59233000
H	3.51461000	2.60415000	-1.33888000
H	0.12650000	-6.58817000	-1.73128000
H	-1.53250000	-5.97052000	-1.66035000
H	-0.84216000	-6.83518000	-0.26864000
H	-1.68754000	6.01750000	1.41844000
H	-0.91115000	6.84857000	0.05223000
H	-0.03680000	6.64102000	1.57868000
H	-4.79969000	-1.13201000	1.82739000
H	-7.23991000	-1.16109000	1.88037000
H	-7.31750000	1.02967000	-1.88111000
H	-4.87647000	1.07197000	-1.88782000
H	-10.67974000	-0.59368000	0.99058000
H	-9.39658000	0.02673000	2.07080000
H	-10.71844000	0.47551000	-0.84018000
H	-9.38708000	0.37298000	-2.01214000

Dy Complex

C	-2.00661000	-5.89139000	-0.45974000
C	-1.22924000	-4.71702000	-0.26075000
C	-1.76535000	-3.45369000	-0.65873000
C	-3.05038000	-3.41912000	-1.26569000
C	-3.77621000	-4.57700000	-1.45873000
C	-3.25431000	-5.82789000	-1.04763000
C	0.07530000	-4.76793000	0.32067000
C	0.80805000	-3.59123000	0.37878000
C	0.19079000	-2.37650000	-0.04431000
N	-1.06185000	-2.28422000	-0.49305000
C	2.21171000	-3.49985000	0.91858000
C	3.05150000	-2.52357000	0.10287000
C	2.38951000	-1.17741000	0.02463000
C	0.98551000	-1.12354000	0.01059000
C	3.11189000	0.03254000	-0.01748000
C	2.39283000	1.24349000	-0.07447000
C	0.98897000	1.19369000	-0.06564000
N	0.31025000	0.03644000	-0.01375000
C	0.19569000	2.44835000	-0.09032000

C	0.82080000	3.63961000	-0.56613000
C	2.25114000	3.54418000	-1.03052000
C	3.05656000	2.58826000	-0.15777000
N	-1.07168000	2.37769000	0.31717000
C	-1.78432000	3.55032000	0.38978000
C	-1.25050000	4.78523000	-0.09090000
C	0.07141000	4.80554000	-0.63249000
C	-3.07832000	3.54917000	0.97883000
C	-3.81874000	4.71045000	1.06828000
C	-3.30242000	5.93039000	0.56657000
C	-2.04382000	5.96219000	-0.00048000
C	4.59518000	0.03178000	-0.00862000
C	5.33210000	-0.62903000	-1.00633000
C	6.72502000	-0.63003000	-1.01033000
C	7.46073000	0.03143000	0.00880000
C	6.71284000	0.67936000	1.02785000
C	5.32017000	0.68691000	1.00160000
N	8.83623000	0.05116000	0.00403000
C	9.54451000	0.54984000	1.16951000
Dy	-2.10133000	0.02207000	0.06533000
O	-4.40707000	0.90971000	0.16383000
N	-4.92649000	-0.19761000	0.50065000
O	-6.12536000	-0.32769000	0.67917000
C	0.60490000	6.07751000	-1.23201000
C	0.60116000	-6.08175000	0.82973000
O	-4.11501000	-1.16895000	0.64254000
O	-3.22740000	-0.34989000	-2.09010000
N	-2.39868000	0.31022000	-2.78992000
O	-2.51454000	0.42230000	-3.99877000
N	-1.94906000	-0.38089000	2.91296000
O	-1.87229000	-0.54911000	4.11852000
O	-2.53023000	0.62834000	2.40683000
C	9.55677000	-0.79572000	-0.93002000
O	-1.44247000	0.84672000	-2.14876000
O	-1.45387000	-1.20438000	2.08206000
H	9.34053000	-1.87052000	-0.78019000
H	9.29109000	1.60432000	1.36724000
H	-3.47613000	2.62004000	1.38160000
H	-4.80708000	4.68564000	1.53437000
H	-3.89607000	6.84523000	0.63844000
H	-1.64473000	6.90844000	-0.36865000
H	2.73732000	4.53147000	-1.01016000
H	2.27087000	3.19133000	-2.08171000
H	3.15723000	3.01076000	0.86225000
H	4.07578000	2.48282000	-0.56234000
H	3.19725000	-2.92272000	-0.92105000
H	4.05282000	-2.42451000	0.55217000
H	2.17375000	-3.16196000	1.97408000
H	2.70621000	-4.48251000	0.90951000
H	-1.60558000	-6.85921000	-0.15573000
H	-3.83651000	-6.73995000	-1.20167000

H	-4.75881000	-4.52485000	-1.93463000
H	-3.45189000	-2.46371000	-1.59432000
H	-0.12434000	6.50573000	-1.93448000
H	1.54072000	5.92014000	-1.77616000
H	0.78523000	6.83319000	-0.45066000
H	1.53926000	-5.97178000	1.38088000
H	0.77189000	-6.78291000	-0.00255000
H	-0.13076000	-6.55116000	1.50293000
H	4.78345000	1.19878000	1.80562000
H	7.22115000	1.18405000	1.84930000
H	7.24342000	-1.15264000	-1.81417000
H	4.80554000	-1.14833000	-1.81213000
H	10.62442000	0.49820000	0.97994000
H	9.32292000	-0.03566000	2.08197000
H	10.63477000	-0.63846000	-0.79576000
H	9.30993000	-0.53722000	-1.97287000

Yb Complex

C	-2.02940800	-5.89472700	-0.23337900
C	-1.23624100	-4.72203900	-0.10136700
C	-1.76333900	-3.47039100	-0.54869400
C	-3.05224100	-3.44850800	-1.14694600
C	-3.79009500	-4.60692500	-1.27755700
C	-3.28197000	-5.84277800	-0.80943600
C	0.08054800	-4.76389400	0.44829500
C	0.83716800	-3.60223300	0.41108000
C	0.21810300	-2.39636500	-0.02707800
N	-1.04867900	-2.30222300	-0.43193500
C	2.27122200	-3.53289000	0.86957900
C	3.07539700	-2.54979100	0.02706600
C	2.41722200	-1.19960600	-0.00858000
C	1.01500300	-1.14523600	-0.01187600
C	3.14400700	0.00825200	-0.01854900
C	2.42443100	1.22034200	-0.02543500
C	1.02246800	1.17173800	-0.03809600
N	0.33633600	0.01527000	-0.03428000
C	0.22774100	2.42268800	-0.01409200
C	0.85369600	3.63919600	-0.41110000
C	2.29445800	3.57777800	-0.85051200
C	3.08858000	2.56786500	-0.03056800
N	-1.04664900	2.31762600	0.36120500
C	-1.77807200	3.47581800	0.46023100
C	-1.23888800	4.74047200	0.06844700
C	0.09770200	4.80191100	-0.43032300
C	-3.10256800	3.42649700	0.97147500
C	-3.85901900	4.57489200	1.08493100
C	-3.33089100	5.82763000	0.69013500
C	-2.04694800	5.90376200	0.19068800
C	4.62565900	0.00137300	-0.02175000
C	5.34885600	-0.63333100	-1.04676500

C	6.74009000	-0.64041800	-1.06756100
C	7.48983500	-0.02020400	-0.03276400
C	6.75724200	0.60958800	1.00852700
C	5.36574000	0.62437500	0.99814800
N	8.85997600	-0.02889000	-0.03918500
C	9.59350600	0.59566000	1.04287200
Yb	-2.01910200	0.01868000	0.00017100
O	-4.22297100	0.83587200	-0.20980300
N	-4.79701800	-0.23258900	0.18786600
O	-6.00355200	-0.33127000	0.27463400
C	0.63800500	6.10722700	-0.94638000
C	0.60707100	-6.04958700	1.02423500
O	-4.00439500	-1.18414100	0.48435900
O	-2.84029500	-0.60878600	-2.22127500
N	-2.46124200	0.46523100	-2.78062200
O	-2.65575600	0.70593300	-3.95518600
N	-2.10519000	-0.28819600	2.82304800
O	-2.13866400	-0.44469100	4.02711000
O	-2.71601600	0.65617600	2.23154000
C	9.57504900	-0.70163600	-1.10462800
O	-1.85350000	1.27772800	-2.00476000
O	-1.45185800	-1.05955300	2.04661700
H	9.33464700	-1.77570700	-1.14765100
H	9.36907900	1.67072400	1.12161500
H	-3.51812900	2.48016200	1.29625400
H	-4.86979700	4.51441900	1.48754700
H	-3.93573600	6.72882000	0.78654200
H	-1.64206000	6.87097600	-0.09891300
H	2.77394300	4.55609200	-0.75076100
H	2.34134100	3.30455500	-1.91646400
H	3.18152100	2.93130400	1.00477200
H	4.10612500	2.48341900	-0.42622700
H	3.16868700	-2.93953300	-0.99859000
H	4.09214300	-2.46125300	0.42363600
H	2.30694300	-3.22711700	1.92705900
H	2.74800300	-4.51558700	0.80441400
H	-1.63435700	-6.85053200	0.10400400
H	-3.87468900	-6.75099000	-0.91531300
H	-4.77093000	-4.56823300	-1.75089400
H	-3.44386600	-2.51615200	-1.53337100
H	-0.08237200	6.58177600	-1.62340900
H	1.57157200	5.98265700	-1.49893300
H	0.82224500	6.80961100	-0.12091800
H	1.51248700	-5.89968900	1.61631700
H	0.83662900	-6.77282400	0.22857000
H	-0.14005400	-6.51252600	1.67983600
H	4.84437300	1.11439900	1.82161100
H	7.27680300	1.09138000	1.83325500
H	7.24591500	-1.13292200	-1.89449200
H	4.81360600	-1.11762200	-1.86477000
H	10.66644300	0.49267900	0.85914000

H	9.37222200	0.12745100	2.01513600
H	10.65091300	-0.60682300	-0.93419700
H	9.35214300	-0.26132000	-2.08900800

Lu Complex

C	-2.00224000	-5.90872000	-0.22946000
C	-1.21243000	-4.73199000	-0.11429000
C	-1.76652000	-3.47795000	-0.51856000
C	-3.08500000	-3.45839000	-1.04742000
C	-3.82297000	-4.61861000	-1.15916000
C	-3.28233000	-5.85847000	-0.74215000
C	0.12546000	-4.77339000	0.38316000
C	0.86888000	-3.60267000	0.34993000
C	0.22601000	-2.39445000	-0.05185000
N	-1.05188000	-2.30895000	-0.42095000
C	2.30957000	-3.52627000	0.78232000
C	3.08994000	-2.51626000	-0.04892000
C	2.41543000	-1.17589000	-0.04301000
C	1.01167000	-1.13580000	-0.02966000
C	3.12522000	0.04074000	-0.03843000
C	2.39573000	1.24551000	-0.03697000
C	0.99298000	1.18235000	-0.03894000
N	0.32595000	0.01789000	-0.02641000
C	0.18793000	2.42839000	-0.02204000
C	0.80735000	3.64367000	-0.43925000
C	2.24724000	3.58818000	-0.87774000
C	3.04789000	2.59706000	-0.04243000
N	-1.08468000	2.32522000	0.35735000
C	-1.81799000	3.48200000	0.45245000
C	-1.29110000	4.74080000	0.02762000
C	0.04260000	4.80034000	-0.47992000
C	-3.12790000	3.44328000	1.00121000
C	-3.88698000	4.59052000	1.10605000
C	-3.37607000	5.83430000	0.66341000
C	-2.10276000	5.90328000	0.13573000
C	4.60933000	0.05459000	-0.03148000
C	5.35205000	-0.50204000	-1.08513000
C	6.74500000	-0.48887000	-1.08642000
C	7.47311000	0.08435000	-0.01142000
C	6.71863000	0.62179000	1.06393000
C	5.32600000	0.61612000	1.03774000
N	8.85126000	0.12800000	-0.01704000
C	9.54922000	0.48229000	1.20625000
Lu	-2.02799000	-0.00743000	0.01389000
O	-4.19512000	0.93611000	-0.22069000
N	-4.80646000	-0.10403000	0.17692000
O	-6.02210000	-0.15853000	0.24339000
C	0.56954000	6.09841000	-1.02610000
C	0.67776000	-6.06769000	0.91347000
O	-4.06623000	-1.08606000	0.50170000

O	-2.88592000	-0.59379000	-2.17282000
N	-2.25678000	0.31296000	-2.79462000
O	-2.34737000	0.46312000	-4.00193000
N	-2.05912000	-0.33297000	2.82853000
O	-2.07176000	-0.48317000	4.03939000
O	-2.63958000	0.63874000	2.25809000
C	9.57651000	-0.65735000	-1.00012000
O	-1.52272000	1.05593000	-2.07142000
O	-1.46101000	-1.13881000	2.05058000
H	9.37492000	-1.74275000	-0.90789000
H	9.27294000	1.49491000	1.54182000
H	-3.53065000	2.50265000	1.36109000
H	-4.88926000	4.53462000	1.53967000
H	-3.98553000	6.73798000	0.74883000
H	-1.70654000	6.86691000	-0.18854000
H	2.72127000	4.57842000	-0.79679000
H	2.29164000	3.29138000	-1.94634000
H	3.12556000	2.96750000	1.00064000
H	4.07532000	2.52278000	-0.43331000
H	3.17002000	-2.87810000	-1.09485000
H	4.11730000	-2.42767000	0.33891000
H	2.35356000	-3.23661000	1.85289000
H	2.79947000	-4.50786000	0.69182000
H	-1.58352000	-6.86835000	0.07783000
H	-3.87470000	-6.77285000	-0.83356000
H	-4.83235000	-4.57544000	-1.57748000
H	-3.51216000	-2.52097000	-1.38577000
H	-0.14482000	6.52992000	-1.74240000
H	1.52669000	5.97535000	-1.54120000
H	0.70563000	6.83699000	-0.21931000
H	1.63579000	-5.93342000	1.42406000
H	0.82140000	-6.79602000	0.09872000
H	-0.02493000	-6.51786000	1.62979000
H	4.78396000	1.04408000	1.88628000
H	7.22015000	1.05203000	1.93108000
H	7.26797000	-0.93115000	-1.93472000
H	4.83130000	-0.95208000	-1.93552000
H	10.63013000	0.48112000	1.01374000
H	9.34047000	-0.22449000	2.03343000
H	10.65348000	-0.49206000	-0.86506000
H	9.31878000	-0.34598000	-2.02533000

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