
Supplementary Information – Theoretical Insights into the Vibrational Spectra and Chemical Bonding of Ln(III) Complexes with a Tripodal N₄O₃ Ligand Along the Lanthanide Series

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1 Structural Parameters: Experiment versus Theory

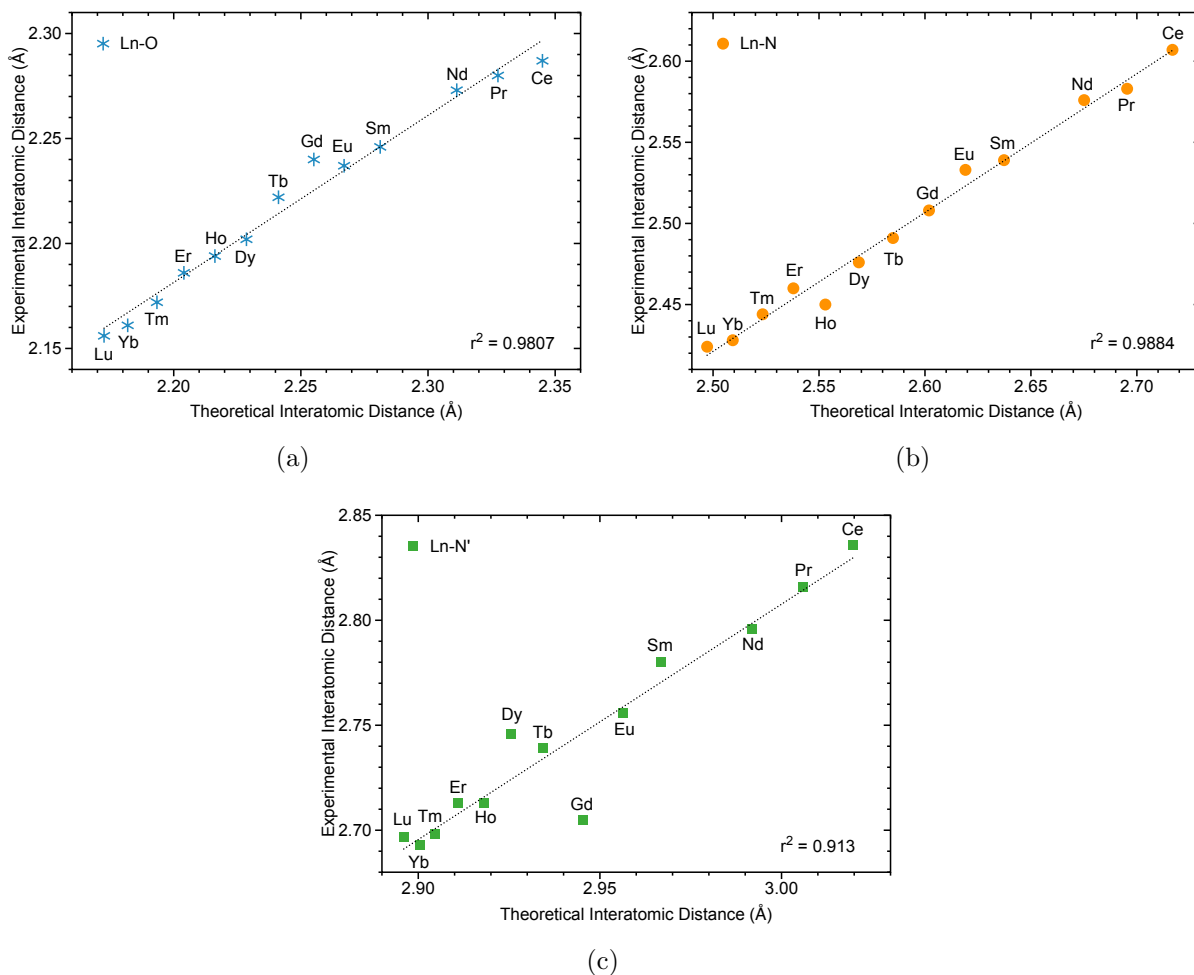


Figure S1: Correlation of experimental [1] interatomic distances for Ln-O (a), Ln-N (b), and Ln-N' (c) with the corresponding B3LYP/MWBn(Ln)/6-311++G** interatomic distances along the series. [La(trensal)] and [Pm(trensal)] have not been included (see text).

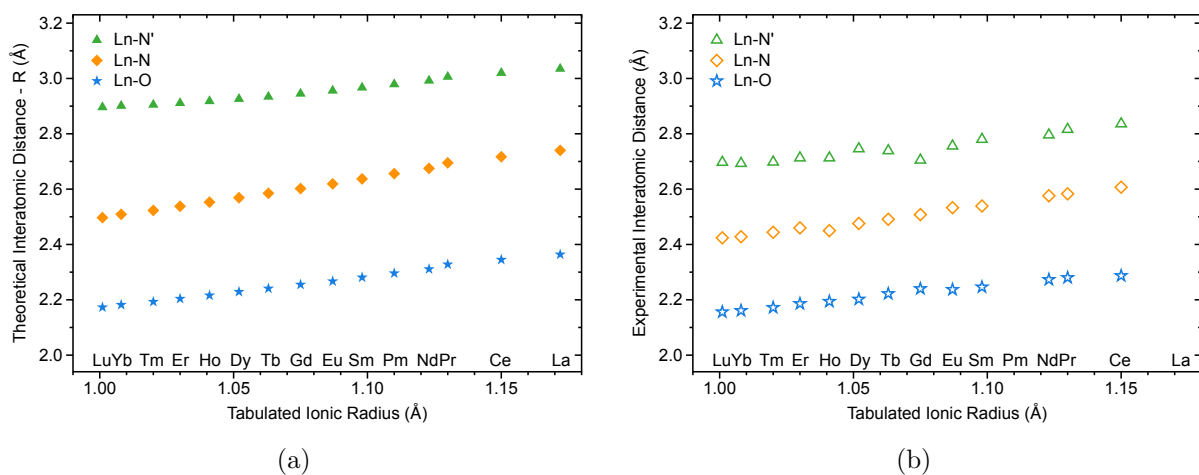


Figure S2: B3LYP/MWBn(Ln)/6-311++G** interatomic distances (a) and experimental interatomic distances [1] (b) versus tabulated ionic radius [2]. [La(trensal)] and [Pm(trensal)] have not been included in (b) – see text.

2 Cartesian coordinates of [M(trensal)]

Equilibrium geometries of [M(trensal)] were obtained at the B3LYP/MWBn(Ln)/6-311++G** level for M being the trivalent ions of La–Lu, and at the UB3LYP/6-311++G** level for M being the trivalent ion of Fe.

2.1 [La(trensal)]

La	0.000000000	0.000000000	-0.019189000
N	0.000000000	0.000000000	3.015987000
O	0.000000000	2.064712000	-1.170157000
N	-1.483560000	1.913231000	1.263144000
O	1.788093000	-1.032356000	-1.170157000
O	-1.788093000	-1.032356000	-1.170157000
N	-0.915127000	-2.241416000	1.263144000
C	3.610825000	-1.791516000	-2.460920000
C	4.973589000	-1.915721000	-2.641054000
C	5.882915000	-1.402322000	-1.697314000
C	5.387125000	-0.767982000	-0.577492000
C	3.997505000	-0.615330000	-0.358899000
C	3.069917000	-1.137647000	-1.321786000
H	2.908539000	-2.186115000	-3.185829000
H	5.349221000	-2.418440000	-3.526713000
H	6.950493000	-1.504905000	-1.848350000
H	6.073297000	-0.367812000	0.163919000
C	3.593687000	0.044400000	0.855828000
N	2.398687000	0.328185000	1.263144000
C	2.281570000	0.949096000	2.578939000
H	1.842790000	1.948005000	2.467294000
C	1.402822000	0.087780000	3.487360000
C	-1.727012000	5.795915000	-1.697314000
C	-2.028470000	5.049379000	-0.577492000
C	-1.465861000	3.769606000	-0.358899000
C	-0.549727000	3.227450000	-1.321786000
C	-0.253914000	4.022824000	-2.460920000
C	-0.827731000	5.265115000	-2.641054000
H	-2.171961000	6.771756000	-1.848350000
H	-2.718114000	5.443536000	0.163919000
H	0.438961000	3.611926000	-3.185829000
H	-0.580180000	5.841781000	-3.526713000
C	-1.835295000	3.090024000	0.855828000
H	-2.498125000	3.680200000	1.504756000
C	-1.962726000	1.501349000	2.578939000
C	-0.777431000	1.170990000	3.487360000
C	-0.318844000	-2.450445000	2.578939000

H	0.765627000	-2.569906000	2.467294000
C	-0.625391000	-1.258770000	3.487360000
H	-1.708514000	-1.121217000	3.504816000
C	-1.758392000	-3.134424000	0.855828000
C	-4.145858000	-3.349393000	-2.641054000
C	-4.155904000	-4.393593000	-1.697314000
C	-3.358655000	-4.281396000	-0.577492000
C	-2.531644000	-3.154276000	-0.358899000
C	-2.520190000	-2.089803000	-1.321786000
C	-3.356911000	-2.231308000	-2.460920000
H	-4.769041000	-3.423341000	-3.526713000
H	-4.778532000	-5.266851000	-1.848350000
H	-3.355184000	-5.075723000	0.163919000
H	-3.347500000	-1.425811000	-3.185829000
H	-1.938084000	-4.003540000	1.504756000
H	1.825259000	-0.919008000	3.504816000
H	-2.567398000	2.284392000	3.058646000
H	-1.124310000	1.009373000	4.520037000
H	4.436210000	0.323340000	1.504756000
H	3.262040000	1.081236000	3.058646000
H	-2.608417000	0.621901000	2.467294000
H	-0.116745000	2.040225000	3.504816000
H	1.436297000	0.468995000	4.520037000
H	-0.311987000	-1.478367000	4.520037000
H	-0.694642000	-3.365628000	3.058646000

2.2 [Ce(trensal)]

Ce	0.000000000	0.000000000	-0.000953000
N	0.000000000	0.000000000	3.018718000
O	0.000000000	2.043564000	-1.151150000
N	-1.510242000	1.874053000	1.259218000
O	1.769779000	-1.021782000	-1.151150000
O	-1.769779000	-1.021782000	-1.151150000
N	-0.867857000	-2.244934000	1.259218000
C	3.592123000	-1.759832000	-2.454875000
C	4.955173000	-1.860611000	-2.648207000
C	5.864692000	-1.321926000	-1.719030000
C	5.369188000	-0.686385000	-0.599595000
C	3.979472000	-0.557023000	-0.368182000
C	3.051616000	-1.105142000	-1.316360000
H	2.889875000	-2.173999000	-3.168790000
H	5.330697000	-2.364552000	-3.533219000
H	6.932332000	-1.406498000	-1.880455000
H	6.055680000	-0.267101000	0.130864000
C	3.574739000	0.104820000	0.844967000
N	2.378099000	0.370881000	1.259218000
C	2.258333000	0.995320000	2.572915000
H	1.799878000	1.985192000	2.460171000
C	1.400794000	0.120178000	3.488410000
C	-1.787524000	5.739935000	-1.719030000
C	-2.090167000	4.993045000	-0.599595000
C	-1.507339000	3.724835000	-0.368182000
C	-0.568727000	3.195348000	-1.316360000
C	-0.272002000	3.990786000	-2.454875000
C	-0.866250000	5.221611000	-2.648207000
H	-2.248103000	6.706825000	-1.880455000
H	-2.796524000	5.377923000	0.130864000
H	0.437801000	3.589705000	-3.168790000
H	-0.617587000	5.798795000	-3.533219000
C	-1.878147000	3.043404000	0.844967000
H	-2.557058000	3.624260000	1.485536000
C	-1.991139000	1.458114000	2.572915000
C	-0.804474000	1.153034000	3.488410000
C	-0.267194000	-2.453434000	2.572915000
H	0.819288000	-2.551337000	2.460171000
C	-0.596320000	-1.273212000	3.488410000
H	-1.682104000	-1.159039000	3.510133000
C	-1.696592000	-3.148225000	0.844967000
C	-4.088923000	-3.361000000	-2.648207000
C	-4.077167000	-4.418009000	-1.719030000

C	-3.279020000	-4.306661000	-0.599595000
C	-2.472132000	-3.167812000	-0.368182000
C	-2.482889000	-2.090206000	-1.316360000
C	-3.320121000	-2.230953000	-2.454875000
H	-4.713111000	-3.434243000	-3.533219000
H	-4.684229000	-5.300326000	-1.880455000
H	-3.259156000	-5.110822000	0.130864000
H	-3.327676000	-1.415706000	-3.168790000
H	-1.860172000	-4.026607000	1.485536000
H	1.844809000	-0.877226000	3.510133000
H	-2.613134000	2.231497000	3.045961000
H	-1.153307000	0.982768000	4.518971000
H	4.417230000	0.402347000	1.485536000
H	3.239100000	1.147292000	3.045961000
H	-2.619166000	0.566144000	2.460171000
H	-0.162705000	2.036265000	3.510133000
H	1.427755000	0.507409000	4.518971000
H	-0.274449000	-1.490177000	4.518971000
H	-0.625966000	-3.378789000	3.045961000

2.3 [Pr(trensal)]

Pr	0.000000000	0.000000000	0.015324000
N	0.000000000	0.000000000	3.021268000
O	-2.021879000	0.091452000	-1.133986000
N	-1.904409000	-1.449306000	1.255359000
O	1.090139000	1.705273000	-1.133986000
O	0.931740000	-1.796725000	-1.133986000
N	2.207341000	-0.924613000	1.255359000
C	1.891227000	3.492832000	-2.448586000
C	2.031973000	4.850562000	-2.654146000
C	1.511041000	5.784106000	-1.738742000
C	0.852125000	5.317950000	-0.620206000
C	0.681532000	3.934801000	-0.376848000
C	1.211329000	2.982522000	-1.311004000
H	2.291583000	2.772151000	-3.151919000
H	2.553993000	5.202998000	-3.538175000
H	1.627176000	6.847268000	-1.909826000
H	0.446233000	6.023140000	0.099928000
C	0.000000000	3.559487000	0.834636000
N	-0.302932000	2.373920000	1.255359000
C	-0.936184000	2.279936000	2.566827000
H	-1.937559000	1.847662000	2.452616000
C	-0.087416000	1.403628000	3.489285000
C	-5.764703000	-1.583453000	-1.738742000
C	-5.031542000	-1.921013000	-0.620206000
C	-3.748404000	-1.377176000	-0.376848000
C	-3.188604000	-0.442220000	-1.311004000
C	-3.970495000	-0.108566000	-2.448586000
C	-5.216697000	-0.665541000	-2.654146000
H	-6.743496000	-2.014458000	-1.909826000
H	-5.439309000	-2.625121000	0.099928000
H	-3.546544000	0.598494000	-3.151919000
H	-5.782924000	-0.389676000	-3.538175000
C	-3.082606000	-1.779744000	0.834636000
H	-3.684835000	-2.447276000	1.467256000
C	-1.506391000	-1.950727000	2.566827000
C	-1.171869000	-0.777519000	3.489285000
C	2.442574000	-0.329209000	2.566827000
H	2.568901000	0.754144000	2.452616000
C	1.259286000	-0.626109000	3.489285000
H	1.118241000	-1.708662000	3.515085000
C	3.082606000	-1.779744000	0.834636000
C	3.184724000	-4.185022000	-2.654146000
C	4.253662000	-4.200653000	-1.738742000

C	4.179418000	-3.396937000	-0.620206000
C	3.066872000	-2.557625000	-0.376848000
C	1.977275000	-2.540302000	-1.311004000
C	2.079268000	-3.384267000	-2.448586000
H	3.228932000	-4.813321000	-3.538175000
H	5.116320000	-4.832810000	-1.909826000
H	4.993076000	-3.398019000	0.099928000
H	1.254961000	-3.370644000	-3.151919000
H	3.961821000	-1.967522000	1.467256000
H	0.920624000	1.822756000	3.515085000
H	-2.298155000	-2.554157000	3.033333000
H	-1.009286000	-1.135772000	4.517785000
H	-0.276986000	4.414798000	1.467256000
H	-1.062887000	3.267339000	3.033333000
H	-0.631343000	-2.601806000	2.452616000
H	-2.038865000	-0.114094000	3.515085000
H	-0.478964000	1.441953000	4.517785000
H	1.488250000	-0.306181000	4.517785000
H	3.361043000	-0.713182000	3.033333000

2.4 [Nd(trensal)]

Nd	0.000000000	0.000000000	0.031576000
N	0.000000000	0.000000000	3.023418000
O	-2.001881000	0.120874000	-1.117248000
N	-1.892487000	-1.444108000	1.251846000
O	1.105620000	1.673243000	-1.117248000
O	0.896261000	-1.794117000	-1.117248000
N	2.196878000	-0.916887000	1.251846000
C	1.915292000	3.448598000	-2.443042000
C	2.055807000	4.804379000	-2.660899000
C	1.526461000	5.746318000	-1.758864000
C	0.859513000	5.290477000	-0.640908000
C	0.688640000	3.909535000	-0.385503000
C	1.226731000	2.948774000	-1.305965000
H	2.322010000	2.721426000	-3.135962000
H	2.584298000	5.148823000	-3.544230000
H	1.642623000	6.807870000	-1.939660000
H	0.447277000	6.002092000	0.069239000
C	0.000000000	3.543920000	0.824683000
N	-0.304391000	2.360996000	1.251846000
C	-0.942438000	2.274141000	2.561433000
H	-1.942666000	1.839544000	2.446196000
C	-0.094578000	1.403573000	3.490020000
C	-5.739688000	-1.551205000	-1.758864000
C	-5.011445000	-1.900878000	-0.640908000
C	-3.730077000	-1.358388000	-0.385503000
C	-3.167079000	-0.412007000	-1.305965000
C	-3.944220000	-0.065608000	-2.443042000
C	-5.188618000	-0.621808000	-2.660899000
H	-6.717100000	-1.981382000	-1.939660000
H	-5.421603000	-2.613692000	0.069239000
H	-3.517829000	0.650206000	-3.135962000
H	-5.751160000	-0.336344000	-3.544230000
C	-3.069124000	-1.771960000	0.824683000
H	-3.673046000	-2.444973000	1.449679000
C	-1.498245000	-1.953246000	2.561433000
C	-1.168241000	-0.783694000	3.490020000
C	2.440683000	-0.320895000	2.561433000
H	2.564425000	0.762626000	2.446196000
C	1.262819000	-0.619880000	3.490020000
H	1.125932000	-1.702897000	3.519361000
C	3.069124000	-1.771960000	0.824683000
C	3.132811000	-4.182571000	-2.660899000
C	4.213227000	-4.195113000	-1.758864000

C	4.151931000	-3.389599000	-0.640908000
C	3.041437000	-2.551147000	-0.385503000
C	1.940348000	-2.536767000	-1.305965000
C	2.028928000	-3.382991000	-2.443042000
H	3.166863000	-4.812479000	-3.544230000
H	5.074477000	-4.826488000	-1.939660000
H	4.974325000	-3.388399000	0.069239000
H	1.195819000	-3.371632000	-3.135962000
H	3.953931000	-1.958464000	1.449679000
H	0.911786000	1.826534000	3.519361000
H	-2.290740000	-2.560282000	3.021848000
H	-1.003331000	-1.145878000	4.516695000
H	-0.280886000	4.403437000	1.449679000
H	-1.071899000	3.263980000	3.021848000
H	-0.621759000	-2.602170000	2.446196000
H	-2.037718000	-0.123637000	3.519361000
H	-0.490694000	1.441850000	4.516695000
H	1.494025000	-0.295971000	4.516695000
H	3.362639000	-0.703698000	3.021848000

2.5 [Pm(trensal)]

Pm	-0.000042000	-0.000039000	0.047761000
N	-0.000116000	0.000253000	3.026220000
O	-1.648411000	1.112152000	-1.099309000
N	-2.347002000	-0.318481000	1.249243000
O	1.787340000	0.871292000	-1.099361000
O	-0.139164000	-1.983551000	-1.099381000
N	1.449225000	-1.873191000	1.249028000
C	3.368981000	1.998894000	-2.438208000
C	4.160181000	3.106191000	-2.669079000
C	4.163576000	4.197925000	-1.780652000
C	3.357620000	4.144536000	-0.662594000
C	2.527276000	3.031035000	-0.394482000
C	2.522047000	1.918531000	-1.301155000
H	3.364722000	1.157120000	-3.120641000
H	4.790721000	3.134103000	-3.552178000
H	4.788623000	5.061564000	-1.971765000
H	3.349618000	4.975572000	0.037372000
C	1.747352000	3.065864000	0.814887000
N	0.897730000	2.191749000	1.249095000
C	0.300430000	2.440750000	2.557051000
H	-0.783863000	2.556675000	2.441253000
C	0.607332000	1.269528000	3.491400000
C	-5.717539000	1.506205000	-1.780585000
C	-5.268220000	0.835069000	-0.662484000
C	-3.888703000	0.672895000	-0.394409000
C	-2.922719000	1.224640000	-1.301147000
C	-3.415882000	1.917723000	-2.438277000
C	-4.770454000	2.049120000	-2.669108000
H	-6.778013000	1.615578000	-1.971661000
H	-5.983853000	0.412628000	0.037556000
H	-2.684814000	2.334930000	-3.120767000
H	-5.109982000	2.581103000	-3.552248000
C	-3.528823000	-0.019824000	0.815006000
H	-4.391072000	-0.309221000	1.432190000
C	-2.264022000	-0.959960000	2.557353000
C	-1.403045000	-0.108448000	3.491491000
C	1.963319000	-1.480428000	2.557092000
H	2.606123000	-0.599514000	2.441471000
C	0.795439000	-1.160496000	3.491303000
H	0.143100000	-2.035674000	3.524062000
C	1.781587000	-3.045970000	0.814745000
C	0.610561000	-5.155597000	-2.669456000
C	1.554382000	-5.704332000	-1.781036000

C	1.910984000	-4.979703000	-0.662901000
C	1.361592000	-3.703979000	-0.394684000
C	0.400654000	-3.143306000	-1.301325000
C	0.046987000	-3.916871000	-2.438492000
H	0.319599000	-5.715582000	-3.552621000
H	1.989956000	-6.677369000	-1.972223000
H	2.634733000	-5.388240000	0.037046000
H	-0.679931000	-3.492355000	-3.120909000
H	2.463454000	-3.647938000	1.431858000
H	1.691429000	1.142149000	3.524238000
H	-3.255557000	-1.096327000	3.011941000
H	-1.439140000	-0.509072000	4.516432000
H	1.927824000	3.957320000	1.432032000
H	0.677775000	3.367805000	3.011548000
H	-1.822586000	-1.957135000	2.441874000
H	-1.834853000	0.894052000	3.524261000
H	0.278397000	1.501252000	4.516293000
H	1.160538000	-0.991575000	4.516228000
H	2.577249000	-2.270851000	3.011737000

2.6 [Sm(trensal)]

Sm	0.000000000	0.000000000	0.061924000
N	0.000000000	0.000000000	3.028772000
O	-1.964536000	0.176490000	-1.084014000
N	-1.870519000	-1.433295000	1.246129000
O	1.135113000	1.613093000	-1.084014000
O	0.829423000	-1.789583000	-1.084014000
N	2.176529000	-0.903270000	1.246129000
C	1.957446000	3.364743000	-2.433534000
C	2.095946000	4.716586000	-2.675735000
C	1.551032000	5.674037000	-1.799513000
C	0.870655000	5.237814000	-0.681854000
C	0.700836000	3.861449000	-0.402610000
C	1.254393000	2.884949000	-1.296791000
H	2.376054000	2.625708000	-3.106516000
H	2.635196000	5.045917000	-3.558328000
H	1.666151000	6.732243000	-1.999585000
H	0.446668000	5.961454000	0.008963000
C	0.000000000	3.514223000	0.805630000
N	-0.306010000	2.336564000	1.246129000
C	-0.952628000	2.263817000	2.552297000
H	-1.951102000	1.825669000	2.435680000
C	-0.107084000	1.403504000	3.492379000
C	-5.689376000	-1.493785000	-1.799513000
C	-4.971408000	-1.864897000	-0.681854000
C	-3.694531000	-1.323783000	-0.402610000
C	-3.125636000	-0.356138000	-1.296791000
C	-3.892676000	0.012827000	-2.433534000
C	-5.132656000	-0.543150000	-2.675735000
H	-6.663369000	-1.923193000	-1.999585000
H	-5.386105000	-2.593901000	0.008963000
H	-3.461957000	0.744870000	-3.106516000
H	-5.687491000	-0.240812000	-3.558328000
C	-3.043406000	-1.757111000	0.805630000
H	-3.650567000	-2.440732000	1.415516000
C	-1.484209000	-1.956909000	2.552297000
C	-1.161928000	-0.794490000	3.492379000
C	2.436837000	-0.306908000	2.552297000
H	2.556627000	0.776869000	2.435680000
C	1.269013000	-0.609014000	3.492379000
H	1.139281000	-1.692749000	3.528352000
C	3.043406000	-1.757111000	0.805630000
C	3.036710000	-4.173436000	-2.675735000
C	4.138344000	-4.180252000	-1.799513000

C	4.100752000	-3.372917000	-0.681854000
C	2.993695000	-2.537666000	-0.402610000
C	1.871243000	-2.528811000	-1.296791000
C	1.935230000	-3.377569000	-2.433534000
H	3.052294000	-4.805106000	-3.558328000
H	4.997218000	-4.809050000	-1.999585000
H	4.939437000	-3.367553000	0.008963000
H	1.085902000	-3.370577000	-3.106516000
H	3.939020000	-1.941118000	1.415516000
H	0.896323000	1.833021000	3.528352000
H	-2.278688000	-2.569832000	3.001055000
H	-0.993054000	-1.164297000	4.515554000
H	-0.288452000	4.381850000	1.415516000
H	-1.086195000	3.258318000	3.001055000
H	-0.605525000	-2.602539000	2.435680000
H	-2.035604000	-0.140272000	3.528352000
H	-0.511784000	1.442159000	4.515554000
H	1.504838000	-0.277862000	4.515554000
H	3.364884000	-0.688486000	3.001055000

2.7 [Eu(trensal)]

Eu	0.000000000	0.000000000	0.074733000
N	0.000000000	0.000000000	3.031115000
O	-1.945910000	0.200688000	-1.070853000
N	-1.859233000	-1.427880000	1.242641000
O	1.146756000	1.584864000	-1.070853000
O	0.799154000	-1.785552000	-1.070853000
N	2.166197000	-0.896203000	1.242641000
C	1.978119000	3.325990000	-2.428238000
C	2.117520000	4.675892000	-2.680288000
C	1.565845000	5.640124000	-1.815676000
C	0.878075000	5.212585000	-0.699247000
C	0.707100000	3.838356000	-0.410290000
C	1.267035000	2.854975000	-1.292772000
H	2.401705000	2.581746000	-3.092304000
H	2.662756000	4.998464000	-3.561700000
H	1.681794000	6.696737000	-2.023530000
H	0.449019000	5.941436000	-0.017088000
C	0.000000000	3.499362000	0.796340000
N	-0.306964000	2.324083000	1.242641000
C	-0.958456000	2.257841000	2.546690000
H	-1.955660000	1.817202000	2.428852000
C	-0.114000000	1.403349000	3.492950000
C	-5.667413000	-1.464000000	-1.815676000
C	-4.953269000	-1.845857000	-0.699247000
C	-3.677664000	-1.306811000	-0.410290000
C	-3.105998000	-0.330203000	-1.292772000
C	-3.869451000	0.050106000	-2.428238000
C	-5.108201000	-0.504120000	-2.680288000
H	-6.640441000	-1.891892000	-2.023530000
H	-5.369944000	-2.581856000	-0.017088000
H	-3.436710000	0.789065000	-3.092304000
H	-5.660175000	-0.193218000	-3.561700000
C	-3.030536000	-1.749681000	0.796340000
H	-3.638862000	-2.438255000	1.399285000
C	-1.476120000	-1.958968000	2.546690000
C	-1.158336000	-0.800401000	3.492950000
C	2.434576000	-0.298873000	2.546690000
H	2.551573000	0.785050000	2.428852000
C	1.272336000	-0.602948000	3.492950000
H	1.146741000	-1.687072000	3.532285000
C	3.030536000	-1.749681000	0.796340000
C	2.990681000	-4.171772000	-2.680288000
C	4.101568000	-4.176124000	-1.815676000

C	4.075193000	-3.366728000	-0.699247000
C	2.970564000	-2.531545000	-0.410290000
C	1.838963000	-2.524772000	-1.292772000
C	1.891332000	-3.376096000	-2.428238000
H	2.997419000	-4.805246000	-3.561700000
H	4.958647000	-4.804845000	-2.023530000
H	4.920925000	-3.359580000	-0.017088000
H	1.035005000	-3.370811000	-3.092304000
H	3.931022000	-1.932220000	1.399285000
H	0.887677000	1.836643000	3.532285000
H	-2.271022000	-2.575549000	2.989488000
H	-0.987400000	-1.174244000	4.514250000
H	-0.292160000	4.370474000	1.399285000
H	-1.094980000	3.254537000	2.989488000
H	-0.595913000	-2.602252000	2.428852000
H	-2.034418000	-0.149571000	3.532285000
H	-0.523225000	1.442236000	4.514250000
H	1.510625000	-0.267992000	4.514250000
H	3.366002000	-0.678988000	2.989488000

2.8 [Gd(trensal)]

Gd	0.000000000	0.000000000	0.087882000
N	0.000000000	0.000000000	3.033275000
O	-1.928571000	0.222831000	-1.059396000
N	-1.849001000	-1.422903000	1.239640000
O	1.157262000	1.558776000	-1.059396000
O	0.771309000	-1.781607000	-1.059396000
N	2.156771000	-0.889830000	1.239640000
C	1.995861000	3.290265000	-2.424340000
C	2.135698000	4.638338000	-2.685611000
C	1.577990000	5.608681000	-1.831674000
C	0.883949000	5.189066000	-0.716161000
C	0.712276000	3.816855000	-0.418047000
C	1.277973000	2.827171000	-1.289842000
H	2.423931000	2.541411000	-3.080290000
H	2.686009000	4.954727000	-3.566117000
H	1.694388000	6.663781000	-2.046838000
H	0.450404000	5.922659000	-0.041972000
C	0.000000000	3.485632000	0.787362000
N	-0.307770000	2.312733000	1.239640000
C	-0.963039000	2.252963000	2.542047000
H	-1.959554000	1.810909000	2.423753000
C	-0.119810000	1.403244000	3.493631000
C	-5.646256000	-1.437761000	-1.831674000
C	-4.935838000	-1.829011000	-0.716161000
C	-3.661631000	-1.291578000	-0.418047000
C	-3.087389000	-0.306828000	-1.289842000
C	-3.847384000	0.083334000	-2.424340000
C	-5.084768000	-0.469600000	-2.685611000
H	-6.618198000	-1.864507000	-2.046838000
H	-5.354375000	-2.571268000	-0.041972000
H	-3.412892000	0.828480000	-3.080290000
H	-5.633924000	-0.151212000	-3.566117000
C	-3.018646000	-1.742816000	0.787362000
H	-3.628290000	-2.435791000	1.383769000
C	-1.469604000	-1.960498000	2.542047000
C	-1.155340000	-0.805381000	3.493631000
C	2.432643000	-0.292465000	2.542047000
H	2.548070000	0.791569000	2.423753000
C	1.275150000	-0.597863000	3.493631000
H	1.152896000	-1.682269000	3.536047000
C	3.018646000	-1.742816000	0.787362000
C	2.949070000	-4.168738000	-2.685611000
C	4.068265000	-4.170920000	-1.831674000

C	4.051888000	-3.360055000	-0.716161000
C	2.949355000	-2.525277000	-0.418047000
C	1.809415000	-2.520343000	-1.289842000
C	1.851523000	-3.373599000	-2.424340000
H	2.947915000	-4.803515000	-3.566117000
H	4.923810000	-4.799274000	-2.046838000
H	4.903971000	-3.351391000	-0.041972000
H	0.988961000	-3.369891000	-3.080290000
H	3.923602000	-1.924295000	1.383769000
H	0.880439000	1.839572000	3.536047000
H	-2.265509000	-2.579508000	2.979467000
H	-0.982510000	-1.182829000	4.513223000
H	-0.295312000	4.360087000	1.383769000
H	-1.101165000	3.251742000	2.979467000
H	-0.588516000	-2.602478000	2.423753000
H	-2.033336000	-0.157303000	3.536047000
H	-0.533105000	1.442293000	4.513223000
H	1.515615000	-0.259464000	4.513223000
H	3.366674000	-0.672234000	2.979467000

2.9 [Tb(trensal)]

Tb	0.000000000	0.000000000	0.102645000
N	0.000000000	0.000000000	3.036945000
O	-1.911067000	0.250005000	-1.041217000
N	-1.839832000	-1.416757000	1.238284000
O	1.172044000	1.530030000	-1.041217000
O	0.739022000	-1.780035000	-1.041217000
N	2.146864000	-0.884963000	1.238284000
C	2.012088000	3.249162000	-2.420886000
C	2.148828000	4.594785000	-2.696035000
C	1.583821000	5.572563000	-1.855405000
C	0.885550000	5.162916000	-0.738848000
C	0.716383000	3.793457000	-0.427208000
C	1.289500000	2.796231000	-1.285315000
H	2.445910000	2.494611000	-3.066439000
H	2.702607000	4.903468000	-3.577100000
H	1.698087000	6.625620000	-2.081456000
H	0.446438000	5.902289000	-0.074644000
C	0.000000000	3.471751000	0.778255000
N	-0.307032000	2.301720000	1.238284000
C	-0.965649000	2.249057000	2.539256000
H	-1.961855000	1.806377000	2.420775000
C	-0.124095000	1.403308000	3.495802000
C	-5.617892000	-1.414652000	-1.855405000
C	-4.913992000	-1.814550000	-0.738848000
C	-3.643422000	-1.276323000	-0.427208000
C	-3.066357000	-0.281376000	-1.285315000
C	-3.819901000	0.117938000	-2.420886000
C	-5.053614000	-0.436452000	-2.696035000
H	-6.586999000	-1.842224000	-2.081456000
H	-5.334751000	-2.564518000	-0.074644000
H	-3.383351000	0.870914000	-3.066439000
H	-5.597831000	-0.111208000	-3.577100000
C	-3.006624000	-1.735875000	0.778255000
H	-3.617933000	-2.434076000	1.366659000
C	-1.464916000	-1.960804000	2.539256000
C	-1.153253000	-0.809124000	3.495802000
C	2.430564000	-0.288252000	2.539256000
H	2.545296000	0.795828000	2.420775000
C	1.277349000	-0.594184000	3.495802000
H	1.157394000	-1.678749000	3.540946000
C	3.006624000	-1.735875000	0.778255000
C	2.904786000	-4.158332000	-2.696035000
C	4.034071000	-4.157911000	-1.855405000

C	4.028442000	-3.348367000	-0.738848000
C	2.927039000	-2.517134000	-0.427208000
C	1.776857000	-2.514855000	-1.285315000
C	1.807813000	-3.367100000	-2.420886000
H	2.895224000	-4.792260000	-3.577100000
H	4.888912000	-4.783397000	-2.081456000
H	4.888313000	-3.337771000	-0.074644000
H	0.937442000	-3.365525000	-3.066439000
H	3.916938000	-1.916184000	1.366659000
H	0.875142000	1.841707000	3.540946000
H	-2.262360000	-2.581539000	2.971269000
H	-0.979102000	-1.189941000	4.513850000
H	-0.299005000	4.350260000	1.366659000
H	-1.104498000	3.250031000	2.971269000
H	-0.583441000	-2.602205000	2.420775000
H	-2.032536000	-0.162958000	3.540946000
H	-0.540968000	1.442898000	4.513850000
H	1.520070000	-0.252957000	4.513850000
H	3.366859000	-0.668492000	2.971269000

2.10 [Dy(trensal)]

Dy	0.000000000	0.000000000	0.114761000
N	0.000000000	0.000000000	3.040398000
O	-1.894084000	0.272230000	-1.027619000
N	-1.830103000	-1.411158000	1.236364000
O	1.182800000	1.504210000	-1.027619000
O	0.711284000	-1.776440000	-1.027619000
N	2.137150000	-0.879337000	1.236364000
C	2.026696000	3.212990000	-2.417763000
C	2.162429000	4.556550000	-2.703403000
C	1.591860000	5.540379000	-1.873641000
C	0.889000000	5.138966000	-0.756956000
C	0.720565000	3.771860000	-0.434991000
C	1.299294000	2.768453000	-1.282029000
H	2.464774000	2.453851000	-3.055002000
H	2.719845000	4.858865000	-3.584385000
H	1.705548000	6.591690000	-2.107968000
H	0.445628000	5.883091000	-0.100942000
C	0.000000000	3.457998000	0.769879000
N	-0.307047000	2.290495000	1.236364000
C	-0.969305000	2.244412000	2.535698000
H	-1.964874000	1.800473000	2.416732000
C	-0.129229000	1.403208000	3.497513000
C	-5.594039000	-1.391598000	-1.873641000
C	-4.894975000	-1.799586000	-0.756956000
C	-3.626809000	-1.261902000	-0.434991000
C	-3.047198000	-0.259005000	-1.282029000
C	-3.795879000	0.148675000	-2.417763000
C	-5.027303000	-0.405557000	-2.703403000
H	-6.561345000	-1.818797000	-2.107968000
H	-5.317720000	-2.555620000	-0.100942000
H	-3.357484000	0.907631000	-3.055002000
H	-5.567823000	-0.073977000	-3.584385000
C	-2.994714000	-1.728999000	0.769879000
H	-3.607342000	-2.431662000	1.351423000
C	-1.459066000	-1.961649000	2.535698000
C	-1.150600000	-0.813520000	3.497513000
C	2.428370000	-0.282764000	2.535698000
H	2.541692000	0.801395000	2.416732000
C	1.279829000	-0.589689000	3.497513000
H	1.162802000	-1.674465000	3.545536000
C	2.994714000	-1.728999000	0.769879000
C	2.864874000	-4.150993000	-2.703403000
C	4.002179000	-4.148780000	-1.873641000

C	4.005975000	-3.339380000	-0.756956000
C	2.906244000	-2.509957000	-0.434991000
C	1.747904000	-2.509448000	-1.282029000
C	1.769183000	-3.361665000	-2.417763000
H	2.847978000	-4.784887000	-3.584385000
H	4.855797000	-4.772893000	-2.107968000
H	4.872092000	-3.327471000	-0.100942000
H	0.892710000	-3.361482000	-3.055002000
H	3.909552000	-1.908219000	1.351423000
H	0.868728000	1.844249000	3.545536000
H	-2.257601000	-2.584634000	2.962257000
H	-0.974985000	-1.197981000	4.513896000
H	-0.302210000	4.339881000	1.351423000
H	-1.109558000	3.247457000	2.962257000
H	-0.576818000	-2.601867000	2.416732000
H	-2.031531000	-0.169784000	3.545536000
H	-0.549989000	1.443352000	4.513896000
H	1.524974000	-0.245371000	4.513896000
H	3.367159000	-0.662823000	2.962257000

2.11 [Ho(trensal)]

Ho	0.000000000	0.000000000	0.126249000
N	0.000000000	0.000000000	3.044250000
O	-1.877071000	0.293381000	-1.014828000
N	-1.820409000	-1.405517000	1.234703000
O	1.192610000	1.478901000	-1.014828000
O	0.684460000	-1.772281000	-1.014828000
N	2.127418000	-0.873762000	1.234703000
C	2.039936000	3.177679000	-2.415036000
C	2.174771000	4.519162000	-2.710783000
C	1.599088000	5.508734000	-1.891435000
C	0.892044000	5.115235000	-0.774561000
C	0.724265000	3.750475000	-0.442644000
C	1.308085000	2.741198000	-1.279105000
H	2.481932000	2.414194000	-3.044321000
H	2.735526000	4.815304000	-3.591746000
H	1.712228000	6.558303000	-2.133708000
H	0.444790000	5.863866000	-0.126358000
C	0.000000000	3.444248000	0.761799000
N	-0.307009000	2.279279000	1.234703000
C	-0.972661000	2.239802000	2.532475000
H	-1.967666000	1.794722000	2.413197000
C	-0.134062000	1.403116000	3.499474000
C	-5.570248000	-1.369517000	-1.891435000
C	-4.875945000	-1.785085000	-0.774561000
C	-3.610139000	-1.248006000	-0.442644000
C	-3.027990000	-0.237764000	-1.279105000
C	-3.771919000	0.177797000	-2.415036000
C	-5.001095000	-0.376174000	-2.710783000
H	-6.535771000	-1.796318000	-2.133708000
H	-5.300652000	-2.546733000	-0.126358000
H	-3.331720000	0.942319000	-3.044321000
H	-5.537938000	-0.038617000	-3.591746000
C	-2.982806000	-1.722124000	0.761799000
H	-3.596807000	-2.428917000	1.336711000
C	-1.453395000	-1.962250000	2.532475000
C	-1.148103000	-0.817659000	3.499474000
C	2.426056000	-0.277552000	2.532475000
H	2.538108000	0.806688000	2.413197000
C	1.282165000	-0.585457000	3.499474000
H	1.167934000	-1.670428000	3.550211000
C	2.982806000	-1.722124000	0.761799000
C	2.826324000	-4.142988000	-2.710783000
C	3.971160000	-4.139218000	-1.891435000

C	3.983901000	-3.330150000	-0.774561000
C	2.885875000	-2.502469000	-0.442644000
C	1.719905000	-2.503434000	-1.279105000
C	1.731983000	-3.355476000	-2.415036000
H	2.802413000	-4.776687000	-3.591746000
H	4.823543000	-4.761985000	-2.133708000
H	4.855861000	-3.317133000	-0.126358000
H	0.849788000	-3.356513000	-3.044321000
H	3.901907000	-1.900468000	1.336711000
H	0.862666000	1.846675000	3.550211000
H	-2.253102000	-2.587335000	2.953565000
H	-0.971245000	-1.205740000	4.514228000
H	-0.305100000	4.329385000	1.336711000
H	-1.114147000	3.244910000	2.953565000
H	-0.570442000	-2.601410000	2.413197000
H	-2.030600000	-0.176247000	3.550211000
H	-0.558579000	1.443993000	4.514228000
H	1.529824000	-0.238253000	4.514228000
H	3.367248000	-0.657576000	2.953565000

2.12 [Er(trensal)]

Er	0.000000000	0.000000000	0.137165000
N	0.000000000	0.000000000	3.048127000
O	-1.860334000	0.313406000	-1.002369000
N	-1.811090000	-1.399799000	1.233162000
O	1.201585000	1.454393000	-1.002369000
O	0.658749000	-1.767800000	-1.002369000
N	2.117807000	-0.868550000	1.233162000
C	2.052161000	3.143259000	-2.412508000
C	2.186174000	4.482619000	-2.718153000
C	1.605789000	5.477757000	-1.908896000
C	0.894873000	5.092040000	-0.791759000
C	0.727709000	3.729657000	-0.450086000
C	1.316193000	2.714712000	-1.276279000
H	2.497734000	2.375542000	-3.034069000
H	2.750024000	4.772717000	-3.599153000
H	1.718438000	6.525550000	-2.158966000
H	0.444022000	5.845032000	-0.151145000
C	0.000000000	3.430854000	0.753968000
N	-0.306717000	2.268349000	1.233162000
C	-0.975783000	2.235247000	2.529319000
H	-1.970210000	1.789021000	2.409635000
C	-0.138736000	1.403020000	3.501445000
C	-5.546771000	-1.348224000	-1.908896000
C	-4.857272000	-1.771037000	-0.791759000
C	-3.593832000	-1.234614000	-0.450086000
C	-3.009106000	-0.217499000	-1.276279000
C	-3.748223000	0.205594000	-2.412508000
C	-4.975149000	-0.348027000	-2.718153000
H	-6.510511000	-1.774564000	-2.158966000
H	-5.283957000	-2.537981000	-0.151145000
H	-3.306147000	0.975330000	-3.034069000
H	-5.508306000	-0.004768000	-3.599153000
C	-2.971207000	-1.715427000	0.753968000
H	-3.586425000	-2.426302000	1.322364000
C	-1.447889000	-1.962677000	2.529319000
C	-1.145683000	-0.821659000	3.501445000
C	2.423672000	-0.272570000	2.529319000
H	2.534442000	0.811741000	2.409635000
C	1.284419000	-0.581362000	3.501445000
H	1.172899000	-1.666504000	3.554852000
C	2.971207000	-1.715427000	0.753968000
C	2.788975000	-4.134591000	-2.718153000
C	3.940982000	-4.129533000	-1.908896000

C	3.962399000	-3.321003000	-0.791759000
C	2.866124000	-2.495043000	-0.450086000
C	1.692913000	-2.497213000	-1.276279000
C	1.696062000	-3.348853000	-2.412508000
H	2.758282000	-4.767949000	-3.599153000
H	4.792073000	-4.750986000	-2.158966000
H	4.839935000	-3.307051000	-0.151145000
H	0.808413000	-3.350872000	-3.034069000
H	3.894452000	-1.892784000	1.322364000
H	0.856786000	1.849012000	3.554852000
H	-2.248672000	-2.589857000	2.945050000
H	-0.967624000	-1.213338000	4.514570000
H	-0.308026000	4.319086000	1.322364000
H	-1.118546000	3.242336000	2.945050000
H	-0.564232000	-2.600762000	2.409635000
H	-2.029684000	-0.182508000	3.554852000
H	-0.566969000	1.444656000	4.514570000
H	1.534593000	-0.231318000	4.514570000
H	3.367218000	-0.652479000	2.945050000

2.13 [Tm(trensal)]

Tm	0.000000000	0.000000000	0.146421000
N	0.000000000	0.000000000	3.051016000
O	-1.844948000	0.331499000	-0.992493000
N	-1.801692000	-1.394805000	1.230743000
O	1.209560000	1.432022000	-0.992493000
O	0.635388000	-1.763521000	-0.992493000
N	2.108783000	-0.862909000	1.230743000
C	2.065345000	3.112418000	-2.409334000
C	2.199769000	4.449913000	-2.722793000
C	1.614955000	5.449803000	-1.922562000
C	0.899338000	5.070734000	-0.806173000
C	0.731611000	3.710392000	-0.456756000
C	1.324322000	2.690584000	-1.273881000
H	2.514231000	2.341113000	-3.024026000
H	2.767381000	4.734845000	-3.603069000
H	1.728023000	6.496052000	-2.178836000
H	0.445182000	5.827423000	-0.172284000
C	0.000000000	3.418018000	0.746296000
N	-0.307090000	2.257714000	1.230743000
C	-0.979715000	2.230343000	2.525177000
H	-1.973341000	1.782533000	2.404911000
C	-0.143963000	1.402846000	3.502404000
C	-5.527145000	-1.326310000	-1.922562000
C	-4.841053000	-1.756518000	-0.806173000
C	-3.579099000	-1.221602000	-0.456756000
C	-2.992275000	-0.198395000	-1.273881000
C	-3.728106000	0.232432000	-2.409334000
C	-4.953622000	-0.319900000	-2.722793000
H	-6.489757000	-1.751514000	-2.178836000
H	-5.269287000	-2.528172000	-0.172284000
H	-3.284579000	1.006831000	-3.024026000
H	-5.484186000	0.029200000	-3.603069000
C	-2.960090000	-1.709009000	0.746296000
H	-3.576254000	-2.423511000	1.308937000
C	-1.441676000	-1.963630000	2.525177000
C	-1.142919000	-0.826099000	3.502404000
C	2.421392000	-0.266713000	2.525177000
H	2.530390000	0.817697000	2.404911000
C	1.286882000	-0.576747000	3.502404000
H	1.178526000	-1.662090000	3.558539000
C	2.960090000	-1.709009000	0.746296000
C	2.753853000	-4.130013000	-2.722793000
C	3.912191000	-4.123493000	-1.922562000

C	3.941716000	-3.314216000	-0.806173000
C	2.847488000	-2.488790000	-0.456756000
C	1.667953000	-2.492189000	-1.273881000
C	1.662761000	-3.344850000	-2.409334000
H	2.716806000	-4.764044000	-3.603069000
H	4.761734000	-4.744537000	-2.178836000
H	4.824105000	-3.299251000	-0.172284000
H	0.770348000	-3.347945000	-3.024026000
H	3.886949000	-1.885371000	1.308937000
H	0.850149000	1.851679000	3.558539000
H	-2.243124000	-2.593250000	2.935730000
H	-0.963461000	-1.221322000	4.513869000
H	-0.310695000	4.308882000	1.308937000
H	-1.124258000	3.239227000	2.935730000
H	-0.557048000	-2.600230000	2.404911000
H	-2.028675000	-0.189589000	3.558539000
H	-0.575965000	1.445043000	4.513869000
H	1.539426000	-0.223721000	4.513869000
H	3.367382000	-0.645977000	2.935730000

2.14 [Yb(trensal)]

Yb	0.000000000	0.000000000	0.155863000
N	0.000000000	0.000000000	3.056436000
O	-1.829045000	0.349840000	-0.981217000
N	-1.792608000	-1.388770000	1.230217000
O	1.217493000	1.409080000	-0.981217000
O	0.611552000	-1.758920000	-0.981217000
N	2.099015000	-0.858059000	1.230217000
C	2.073523000	3.080619000	-2.408272000
C	2.206271000	4.416061000	-2.731116000
C	1.617644000	5.420712000	-1.939673000
C	0.899891000	5.048510000	-0.822344000
C	0.733722000	3.690425000	-0.463637000
C	1.330334000	2.665788000	-1.271706000
H	2.525335000	2.305693000	-3.016229000
H	2.775549000	4.695593000	-3.612045000
H	1.729484000	6.465269000	-2.203284000
H	0.442759000	5.808920000	-0.195086000
C	0.000000000	3.404762000	0.739575000
N	-0.306406000	2.246830000	1.230217000
C	-0.982090000	2.225845000	2.523179000
H	-1.975269000	1.777146000	2.402701000
C	-0.148137000	1.402734000	3.505575000
C	-5.503297000	-1.309435000	-1.939673000
C	-4.822083000	-1.744927000	-0.822344000
C	-3.562863000	-1.209790000	-0.463637000
C	-2.973807000	-0.180791000	-1.271706000
C	-3.704656000	0.255414000	-2.408272000
C	-4.927557000	-0.297344000	-2.731116000
H	-6.463829000	-1.734857000	-2.203284000
H	-5.252052000	-2.521020000	-0.195086000
H	-3.259456000	1.034158000	-3.016229000
H	-5.454278000	0.055899000	-3.612045000
C	-2.948611000	-1.702381000	0.739575000
H	-3.565947000	-2.420418000	1.296243000
C	-1.436593000	-1.963437000	2.523179000
C	-1.140735000	-0.829657000	3.505575000
C	2.418683000	-0.262408000	2.523179000
H	2.526688000	0.822060000	2.402701000
C	1.288871000	-0.573077000	3.505575000
H	1.182902000	-1.658542000	3.564242000
C	2.948611000	-1.702381000	0.739575000
C	2.721286000	-4.118718000	-2.731116000
C	3.885652000	-4.111277000	-1.939673000

C	3.922192000	-3.303583000	-0.822344000
C	2.829140000	-2.480634000	-0.463637000
C	1.643473000	-2.484997000	-1.271706000
C	1.631133000	-3.336033000	-2.408272000
H	2.678729000	-4.751493000	-3.612045000
H	4.734345000	-4.730412000	-2.203284000
H	4.809293000	-3.287901000	-0.195086000
H	0.734121000	-3.339851000	-3.016229000
H	3.879117000	-1.877991000	1.296243000
H	0.844889000	1.853694000	3.564242000
H	-2.239231000	-2.594949000	2.928293000
H	-0.960475000	-1.228644000	4.515409000
H	-0.313170000	4.298409000	1.296243000
H	-1.127676000	3.236705000	2.928293000
H	-0.551419000	-2.599206000	2.402701000
H	-2.027791000	-0.195152000	3.564242000
H	-0.583799000	1.446117000	4.515409000
H	1.544274000	-0.217474000	4.515409000
H	3.366907000	-0.641757000	2.928293000

2.15 [Lu(trensal)]

Lu	0.000000000	0.000000000	0.163555000
N	0.000000000	0.000000000	3.059575000
O	-1.815730000	0.363759000	-0.972573000
N	-1.784990000	-1.383862000	1.228712000
O	1.222890000	1.390589000	-0.972573000
O	0.592840000	-1.754348000	-0.972573000
N	2.090955000	-0.853916000	1.228712000
C	2.082116000	3.054459000	-2.406614000
C	2.214702000	4.388194000	-2.736503000
C	1.622977000	5.396861000	-1.952454000
C	0.902268000	5.030491000	-0.835096000
C	0.736244000	3.674297000	-0.469346000
C	1.335791000	2.645594000	-1.269969000
H	2.536129000	2.276475000	-3.008993000
H	2.786332000	4.663273000	-3.617313000
H	1.734803000	6.439983000	-2.221700000
H	0.442736000	5.794054000	-0.213449000
C	0.000000000	3.393902000	0.733365000
N	-0.305964000	2.237778000	1.228712000
C	-0.984576000	2.221819000	2.520211000
H	-1.977226000	1.772090000	2.399329000
C	-0.151955000	1.402614000	3.506895000
C	-5.485308000	-1.292892000	-1.952454000
C	-4.807667000	-1.733859000	-0.835096000
C	-3.550156000	-1.199543000	-0.469346000
C	-2.959047000	-0.165968000	-1.269969000
C	-3.686297000	0.275936000	-2.406614000
C	-4.907638000	-0.276109000	-2.736503000
H	-6.444590000	-1.717608000	-2.221700000
H	-5.239166000	-2.513607000	-0.213449000
H	-3.239549000	1.058115000	-3.008993000
H	-5.431679000	0.081398000	-3.617313000
C	-2.939205000	-1.696951000	0.733365000
H	-3.557113000	-2.418201000	1.285099000
C	-1.431864000	-1.963577000	2.520211000
C	-1.138722000	-0.832904000	3.506895000
C	2.416439000	-0.258242000	2.520211000
H	2.523288000	0.826283000	2.399329000
C	1.290677000	-0.569710000	3.506895000
H	1.187072000	-1.655296000	3.567714000
C	2.939205000	-1.696951000	0.733365000
C	2.692936000	-4.112085000	-2.736503000
C	3.862331000	-4.103970000	-1.952454000

C	3.905399000	-3.296632000	-0.835096000
C	2.813913000	-2.474754000	-0.469346000
C	1.623256000	-2.479626000	-1.269969000
C	1.604181000	-3.330395000	-2.406614000
H	2.645346000	-4.744671000	-3.617313000
H	4.709787000	-4.722375000	-2.221700000
H	4.796430000	-3.280448000	-0.213449000
H	0.703420000	-3.334590000	-3.008993000
H	3.872780000	-1.871450000	1.285099000
H	0.839992000	1.855682000	3.567714000
H	-2.235281000	-2.596856000	2.920849000
H	-0.957568000	-1.234957000	4.515328000
H	-0.315667000	4.289651000	1.285099000
H	-1.131303000	3.234238000	2.920849000
H	-0.546062000	-2.598373000	2.399329000
H	-2.027064000	-0.200386000	3.567714000
H	-0.590720000	1.446757000	4.515328000
H	1.548288000	-0.211800000	4.515328000
H	3.366584000	-0.637382000	2.920849000

2.16 [Fe(trensal)]

Fe	-0.057454000	-0.092760000	0.043852000
N	-0.678901000	0.013478000	3.595322000
O	-1.248122000	0.394562000	-1.372397000
N	-1.501687000	-1.220697000	0.925569000
O	1.308980000	0.772944000	-0.993078000
O	0.344709000	-1.709679000	-0.864751000
N	1.457731000	-0.430365000	1.360768000
C	2.631075000	2.443539000	-1.951428000
C	2.969824000	3.770192000	-2.081663000
C	2.301279000	4.775236000	-1.347430000
C	1.294366000	4.405052000	-0.487507000
C	0.919861000	3.046889000	-0.314897000
C	1.592063000	2.025740000	-1.066486000
H	3.133714000	1.671557000	-2.521551000
H	3.763520000	4.049958000	-2.767188000
H	2.575281000	5.816290000	-1.465359000
H	0.763213000	5.161676000	0.083022000
C	-0.138190000	2.760979000	0.597933000
N	-0.616271000	1.605225000	0.954089000
C	-1.727579000	1.632781000	1.911026000
H	-2.496133000	0.942387000	1.567422000
C	-1.323597000	1.283813000	3.361795000
C	-5.144463000	-0.685797000	-2.269848000
C	-4.532661000	-1.221212000	-1.157568000
C	-3.210580000	-0.868519000	-0.795010000
C	-2.470053000	0.046797000	-1.607268000
C	-3.127364000	0.583684000	-2.750348000
C	-4.421266000	0.227285000	-3.064365000
H	-6.157750000	-0.962725000	-2.533098000
H	-5.067449000	-1.931050000	-0.532715000
H	-2.565300000	1.274582000	-3.367131000
H	-4.889071000	0.655002000	-3.945477000
C	-2.647684000	-1.466164000	0.376534000
H	-3.283399000	-2.215614000	0.858403000
C	-1.178602000	-1.997304000	2.124159000
C	-1.415862000	-1.216587000	3.432138000
C	1.633459000	0.371438000	2.577093000
H	1.438661000	1.414727000	2.327582000
C	0.752279000	-0.039896000	3.772100000
H	1.015852000	-1.058798000	4.073557000
C	2.461032000	-1.186803000	1.032457000
C	2.905240000	-3.860132000	-2.206895000
C	3.978997000	-3.632586000	-1.321760000

C	3.806045000	-2.745414000	-0.282022000
C	2.585531000	-2.053131000	-0.096969000
C	1.500768000	-2.276617000	-1.000014000
C	1.698645000	-3.211764000	-2.051324000
H	3.030525000	-4.557796000	-3.028751000
H	4.921193000	-4.149045000	-1.457649000
H	4.617300000	-2.562022000	0.416573000
H	0.871906000	-3.381589000	-2.730356000
H	3.330951000	-1.176896000	1.695408000
H	-0.658032000	2.068465000	3.738120000
H	-1.787232000	-2.909577000	2.157458000
H	-1.180801000	-1.903692000	4.259442000
H	-0.596484000	3.645479000	1.050016000
H	-2.177876000	2.633188000	1.928450000
H	-0.134949000	-2.307656000	2.061426000
H	-2.483149000	-0.984866000	3.515800000
H	-2.245236000	1.347806000	3.960588000
H	1.050715000	0.616387000	4.605390000
H	2.677823000	0.310471000	2.907446000

3 B3LYP versus PBE0

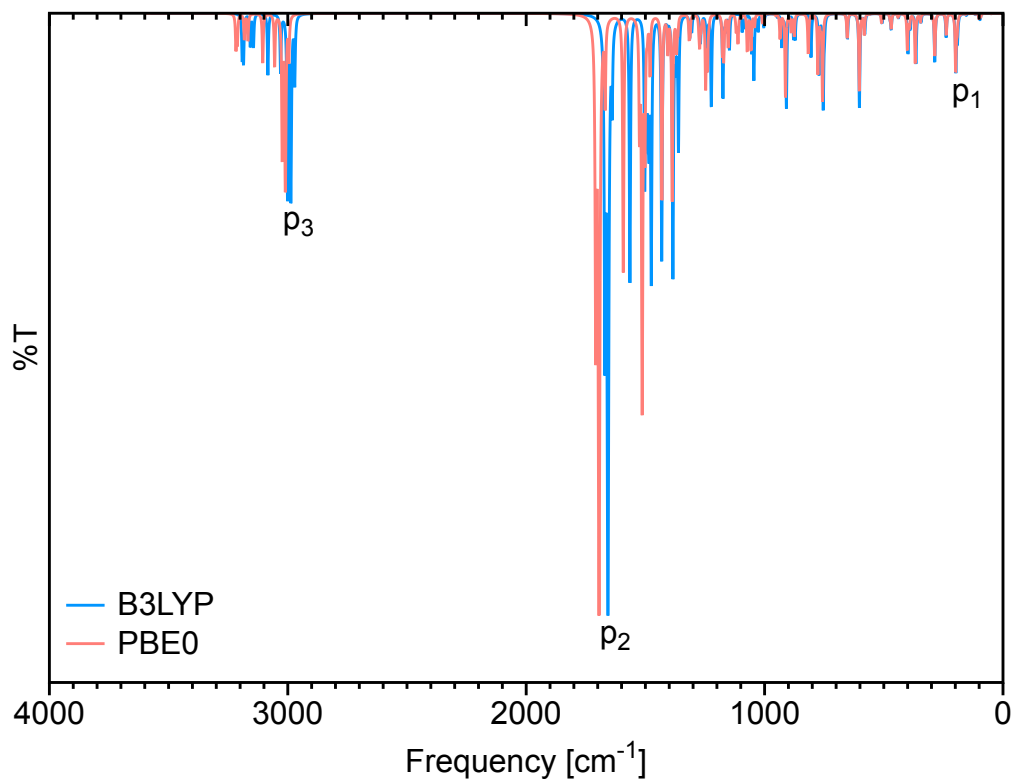


Figure S3: Comparison of the calculated IR spectra of [Eu(trensal)] at the B3LYP/MWB52/6-311++G** and PBE0/MWB52/6-311++G** levels of theory.

References

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