

*Electronic Supplementary Information for*

**N-oxide ligands for selective separations of lanthanides: Insights from  
computation**

Tongyu Liu,<sup>1</sup> Alexander S. Ivanov,<sup>2</sup> Ilja Popovs,<sup>2</sup> Santa Jansone-Popova,<sup>2</sup> and De-en Jiang<sup>3,4\*</sup>

<sup>1</sup>Department of Chemistry, University of California, Riverside, CA 92521, USA

<sup>2</sup>Chemical Sciences Division, Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge,  
TN 37831, USA

<sup>3</sup>Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN  
37235, USA

<sup>4</sup>Department of Chemistry, Vanderbilt University, Nashville, TN 37235, USA

\*To whom correspondence should be addressed. E-mail: [de-en.jiang@vanderbilt.edu](mailto:de-en.jiang@vanderbilt.edu).

Table S1. Average distance between Ln(III) and N-donor in complexes

Complexes	[Eu( <b>1a</b> )](NO <sub>3</sub> ) <sub>3</sub>	[Eu( <b>2a</b> )](NO <sub>3</sub> ) <sub>3</sub>	[Eu( <b>2b</b> )](NO <sub>3</sub> ) <sub>3</sub>	[Eu( <b>2c</b> )](NO <sub>3</sub> ) <sub>3</sub>
Eu-N distance (Å)	2.66	2.67	2.64	2.67
Complexes	[Lu( <b>1a</b> )](NO <sub>3</sub> ) <sub>3</sub>	[Lu( <b>2a</b> )](NO <sub>3</sub> ) <sub>3</sub>	[Lu( <b>2b</b> )](NO <sub>3</sub> ) <sub>3</sub>	[Lu( <b>2c</b> )](NO <sub>3</sub> ) <sub>3</sub>
Lu-N distance (Å)	2.57	2.57	2.55	2.57

Table S2. NBO charges of N and O atoms in ligands **2a-2d**

	<b>2a</b>	<b>2b</b>	<b>2c</b>	<b>2d</b>
N (pyridine)	-0.43	-0.43	-0.44	-0.44
O (N-Oxide)	-0.54	-0.55	-0.54	-0.55

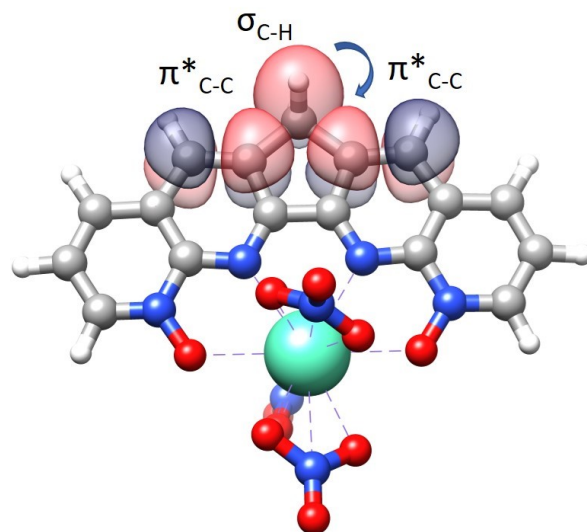


Figure S1. Natural bond orbital (NBO) analysis of the  $[\text{Eu}(\mathbf{2b})](\text{NO}_3)_3$  complex:  $\sigma_{\text{C-H}} \rightarrow \pi^*_{\text{C-C}}$  interactions characterized by the overlap of the C-H  $\sigma$ -bond orbitals with adjacent C=C  $\pi^*$  orbitals.

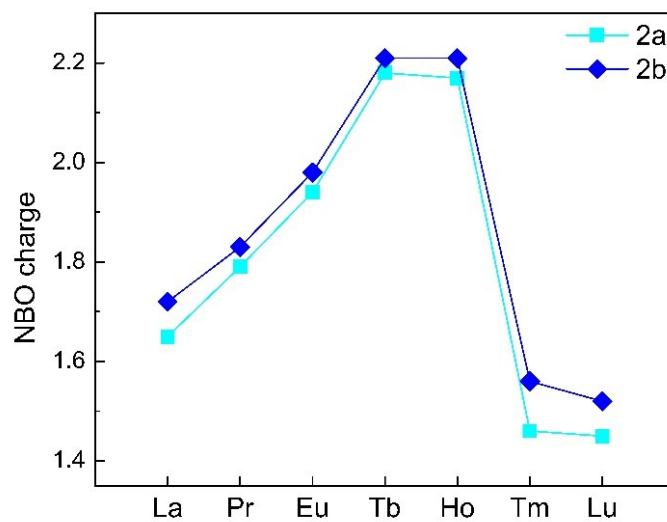


Figure S2. NBO charge on Ln in  $[\text{Ln}(\mathbf{2a})](\text{NO}_3)_3$  and  $[\text{Ln}(\mathbf{2b})](\text{NO}_3)_3$  complexes.

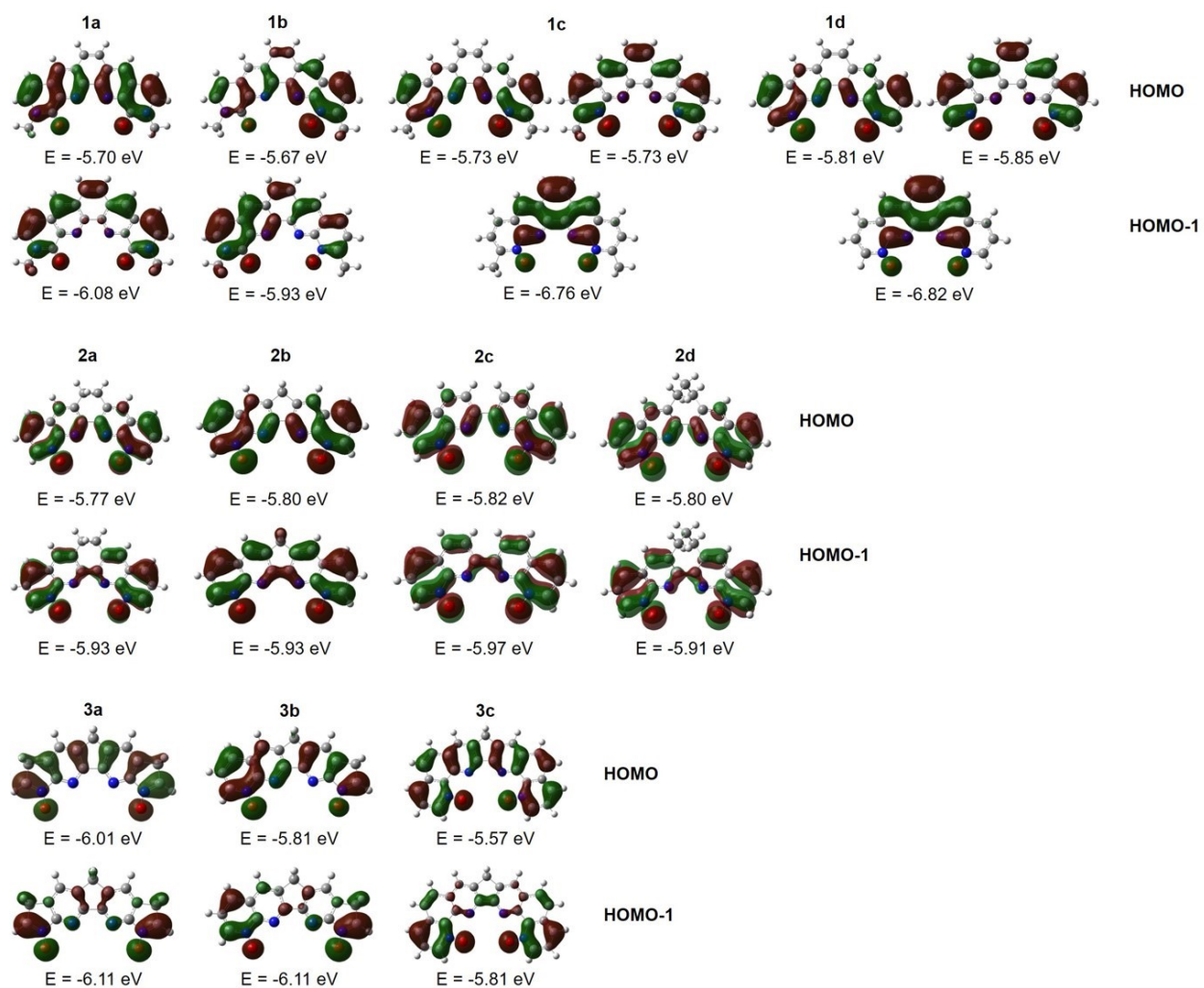


Figure S3. HOMO and HOMO-1 (isovalue = 0.02 a.u.) of all ligands and their energies.

## Sample Gaussian Input

```
#N B3LYP/gen gfinput pseudo=read scf=(MaxCycle=1000) integral=(grid=199302) opt=(maxcycle=999)  
freq scrf=(iefpcm,solvent=water) nosymm
```

*Ln-ligand*

0 1

.....

.....

C,H,N,O 0

6-31+G(d)

\*\*\*\*

*La 0*

S 3 1.00

5.0873990 -0.4172430

4.2709780 0.8860100

1.9154580 -1.4197520

S 1 1.00

0.5255960 1.0

S 1 1.00

0.2634740 1.0

S 1 1.00

0.0488200 1.0

S 1 1.00

0.0228360 1.0

P 3 1.00

3.0251610 0.5381960

2.3820950 -0.9816400

0.5844260 1.2395900

P 1 1.00

0.2603600 1.0

P 1 1.00

0.0833340 1.0

P 1 1.00

0.0302750 1.0

D 3 1.00

1.5768240 -0.0969440

0.5923900 0.4074660

0.2495000 0.7043630

D 1 1.00

0.1065130 1.0

D 1 1.00

0.0458310 1.0

\*\*\*\*

La 0

ECP46MWB 4 46

G-Komponente

1

2 1.000000 0.000000

S-G

2

2 3.309900 91.932177

2 1.655000 -3.788764

P-G

2

2 2.836800 63.759486

2 1.418400 -0.647958

D-G

2

2 2.021300 36.116173

2 1.010700 0.219114

F-G

1

2 4.028600 -36.010016

*Cartesian Coordinates for the La(1a)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -2012.99362831Hartree*

O	0.44385600	10.07006500	10.91927500
C	1.10622500	11.13706400	10.96536400
N	1.61463000	11.70250600	9.82799300
C	1.35805000	11.01604900	8.55039300
H	0.28156400	10.94547700	8.38065400
H	1.82288600	11.58847400	7.74896200
O	-1.62025300	7.77698200	15.13977300
C	-1.49886600	8.23977300	16.29859700
N	-2.09081500	7.62502700	17.37006000
C	-2.87519500	6.40670500	17.10683300
H	-3.69883600	6.63912600	16.42794000
H	-3.26842300	6.03453200	18.05192900
O	0.43915300	6.91221500	11.35621300
N	-0.45538700	6.03394000	11.59866500
O	-1.35549300	6.35135600	12.44485500
O	-0.44667800	4.93242300	11.04450200
O	3.37151000	7.11655600	14.20535500
N	2.28952200	7.62740600	13.90891200
O	1.18653400	7.17978600	14.36873000
O	2.21473200	8.63356800	13.12783000
O	-2.76066700	9.18846700	11.60036700
N	-2.98291500	10.38510800	11.98181900
O	-3.96085600	11.02070500	11.58581900
O	-2.13858900	10.89644000	12.79492200
C	2.35321600	12.87599800	9.85623500
C	2.62264300	13.54532200	11.00711500
C	2.13307300	13.03284400	12.25205900
C	1.37579300	11.83174600	12.22543900
C	2.34607400	13.62898600	13.50683400
H	2.91773300	14.55016400	13.58027000
C	1.82253000	13.03767100	14.65898500
C	1.07806700	11.82500000	14.50897100
N	0.86759500	11.25301400	13.31990600
C	0.51383500	11.17944300	15.68310300
C	1.99750500	13.59691700	15.97978100
H	2.56817200	14.51578800	16.07731100

C	1.46167300	12.99883000	17.07701900
H	1.59724100	13.43365300	18.06293400
C	0.69806700	11.77664000	16.97004700
C	0.12074800	11.14391000	18.07297800
H	0.23803800	11.56838900	19.06636400
C	-0.62084200	9.96321600	17.89776400
C	-0.73169000	9.45655400	16.57611100
N	-0.17329300	10.04391200	15.50794200
C	-1.27220300	9.24436100	18.95198100
C	-1.97435900	8.11900600	18.65971400
La	-0.46216900	8.83084600	13.02299800
H	3.20616900	14.45808400	10.97549300
H	2.70169500	13.21989200	8.89062700
H	1.78182600	10.00998500	8.58217200
H	-2.23617400	5.65022100	16.64655000
H	-2.48735900	7.54250900	19.41892800
H	-1.21257500	9.59181700	19.97672600

*Cartesian Coordinates for the La(1b)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -2012.93110219 Hartree*

O	0.43119800	10.06836600	10.92855600
C	1.10647000	11.12451400	10.98247400
N	1.61684100	11.69477500	9.84698400
C	1.34443400	11.02267000	8.56501700
H	0.26634900	10.97513400	8.39663200
H	1.81941200	11.59124800	7.76680200
O	-1.54002700	7.82433700	15.13630400
N	-1.47851300	8.29658000	16.36488700
C	-2.09895400	7.64025100	17.36649000
C	-2.84440900	6.39814300	17.01174800
H	-3.62011000	6.61596300	16.26838900
H	-3.30556600	5.96839900	17.90286500
O	0.35332900	6.81312200	11.40617900
N	-0.54032700	5.95491600	11.71448300
O	-1.39343900	6.30629000	12.59495800
O	-0.57273300	4.83899600	11.18962400
O	3.51537300	7.12980800	13.91669500

N	2.41890400	7.64769600	13.68612600
O	1.36769400	7.29418800	14.32224700
O	2.27801000	8.55543800	12.80570100
O	-2.74861900	9.19690300	11.65360000
N	-2.95408300	10.40050800	12.02443500
O	-3.92832700	11.04217200	11.62743100
O	-2.09943400	10.91040600	12.82573800
C	2.36282300	12.86249100	9.88059200
C	2.63714900	13.52529400	11.03417800
C	2.14436700	13.01108000	12.27657700
C	1.38524500	11.80988600	12.24766500
C	2.35364500	13.60737500	13.53073500
H	2.92855400	14.52632400	13.60571800
C	1.81785300	13.02380100	14.68159200
C	1.07144500	11.81206200	14.53059700
N	0.87563700	11.23251800	13.34142200
C	0.48547800	11.17974300	15.70285500
C	1.98490400	13.59498300	15.99765500
H	2.56073600	14.51076800	16.09202100
C	1.43331000	13.00956100	17.09262900
H	1.55999200	13.44915800	18.07747400
C	0.66287400	11.79206000	16.98439900
C	0.06954400	11.17375600	18.08400200
H	0.17380700	11.60472300	19.07579200
C	-0.67154600	9.99058500	17.92020400
C	-0.76502100	9.47359500	16.59646200
N	-0.20880000	10.04618000	15.52765600
C	-1.32038200	9.29492100	18.97521400
C	-2.01687100	8.14830400	18.68675400
La	-0.43967700	8.80892400	13.04531700
H	3.22487300	14.43540400	11.00622000
H	2.71210300	13.20972800	8.91641500
H	1.74768000	10.00809300	8.58903200
H	-2.17092200	5.66186400	16.55801500
H	-2.52596300	7.59440400	19.46727900
H	-1.25959500	9.67605800	19.98928300



*Cartesian Coordinates for the La(1c)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -2012.86733197 Hartree*

O	0.41896400	10.09381600	11.00449200
N	1.12251300	11.20762200	11.00807700
C	1.59164300	11.70813100	9.84826200
C	1.27872200	10.95334300	8.60063400
H	0.19423600	10.86680400	8.46642900
H	1.71273300	11.45783400	7.73558400
O	-1.60125500	7.86369500	15.10753400
N	-1.48611000	8.30719100	16.34030500
C	-2.09503000	7.64849300	17.34757900
C	-2.88346100	6.43408400	16.99054500
H	-3.67350600	6.68791600	16.27410400
H	-3.33110400	5.99864700	17.88574400
O	0.43898000	6.89533000	11.36099700
N	-0.43362400	6.00616400	11.63927400
O	-1.32513100	6.32397800	12.49404500
O	-0.41262500	4.89230500	11.10968000
O	3.40083100	7.13423400	14.21693300
N	2.31147300	7.63337900	13.92099800
O	1.21296000	7.15340200	14.35283100
O	2.22871800	8.66007100	13.16777000
O	-2.75503900	9.17208600	11.58370000
N	-2.98388800	10.37559500	11.94112900
O	-3.94926800	11.00655000	11.50515800
O	-2.16405800	10.89850500	12.76896200
C	2.35084200	12.90599000	9.86426300
C	2.62414000	13.57092000	11.03221900
C	2.13141400	13.04384600	12.25667200
C	1.36664000	11.84187400	12.22937700
C	2.34690000	13.62437100	13.51728000
H	2.92427200	14.54155500	13.59161400
C	1.82562600	13.02960200	14.66632100
C	1.07399200	11.82244900	14.50368200
N	0.85596900	11.25594500	13.31067400
C	0.50990800	11.17334900	15.67925100
C	2.01630300	13.58480100	15.98561100
H	2.59425000	14.49908200	16.07998200

C	1.48538800	12.98379200	17.08096800
H	1.62835600	13.40720800	18.07046100
C	0.71418900	11.76820500	16.96450500
C	0.14363400	11.13378000	18.06761000
H	0.27215100	11.54908000	19.06314800
C	-0.60914400	9.96029800	17.90185300
C	-0.73694500	9.46348000	16.57235000
N	-0.18874400	10.04171300	15.50129900
C	-1.24341400	9.25939400	18.96279200
C	-1.96654800	8.13039400	18.67432100
La	-0.46209400	8.82879800	13.01853700
H	3.20874900	14.48498100	11.03523900
H	2.71349000	13.27989800	8.91349400
H	1.67176900	9.93188300	8.66223400
H	-2.24340600	5.68960900	16.50304200
H	-2.46667200	7.57351000	19.45851900
H	-1.15197200	9.62548300	19.98003600

*Cartesian Coordinates for the La(1d)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -1934.21848638 Hartree*

O	0.45195400	10.06053300	10.99801800
N	1.14298800	11.17911500	11.01271700
C	1.61866500	11.69667500	9.87433000
H	1.38641300	11.12668600	8.98377100
O	-1.56172500	7.81460100	15.12327000
N	-1.44549100	8.27362500	16.34746000
C	-2.02665900	7.63036100	17.36805900
H	-2.57241700	6.73825100	17.08846400
O	0.47084300	6.85736300	11.37193200
N	-0.39360900	5.96387100	11.66325100
O	-1.27949700	6.28223300	12.52434000
O	-0.37027700	4.84741100	11.14099700
O	3.44736900	7.15533900	14.22352800
N	2.35267000	7.63875900	13.92366200
O	1.26007800	7.15686500	14.36955200
O	2.25631100	8.65036400	13.15171500
O	-2.72511400	9.14574500	11.59153600

N	-2.95146000	10.34653000	11.95964200
O	-3.91879100	10.98129100	11.53509700
O	-2.12561200	10.86212300	12.78671700
C	2.36445500	12.89053500	9.85942900
C	2.62643600	13.56316400	11.03017200
C	2.13104400	13.03193900	12.25136100
C	1.37755400	11.82074300	12.23207200
C	2.33401900	13.62138900	13.51262900
H	2.90097500	14.54507900	13.58503400
C	1.81368800	13.02754500	14.66102400
C	1.07560200	11.81028300	14.50230800
N	0.86913300	11.23464200	13.31410800
C	0.51254400	11.16109400	15.67933600
C	1.99017900	13.59187700	15.97928600
H	2.55706400	14.51314700	16.07186300
C	1.45999900	12.99164000	17.07502800
H	1.59288100	13.42291400	18.06245200
C	0.70322400	11.76567000	16.96340000
C	0.13706800	11.13116900	18.06708700
H	0.25613300	11.55369100	19.06060800
C	-0.60002000	9.94418000	17.90613600
C	-0.71418800	9.44233400	16.57552900
N	-0.17053700	10.02225000	15.50326900
C	-1.22257100	9.24340500	18.97360500
C	-1.92660300	8.09600500	18.69184700
La	-0.43366300	8.78988100	13.01905300
H	3.20153400	14.48299600	11.03696400
H	2.72221500	13.25468100	8.90330600
H	-2.42089900	7.52665900	19.47044800
H	-1.13680600	9.62097000	19.98695300

*Cartesian Coordinates for the La(2a)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -1935.42839722 Hartree*

La	1.05020600	-0.00441400	-0.10938300
O	0.85114100	2.53809800	0.08649100
C	-0.15754400	4.56877000	-0.32321800
N	-0.23140600	3.23911600	-0.17141300

O	1.02512300	-2.54313800	0.22163400
N	-1.44426200	1.26228800	-0.09079200
C	-1.46067000	2.58887000	-0.26888500
O	0.26575700	0.19967600	2.45082100
N	-1.36496100	-1.42613800	0.16174600
C	-2.63570400	3.34224300	-0.53123200
O	2.34590000	0.72612300	2.09831300
C	0.12604600	-4.61464100	0.67430800
O	1.51024400	0.89126500	4.11622800
N	4.13296400	-0.00588600	-0.63820700
O	3.54250400	-1.03348500	-0.16991900
N	1.08640700	0.03454300	-3.24234800
O	5.34918900	0.00822100	-0.84169100
N	1.37792300	0.61295100	2.92393500
O	3.40105700	1.01139300	-0.88820200
O	1.47792100	-0.99466400	-2.59828500
O	1.10342400	0.07442000	-4.47408100
O	0.67827700	1.02680900	-2.54731600
C	-3.84298300	2.60568000	-0.61912400
H	-4.76725700	3.13304000	-0.83870200
C	-3.84835100	1.23837700	-0.42891300
C	-2.60354900	0.60698400	-0.13967700
C	-2.56500400	-0.84723800	0.13096100
C	-3.78006200	-1.55162800	0.37508300
C	-5.08345700	-0.78977300	0.41680400
H	-5.23222500	-0.41471000	1.43963500
C	-5.08998800	0.38997500	-0.56483100
H	-5.13826400	0.00782700	-1.59466900
C	-3.69423400	-2.90779100	0.61977000
H	-4.59218200	-3.48963600	0.80865900
C	-2.43723800	-3.56055300	0.64077200
C	-1.30131300	-2.74018000	0.40881000
N	-0.02752400	-3.30486900	0.43535800
H	0.83780000	4.98278500	-0.22571400
C	-1.29981400	5.34245400	-0.58741800
C	-2.53818200	4.74626900	-0.69367100
C	-2.25667100	-4.94393700	0.88785000
C	-0.97637300	-5.45446700	0.90192700

H	-0.78703700	-6.50528800	1.08826300
H	1.15228500	-4.95888300	0.67478300
H	-3.11914900	-5.57789000	1.06476600
H	-3.42957900	5.33013700	-0.89751600
H	-5.98265000	1.00322700	-0.41224800
H	-5.91784500	-1.46385400	0.20273500
H	-1.17469100	6.41291100	-0.70280000

*Cartesian Coordinates for the La(2b)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -1896.09473138 Hartree*

La	1.20823400	-0.00157600	0.03023400
O	0.92795100	2.69674700	-0.17973500
C	-0.27769500	4.67151500	-0.41193500
N	-0.21821400	3.33892300	-0.27163800
O	1.04497000	-2.80153200	0.39882200
N	-1.22966400	1.29306400	-0.06755400
C	-1.39957200	2.60805200	-0.21096300
O	0.38257200	0.78116400	2.46924000
N	-1.17153400	-1.48985100	0.27763100
C	-2.67854100	3.23627500	-0.28940200
O	2.48652300	1.15225300	2.06519500
C	-0.07797900	-4.82801600	0.59995300
O	1.62150800	1.77305500	3.97917000
N	4.26069000	0.00576000	-0.50527100
O	3.70118600	-0.96447700	0.10576100
N	1.24851200	-0.31740200	-3.09297400
O	5.47108800	0.02021500	-0.72856100
N	1.50042800	1.24927700	2.87155500
O	3.49984800	0.96488800	-0.87586800
O	1.82014000	-1.18305900	-2.35384300
O	1.25942700	-0.40114500	-4.32209300
O	0.66105300	0.65077800	-2.49543300
C	-3.84379500	2.40323900	-0.20677200
H	-4.82407800	2.86696000	-0.26843700
C	-3.67197400	1.04304500	-0.04738700
C	-2.33698600	0.58861700	0.01505600
C	-2.30760100	-0.83315200	0.18716500

C	-3.62203000	-1.34508200	0.22932200
C	-4.60024300	-0.17183000	0.08454000
C	-3.73546500	-2.71296300	0.37615500
H	-4.69525400	-3.21982800	0.41900800
C	-2.53609500	-3.49543600	0.46678200
C	-1.28418000	-2.81220500	0.40885100
N	-0.07152100	-3.49201100	0.47324000
H	0.67925400	5.17615900	-0.44898100
C	-1.51330200	5.33763300	-0.49909000
C	-2.70762800	4.64542100	-0.44049100
C	-2.50737100	-4.90625600	0.60150400
C	-1.28502900	-5.54698100	0.66638000
H	-1.22399200	-6.62465700	0.76728300
H	0.89876100	-5.29282800	0.64188000
H	-3.43530300	-5.46665800	0.64905000
H	-3.65793100	5.16504800	-0.50635100
H	-1.49724300	6.41567100	-0.61207800
H	-5.26097100	-0.08516300	0.95495200
H	-5.24325100	-0.28675600	-0.79587000

*Cartesian Coordinates for the La(2c)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -1857.99025441 Hartree*

La	1.10530500	0.13186400	0.02354800
O	0.91511700	2.65996100	0.08448900
C	-0.10554700	4.71004700	-0.13180400
N	-0.17894400	3.37330300	-0.07395900
O	1.10383500	-2.23648900	0.88971300
N	-1.38815700	1.38865200	-0.09343600
C	-1.40945000	2.72607400	-0.18063600
O	0.17704000	0.50875100	2.51460100
N	-1.26791200	-1.27131800	0.23160800
C	-2.58380600	3.50288000	-0.36658900
O	2.34398200	0.37164100	2.41289600
C	0.27849200	-4.37647600	1.04786100
O	1.36207800	0.65225900	4.35146900
N	3.99246300	-0.11786300	-1.19626800
O	3.59924900	-0.84945900	-0.22736000

N	0.47387500	-0.75374200	-2.91916200
O	5.12258900	-0.23338600	-1.67615600
N	1.29644900	0.51537700	3.12852600
O	3.15930100	0.73775100	-1.64780500
O	1.02276100	-1.53952100	-2.07541200
O	0.28650100	-1.08936800	-4.08988200
O	0.12618500	0.39526300	-2.48644700
C	-3.79312600	2.77362100	-0.47352400
H	-4.72734700	3.30611600	-0.62187700
C	-3.77650400	1.40077800	-0.38179000
C	-2.54385900	0.72636100	-0.18061300
C	-2.47470400	-0.75333800	-0.01698000
C	-3.63493700	-1.56786600	-0.08374000
C	-3.52752100	-2.92364300	0.12307500
H	-4.40327300	-3.56261700	0.06934500
C	-2.26706600	-3.49412600	0.42546900
C	-1.17337500	-2.58937800	0.47010300
N	0.09182500	-3.07183100	0.80098600
H	0.89443500	5.11327900	-0.03587000
C	-1.25004800	5.50337200	-0.31019800
C	-2.49003500	4.91442300	-0.43145800
C	-2.05368000	-4.86960600	0.68475700
C	-0.77940900	-5.29682300	0.98943700
H	-0.56269600	-6.33839700	1.19650500
H	1.29625400	-4.64796800	1.29728100
H	-2.88813900	-5.56168900	0.64418800
H	-3.38619600	5.50891800	-0.57412800
H	-1.12492200	6.57910100	-0.35157900
H	-4.70686400	0.85484900	-0.45819100
H	-4.60481700	-1.13963700	-0.29609400

*Cartesian Coordinates for the La(2d)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -1974.73098908 Hartree*

La	0.97787200	0.02048700	-0.11728300
O	0.70730400	2.50210100	0.50662900
C	-0.25632200	4.54142600	0.01383600
N	-0.33869400	3.20957300	0.13297500

O	0.99708800	-2.52241900	-0.04124200
N	-1.54848100	1.23406600	0.06119600
C	-1.54092600	2.55720400	-0.13393800
O	0.25093900	-0.32872600	2.43583900
N	-1.41427100	-1.45802000	0.08218800
C	-2.66146300	3.29723900	-0.58787500
O	2.27650600	0.42272600	2.18994700
C	0.18001600	-4.61261300	0.47965300
O	1.47158300	0.10714200	4.20250800
N	4.04630200	0.18886000	-0.67718900
O	3.48509500	-0.92342000	-0.40780100
N	1.00573000	0.64849300	-3.19560200
O	5.25517000	0.26703800	-0.90782200
N	1.33778300	0.06785900	2.97921400
O	3.29379600	1.22127200	-0.69686100
O	1.56551400	-0.40633000	-2.75259700
O	1.01272600	0.93438200	-4.39416900
O	0.43674100	1.40456800	-2.33403800
C	-3.80196300	2.53310600	-0.93848700
H	-4.65830000	3.04137200	-1.37297800
C	-3.82445600	1.16032500	-0.77178200
C	-2.66929300	0.55661100	-0.18144700
C	-2.61799200	-0.89079000	0.17261700
C	-3.77238100	-1.59157100	0.64674100
C	-3.63254100	-2.94566100	0.88857600
H	-4.48158200	-3.52461700	1.24106700
C	-2.38525500	-3.59534000	0.72621400
C	-1.29814900	-2.76353800	0.35471600
N	-0.01832400	-3.30553400	0.26191100
H	0.71261200	4.96182900	0.25093600
C	-1.35721700	5.30977600	-0.40233000
C	-2.55597600	4.70467800	-0.71541100
C	-2.15919100	-4.97521100	0.95665100
C	-0.87926900	-5.46906900	0.82230200
H	-0.65504700	-6.51671200	0.98662400
H	1.20694400	-4.93947500	0.37827400
H	-2.98581800	-5.61885500	1.23923300
H	-3.40660200	5.28341300	-1.06024500



H	-1.22738900	6.38297400	-0.48180400
C	-4.95970100	0.31133500	-1.29747600
C	-5.05078500	-0.85931600	0.98775200
C	-5.85207900	-0.33012500	-0.21711900
H	-6.41922300	-1.14470600	-0.68159900
H	-6.57934900	0.40084000	0.15419400
H	-4.52271500	-0.48462600	-1.91438600
H	-5.57566500	0.91766700	-1.96877600
H	-4.78888300	-0.01323600	1.63643800
H	-5.68641600	-1.51954200	1.58573100

*Cartesian Coordinates for the La(3a)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -1819.84807277 Hartree*

La	1.77267300	-0.32827800	0.33734200
O	0.25352500	4.36822600	0.06431400
N	-1.00810400	4.41518700	-0.18342900
O	1.18627300	-2.72172300	0.92940800
N	-1.36210100	2.00799700	-0.01715200
C	-1.83538100	3.21908800	-0.22585300
O	0.95651500	-0.29479600	2.94637700
N	-0.95810500	-1.02336400	0.33342500
C	-3.15303600	3.59644000	-0.51179700
O	3.01519900	-0.91569200	2.61846200
O	2.19099300	-0.90900200	4.64783300
N	4.42293800	-1.15348600	-1.09054200
O	3.88303000	-1.85620700	-0.16893700
N	0.86458400	-0.71288600	-2.62978400
O	5.46148900	-1.50885500	-1.64751700
N	2.05666300	-0.70977900	3.43931700
O	3.82829400	-0.06908400	-1.40351400
O	1.23098800	-1.67535500	-1.86809500
O	0.56222900	-0.90643100	-3.80799400
O	0.82647200	0.44494700	-2.10369300
C	-4.12272500	2.60097800	-0.58551900
H	-5.16481400	2.82634200	-0.79454500
C	-3.67637900	1.29449600	-0.37046200
C	-2.30922500	1.05995900	-0.10472600

C	-2.11580000	-0.38099700	0.07737100
C	-3.36871400	-1.02642100	-0.05132700
C	-4.44202800	-0.00738100	-0.35762300
C	-3.47298400	-2.40940100	0.10611200
H	-4.42296100	-2.92744900	0.01209400
C	-2.28711800	-3.08358100	0.39515900
C	-1.12271000	-2.32771800	0.48338300
N	-0.02197900	-3.19559200	0.77987600
H	-4.92804900	-0.20939000	-1.32112200
H	-5.23458300	-0.00934200	0.40184400
C	-1.75847000	5.46595800	-0.43091000
C	-3.18994200	5.09214400	-0.66891500
H	-1.32115800	6.45477100	-0.44513700
H	-3.52909600	5.40206400	-1.66726200
H	-3.86134200	5.57578900	0.05400800
C	-1.91321600	-4.52099100	0.64853800
C	-0.43376000	-4.43200000	0.87808900
H	-2.42196000	-4.94760900	1.52378800
H	-2.14245700	-5.17982300	-0.19995400
H	0.25803000	-5.23205400	1.10396900

*Cartesian Coordinates for the La(3b)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -1857.97368932 Hartree*

La	1.50970400	-0.03428800	0.19082500
O	0.57582800	3.99377200	0.06147700
N	-0.68827200	4.13304500	-0.13041500
O	1.25788500	-2.45896800	0.89577800
N	-1.18785200	1.75116500	-0.01722500
C	-1.58694200	2.99709900	-0.17248200
O	0.48206500	0.19438300	2.67019600
N	-0.93691600	-1.18914500	0.28309900
C	-2.89420600	3.45692800	-0.39459400
O	2.58419000	-0.35862600	2.65236500
C	0.17237300	-4.49872900	0.94554000
O	1.52123900	-0.18825800	4.55984800
N	4.28440200	-0.59581400	-1.13277400
O	3.83317400	-1.23320200	-0.11775300

N	0.68815900	-0.85467700	-2.72385500
O	5.37560100	-0.87471000	-1.63106800
N	1.53100800	-0.11783500	3.32910400
O	3.54848500	0.33313500	-1.59877100
O	1.28422300	-1.65524500	-1.92882600
O	0.41899300	-1.17250700	-3.88372300
O	0.37994900	0.28966100	-2.25166700
C	-3.93180700	2.53187700	-0.46682000
H	-4.96125000	2.83611300	-0.63268500
C	-3.56507500	1.19022600	-0.30802000
C	-2.20936800	0.88071500	-0.09649900
C	-2.07505500	-0.55443900	0.05800600
C	-3.35863900	-1.15865600	-0.04720800
C	-4.39530600	-0.08091300	-0.30492900
C	-3.44525700	-2.52057000	0.09850900
H	-4.38850100	-3.05409000	0.02400900
C	-2.24976300	-3.25473600	0.37285000
C	-1.03383700	-2.51957400	0.46109500
N	0.15263100	-3.16934400	0.76425600
C	-2.20855400	-4.65601300	0.56651900
C	-0.99908400	-5.26245600	0.84517300
H	-0.92604500	-6.33270800	0.99985300
H	1.14470300	-4.91366500	1.17812000
H	-3.12295800	-5.23620100	0.49738900
H	-4.91211700	-0.23407000	-1.26067800
H	-5.16705100	-0.06282700	0.47455200
C	-1.38234900	5.23522300	-0.31387500
C	-2.84246200	4.95690700	-0.50166000
H	-0.88639100	6.19604300	-0.31600900
H	-3.20378700	5.32128500	-1.47330800
H	-3.45236700	5.45329000	0.26578000

*Cartesian Coordinates for the La(3c)(NO<sub>3</sub>)<sub>3</sub> complex at B3LYP/LC/6-31+G(d);*

*E = -2203.38581695 Hartree*

C	-0.66225400	1.26195700	-0.28482300
C	-1.11664500	2.57249700	-0.56796200
C	1.23186300	2.60384800	-0.52006000

C	0.80847800	1.27187800	-0.29040200
C	2.57739100	2.86199900	-0.46833100
C	3.46336400	1.79609100	-0.18264500
C	2.94816900	0.46255000	-0.02810100
N	1.60334900	0.22445400	-0.08970500
C	4.85300700	2.08671300	-0.00079800
C	5.72329600	1.11641800	0.37768900
C	5.28404300	-0.23793400	0.53242000
C	3.92282800	-0.58218000	0.26913700
N	-1.43850000	0.21343700	-0.03529800
C	-2.78933400	0.40753800	-0.05322300
C	-3.34000400	1.67958900	-0.42605800
C	-2.47100400	2.77188300	-0.66445200
C	-3.73226800	-0.65740100	0.25684000
C	-5.12624300	-0.46526400	0.02186100
C	-5.60597700	0.81133400	-0.41949500
C	-4.75112200	1.85200900	-0.59649500
H	2.97783500	3.86232300	-0.60823300
H	5.18560700	3.11174600	-0.13461800
H	6.76918900	1.34057000	0.56159700
H	-2.89180500	3.73909500	-0.92575600
H	-6.67263800	0.92937000	-0.58194900
H	-5.11853600	2.82859900	-0.89746500
C	0.04910700	3.51541800	-0.74412500
H	0.02262500	4.34056700	-0.02155500
H	0.06482200	3.96794300	-1.74388900
N	-3.34777000	-1.86825800	0.81216000
C	-4.23006800	-2.86686900	1.02505300
C	-5.58349100	-2.72507700	0.73779200
C	-6.03932700	-1.51530600	0.25303200
C	6.20975900	-1.22541500	0.92957100
C	5.80445800	-2.53947300	1.04849700
C	4.49484000	-2.86606600	0.71770100
N	3.60583500	-1.93114300	0.31899100
O	-2.11147000	-2.08346000	1.22022800
H	-3.79095200	-3.75712900	1.45491100
H	-6.25038300	-3.55871800	0.92556300
H	-7.09391000	-1.35421400	0.05440800

H	7.23505000	-0.93595100	1.13553200
H	6.48067900	-3.32676300	1.36109600
H	4.10056800	-3.87341100	0.71920900
O	2.43873100	-2.38130400	-0.08153000
La	0.01099900	-2.13565600	-0.06329400
O	0.60631800	-1.25191500	2.41839600
O	0.39517000	-3.41121600	2.30130600
O	0.81383600	-2.46361200	4.23178900
N	-0.38608600	-4.98158800	-1.33612500
O	-0.99012700	-4.63391500	-0.26838700
N	-1.36774400	-1.52864500	-2.83666100
O	-0.57524100	-6.08490500	-1.85658800
N	0.61005800	-2.37859700	3.01656300
O	0.42215200	-4.13453900	-1.84304900
O	-1.93869600	-2.23263000	-1.93985000
O	-1.89364100	-1.33099300	-3.93559500
O	-0.22919200	-1.03518100	-2.54302200