Supporting Information File

The Fascinating Role of the Number of f Electrons in Dipolar and Octupolar Contributions to Quadratic Hyperpolarizability of trinuclear lanthanides-*bis*copper Schiff base complexes.

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Complete ref 11: Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Synthesis of $[La(NO_3)_3(CuL)_2]$

0.24 g ($6.98x10^{-4}$ mol) of CuL were dissolved in 100 mL of EtOH at 70°C. 25 mL of a warm (50°C) EtOH solution containing 0.151 g ($3.49\ x10^{-4}$ mol) of $La(NO_3)_3 \cdot 6H_2O$ have been dropwise added to the above solution under stirring. At the end of this addition a pale yellow-green precipitate appeared. The whole suspension was left to digest at 60°C for two hours. Afterward, the suspension was left to cool to room temperature and the precipitate was filtered under vacuum and repeatedly washed using cold EtOH; yield 68%. Elemental analysis for $C_{34}H_{32}Cu_2LaN_7O_{13}$: C=40.33; H=3.19; N=9.68; Found: C=40.32; H=3.12; N=9.56 %. EDX Cu/La=1.93. Exact mass of $[La(NO_3)_3(CuL)_2]$ = 1011 (molecular weight = 1012.65); MS ($MALDI^+$, m/z fragments: M*= $[La(NO_3)_3(CuL)_2]$, 949 (M* - NO_3^-), 1074 (M* + Cu^+), IR (Nujol; ν/cm^{-1}): 1622 (s), 1550 (s), 1475 (s), 1280 (s), 1030 (m), 822 (m). UV-vis in C_2H_5OH: 226.4 nm, 273.4 nm, 362.2 nm.

Synthesis of $[Ce(NO_3)_3(CuL)_2]$

0. 687 g ($2.00x10^{-3}$ mol) of CuL were dissolved in 100 mL of EtOH at 70°C. 25 mL of a warm (50°C) EtOH solution containing 0.435 g ($1.00\ x10^{-3}$ mol) of $Ce(NO_3)_3 \cdot 6H_2O$ have been dropwise added to the above solution under stirring. At the end of this addition a pale yellow-green precipitate appeared. The whole suspension was left to digest at 60°C for two hours. Afterward, the suspension was left to cool to room temperature and the precipitate was filtered under vacuum and repeatedly washed using cold EtOH; yield 65%. Elemental analysis for $C_{34}H_{32}Cu_2CeN_7O_{13}$: C=40.28; H=3.18; N=9.67; Found: C=40.32; H=3.12; N=9.58 %. EDX Cu/Ce=1.91. Exact mass of $[(CuL)_2Ce(NO_3)_3]$ =1012 (molecular weight = 1013.87); MS ($MALDI^+$, m/z fragments: M*= $[Ce(NO_3)_3(CuL)_2]$, 950 (M* - NO_3^-), 1075 (M* + Cu^+). IR (Nujol; ν/cm^{-1}): 1620 (s), 1552 (s), 1477 (s), 1280 (s), 1028 (m), 820 (m). UV-vis in C_2H_5OH: 227.5 nm, 274.0 nm, 361.5 nm.

Synthesis of $[Sm(NO_3)_3(CuL)_2]$

0.688 g ($2.00x10^{-3}$ mol) of CuL were dissolved in 100 mL of EtOH at 70°C. 25 mL of a warm (50°C) EtOH solution containing 0.45 g ($1.01\ x10^{-3}$ mol) of $Sm(NO_3)_3 \cdot 6H_2O$ have been dropwise added to the above solution under stirring. At the end of this addition a pale yellow-green precipitate appeared. The whole suspension was left to digest at 60°C for two hours. Afterward, the suspension was left to cool to room temperature and the precipitate was filtered under

vacuum and repeatedly washed using cold EtOH; yield 62%. Elemental analysis for $C_{34}H_{32}Cu_2SmN_7O_{13}$: C=39.88; H=3.15; N=9.57; Found: C=40.03; H=3.12; N=9.35 %. EDX Cu/Sm=1.83. Exact mass of $[Sm(NO_3)_3(CuL)_2]$ = 1024 (molecular weight = 1024.11); MS ($MALDI^+$, m/z fragments: M*= $[Sm(NO_3)_3(CuL)_2]$, 962 (M* - NO_3^-). IR (Nujol; ν/cm^{-1}): 1622 (s), 1555 (s), 1475 (s), 1285 (s), 1030 (m), 822 (m). UV-vis in C_2H_5OH: 226.0 nm, 274.0 nm, 364.8 nm.

Synthesis of $[Eu(NO_3)_3(CuL)_2]$

0. 685 g ($1.99x10^{-3}$ mol) of CuL were dissolved in 100 mL of EtOH at 70°C. 25 mL of a warm (50°C) EtOH solution containing 0.43 g ($1.00\ x10^{-3}$ mol) of $Eu(NO_3)_3{\cdot}5H_2O$ have been dropwise added to the above solution under stirring. At the end of this addition a pale yellow-green precipitate appeared. The whole suspension was left to digest at 60°C for two hours. Afterward, the suspension was left to cool to room temperature and the precipitate was filtered under vacuum and repeatedly washed using cold EtOH; yield 66%. Elemental analysis for $C_{34}H_{32}Cu_2EuN_7O_{13}$: C=39.81; H=3.14; N=9.56; Found: C=39.98; H=3.12; N=9.56 %. EDX Cu/Eu=1.92. Exact mass of $[Eu(NO_3)_3(CuL)_2]$ = 1025 (molecular weight = 1025.71); MS ($MALDI^+$, m/z fragments: M*= $[Eu(NO_3)_3(CuL)_2]$, 963 (M* - NO_3^-), IR (Nujol; ν/cm^{-1}): 1620 (s), 1560 (s), 1480 (s), 1285 (s), 1028 (m), 820 (m). UV-vis in C_2H_5OH: 226.6 nm, 273.0 nm, 364.4 nm.

Synthesis of $[Er(NO_3)_3(CuL)_2]$

0. 181 g ($5.26x10^{-4}$ mol) of CuL were dissolved in 100 mL of EtOH at 70°C. 25 mL of a warm (50°C) EtOH solution containing 0.118 g ($2.66\ x10^{-4}$ mol) of $Er(NO_3)_3{\cdot}5H_2O$ have been dropwise added to the above solution under stirring. At the end of this addition a pale yellow-green precipitate appeared. The whole suspension was left to digest at 60°C for two hours. Afterward, the suspension was left to cool to room temperature and the precipitate was filtered under vacuum and repeatedly washed using cold EtOH; yield 64%. Elemental analysis for $C_{34}H_{32}Cu_2ErN_7O_{13}$: C=39.23; H=3.01; N=9.42; Found: C=38.30; H=2.99; N=9.39 %. EDX Cu/Er=2.00. Exact mass of $[Er(NO_3)_3(CuL)_2]$ = 1038 (molecular weight = 1041.01); MS ($MALDI^+$, m/z fragments: M*= $[Er(NO_3)_3(CuL)_2]$, 976 (M* - NO_3^-), IR (Nujol; ν/cm^{-1}): 1618 (s), 1555 (s), 1480 (s), 1280 (s), 1030 (m), 820 (m). UV-vis in C_2H_5OH: 227.0 nm, 273.3 nm, 363.0 nm.

Cartesian coordinates (Å) of the CuL optimized structure (L=N,N'-1,3-propylen-bis(salicylideniminato)

O	2.682612000	1.712988000	-2.084479000
O	2.829361000	-0.868168000	-1.707566000
N	4.056594000	2.207998000	0.346669000
N	5.202024000	-0.542650000	-0.167623000
C	2.005884000	2.782887000	-1.790478000
C	1.008304000	3.248902000	-2.706686000
C	0.253195000	4.379184000	-2.433215000
C	0.443558000	5.124925000	-1.241236000
C	1.413801000	4.712833000	-0.342766000
C	2.209413000	3.555838000	-0.584846000
C	3.243969000	3.243023000	0.346100000
C	5.161352000	2.269639000	1.313934000
C	5.644564000	0.905667000	1.802186000
C	6.240375000	0.039008000	0.685926000
C	5.261961000	-1.839039000	-0.376307000
C	4.365208000	-2.655082000	-1.127959000
C	4.656467000	-4.046024000	-1.233863000
C	3.831646000	-4.907810000	-1.937457000
C	2.670575000	-4.384921000	-2.562795000
C	2.352522000	-3.037796000	-2.483128000
C	3.181343000	-2.118949000	-1.761488000
H	0.862718000	2.668841000	-3.621754000
H	-0.508353000	4.699894000	-3.152164000
H	-0.162087000	6.012233000	-1.040745000
H	1.590004000	5.280216000	0.578868000
H	3.389130000	3.990303000	1.149625000
H	4.864443000	2.893446000	2.180174000
H	6.015966000	2.785357000	0.830345000
H	4.824385000	0.356789000	2.297933000
H	6.425732000	1.081719000	2.562666000
H	6.859758000	-0.767446000	1.124658000
H	6.912819000	0.662416000	0.064066000
H	6.109247000	-2.378118000	0.088067000
H	5.559953000	-4.425237000	-0.741583000
H	4.069458000	-5.971883000	-2.011717000
H	2.011412000	-5.057545000	-3.122046000
H	1.458999000	-2.629909000	-2.963018000
Cu	3.761887000	0.632529000	-0.872571000

Cartesian coordinates (Å) of the $[La(NO_3)_3(CuL)_2]$ optimized structure (L=N,N'-1,3-propylen-bis(salicylideniminato)

Cu	-3.068553000	0.410127000	-0.344107000
O	1.347297000	1.262442000	-0.403053000
O	2.311355000	-1.074161000	-1.103149000
O	-2.477062000	-1.100340000	0.846724000
O	-1.601104000	1.369711000	0.610782000
O	0.066140000	-2.385805000	2.386910000
O	0.905878000	-3.197172000	0.530559000
O	0.884796000	-4.436645000	2.358257000
O	0.611671000	0.397392000	2.631758000
O	2.340088000	-0.593694000	1.719134000
O	2.615378000	0.678049000	3.508511000
O	-2.098516000	-1.640869000	-3.271060000
O	-0.875948000	-2.320562000	-1.564871000
O	-1.313562000	-0.184522000	-1.799932000
N	3.757188000	2.183036000	0.662990000
N	5.004503000	-0.275533000	-0.367287000
N	-4.507941000	-0.733950000	-1.128766000
N	-3.624647000	2.109091000	-1.235767000
N	0.631476000	-3.388491000	1.782054000
N	1.874907000	0.180245000	2.659864000
N	-1.448174000	-1.405314000	-2.252552000
C	1.250189000	2.459429000	-0.965535000
C	0.213864000	2.734364000	-1.897478000
C	0.065289000	4.009770000	-2.439825000
C	0.934477000	5.064733000	-2.088654000
C	1.970163000	4.811051000	-1.196398000
C	2.165644000	3.520950000	-0.639414000
C	3.278826000	3.325652000	0.253545000
C	4.834183000	2.206284000	1.666835000
C	5.634357000	0.902044000	1.711851000
C	6.092726000	0.419170000	0.328379000
C	5.261108000	-1.414954000	-0.952978000
C	4.354282000	-2.281776000	-1.648831000
C	4.929322000	-3.406088000	-2.307913000
C	4.154847000	-4.311534000	-3.015255000
C	2.757220000	-4.110326000	-3.067256000
C	2.157069000	-3.028979000	-2.432739000
C	2.928024000	-2.084321000	-1.700462000
C	-3.319466000	-1.984326000	1.375174000
C	-2.995401000	-2.624445000	2.601281000
C	-3.843845000	-3.580231000	3.155169000
C	-5.054298000	-3.943305000	2.526513000
C	-5.392936000	-3.328916000	1.328988000
C	-4.558822000	-2.341133000	0.738248000

C	-4.997724000	-1.771298000	-0.505881000
C	-5.062336000	-0.394870000	-2.441497000
C	-5.483290000	1.074651000	-2.548464000
C	-4.305496000	2.054269000	-2.529166000
C	-3.376152000	3.281374000	-0.716813000
C	-2.601918000	3.571104000	0.456607000
C	-2.659684000	4.895007000	0.969209000
C	-1.919776000	5.275939000	2.079766000
C	-1.082633000	4.319056000	2.696221000
C	-0.988128000	3.016155000	2.216448000
C	-1.737726000	2.597661000	1.079285000
H	-0.459897000	1.917691000	-2.166565000
H	-0.741589000	4.190885000	-3.158155000
H	0.802951000	6.061060000	-2.518175000
H	2.667797000	5.609468000	-0.918747000
H	3.772004000	4.248821000	0.613999000
H	4.373233000	2.368368000	2.656802000
H	5.507624000	3.061843000	1.455338000
H	5.027140000	0.115320000	2.190562000
H	6.517166000	1.070100000	2.351984000
H	6.962935000	-0.257635000	0.424122000
H	6.413875000	1.284027000	-0.285286000
H	6.309283000	-1.767371000	-0.922456000
H	6.015558000	-3.538820000	-2.247601000
H	4.614649000	-5.166180000	-3.517582000
H	2.125847000	-4.819946000	-3.611436000
H	1.072704000	-2.898726000	-2.454588000
H	-2.043473000	-2.377349000	3.075547000
H	-3.556101000	-4.057917000	4.097122000
H	-5.709467000	-4.696528000	2.971093000
H	-6.325247000	-3.593722000	0.817398000
H	-5.856756000	-2.282917000	-0.979980000
H	-3.796919000	4.163448000	-1.236638000
H	-3.315930000	5.616485000	0.468864000
H	-1.984851000	6.294622000	2.470338000
H	-0.494844000	4.601003000	3.576169000
H	-0.335333000	2.281685000	2.693855000
H	-5.928185000	-1.050651000	-2.659659000
H	-4.281682000	-0.612645000	-3.194390000
H	-6.199166000	1.327825000	-1.746056000
H	-6.011931000	1.204027000	-3.509213000
H	-4.650985000	3.068530000	-2.812447000
H	-3.563422000	1.734613000	-3.286357000
Cu	3.190614000	0.463528000	-0.212695000
La	0.076824000	-0.822852000	0.395216000

Cartesian coordinates (Å) of the $[Ce(NO_3)_3(CuL)_2]$ optimized structure (L=N,N'-1,3-propylen-bis(salicylideniminato)

Cu	-3.041190000	0.389455000	-0.194861000
O	1.471657000	1.278456000	-0.386803000
O	2.212932000	-1.188418000	-0.944719000
O	-2.233179000	-0.979272000	1.070398000
O	-1.477365000	1.418899000	0.567179000
O	0.365843000	-2.856312000	1.174910000
O	-0.746808000	-2.754553000	-0.708379000
O	-0.438216000	-4.708383000	0.274688000
O	0.318417000	0.164683000	2.658665000
O	2.143200000	-0.671132000	1.790582000
O	2.258580000	0.498709000	3.665706000
O	-2.602178000	-0.583294000	-3.406703000
O	-0.497534000	-1.222291000	-3.435639000
O	-1.285940000	-0.090896000	-1.704680000
N	3.908727000	2.000805000	0.804550000
N	4.953478000	-0.646534000	-0.065347000
N	-4.598644000	-0.799563000	-0.553476000
N	-3.737037000	2.034875000	-1.073939000
N	-0.283164000	-3.498792000	0.247455000
N	1.597801000	0.014274000	2.750966000
N	-1.467797000	-0.672686000	-2.904385000
C	1.496374000	2.486225000	-0.946486000
C	0.486321000	2.861378000	-1.867806000
C	0.483785000	4.131833000	-2.440838000
C	1.477100000	5.081287000	-2.119710000
C	2.476845000	4.730059000	-1.220547000
C	2.523953000	3.439785000	-0.628976000
C	3.592972000	3.162529000	0.298471000
C	4.964789000	1.964269000	1.828213000
C	5.614377000	0.583805000	1.974883000
C	6.078653000	-0.031285000	0.645001000
C	5.104074000	-1.844961000	-0.561278000
C	4.143378000	-2.637174000	-1.281129000
C	4.630437000	-3.851835000	-1.842601000
C	3.820510000	-4.686069000	-2.598526000
C	2.478327000	-4.307936000	-2.818205000
C	1.960461000	-3.134289000	-2.278338000
C	2.761338000	-2.279503000	-1.475563000
C	-2.916785000	-1.887393000	1.757043000
C	-2.337795000	-2.468258000	2.915567000
C	-3.019580000	-3.438697000	3.645411000
C	-4.304893000	-3.874377000	3.258434000
C	-4.891223000	-3.312861000	2.131733000
C	-4.232024000	-2.312037000	1.367702000

C	-4.927459000	-1.803357000	0.213447000
C	-5.436028000	-0.533113000	-1.726750000
C	-5.838873000	0.941254000	-1.857544000
C	-4.672873000	1.883288000	-2.188347000
C	-3.416350000	3.238328000	-0.684919000
C	-2.462490000	3.615448000	0.326460000
C	-2.429823000	4.982869000	0.711702000
C	-1.544952000	5.448563000	1.675428000
C	-0.658992000	4.532028000	2.282507000
C	-0.648385000	3.187657000	1.920713000
C	-1.533952000	2.691790000	0.924677000
H	-0.283485000	2.122335000	-2.106516000
H	-0.304776000	4.392568000	-3.154258000
H	1.461490000	6.076383000	-2.571347000
H	3.259307000	5.450932000	-0.957275000
H	4.195263000	4.040839000	0.602829000
H	4.509335000	2.237659000	2.797305000
H	5.735960000	2.726791000	1.593543000
H	4.907225000	-0.107293000	2.464400000
H	6.482204000	0.692554000	2.647826000
H	6.867744000	-0.786878000	0.823426000
H	6.517187000	0.755968000	0.000303000
H	6.096470000	-2.319226000	-0.438460000
H	5.680796000	-4.113594000	-1.670645000
H	4.215973000	-5.612944000	-3.021431000
H	1.825594000	-4.943096000	-3.425318000
H	0.925210000	-2.839614000	-2.461846000
H	-1.342926000	-2.131048000	3.215377000
H	-2.543731000	-3.868088000	4.532623000
H	-4.828635000	-4.641669000	3.833816000
H	-5.888504000	-3.635618000	1.811875000
H	-5.858720000	-2.344540000	-0.040692000
H	-3.931780000	4.083141000	-1.181139000
H	-3.134036000	5.672489000	0.231895000
H	-1.540220000	6.502709000	1.963784000
H	0.031478000	4.878179000	3.058730000
H	0.015876000	2.471271000	2.409719000
H	-6.344686000	-1.165586000	-1.687224000
H	-4.852676000	-0.827255000	-2.617690000
H	-6.353516000	1.281586000	-0.940702000
H	-6.568457000	1.012159000	-2.683413000
H	-5.062928000	2.876058000	-2.488962000
H	-4.106158000	1.462638000	-3.039955000
Cu	3.234629000	0.303920000	-0.043190000
Ce	0.054350000	-0.592059000	0.241406000

Cartesian coordinates (Å) of the $[Sm(NO_3)_3(CuL)_2]$ optimized structure (L=N,N'-1,3-propylen-bis(salicylideniminato)

Cu	-3.040978000	0.446288000	-0.169183000
O	1.487353000	1.271919000	-0.377194000
O	2.254994000	-1.119181000	-1.016618000
O	-2.323483000	-0.925520000	1.089254000
O	-1.467147000	1.411131000	0.630364000
O	0.575547000	-2.895413000	1.123999000
O	-0.812389000	-2.795262000	-0.563472000
O	-0.278351000	-4.756934000	0.296041000
O	0.331701000	0.043147000	2.704171000
O	2.178249000	-0.620256000	1.740322000
O	2.279895000	0.533861000	3.625052000
O	-2.689225000	-0.536335000	-3.332682000
O	-0.634035000	-1.314269000	-3.383176000
O	-1.315927000	-0.112615000	-1.658731000
N	3.935284000	2.027657000	0.699927000
N	4.950923000	-0.611567000	-0.101667000
N	-4.656230000	-0.652675000	-0.558172000
N	-3.650600000	2.129113000	-1.037081000
N	-0.177837000	-3.538274000	0.286526000
N	1.619135000	0.002962000	2.732096000
N	-1.553538000	-0.691004000	-2.838335000
C	1.476691000	2.459437000	-0.966658000
C	0.429712000	2.804663000	-1.861097000
C	0.394413000	4.062652000	-2.458594000
C	1.384200000	5.033355000	-2.189687000
C	2.415452000	4.716970000	-1.313768000
C	2.498524000	3.438081000	-0.702682000
C	3.576418000	3.187198000	0.217610000
C	4.955901000	2.006302000	1.760553000
C	5.613508000	0.633311000	1.927607000
C	6.076348000	0.013156000	0.601151000
C	5.109199000	-1.812221000	-0.595997000
C	4.152453000	-2.615449000	-1.299530000
C	4.616445000	-3.856131000	-1.823431000
C	3.783210000	-4.699085000	-2.542048000
C	2.443420000	-4.305420000	-2.762588000
C	1.950506000	-3.103508000	-2.266233000
C	2.778201000	-2.235944000	-1.502067000
C	-2.995809000	-1.897806000	1.680398000
C	-2.397685000	-2.592903000	2.766934000
C	-3.074707000	-3.621084000	3.415435000
C	-4.374876000	-4.005129000	3.018563000
C	-4.976836000	-3.339454000	1.959313000
C	-4.319260000	-2.281651000	1.274203000

C	-5.009247000	-1.683434000	0.163990000
C	-5.488131000	-0.328831000	-1.723023000
C	-5.795052000	1.166274000	-1.857114000
C	-4.563246000	2.023332000	-2.175580000
C	-3.292530000	3.316759000	-0.630855000
C	-2.352946000	3.647509000	0.407315000
C	-2.272868000	5.005435000	0.814958000
C	-1.391270000	5.416102000	1.806816000
C	-0.559045000	4.452547000	2.419240000
C	-0.595401000	3.115167000	2.035990000
C	-1.478306000	2.673569000	1.009334000
H	-0.336499000	2.050095000	-2.060070000
H	-0.418019000	4.297821000	-3.154153000
H	1.340326000	6.017314000	-2.663277000
H	3.193894000	5.454513000	-1.087330000
H	4.140357000	4.079127000	0.551413000
H	4.467160000	2.280018000	2.712772000
H	5.724389000	2.775389000	1.541835000
H	4.909221000	-0.056227000	2.423006000
H	6.480923000	0.753669000	2.598703000
H	6.865552000	-0.740909000	0.781369000
H	6.512722000	0.796943000	-0.049141000
H	6.106289000	-2.274636000	-0.473832000
H	5.662584000	-4.132291000	-1.648509000
H	4.156325000	-5.647939000	-2.935386000
H	1.774324000	-4.953390000	-3.337453000
H	0.919411000	-2.791743000	-2.451812000
H	-1.393456000	-2.292567000	3.077610000
H	-2.585649000	-4.138113000	4.246998000
H	-4.895219000	-4.816838000	3.532810000
H	-5.981716000	-3.625619000	1.628549000
H	-5.957788000	-2.181822000	-0.110596000
H	-3.759742000	4.182960000	-1.136808000
H	-2.936047000	5.732412000	0.331977000
H	-1.349039000	6.464017000	2.114238000
H	0.124816000	4.757040000	3.218440000
H	0.025359000	2.362998000	2.528555000
H	-6.434799000	-0.900995000	-1.670986000
H	-4.934479000	-0.662190000	-2.618971000
H	-6.294228000	1.543534000	-0.946237000
H	-6.509995000	1.282541000	-2.690562000
H	-4.877739000	3.035697000	-2.497243000
H	-4.002902000	1.551576000	-3.004030000
Cu	3.230999000	0.333444000	-0.101969000
Sm	0.040021000	-0.640563000	0.292889000

Cartesian coordinates (Å) of the $[Eu(NO_3)_3(CuL)_2]$ optimized structure (L=N,N'-1,3-propylen-bis(salicylideniminato)

Cu	-3.063478000	0.310532000	-0.276195000
O	1.509518000	1.261421000	-0.421101000
O	2.364443000	-1.134391000	-0.930746000
O	-2.286018000	-1.069708000	0.962825000
O	-1.597843000	1.372319000	0.565083000
O	0.317571000	-2.883974000	1.328888000
O	-0.516565000	-2.855627000	-0.694845000
O	-0.310158000	-4.772684000	0.375690000
O	0.360540000	0.246335000	2.664769000
O	2.179619000	-0.603028000	1.792471000
O	2.315010000	0.643801000	3.615120000
O	-2.527561000	-0.663579000	-3.456543000
O	-0.414723000	-1.260062000	-3.355918000
O	-1.330669000	-0.167638000	-1.672609000
N	3.879335000	2.091105000	0.785910000
N	5.019028000	-0.489657000	-0.008120000
N	-4.626809000	-0.870789000	-0.639533000
N	-3.782660000	1.932929000	-1.174593000
N	-0.176537000	-3.555284000	0.338447000
N	1.635250000	0.115644000	2.732911000
N	-1.425474000	-0.730707000	-2.873030000
C	1.469972000	2.468544000	-0.966682000
C	0.422216000	2.804350000	-1.863956000
C	0.353257000	4.075767000	-2.427768000
C	1.308673000	5.070266000	-2.121215000
C	2.334977000	4.765622000	-1.236789000
C	2.450097000	3.474318000	-0.655197000
C	3.505040000	3.242562000	0.294035000
C	4.860107000	2.095949000	1.884505000
C	5.565306000	0.748497000	2.059310000
C	6.095834000	0.166721000	0.741564000
C	5.245886000	-1.669498000	-0.524813000
C	4.346536000	-2.497177000	-1.273654000
C	4.889261000	-3.680660000	-1.850294000
C	4.114999000	-4.532976000	-2.622294000
C	2.756884000	-4.207089000	-2.841551000
C	2.186614000	-3.063845000	-2.292532000
C	2.953414000	-2.188513000	-1.474164000
C	-3.000719000	-1.878648000	1.720858000
C	-2.435678000	-2.410142000	2.914419000
C	-3.156812000	-3.291147000	3.713303000
C	-4.466438000	-3.690971000	3.364832000
C	-5.037720000	-3.185786000	2.203181000
C	-4.342035000	-2.269706000	1.371524000

C	-5.002718000	-1.819601000	0.174791000
C	-5.407664000	-0.658994000	-1.860285000
C	-5.823764000	0.803868000	-2.059313000
C	-4.650137000	1.751595000	-2.339086000
C	-3.511282000	3.146579000	-0.776488000
C	-2.614261000	3.549355000	0.272569000
C	-2.619338000	4.918813000	0.651907000
C	-1.775922000	5.402727000	1.643107000
C	-0.892682000	4.503882000	2.283335000
C	-0.845645000	3.159181000	1.930808000
C	-1.692337000	2.640324000	0.907801000
H	-0.319432000	2.032609000	-2.087978000
H	-0.459374000	4.304062000	-3.125259000
H	1.238831000	6.064268000	-2.569944000
H	3.083168000	5.522867000	-0.976216000
H	4.033710000	4.146228000	0.652267000
H	4.324084000	2.335179000	2.819876000
H	5.604293000	2.897585000	1.702099000
H	4.871423000	0.027169000	2.523070000
H	6.404296000	0.894017000	2.760806000
H	6.907040000	-0.559573000	0.936618000
H	6.521357000	0.976681000	0.116632000
H	6.260702000	-2.086695000	-0.388184000
H	5.948489000	-3.902133000	-1.676726000
H	4.548121000	-5.436349000	-3.058873000
H	2.134064000	-4.862828000	-3.458144000
H	1.138619000	-2.812082000	-2.466962000
H	-1.420288000	-2.106148000	3.178437000
H	-2.695050000	-3.681221000	4.625709000
H	-5.019705000	-4.390130000	3.996698000
H	-6.049799000	-3.488062000	1.911157000
H	-5.938552000	-2.354705000	-0.074074000
H	-4.022321000	3.974551000	-1.303913000
H	-3.317974000	5.594661000	0.145045000
H	-1.799988000	6.457579000	1.928083000
H	-0.234797000	4.867119000	3.079949000
H	-0.183929000	2.454720000	2.441599000
H	-6.306757000	-1.305761000	-1.844715000
H	-4.772120000	-0.971181000	-2.708822000
H	-6.401009000	1.160465000	-1.186939000
H	-6.499019000	0.840324000	-2.932281000
H	-5.031267000	2.735172000	-2.677986000
H	-4.029889000	1.322186000	-3.147871000
Cu	3.259006000	0.382049000	-0.037885000
Eu	0.097603000	-0.659660000	0.285428000

Cartesian coordinates (Å) of the $[Er(NO_3)_3(CuL)_2]$ optimized structure (L=N,N'-1,3-propylen-bis(salicylideniminato)

Cu	-2.991720000	0.323172000	-0.257054000
O	1.422799000	1.263408000	-0.370809000
O	2.244558000	-1.130290000	-0.923160000
O	-2.180096000	-1.020706000	0.991228000
O	-1.481236000	1.378780000	0.528094000
O	0.410990000	-2.727546000	1.261599000
O	-0.568641000	-2.695231000	-0.686282000
O	-0.250000000	-4.627315000	0.340163000
O	0.206921000	0.119903000	2.592377000
O	2.089414000	-0.569044000	1.737958000
O	2.103354000	0.553519000	3.646904000
O	-2.492688000	-0.634368000	-3.381217000
O	-0.365878000	-1.190814000	-3.403589000
O	-1.211206000	-0.124064000	-1.660568000
N	3.820145000	2.087333000	0.785488000
N	4.932660000	-0.500487000	-0.023134000
N	-4.535067000	-0.873701000	-0.623433000
N	-3.723469000	1.949108000	-1.128108000
N	-0.142438000	-3.411053000	0.307614000
N	1.487954000	0.053156000	2.707033000
N	-1.358822000	-0.689527000	-2.864643000
C	1.401784000	2.454444000	-0.960286000
C	0.379894000	2.775443000	-1.889754000
C	0.332571000	4.033739000	-2.486389000
C	1.28129000	5.029038000	-2.181553000
C	2.293287000	4.736165000	-1.270591000
C	2.388124000	3.457693000	-0.659474000
C	3.443617000	3.236809000	0.294124000
C	4.812500000	2.087572000	1.872066000
C	5.518746000	0.737704000	2.033478000
C	6.024447000	0.152256000	0.706799000
C	5.139528000	-1.684810000	-0.537372000
C	4.221717000	-2.506148000	-1.271402000
C	4.756089000	-3.696611000	-1.843850000
C	3.976600000	-4.550622000	-2.607379000
C	2.620309000	-4.217826000	-2.823438000
C	2.057911000	-3.069400000	-2.276403000
C	2.828056000	-2.192946000	-1.464556000
C	-2.864935000	-1.895158000	1.713768000
C	-2.289936000	-2.435408000	2.895082000
C	-2.978239000	-3.374465000	3.657994000
C	-4.265177000	-3.820482000	3.285409000
C	-4.847505000	-3.300426000	2.137434000
C	-4.182490000	-2.330308000	1.339460000

C	-4.866611000	-1.861315000	0.163888000
C	-5.346590000	-0.644540000	-1.821504000
C	-5.774881000	0.819089000	-1.984673000
C	-4.613980000	1.779494000	-2.276320000
C	-3.445600000	3.156762000	-0.717450000
C	-2.532059000	3.544864000	0.324196000
C	-2.550861000	4.903933000	0.738537000
C	-1.701425000	5.374496000	1.730983000
C	-0.799539000	4.471434000	2.336370000
C	-0.737414000	3.136927000	1.946227000
C	-1.586596000	2.634053000	0.919902000
H	-0.360467000	2.003310000	-2.112373000
H	-0.461692000	4.249197000	-3.208738000
H	1.233157000	6.013148000	-2.653860000
H	3.044097000	5.492448000	-1.014798000
H	3.972291000	4.143848000	0.644480000
H	4.288923000	2.325568000	2.815334000
H	5.555748000	2.889381000	1.686342000
H	4.833989000	0.015200000	2.509002000
H	6.370419000	0.881447000	2.719919000
H	6.836206000	-0.576734000	0.889644000
H	6.443210000	0.959923000	0.074417000
H	6.151695000	-2.112487000	-0.413133000
H	5.815101000	-3.921101000	-1.672635000
H	4.404013000	-5.458676000	-3.039860000
H	1.991622000	-4.871528000	-3.436285000
H	1.013027000	-2.810297000	-2.455094000
H	-1.293303000	-2.092951000	3.180854000
H	-2.506469000	-3.771851000	4.562213000
H	-4.792487000	-4.563403000	3.888878000
H	-5.845410000	-3.631033000	1.827721000
H	-5.788420000	-2.417029000	-0.091818000
H	-3.968111000	3.991795000	-1.221882000
H	-3.266636000	5.581824000	0.259102000
H	-1.736579000	6.420990000	2.044045000
H	-0.138521000	4.821255000	3.136368000
H	-0.063633000	2.431192000	2.436599000
H	-6.242631000	-1.295014000	-1.793351000
H	-4.733676000	-0.940250000	-2.691640000
H	-6.332383000	1.157818000	-1.092568000
H	-6.471455000	0.867174000	-2.840146000
H	-5.008208000	2.765338000	-2.592925000
H	-4.007808000	1.365845000	-3.103778000
Cu	3.183766000	0.378283000	-0.040338000
Er	0.060546000	-0.602631000	0.260839000