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Optical and Nonlinear Optical Properties of $Ln(Tp)_2$ where Ln= La, …, Lu, and Tp= tris (pyrazolyl) borate: a DFT+TD-DFT Study

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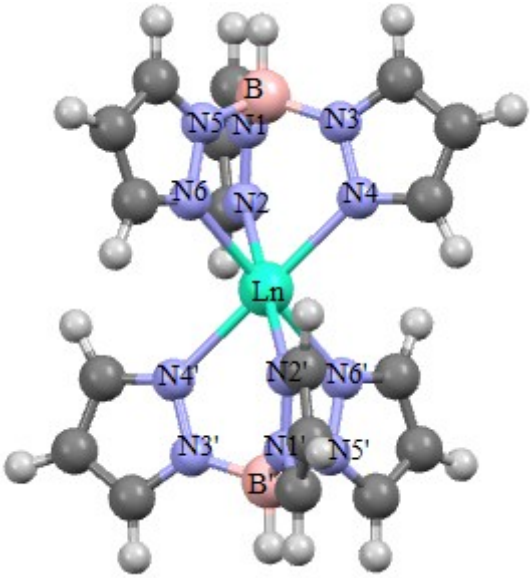
Supporting Information



Scheme 1-S $Ln(Tp)_2$

Topological study of electron density: QTAIM analysis

In order to have a better insight of the electronic structure of linear and bent geometry of $Ln(Tp)_2$ complexes, a topological analysis of the electron density at DFT optimized structures of $Ln(Tp)_2$ complexes where Ln= La, Lu was performed via Bader's Quantum Theory of Atoms in Molecules (QTAIM)[1]. We used the Dgrid 4.5[2] program for calculating the topological properties of electron density (ρ), the ellipticity (ε), Laplacian ($\nabla^2\rho$), the ratio (V/G) (where (V) is the electronic potential energy density and (G) is the energy density) and local total electronic energy density (H) at each hydrogen bond (HB), bond critical points (BCPs between Lanthanide-atom, atom-atom), ring critical points (RCPs) and cage critical points (CCPs) of various lanthanide complexes. The results of the calculations are gathered in Table 1-S.

It is important to stress that the bond strength and the type of interactions existing between the atoms in a molecule are correlated by the electron density and its Laplacian at BCPs. Precisely, values of $\rho < 0.1$ together with $\nabla^2\rho > 0$ are significant of closed-shell interactions whereas if $\rho > 0.1$ and $\nabla^2\rho < 0$ are indicative of an open-shell interaction[1-3-4]. Espinosa et al.[5] found that the ($|v|/G$) ratio is a good reliable indicator for classifying the atomic interactions. On the basis of this suggested indicator, closed-shell type interactions are associated with ($|v|/G \leq 1$), intermediate interactions $1 < |v|/G < 2$,

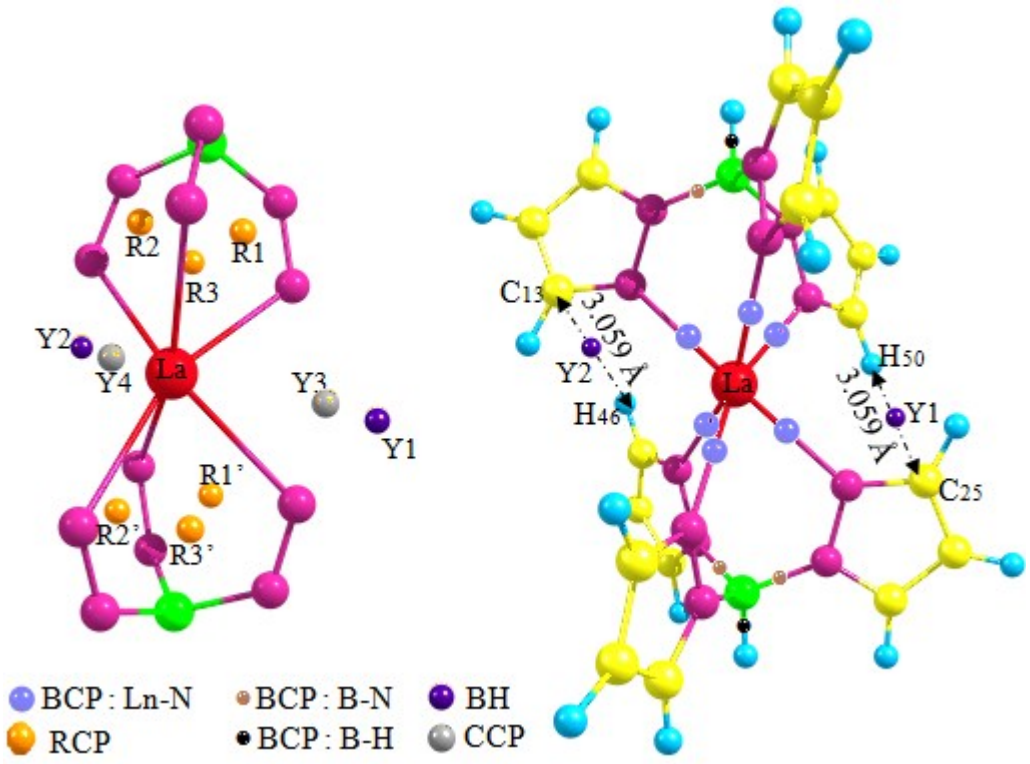
and open-shell type interaction |v|/G >2. According to the classification of Cremer and Kraka,[6-7] the local total electronic energy density (H) defined at BCPs as: H= G + V has a positive value for closed-shell type interactions, and it is negative for open-shell type interactions.

On the other hand, Rozas et al.[8] classified hydrogen bonds on the basis of H and $\nabla^2\rho$ values as follows: (i) strong hydrogen bonds are characterized by H<0 and $\nabla^2\rho$ <0 (ii) weak hydrogen bonds are characterized by H> 0 and $\nabla^2\rho$>0 (iii) intermediate hydrogen bonds are characterized by H< 0 and $\nabla^2\rho$> 0.

The calculated electron density properties of $La(Tp)_2$ and $Lu(Tp)_2$ complexes at $Ln-N$ bonds exhibit positive values of $\nabla^2\rho_{(BCP:Ln\text{-}N)}$ and $\rho_{(BCP:Ln\text{-}N)}$ values higher than 0.1 (Table 1-S). Values of |V|/G ~1 at BCP: Ln-N are typical of closed-shell interactions (i.e. electrostatic interaction between the lanthanide and the nitrogen atoms of the ligands). The small negative values for the energy density (-0.001 and -0.005 a.u.) at the BCP: Ln-N indicate a partial covalent character of the bond in $La(Tp)_2$ and $Lu(Tp)_2$, respectively. The values of ρ and $\nabla^2\rho$ at bond critical points of B-N are characteristics of closed-shell interactions (see Table 1-S).

The molecular graph of the $La(Tp)_2$ is shown on Scheme SI-2. There are two hydrogen bond Y1 and Y2 contacts between C25 and H50 (3.059 Å) and between C13 and H46 (3.095 Å), respectively and two cages Y3 and Y4.

According to the Rozas et al.[8] criteria all intramolecular hydrogen bonds (Y1 and Y2) in the discussed $La(TP)_2$ complex appear as weak interactions (see Scheme 2-S and Table 1-S) which correspond to electrostatic interactions whereas the distance between interacting atoms is less than the sum of their van der Waals' radii.



Scheme 2-S molecular topology of La $(Tp)_2$.

	La(Tp)$_2$				Lu(Tp)$_2$			
	$\rho(r)$	$\nabla^2\rho(r)$	|V|/G	H(r)	$\rho(r)$	$\nabla^2\rho(r)$	|V|/G	H(r)
BCP : Ln-N	0.250	0.126	1.033	-0.001	0.193	0.213	1.096	-0.005
BCP : B-N	0.06	0.106	1.837	-0.136	0.05	0.108	1.833	-0.136
BCP : B-H	0.000	-0.442	3.447	-0.187	0.000	-0.445	3.464	-0.187
BH : Y1=Y2	0.95	0.013	0.650	0.0009				
CCP : Y3=Y4	5.130	0.012	0.657	0.0008				
RCP : R1=R1'	1.770	0.037	0.771	0.001	1.59	0.042	0.771	0.002
RCP : R2=R2'	2.660	0.033	0.757	0.001	1.32	0.044	0.778	0.002
RCP : R3=R3'	2.460	0.030	0.757	0.001	1.35	0.046	0.781	0.002

Table 1-S QTAIM calculated values of: ρ (r): electronic density. $\nabla^2\rho$ (r): Density laplacian (a.u.); |V|/G : Where, V: the electronic potential energy density. G: the electronic kinetic energy density (a.u); H(r): Local total energy density (a.u.).

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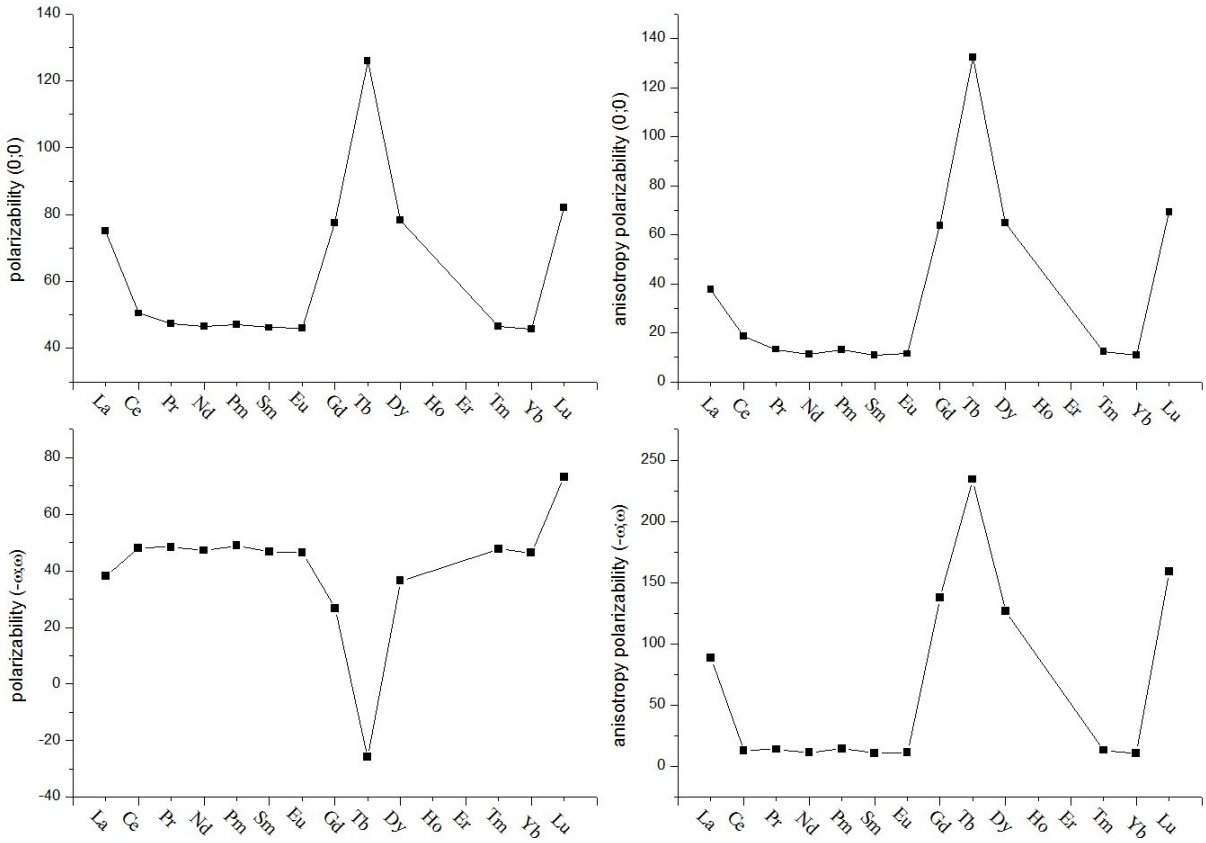

Fig. 1-S Variation of static and dynamic polarizability (α and $\Delta\alpha$ 10^{-24}esu) of $Ln(Tp)_2$ complexes (where, Ln= La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Tm, Yb and Lu). Calculations at B3LYP/CEP-121G level.

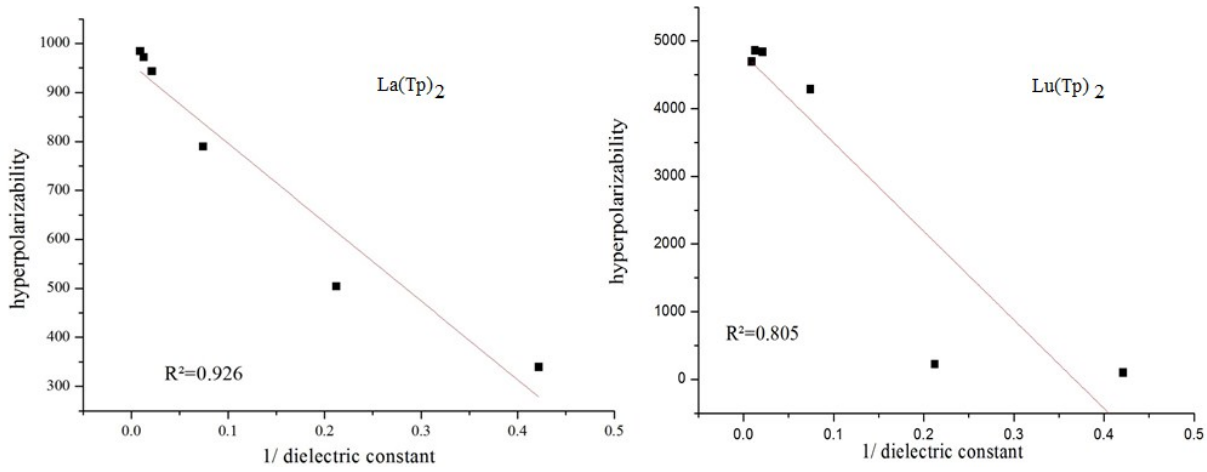

Fig. 2-S Correlation between the hyperpolarizabilities $\beta(0;0,0)$ and inverse dielectric constant $(1/\varepsilon)$ of $La(Tp)_2$ and $Lu(Tp)_2$.

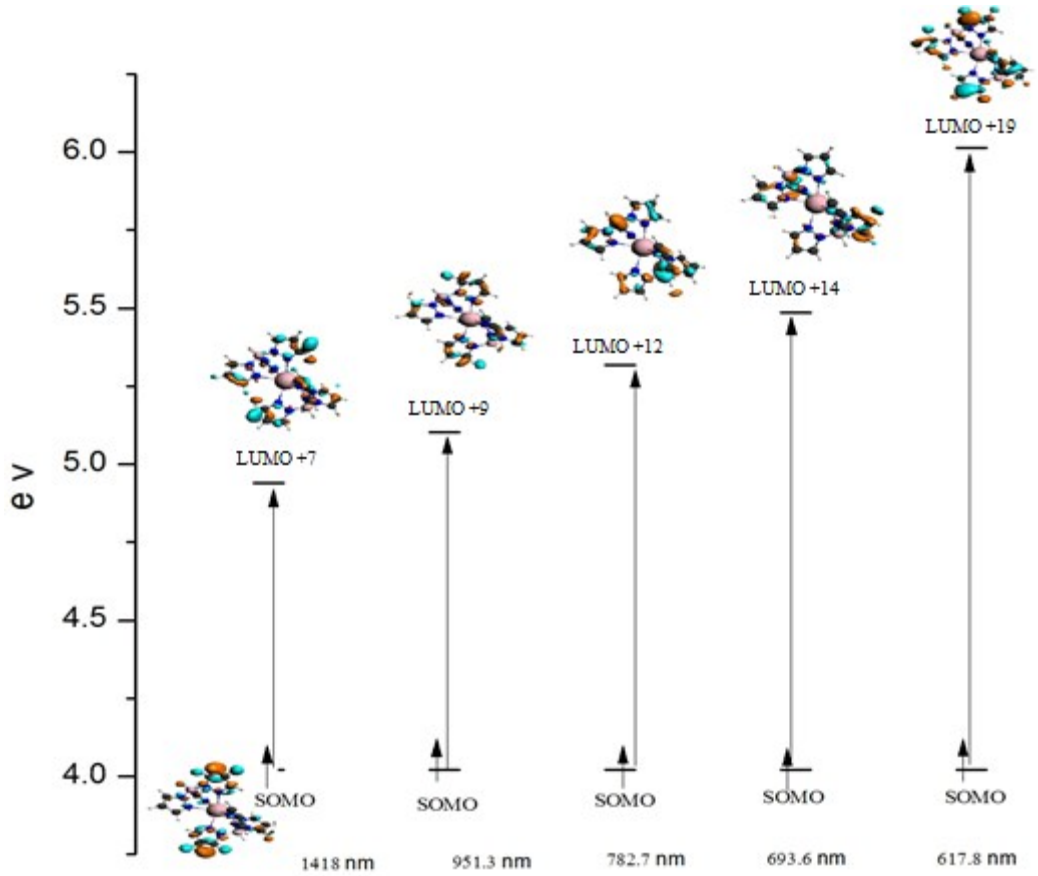

Fig. 3-S Orbital energy level diagrams of the molecular orbitals involved in the excitation transitions for $La(Tp)_2$ calculated by TD-DFT in gas phase. PBE/TZP level of theory.

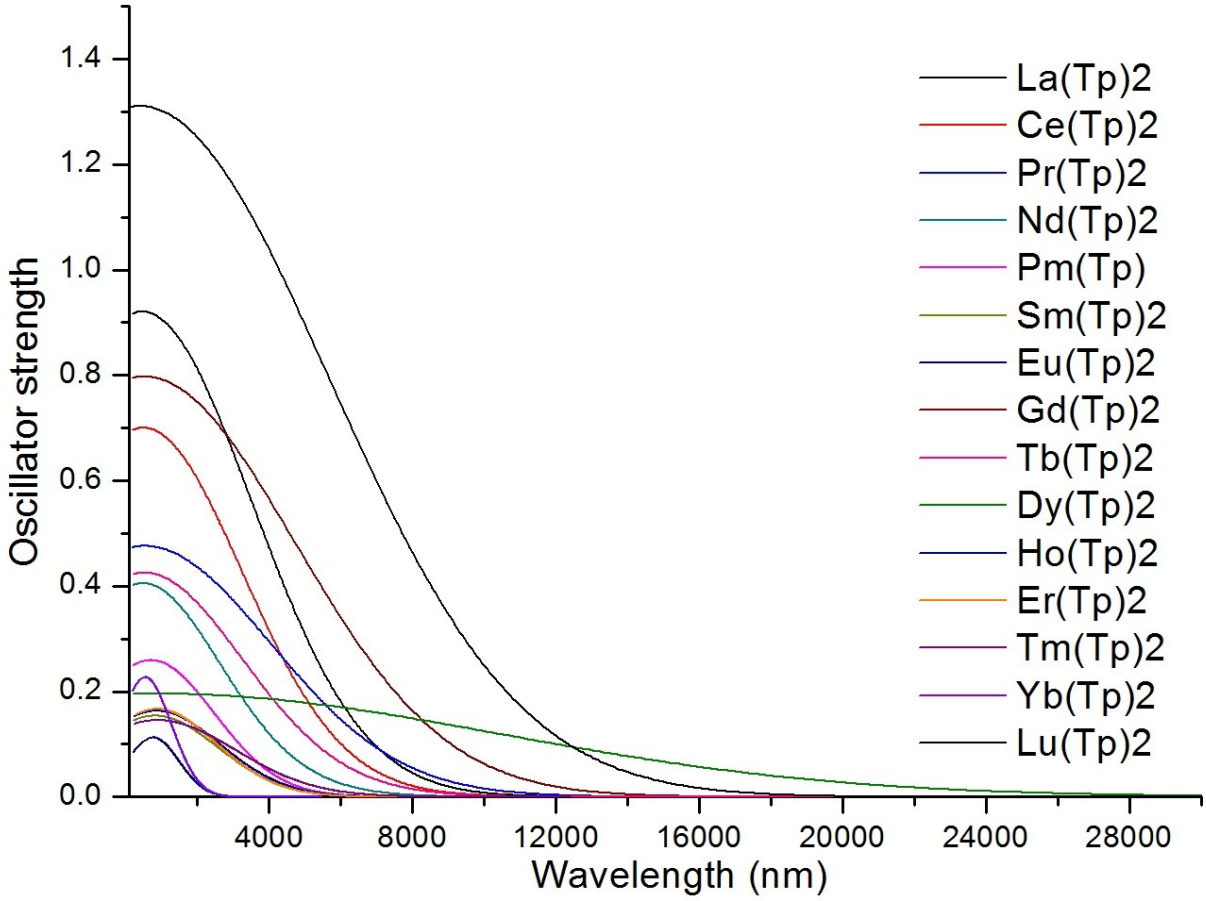

Fig. 4-S TD-DFT calculation of the electronic transition of the compounds $Ln(Tp)_2$ (Ln = La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Lu and Yb) PBE/TZP level of theory.

Table 2-S Interatomic Distances (Å) and Angles (deg) for $Ln(Tp)_2$ where Ln = La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Tm, Yb and Lu. Experimental interatomic distances of $Sm(Tp^{iPr_2})_2$ and $Yb\ (Tp^{iPr_2})_2$ are given in italic. Calculations at B3LYP/CEP-121G level. $Ln^{-}-N$: Average value

	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Tm	Yb	Lu
Distances													
Ln-B	3.718	3.777	3.749	3.746	3.710	3.701; 3.632	3.686	3.519	3.492	3.488	3.608	3.563 ; 3.435	3.429
Ln-B'	3.718	3.778	3.750	3.746	3.714	3.701 ; 3.644	3.686	3.521	3.493	3.488	3.608	3.563 ; 3.486	3.429
Ln -N_2	2.651	2.738	2.718	2.717	2.686	2.686 ; 2.638	2.661	2.491	2.462	2.464	2.550	2.540 ; 2.528	2.388
Ln -N_4	2.634	2.747	2.725	2.709	2.677	2.687 ; 2.668	2.660	2.450	2.414	2.402	2.536	2.538 ; 2.530	2.352
Ln -N_6	2.655	2.736	2.727	2.715	2.685	2.679 ; 2.645	2.661	2.443	2.419	2.408	2.553	2.535 ; 2.550	2.342
Ln –N_2'	2.651	2.747	2.73	2.714	2.682	2.675 ; 2.587	2.661	2.491	2.462	2.464	2.536	2.539 ; 2.487	2.388
Ln –N_4'	2.655	2.745	2.715	2.706	2.676	2.682 ; 2.680	2.660	2.451	2.414	2.402	2.550	2.541 ; 2.589	2.348
Ln –N_6'	2.634	2.733	2.725	2.723	2.688	2.680 ; 2.605	2.661	2.445	2.419	2.408	2.553	2.544 ; 2.478	2.343
$Ln^{-}-N$	2.646	2.741	2.723	2.714	2.682	6.815 ; *2.656*	2.660	2.461	2.431	2.424	2.546	2.539 ; ***2.527***	2.359
Angles													
B-Ln-B'	157.06	175.69	175.68	175.90	179.33	178.16 ; 148.34	179.64	179.95	179.99	179.98	179.96	179.61 ; 151.07	179.02
N_6-Ln-N_6'	158.94	174.84	156.68	176.36	157.91	179.49 ; 161.18	163.57	179.99	179.99	179.99	175.14	174.95 ; 164.13	176.42
N_2-Ln-N_6'	84.76	100.98	92.94	107.31	93.33	104.46 ; 101.05	95.58	100.03	99.29	99.43	103.85	97.82 ; 99.25	99.67
N_4-Ln-N_6'	98.80	104.77	121.63	103.42	120.38	104.43 ; 84.93	116.02	100.19	99.72	99.46	97.45	104.49; 83.57	95.39
N_2'-Ln-N_6'	76.69	74.13	74.80	74.54	75.05	76.15 ; 81.41	75.90	79.89	80.70	80.53	79.64	78.77 ; 86.51	82.27
N_4'-Ln-N_6'	73.90	73.75	74.34	74.76	75.50	75.96 ; 72.96	75.96	79.75	80.28	80.53	79.28	78.50 ; 73.51	81.78
N_2-Ln-N_4'	121.20	108.14	116.49	108.78	120.98	106.86; 127.86	116.07	100.19	99.27	99.20	101.00	105.01; 118.34	94.99
N_6-Ln-N_4'	119.48	107.67	93.29	107.45	94.16	103.70 ; 125.83	95.00	100.26	99.72	99.47	103.91	98.55 ; 122.11	101.12
N_4-Ln-N_4'	158.94	177.47	161.53	176.21	158.13	177.64 ; 147.68	163.18	179.92	179.99	179.99	174.58	174.8 ; 151.17	175.79
N_2'-Ln-N_4'	74.38	74.10	74.57	74.74	75.59	75.28 ; 69.70	75.89	79.86	90.72	80.78	75.47	78.73 ; 76.31	82.35
N_2-Ln-N_6	74.39	73.87	74.68	74.89	75.08	75.99 ; 69.08	75.86	79.97	80.71	80.57	79.28	97.82 ; 71.62	82.24
N_2-Ln-N_4	76.70	74.07	74.41	74.89	75.57	75.35 ; 78.69	75.96	79.88	80.73	80.80	75.46	78.93 ; 81.94	82.37
N_2-Ln-N_2'	151.41	174.02	161.11	176.29	157.29	177.85; 162.34	163.63	179.90	179.99	179.96	174.63	174.45; 165.21	176.50
N_6-Ln-N_4	73.90	73.99	74.68	74.19	75.52	75.90 ; 77.52	75.98	79.80	80.28	80.53	79.64	78.76 ; 82.31	81.82
N_6-Ln-N_2'	121.21	111.01	121.61	103.09	121.86	103.41; 103.24	115.67	100.11	99.30	99.47	97.52	104.80; 99.47	95.99

φ	3.72	3.78	3.75	3.75	3.71	3.70	3.69	3.52	3.49	3.49	3.61	3.56	3.43
θ	40.38	55.65	31.33	60.65	28.21	58.26	36.58	60.63	60.93	60.88	65.65	52.94	60.95

Table 3-S Interatomic Distances (Å) and Angles (deg) for $Ln(Tp)_2$ where Ln = La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu. Experimental Interatomic Distances of $Sm(Tp^{iPr_2})_2$ and $Yb\ (Tp^{iPr_2})_2$ are given in italic. Calculations at PBE/TZP level. $\bar{Ln-N}$: Average value

	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Distances															
Ln-B	3.647	3.620	3.645	3.641	3.621	3.614;*3.632*	3.602	3.384	3.523	3.454	3.511	3.502	3.484	3.476;*3.435*	3.384
Ln-B'	3.646	3.620	3.645	3.640	3.626	3.613;*3.644*	3.600	3.384	3.521	3.454	3.510	3.502	3.482	3.476;*3.486*	3.384
Ln -N_2	2.621	2.578	2.585	2.590	2.569	2.585;*2.638*	2.585	2.351	2.491	2.384	2.492	2.469	2.467	2.457;*2.528*	2.351
Ln -N_4	2.575	2.556	2.593	2.589	2.590	2.588;*2.668*	2.586	2.352	2.492	2.423	2.476	2.481	2.467	2.456;*2.530*	2.352
Ln -N_6	2.584	2.575	2.586	2.588	2.579	2.587;*2.645*	2.587	2.319	2.478	2.428	2.477	2.463	2.459	2.456;*2.550*	2.319
Ln –N_2'	2.618	2.563	2.584	2.587	2.574	2.588;*2.587*	2.588	2.350	2.481	2.384	2.473	2.475	2.467	2.456;2.487	2.350
Ln –N_4'	2.585	2.581	2.590	2.588	2.577	2.587;*2.680*	2.584	2.253	2.482	2.423	2.492	2.461	2.463	2.456;*2.589*	2.353
Ln –N_6'	2.573	2.563	2.587	2.590	2.589	2.584;*2.605*	2.586	2.320	2.495	2.428	2.487	2.477	2.458	2.456;*2.478*	2.320
$\bar{Ln-N}$	2.593	2.569	2.588	2.593	2.58	2.586 ; *2.656*	2.586	2.454	2.463	2.411	2.483	2.471	2.463	2.456 ; *2.527*	2.341
Angles															
B-Ln-B'	165.3	179.31	179.1	179.33	171.62	177.6;*148.34*	179.1	178.8	179.40	179.99	176.33	177.47	179.44	179.9;*151.07*	178.8
N_6-Ln-N_6'	166.4	158.53	172	160.34	160.92	156.1;*161.18*	157.5	171.6	161.13	171.6	162.81	161.10	172	160.9;*164.13*	171.6
N_2-Ln-N_6'	91.3	94.18	92.5	94.09	89.19	91.5;*101.05*	120.1	93.1	114.80	92.9	92.59	89.91	93.1	90.2;*99.25*	93.1
N_4-Ln-N_6'	98.5	119.59	104	118.55	112.37	120.5;*84.93*	92	104.5	91.68	105.1	114.83	113.70	104.5	114.8;*83.57*	104.5
N_2'-Ln-N_6'	75.1	76.79	82.1	75.35	75.33	76.6;*81.41*	76.5	81.4	77.97	81.2	78.13	78.70	81.4	79.4;*86.51*	81.4
N_4'-Ln-N_6'	75.5	75.58	82	75.50	75.98	75.9;*72.96*	76.7	81.7	77.91	81.7	78.90	78.77	81.7	79.3;*73.51*	81.7
N_2-Ln-N_4'	116.5	118.45	102.4	118.44	122.79	117.6;*127.86*	91.5	102.4	91.03	102.4	119.34	116.97	102.4	114.8;*118.34*	102.4
N_6-Ln-N_4'	112.8	92.90	92.8	94.86	101.68	92.1;*125.83*	120.6	92.8	116.15	92.8	92.49	93.21	92.8	90.4;*122.11*	92.8
N_4-Ln-N_4'	166.6	159.53	159.51	160.83	160.82	159.7;*147.68*	156.7	172.1	159.76	172.1	157.95	160.83	172.1	160.9;*151.17*	172.1
N_2'-Ln-N_4'	75.4	75.64	82.3	75.25	75.85	76;*69.70*	76.4	82.3	79.04	82.3	78.68	78.57	82.3	79.4;*76.31*	82.3

N_2-Ln-N_6	75.4	75.17	81.7	75.22	76.07	75.7;*69.08*	76.5	81.7	78.95	81.7	78.57	78.41	81.7	79.4;*71.62*	81.7
N_2-Ln-N_4	75.2	76.25	82.2	75.50	75.56	76.2;*78.69*	76.5	82.2	77.49	82.2	78.73	78.80	82.2	79.4;*81.94*	82.2
N_2-Ln-N_2'	159.6	161.26	172.3	160.57	152.53	159.6;*162.34*	157.1	172.3	162.04	172.3	158.10	158.80	172.3	90.2;*165.21*	172.3
N_6-Ln-N_4	75.4	76.56	82	75.29	76	76.5;*77.52*	76.4	81.5	78.34	81.5	78.19	78.84	81.5	79.3;*82.31*	81.5
N_6-Ln-N_2'	116.7	118.40	105	119.30	122.89	121;*103.24*	92.8	104.3	91.93	104.3	115.03	116.77	104.3	114.8;*99.47*	104.3

Table 4-S Thermodynamic parameters of the lanthanide complexes in the gas phase calculated byB3LYP/ CEP-121G for $Ln(Tp)_2$.

$Ln(Tp)_2$	H (atomic units)	S (Cal/Mol K)	G (atomic units)
La	-269.12	194.61	-269.21
Ce	-276.42	205.16	-276.52
Pr	-284.95	202.58	-285.05
Nd	-294.88	204.13	-294.97
Pm	-306.20	201.39	-306.29
Sm	-319.09	200.71	-319.19
Eu	-333.63	203.99	-333.73
Gd	-349.66	201.13	-349.76
Tb	-367.41	199.86	-367.51
Dy	-386.98	198.09	-387.08
Tm	-457.49	191.94	-457.59
Yb	-485.22	201.99	-485.32
Lu	-515.03	191.54	-515.12

Table 5-S Interatomic Distances (Å) for $Ln(Tp)_2$ where Ln =La, Yb and Lu in six solvents. Calculations at CPCM/ B3LYP/ CEP-121G level. $\bar{Ln-N}$: Average value

$Ln(Tp)_2$	Formamide	Water	DMSO	Butanal	Chloroform	Toluene
La-N2	2.675	2.697	2.622	2.692	2.683	2.669
La-N4	2.697	2.674	2.673	2.666	2.653	2.649
La-N6	2.622	2.622	2.622	2.622	2.622	2.622
La-N'2	2.675	2.697	2.673	2.692	2.653	2.649
La-N'4	2.698	2.674	2.696	2.666	2.683	2.669
La-N'6	2.622	2.622	2.622	2.622	2.622	2.621
$\bar{La-N}$	2.664	2.664	2.651	2.66	2.652	2.647
Yb-N2	2.584	2.594	2.58	2.575	2.61	2.565
Yb-N4	2.586	2.58	2.576	2.61	2.557	2.563
Yb-N6	2.582	2.597	2.583	2.596	2.612	2.562
Yb-N'2	2.585	2.589	2.582	2.602	2.629	2.565
Yb-N'4	2.586	2.593	2.577	2.561	2.594	2.563
Yb-N'6	2.583	2.576	2.58	2.571	2.573	2.562
$\bar{Yb-N}$	2.584	2.588	2.579	2.585	2.595	2.56
Lu-N2	2.409	2.407	2.409	2.419	2.356	2.348
Lu-N4	2.371	2.377	2.378	2.384	2.398	2.394
Lu-N6	2.287	2.379	2.286	2.258	2.357	2.36
Lu-N'2	2.38	2.285	2.378	2.328	2.354	2.349
Lu-N'4	2.403	2.404	2.404	2.406	2.398	2.397

Lu-N'6	2.408	2.408	2.406	2.431	2.354	2.353
$\overline{Lu - N}$	2.376	2.376	2.376	2.371	2.369	2.366

Table 6-S static and dynamic polarizabilities (α and $\Delta\alpha 10^{-24}$ esu) in solvent phases.

		ε	dipole moment	α(0;0,0)		α(-ω;ω,0)	
				α	Δα	α	Δα
$La(Tp)_2$	Formamide	108.94	5.76	164.346	216.686	70.2806	140.97
	Water	78.35	5.70	134.365	156.696	59.3506	129.661
	DMSO	46.82	5.56	180.756	252.222	180.756	252.222
	Butanal	13.45	4.82	185.167	262.214	185.167	262.214
	Chloroform	4.71	3.43	108.626	109.855	46.5215	124.048
	Toluene	2.37	2.16	183.843	259.228	74.5733	145.312
$Yb(Tp)_2$	Formamide	108.94	0.007	59.3391	14.7224	52.4132	12.5648
	Water	78.35	0.360	60.5775	15.0902	51.7997	12.3481
	DMSO	46.82	1.60	60.4702	14.8889	52.7433	12.7555
	Butanal	13.45	0.78	60.5296	15.0828	52.9851	12.7018
	Chloroform	4.71	0.81	56.9509	14.028	53.2782	12.8673
	Toluene	2.37	0.0005	53.2437	12.9387	53.6086	13.0951
$Lu(Tp)_2$	Formamide	108.94	7.38	138.793	141.028	87.7286	151.726
	Water	78.35	7.34	140.300	147.377	82.6193	134.869
	DMSO	46.82	7.18	141.647	151.479	91.3676	158.996

	Butanal	13.45	5.68	116.715	81.7169	73.3242	114.183
	Chloroform	4.71	0.48	155.598	198.497	172.735	434.845
	Toluene	2.37	0.38	124.118	137.738	238.718	628.517

Table 7-S Calculated Slater's TS and TD-PBE/TZP for $Ln(Tp)_2$ where Ln = La, Ce, Pr, Nd, Pm, Sm,Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu. Experimental values of $Eu(Tp)_2$ are given in bold italic (M: metal, f: f orbital, d: d orbital; *: experimental values from Ref.27 and 109).

	Slater's TS		TD-DFT			
Complexes	λ (nm)	Type	λ(nm)	*f*	%	Type
$La(Tp)_2$	287 263 234 219	HOMOβ→LUMOβ (L♈M(d) : LMCT) HOMOβ→LUMOβ+4 (L→L: π→π*) HOMOβ→LUMOβ+5 (L→M(f)+L: LMCT) HOMOβ→LUMOβ+7 (L→M(f): LMCT)	208 212 220 223 228 230 230 233 244 253 267 290 295 291 564	0.012 0.010 0.011 0.010 0.0013 0.0026 0.0025 0.033 0.0125 0.0234 0.0087 0.0018 0.0001 0.0002 0.0026	20 33 23 68 79 38 81 17.3 20 16 43 64 65 63 99	HOMOα -4→LUMO14α:L→M HOMO β -4→LUMO+12β:-π→π* HOMO β -4→LUMO+11β:L→M HOMOα-11→146α:L→M HOMOβ -9→Lu+5β: L→Mf HOMOβ -7→LU+5β:-L→Mf HOMO α -7→LUMO+6α:L→Mf HOMO-10α-LUMO+3α:L→Mf+L HOMOβ-5S--L+4β:-L→Mf+L HOMOβ-2→LU+4β:-L→Mf+L HOMOβ-2→LUMOβ+2:L→Md+L HOMOβ-1→LUMOβ:L→Md+L HOMOα-2-LUMOα: L→Md HOMOβ→LUMOβ: L→Md+L HOMOα--LUMOα+22: M→L

			617 694 951 1371 1848 7569	0.0063 0.0244 0.084 0.0139 0.0328 0.0001	99 53 52 80 85 99	HOMOα→LUMOα+19:M→L HOMOSα→LUMO+14α:Md→Md HOMOSα→LUMO+9α:Md→Mf HOMOα→LUMO+8α:Md+L→-Mf HOMOα→UMOα+3:Md+L→Mf+L HOMOα→LUMOα:Md+L→Md+L
$Ce(Tp)_2$	281 273	HOMOβ→LUMOβ (L→L :π→π*) HOMOβ→LUMOβ+2 (L→M(f) :LMCT)	226 229 229 234 239 279 460 393 645 671 730 872 892 1258 2862 6662	0.0006 0.0001 0.0006 0.0076 0.0014 0.0003 0.0001 0.0021 0.0085 0.0005 0.002 0.0119 00284 0.0034 0.0001 0.0002	70 90 45 39 43 69 100 100 87 100 78 83 91 40 76 85	HOMOβ-7-LUMOβ+5:L→M HOMOβ-5→LUMOβ+5:L→M HOMOβ-2→LLUMOβ+6:L→M HOMOβ-1→LUMOβ+9:L→M HHOMOβ→LUMOβ+7:L→M HOMOβ→LUMOβ: L→L HOMOα → LUMOα +27α:Mf→L HOMOα -1→ LUMOα +32α:Mf→L HOMOα -1→LUMOα +17:Mf→L+Md HOMOα-1→ LUMOα +15:Mf→L HOMO-1α-→UMO+14α:Mf→Md HOMOα -1→LUMOα +11α:Mf→L HOMOα →LUMOα +10:Mf→L HOMOα -1→LUMOα +9:Mf→Mf HOMOα -1→LUMOα +2:Mf→Mf HOMOα→LUMOα: Mf→M
$Pr(Tp)_2$	272 247	HOMOβ→ LUMOβ (L→L : π→π*) HMOMβ→LUMOβ+4 (L→M (d+s): LMCT)	224 228 238 245 250 271 551 650	0.0014 0.023 0.0002 0.0008 0.03 0.0001 0.001 0.003	69 82 96 70 56 41 98 90	HOMOβ-9→LUMOβ+4:L→M HOMOα-2→LUMOα+2:L→M HOMOβ-2→-LUMOβ+4:L-M HOMOα-3→-LUMOα+4:L→M HOMOβ→LUMOβ+4:L→M(d+s) HOMOβ→LUMOβ:L→L+M HOMOα-2→LUMOα+23:M→L HOMOα-2→LUMOα+18:M→L

			656 732 925 1400 2166 3552 8525	0.009 0.008 0.023 0.0015 0.0057 0.016 0.000	75 46 71 47 44 47 96	HOMOα140→LUMOα+16:M→Md+L HOMOα-2→LUMOα+12:Mf→Md HOMOα-2→LUMOα+9:Mf→L HOMOα-2→LUMOα:M→Mf HOMOα-1→LUMOα147:Mf→Mf+L HOMOα-2→LUMOα: Mf→Mf HOMOα→LUMOα: Mf→Mf
$Nd(Tp)_2$	271 238	HOMOβ→ LUMOβ (L→L:π→π*ILCT) HOMOβ→ LUMOβ+4 (L→M(d+s) : LMCT)	238 248 270 280 303 361 408 535 896 1665	0.0143 0.0777 0.0000 0.0000 0.0011 0.0022 0.0016 0.0006 0.0201 0.0063	25 27 71 76 99 86 98 99 96	HOMOβ-9→-LUMOβ:L→M+L HOMOβ-4→-LUMOβ+1:L→L+Md HOMOβ→LUMOβ:L→M+l LUMOα-5→LUMOα+1:-L→Md+l HOMOα-LUMOα+32: Mf→Md HOMOα+2→LUMOα+35:Mf→Md+L HOMOα+2→LUMOα+30:Mf→L HOMOα→LUMOα+23:Mf→L HOMOα→LUMOα+9:Mf→L HOMOα-2→LUMOα+2:Mf→Md HOMOα→LUMOα:Mf→Md+L
$Pm(Tp)_2$	265 259 236	HOMOβ→ LUMOβ (L→L: π→π*) HOMOβ→ LUMOβ+2 (L→L: π→π*) HOMOβ→ LUMOβ+4 (L→M(d+s): LMCT)	246 265 269 277 346 452 533 580 686 914 1034 2119	32 50 45 88 98 98 94 97 93 77 77 68	0.0076 0.0005 0.0001 0.0002 0.0003 0.0004 0.0010 0.0021 0.0035 0.0132 0.0072 0.0004	HOMOβ-4→LUMOβ:L→L 139β→140β:L→L HOMOα-7→LUMOα:L→M HOMOα-6→LUMOα+1:L→M HOMOα-3-LUMOα+27:Mf→Msd HOMOα-4-LUMOα+13:Mf→M+L HOMOα-3→LUMOα+10:Mf→Md HOMOα-4→-LUMOα+8:Mf→L HOMOα-2→LUMOα+8:Mf→L HOMOα→LUMOα+7:Mf→L HOMOα-4→-LUMOα+2:Mf→Md+L HOMOα→LUMOα+3:Mf→Md+L

			3836	86	0.0002	HOMOα-145α:Mf→Mf
$Sm(Tp)_2$	260 230	HOMOβ→LUMOβ HOMOβ→LUMOβ+4 (L→M (d+s) LMCT)	258 262 262 275 292 346 498 666 704 825 1797 2081 3721	0.0001 0.0005 0.0004 0.0013 0.0002 0.0009 0.001 0.0041 0.0078 0.0053 0.0064 0.0031 0.0001	52 46 50 89 99 99 82 43 99 74 83 77 95	HOMOβ-1→LUMOβ+2:L→L HOMOβ-1→-LUMOβ:L→L HOMOβ→HOMOβ:L→L HOMOα-9→LUMOα:L→Mf HOMOα-6→LUMOα:L→Mf HOMOα-5→LUMOα+26:Mf--L+Msd HOMOα-4→LUMOα+13:M→L HOMOα-4→LUMOα+7:M→L HOMOα-2→-LUMOα+6:M→L HOMOα-5→LUMOα+5:M→L HOMOα-2→LUMOα+2:Mf→L+Md HOMOα-→LUMOα+2:Mf→L+Md HOMOα→LUMO: Mf→Mf
$Eu(Tp)_2$ 220*nm 450*nm	261 260 331 404	HOMOβ→LUMOβ(L→L: π→π*) HOMOβ→LUMOβ +1(L→L: π→π*) HOMOα→LUMOα+4 (M(f)→L : MLCT) HOMOα→LUMOα+2 (M(f) → M (d):IC	230 240 243 247 260 261 295 434 452 455 463 797 801 837 1008 1065	0.002 0.0001 0.0008 0.0034 0.0009 0.0006 0.0012 0.0026 0.0000 0.0000 0.0000 0.0004 0.0036 0.0014 0.0013 0.0021	33 49 41 48 40 50 96 37 74 98 47 93 90 92 46 79	HOMOβ-9→LUMOβ+3: L→L HOMOβ-5→LUMOβ+3: L→L HOMOβ-6→LUMOβ: L→L HOMOβ-2→LUMOβ: L→L HOMOβ→LUMOβ+1:L→L HOMOβ→LUMOβ:L→L HOMOα-2→LUMOα32:Mf→L HOMOα-6→LUMOα+17:αMf→Md HOMOα-4→LUMOα17:Mf→Md HOMOα-2→LUMOα+17:Mf→Md HOMOα→LUMOα+17:Mf→Md HMOMα-5→LUMOα+4:Mf→Md HOMOα-2→LUMOα+4:Mf→Md HOMOα→LUMOα+4:Mf→Md HOMOα-6→LUMOα+3:Mf→L

			1185 1333	0.0215 0.0017	46 88	HOMOα-1→LUMOα+3:Mf→L HOMOα-4→LUMOα+1:Mf→L HOMOα→LUMOα:Mf→L
$Gd(Tp)_2$	279 242	HOMOβ→LUMOβ (L→ M(f): LMCT) HOMOβ→LUMOβ+4 (L→M(f) : LMCT)	217 222 239 258 350 394 528 593 688 793 1135 1746 10630	0.0011 0.019 0.0210 0.0035 0.0047 0.0001 0.0033 0.0054 0.0011 0.09 0.1421 0.0071 0.0001	58 47 25 71 71 99 99 99 90 91 98 98 100	HOMOβ-3→-LUMOβ+13:L→L HOMOα-12→-LUMOα+3:L→L HOMOα-3→-LUMOα+3:-L→L HOMOα-6→-LUMOα+1:L→M HOMOβ-2→-LUMOβ+5:L→M HOMOβ→LUMOβ:L→M HOMOα→LUMOα+16:Md→L HOMOα→LUMOα+12:Md→L+M HOMOα→LUMOα+7:Md→Md HOMOα→LUMα+4:Md→L HOMOα→LUMOα+3:Md→L HOMOα-LUMOα+2:Md→L HOMOα→LUMOα:Md→L
$Tb(Tp)_2$	500 348	HOMOα→LUMOα (M(f)→L :MLCT HOMOα-1→LUMOα+4 (M(f)→L :MLCT	235 270 280 342 410 411 565 676 930 963 995 1343 2514 6326	0.0024 0.0006 0.0106 0.0015 0.0072 0.0009 0.004 0.0004 0.0158 0.0018 0.0238 0.0004 0.0114 0.0001	86 48 83 56 51 83 94 97 62 40 44 81 79 54	HOMOβ-11→LUMOβ-5:L→M HOMOβ-8→LUMOβ+1:L→L HOMOα-6→-LUMOα+4:Mf→Md HOMOα-2→LUMOα:Mf-Md+L HOMOα→LUMOα+1:Mf→L 146α→147α:Mf→Md+L HOMOβ→LUMOβ+23:Mf→Md 140β-159β:Mf→L HOMO-1β-→LUMO+11β:Mf→Mf HOMOβ-1→LUMOβ+10:Mf→Mf+L HOMOβ-1→LUMOβ+11:Mf→Mf HOMOβ→LUMOβ+7:Mf→Msd HOMOβ→LUMOβ+4:Mf→L HOMOβ→LUMO:Mf→L

$Dy(Tp)_2$	404 384	HOMOα→LUMOα (M(f)→ L: MLCT) HOMOα→LUMOα+4 (M(f)→M(d): ICMT	255 270 278 352 375 574 548 678 951 1011 1637 2662 20548	0.0011 0.0006 0.0014 0.0021 0.0001 0.0000 0.001 0.0011 0.0241 0.0102 0.0016 0.0023 0.0000	53 44 95 100 83 98 99 94 65 63 94 78 99	HOMOα-10→LUMOα+1:L→M+L HOMOβ-8→LUMOβ+3:L→L+M HOMOα-4→LUMOα+7:Mf→Md HOMOα-2→LUMOα+6:Mf→L HOMOα-4→-LUMOα+2: Mf→L HOMOα→LUMO7α:Mf-L HOMOα-3→LUMOα+4:Mf→L+M HOMOβ-2→-LUMOβ+15:Mf→L HOMOβ-2→-LUMOβ+7:Mf→L HOMOβ-1→LUMOβ+7:Mf→L HOMOβ→LUMOβ+4:MF→L HOMOβ→LUMOβ+3:Mf→L HOMOβ→LUMOβ:Mf→L
$Ho(Tp)_2$	388 363	HOMOα→LUMOα (M(f)→L: MLCT) HOMOα→LUMOα+4 (M(f)→M(d+s):IC	288 324 394 88 609 629 677 694 712 880 894 918 982 1035 3096	0.0005 0.001 0.0001 0.0016 0.0021 0.0003 0.0001 0.0002 0.0001 0.0039 0.0039 0.0105 0.0005 0.0027 0.0009	95 98 87 88 67 77 97 42 42 45 51 24 64 87 83	HOMOα-6→LUMOα+8:Mf→L HOMOα-5→-HOMOα+6:Mf→Md+L HOMOα-6→LUMOα+3;Mf→L HOMOα-1→-LUMOα+4:Mf→Md HOMOα-2→LUMOα:Mf→L HOMOα→LUMOα:Mf→L HOMOβ→LUMO13β:Mf→L HMOM-2β→LUMO+8β:Mf→Mf HOMO-3β→LUMO+7β:Mf→Mf HMOM-2β-LUMO+7β:Mf→Mf HOMO-1β-151β:Mf→L HOMOβ-LUMO+9β:Mf→Mf+L HOMO-1β-LUMO+5β:Mf→Md-S HMOMβ-LUMO+5β:Mf→Md-s 143β-144β:Mf-L
$Er(Tp)_2$	459 410	HOMOα→LUMO α(M(f)→L :MLCT) HOMOα→LUMOα3 (M(f)→M(d)S	308 379	0.0001 0.0009	60 51	HOMOα-6→LUMOα+6:Mf→L HOMOα-5→LUMOα+3: Mf→L

			406 441 563 640 742 785 843 980 1570 2874	0.0015 0.0016 0.0017 0.0001 0.0031 0.0019 0.003 0.0122 0.0159 0.0085	96 92 51 99 79 39 97 67 83 79	HOMOα-5→LUMOα:Mf→L HOMOα-2→LUMOα+4:Mf→Md-s HOMOα-1→LUMOα+3:Mf→L HOMOα→LUMOα:Mf→L HOMOβ-2→LUMOβ+8:Mf→L HOMOβ-3→LUMOβ+4:Mf→L HOMOβ-1→LUMOβ+6:Mf→Md-s HOMOβ→-LUMOβ+7:Mf→Md-s HOMOβ-2→LUMOβ+2:Mf→L 144β-145β:Mf→Mf-L
$Tm(Tp)_2$	344 314	HOMOα→LUMOα+4 (M(f)→L: MLCT) HOMOα→LUMOα+6 (M(f)→L: MLCT)	366 430 498 535 571 708 840 915 966 1281 1305 2246 2847	0.0003 0.0012 0.0014 0.0010 0.0011 0.029 0.006 0.0015 0.0003 0.0063 0.0025 0.0047 0.001	97 88 98 57 39 92 44 61 63 44 46 53 52	HOMOα-6→LUMOα+5:Mf→L HOMOα-5→-LUMOα+10:Mf→Md HOMOα-6→LUMOα-Mf→L HOMOα-4→HOMOα+5:Mf→L HOMOα-2→HOMOα+4:Mf→Md HOMOβ-5→HOMOβ+4:Mf→Md HOMOα-5→HOMOα+1:Mf→L HOMOα-1→LUMOα+5:Mf→L HOMOα→LUMOα:Mf→L HOMOβ-5→LUMOβ+2:Mf→L HOMOβ-4→LUMOβ+1:Mf→L HOMOβ→LUMOβ+2:Mf→L HOMOβ→LUMOβ:Mf→Mf
$Lu(Tp)_2$	289 234	HOMOβ→LUMOβ (Lη_6L : π→π*) HOMOβ→LUMOβ+5 (Lη_6M (d+s) : LMCT)	197 200 277 294 362 457 523	0.0003 0.0101 0.0401 0.0014 0.0037 0.0001 0.0017	61 67 62 50 99 100 94	HOMOβ-6→LUMOβ+7:L-M HOMOβ-4→LUMOβ+7:L-M HOMOβ-3→LUMOβ+1:L-Md+L HOMOβ→LUMOβ:L-L-Md HOMOα→LUMOα+31:M-L→L HOMOα→LUMOα21:M-L→L HOMOα→LUMOα+17:M-L→L

			647 832 1861 14918	0.0037 0.1231 0.039 0.0000	96 94 100 100	HOMOα→LUMOα+10:Md-L→L HOMOα→LUMOα+4:Md-L→L HOMOα→LUMOα+1:Md-L→L HOMOα→LUMO:Md-L→Md-L
Yb(Tp)2			248 261 293 330 372 433 475 538 666 697 1078 1158 1355	0.0057 0.0007 0.0011 0.0005 0.0001 0.0011 0.0017 0.0001 0.0062 0.0038 0.0169 0.0152 0.0000	71 83 86 71 96 99 58 100 96 98 62 38 91	HOMO-11→LUMO+1:L→L HOMO-12→LUMO+1:L→L HOMO-1→LUMO+23:Mf→Md HOMO-4→LUMO29:Mf→L HOMO-6→LUMO+23:Mf→L HOMO-4→LUMO+17:Mf→L HOMO→LUMO+13:Mf→L HOMO-4→LUMO+7:Mf→L HOMO-6→LUMO+5:Mf→L HOMO-3→LUMO+4:Mf→L HOMO-2→LUMO+2:Mf→L HOMO-4→LUMO+1:Mf→L HOMO→LUMO:Mf→L

The Cartesian coordinates of the optimized geometries in gas phase (B3LYP/ CEP-121G level)

La(Tp)2

N	-3.10920000	-1.49920000	-0.40350000
N	-1.76910000	-1.86290000	-0.20200000
N	-2.94480000	0.91190000	-1.30920000
N	-1.57340000	1.23410000	-1.26130000
N	-3.46460000	0.50900000	1.16310000
N	-2.21050000	0.61180000	1.79080000

N	3.10930000	1.49900000	-0.40380000
N	1.76930000	1.86280000	-0.20210000
N	3.46460000	-0.50890000	1.16320000
N	2.21050000	-0.61150000	1.79090000
N	2.94500000	-0.91220000	-1.30910000
N	1.57350000	-1.23410000	-1.26110000
C	-1.71140000	-3.21900000	-0.37770000
C	-2.99330000	-3.74160000	-0.69560000
H	-3.25920000	-4.77030000	-0.88840000
C	-3.84540000	-2.62090000	-0.70220000
C	-1.35410000	2.08930000	-2.31190000
C	-2.55420000	2.32320000	-3.03650000
H	-2.68620000	2.94620000	-3.90910000
C	-3.53340000	1.55940000	-2.37790000
C	-2.45170000	1.17570000	3.01660000
C	-3.83740000	1.44340000	3.18960000
H	-4.32370000	1.87640000	4.05140000
C	-4.44270000	0.99930000	2.00010000
C	1.71160000	3.21870000	-0.37780000
C	2.99350000	3.74130000	-0.69570000
H	3.25940000	4.77010000	-0.88860000
C	3.84560000	2.62070000	-0.70240000
C	2.45170000	-1.17540000	3.01670000
C	3.83730000	-1.44330000	3.18970000
H	4.32350000	-1.87630000	4.05150000
C	4.44260000	-0.99940000	2.00020000
C	1.35390000	-2.08890000	-2.31190000
C	2.55380000	-2.32290000	-3.03670000
H	2.68550000	-2.94570000	-3.90950000
C	3.53330000	-1.55960000	-2.37800000
B	-3.64390000	-0.02650000	-0.28650000
H	-4.82360000	-0.04990000	-0.54010000
B	3.64400000	0.02630000	-0.28660000

H	4.82380000	0.04970000	-0.54000000
H	4.90650000	2.54640000	-0.89450000
H	0.76860000	3.73920000	-0.27210000
H	5.48100000	-0.99040000	1.69960000
H	1.63040000	-1.33430000	3.70300000
H	4.58540000	-1.42980000	-2.58870000
H	0.35630000	-2.46130000	-2.50090000
H	-0.76840000	-3.73940000	-0.27210000
H	-4.90630000	-2.54660000	-0.89420000
H	-4.58550000	1.42940000	-2.58860000
H	-0.35670000	2.46200000	-2.50090000
H	-5.48110000	0.99010000	1.69950000
H	-1.63050000	1.33490000	3.70280000
La	0.00000000	0.00010000	0.45270000

Ce(Tp)2

N	3.27456500	1.45077600	0.45445100
N	1.92528400	1.82115800	0.54023500
N	3.31163500	-0.29068500	-1.45801600
N	1.97213900	-0.46243800	-1.84162300
N	3.35001100	-1.07369700	1.00354400
N	2.01270600	-1.36359300	1.33831800
N	-3.34436500	-1.34467800	-0.61515200
N	-2.01003100	-1.75987900	-0.76090700
N	-3.33217800	0.21047200	1.46332100
N	-1.99284400	0.23660800	1.89260800
N	-3.25964500	1.22997900	-0.91760800
N	-1.90722900	1.52520400	-1.12640700
C	1.91670600	3.11387800	0.97694600
C	3.24365800	3.59595900	1.16070900
H	3.54987900	4.57841100	1.49891400
C	4.07025800	2.51075500	0.81924800

C	1.99519700	-0.72953800	-3.17766000
C	3.33450100	-0.73872100	-3.67792200
H	3.66053300	-0.91288500	-4.69036900
C	4.12790100	-0.45594900	-2.55755800
C	2.06766800	-2.39773600	2.22748000
C	3.42239600	-2.78092200	2.48368100
H	3.77275800	-3.56130600	3.14334900
C	4.19047700	-1.92572400	1.68962100
C	-2.06127500	-3.01229500	-1.28832300
C	-3.40816200	-3.43435500	-1.48759700
H	-3.76424700	-4.37160100	-1.89638600
C	-4.17991000	-2.34443800	-1.05075000
C	-2.03648400	0.39798000	3.24371600
C	-3.38600600	0.48241700	3.70332800
H	-3.73247600	0.61618000	4.71816600
C	-4.16892100	0.35050800	2.54750100
C	-1.89182900	2.62962700	-1.94016200
C	-3.20643700	3.04784000	-2.26685500
H	-3.50653300	3.87847300	-2.89130900
C	-4.04982500	2.12724000	-1.59367800
B	3.77489700	0.04219000	-0.00549300
H	4.98297300	0.06820000	-0.00594500
B	-3.77488300	0.04853400	-0.03450300
H	-4.98295900	0.07255600	-0.04951900
H	-5.25730200	-2.20839700	-1.01770700
H	-1.15079100	-3.55533300	-1.50566300
H	-5.24304700	0.35657100	2.41598200
H	-1.12185000	0.45569400	3.81566200
H	-5.12532700	2.06173000	-1.55329000
H	-0.94103200	3.05634500	-2.24602100
H	0.98129500	3.62709400	1.12919800

H	5.15263700	2.42463100	0.81102600
H	5.20206800	-0.36159100	-2.46658500
H	1.07033100	-0.89787000	-3.71910300
H	5.26594200	-1.85035800	1.56861400
H	1.15702600	-2.80923000	2.64403000
Ce	0.00000400	-0.06215000	0.01822900

Pr(Tp)2

N	3.23652600	1.06741600	-1.09000700
N	1.88366900	1.28474200	-1.39381800
N	3.33384400	-1.41735600	-0.37866300
N	2.00785600	-1.86918300	-0.46177900
N	3.28331700	0.44048500	1.41770000
N	1.94171400	0.52405600	1.81905300
N	-3.34193700	-1.37839400	0.47683100
N	-2.01801900	-1.82641000	0.60036300
N	-3.23351300	1.15106200	1.00756900
N	-1.87952100	1.39759500	1.28277400
N	-3.27861000	0.34547600	-1.44784500
N	-1.93539400	0.40278700	-1.84889600
C	1.86702000	2.26025700	-2.34858400
C	3.18724800	2.68227400	-2.67489300
H	3.48544200	3.43446300	-3.39048000
C	4.02180200	1.90246100	-1.85596500
C	2.08436100	-3.19092700	-0.79622200
C	3.43808100	-3.60975600	-0.93084700
H	3.80626700	-4.59253000	-1.18637900
C	4.19439800	-2.45670800	-0.65795200
C	1.96757400	0.87582700	3.13813400
C	3.30445700	1.02469400	3.60390600
H	3.63482200	1.29513800	4.59612000
C	4.10408800	0.74013000	2.48316900
C	-2.10056900	-3.12076900	1.02755800

C	-3.45622400	-3.52552200	1.18297700
H	-3.82889700	-4.48668700	1.50545200
C	-4.20732300	-2.39264500	0.82396400
C	-1.86139100	2.43252000	2.17276600
C	-3.18165100	2.86447200	2.48528400
H	-3.47890200	3.65899600	3.15395900
C	-4.01781400	2.02730000	1.72674700
C	-1.95653300	0.65437600	-3.19077300
C	-3.29203600	0.76329300	-3.67197800
H	-3.61887800	0.95737700	-4.68306500
C	-4.09577600	0.56129000	-2.53662400
B	3.74658700	0.04779400	-0.02316700
H	4.95360900	0.09102800	-0.03315800
B	-3.74674700	0.05987000	0.01545700
H	-4.95361000	0.10840600	0.02091700
H	-5.27672900	-2.23964600	0.79223000
H	-1.19630300	-3.68938400	1.20459800
H	-5.09521800	1.99460600	1.64772900
H	-0.91534600	2.81464900	2.53454900
H	-5.17113700	0.55573300	-2.42868200
H	-1.02620900	0.73860700	-3.73805800
H	0.92199900	2.61024800	-2.74398300
H	5.09860400	1.88337100	-1.76492300
H	5.26436100	-2.30496200	-0.64390500
H	1.17746700	-3.76792800	-0.92644900
H	5.17900100	0.72946500	2.37128800
H	1.03924300	0.99810400	3.68166700
Pr	0.00005800	-0.08709700	0.00512100

Nd(Tp)2

N	-3.32037800	-1.19867300	-0.84802200
N	-1.99407100	-1.59607400	-1.07183700
N	-3.22196300	1.37779400	-0.66869400

N	-1.86773900	1.69248200	-0.84118400
N	-3.28961100	-0.05615000	1.48045900
N	-1.94861000	-0.11931500	1.88171300
N	3.23410500	1.26508500	0.83764900
N	1.87427700	1.55344700	1.06791100
N	3.31471100	-1.31890400	0.68066600
N	1.97819400	-1.72635100	0.83539700
N	3.28556100	0.12144400	-1.46905600
N	1.95230500	0.11951300	-1.89469900
C	-2.06031500	-2.73711800	-1.81273100
C	-3.41336500	-3.09819800	-2.07956700
H	-3.78451300	-3.94147800	-2.65034200
C	-4.18155800	-2.09362900	-1.45398300
C	-1.84644000	2.92941500	-1.42034100
C	-3.15366800	3.42148800	-1.63947700
H	-3.44926400	4.37350600	-2.08497600
C	-3.99842900	2.41793000	-1.14525100
C	-1.97026700	-0.21870100	3.24834300
C	-3.30872600	-0.22558500	3.73771900
H	-3.64299700	-0.27870700	4.76266000
C	-4.10556700	-0.10983400	2.57543100
C	1.85602400	2.70963300	1.81153300
C	3.17583700	3.17184800	2.07576000
H	3.47032300	4.05865700	2.63018300
C	4.01086000	2.23611600	1.43733800
C	2.02581700	-2.95049300	1.44479600
C	3.37650000	-3.35103500	1.67773200
H	3.72328500	-4.26338800	2.13521700
C	4.16018300	-2.28505700	1.17798400
C	1.98950900	0.21372200	-3.26197200
C	3.33578500	0.26924900	-3.73332000

H	3.66784000	0.34685500	-4.75216800
C	4.12493300	0.21716400	-2.56742200
B	-3.74448300	0.05435700	-0.01392600
H	-4.95247000	0.10122600	-0.01463700
B	3.74271400	0.03873700	0.02894300
H	4.95078700	0.07636700	0.03900900
H	5.09507700	2.18194200	1.38147200
H	0.91033800	3.13339400	2.12242200
H	5.21952800	-2.15553000	1.15540500
H	1.11800400	-3.48156700	1.66618400
H	5.19198800	0.23182400	-2.45184300
H	1.07023000	0.22567500	-3.82232100
H	-1.14809500	-3.23851700	-2.11923200
H	-5.24789500	-1.95883600	-1.38545300
H	-5.08333300	2.35840800	-1.09687700
H	-0.88748600	3.39724400	-1.65972000
H	-5.18817100	-0.07451500	2.46764800
H	-1.04326000	-0.28467500	3.80050300
Nd	-0.00102000	-0.08624900	-0.00942900

Pm(Tp)2

N	-3.24152200	-0.25754700	1.46887600
N	-1.89715000	-0.32853600	1.86365200
N	-3.23293000	-1.15664300	-0.95243000
N	-1.88655000	-1.44080000	-1.22772200
N	-3.25494900	1.39003100	-0.51800800
N	-1.91490800	1.78887300	-0.63225000
N	3.24501800	-0.52794500	-1.39148500
N	1.90174900	-0.69665400	-1.75905400
N	3.24524200	1.46945300	0.24506900
N	1.90196400	1.87251200	0.28571000

N	3.24052100	-0.94735400	1.15609100
N	1.89547200	-1.18840600	1.47456600
C	-1.91404200	-0.53119000	3.21356000
C	-3.24815700	-0.59623000	3.70612200
H	-3.57219400	-0.74735600	4.72537500
C	-4.05539200	-0.41824800	2.56906200
C	-1.89728800	-2.51310500	-2.07280100
C	-3.22838900	-2.93141500	-2.35593100
H	-3.54678000	-3.74720100	-2.98829500
C	-4.04113000	-2.04605600	-1.62709300
C	-1.94416900	3.05901100	-1.13183800
C	-3.28209000	3.49666100	-1.34336300
H	-3.61539000	4.44970900	-1.72716400
C	-4.07847800	2.40983800	-0.94199500
C	1.92052300	-1.14529200	-3.04832700
C	3.25466700	-1.27474500	-3.52737800
H	3.57997700	-1.60584400	-4.50270000
C	4.06001900	-0.87396900	-2.44693000
C	1.92287800	3.21459400	0.53546000
C	3.25769800	3.69435500	0.65613800
H	3.58388300	4.70532700	0.85171700
C	4.06179900	2.55724800	0.46551700
C	1.91043100	-2.07625900	2.51136700
C	3.24368500	-2.41619500	2.87719500
H	3.56605200	-3.08999800	3.65744100
C	4.05267600	-1.67989400	1.99436500
B	-3.70979000	-0.01303000	-0.00159400
H	-4.91750500	-0.02287500	-0.00246100
B	3.71062000	-0.00272300	0.00461000
H	4.91835700	-0.00416000	0.00581300
H	5.13521800	-0.81088100	-2.35700400

H	0.98945200	-1.34389600	-3.56357200
H	5.13695700	2.44729000	0.47218200
H	0.99254100	3.76118000	0.62260200
H	5.12843400	-1.62715800	1.90449100
H	0.97760200	-2.42783300	2.93330800
H	-0.98201300	-0.61208300	3.75819400
H	-5.13110800	-0.39419500	2.46728400
H	-5.11693000	-1.98791500	-1.54128000
H	-0.96276300	-2.93023700	-2.42565200
H	-5.15279200	2.29242400	-0.92888200
H	-1.01749500	3.58645900	-1.31891600
Pm	0.00028200	0.01269600	-0.00569600

Eu(Tp)2

N	-3.22281800	-0.59234100	-1.36348700
N	-1.87931200	-0.74287500	-1.73904500
N	-3.21530000	1.48268800	0.17313900
N	-1.86980500	1.87730100	0.22514000
N	-3.21458300	-0.88573500	1.20097700
N	-1.86867500	-1.13552300	1.50877400
N	3.21490900	1.07468200	1.03497400
N	1.86903700	1.36978400	1.29990000
N	3.21671300	-1.43176300	0.41691000
N	1.87127300	-1.81147400	0.53565500
N	3.22201300	0.35619000	-1.44496400
N	1.87813400	0.44342000	-1.83875500
C	-1.89937000	-1.30204600	-2.98393500
C	-3.23469700	-1.51828000	-3.42793300
H	-3.56108600	-1.94382200	-4.36554300
C	-4.03924100	-1.05504100	-2.37214800
C	-1.88331300	3.23498500	0.36453100

C	-3.21631300	3.73329600	0.40590700
H	-3.53779500	4.75934200	0.50883800
C	-4.02642500	2.59103500	0.28161300
C	-1.88003000	-1.93685100	2.61358000
C	-3.21217800	-2.21554500	3.03153800
H	-3.53211700	-2.81725400	3.86957700
C	-4.02400800	-1.53118500	2.11003900
C	1.88076700	2.34252700	2.25713800
C	3.21311200	2.68849500	2.62084900
H	3.53326400	3.42086400	3.34739800
C	4.02462100	1.86250100	1.82348000
C	1.88449400	-3.12637200	0.90145300
C	3.21740100	-3.61127400	1.02454700
H	3.53881900	-4.60558800	1.29794700
C	4.02770600	-2.50645700	0.70931100
C	1.89702300	0.78464600	-3.16018400
C	3.23192500	0.92018600	-3.63614200
H	3.55741500	1.18066600	-4.63259600
C	4.03748800	0.64055900	-2.51838000
B	-3.68563500	0.00240200	0.00512400
H	-4.89340100	0.00454800	0.00895600
B	3.68611300	-0.00005900	0.00366700
H	4.89388200	0.00000200	0.00678800
H	5.10065800	1.78081400	1.76339600
H	0.94635500	2.73723700	2.63532700
H	5.10372000	-2.41143400	0.67258400
H	0.95072100	-3.65318800	1.05153700
H	5.11304200	0.62484900	-2.41312100
H	0.96558100	0.91851300	-3.69544700
H	-0.96833800	-1.52266900	-3.49038000
H	-5.11467000	-1.02366900	-2.26910800

H	-5.10241400	2.49088700	0.26257000
H	-0.94970300	3.77995100	0.42301400
H	-5.10007500	-1.45906600	2.03888500
H	-0.94552600	-2.26531600	3.05036400
Eu	-0.00008900	-0.00014200	-0.00716000

Gd(Tp)2

N	-3.02360000	-1.50280000	-0.05440000
N	-1.66390000	-1.85290000	-0.06670000
N	-3.02160000	0.76660000	-1.25340000
N	-1.64870000	0.95750000	-1.53870000
N	-3.01990000	0.67450000	1.30320000
N	-1.64460000	0.84540000	1.59850000
N	3.02370000	1.50280000	0.05430000
N	1.66390000	1.85220000	0.06530000
N	3.02310000	-0.76670000	1.25380000
N	1.65010000	-0.95600000	1.53950000
N	3.02020000	-0.67400000	-1.30270000
N	1.64490000	-0.84620000	-1.59690000
C	-1.61820000	-3.21910000	-0.11550000
C	-2.92940000	-3.76300000	-0.13310000
H	-3.21280000	-4.80430000	-0.17070000
C	-3.78480000	-2.64280000	-0.09410000
C	-1.60460000	1.72710000	-2.68030000
C	-2.91560000	2.04400000	-3.12430000
H	-3.19270000	2.63010000	-3.98860000
C	-3.78050000	1.42090000	-2.20580000
C	-1.59990000	1.52760000	2.79660000
C	-2.91050000	1.80540000	3.26680000
H	-3.18610000	2.32420000	4.17370000
C	-3.77770000	1.25330000	2.30670000

C	1.61740000	3.21860000	0.10930000
C	2.92830000	3.76310000	0.12580000
H	3.21120000	4.80470000	0.15910000
C	3.78440000	2.64340000	0.09100000
C	1.60540000	-1.72650000	2.68060000
C	2.91610000	-2.04510000	3.12390000
H	3.19300000	-2.63220000	3.98760000
C	3.78150000	-1.42220000	2.20560000
C	1.59990000	-1.52820000	-2.79470000
C	2.91040000	-1.80490000	-3.26620000
H	3.18580000	-2.32270000	-4.17360000
C	3.77780000	-1.25170000	-2.30670000
B	-3.51980000	-0.00590000	0.00100000
H	-4.72580000	-0.01630000	0.00030000
B	3.52050000	0.00680000	-0.00090000
H	4.72650000	0.01730000	-0.00030000
H	4.86360000	2.58470000	0.09010000
H	0.66250000	3.72740000	0.12670000
H	4.86110000	-1.39250000	2.16360000
H	0.65070000	-2.00080000	3.11020000
H	4.85740000	-1.22260000	-2.26630000
H	0.64510000	-1.77490000	-3.24050000
H	-0.66350000	-3.72840000	-0.13410000
H	-4.86410000	-2.58370000	-0.09130000
H	-4.86010000	1.39020000	-2.16400000
H	-0.65020000	2.00250000	-3.10970000
H	-4.85740000	1.22470000	2.26550000
H	-0.64520000	1.77260000	3.24360000
Gd	-0.00040000	-0.00010000	0.00150000

Tb(Tp)2

N	2.98999100	1.50617000	0.05557600
N	1.62798400	1.84608900	0.07050700
N	2.99019300	-0.66848200	-1.30155400
N	1.61102900	-0.84151700	-1.58820500
N	2.99097100	-0.76231300	1.25231700
N	1.61373300	-0.96027500	1.52487000
N	-2.99019700	-1.50601900	-0.05561800
N	-1.62820900	-1.84596600	-0.07052100
N	-2.99018600	0.66854900	1.30160300
N	-1.61101900	0.84140600	1.58822100
N	-2.99101300	0.76247900	-1.25227500
N	-1.61378200	0.96017600	-1.52487200
C	1.57018500	3.21233400	0.11398000
C	2.87676300	3.76587200	0.12624700
H	3.15211800	4.80955500	0.15806000
C	3.74134600	2.65207100	0.08872300
C	1.55857200	-1.53129800	-2.78391300
C	2.86569500	-1.81118700	-3.25901200
H	3.13618900	-2.33462200	-4.16483400
C	3.74033700	-1.25391900	-2.30733200
C	1.56224100	-1.73425900	2.66622800
C	2.86986100	-2.04444800	3.12089900
H	3.14179300	-2.63097100	3.98667200
C	3.74237700	-1.41602900	2.21217800
C	-1.57043400	-3.21221200	-0.11396800
C	-2.87702900	-3.76572300	-0.12623900
H	-3.15240800	-4.80940000	-0.15804100
C	-3.74158700	-2.65190400	-0.08874700
C	-1.55843200	1.53108500	2.78395300
C	-2.86550800	1.81108600	3.25913900
H	-3.13590900	2.33447100	4.16501300
C	-3.74023500	1.25398200	2.30743700
C	-1.56216200	1.73407800	-2.66625600

C	-2.86974000	2.04446400	-3.12093400
H	-3.14159200	2.63098400	-3.98673300
C	-3.74233600	1.41623000	-2.21216100
B	3.49251700	0.00872200	0.00017300
H	4.69828300	0.02253700	0.00141000
B	-3.49261200	-0.00856900	-0.00015400
H	-4.69838200	-0.02225200	-0.00136000
H	-4.82125500	-2.60154000	-0.08385600
H	-0.61176100	-3.71380700	-0.13352700
H	-4.82020600	1.22631900	2.27432100
H	-0.60095600	1.77872300	3.22333100
H	-4.82217700	1.38197700	-2.18164600
H	-0.60502800	2.01490000	-3.08593400
H	0.61150000	3.71390500	0.13355000
H	4.82101500	2.60173400	0.08381000
H	4.82030300	-1.22617600	-2.27417200
H	0.60114400	-1.77908600	-3.22330700
H	4.82221300	-1.38160700	2.18168600
H	0.60515000	-2.01525900	3.08588400
Tb	0.00006900	-0.00007000	-0.00003200

Dy(Tp)2

N	-2.99373700	-1.49844400	0.00366700
N	-1.63316800	-1.84462200	0.00892700
N	-2.97776100	0.71942700	-1.28181600
N	-1.59839000	0.89496700	-1.55423800
N	-2.98201400	0.72893000	1.27217800
N	-1.60398900	0.90010000	1.55485500
N	2.99457300	1.49794300	-0.00247100
N	1.63421000	1.84451700	-0.00886700
N	2.97781200	-0.72050500	1.28201600
N	1.59824200	-0.89401400	1.55476300
N	2.98179600	-0.72850400	-1.27200800

N	1.60372700	-0.89945600	-1.55472500
C	-1.58281900	-3.21122200	0.01273100
C	-2.89244100	-3.75928900	0.01052700
H	-3.17271200	-4.80215000	0.01239200
C	-3.75150000	-2.64118300	0.00455800
C	-1.53406600	1.62339600	-2.72437000
C	-2.83711100	1.92592900	-3.19824600
H	-3.09927000	2.47989400	-4.08813400
C	-3.71936200	1.34033000	-2.27105600
C	-1.54628100	1.64101200	2.71701800
C	-2.85181400	1.95701200	3.17541500
H	-3.11911400	2.52350100	4.05582300
C	-3.72875000	1.36581900	2.24688700
C	1.58424900	3.21112300	-0.01426400
C	2.89406300	3.75878400	-0.01160900
H	3.17466000	4.80155700	-0.01472600
C	3.75278100	2.64045900	-0.00435400
C	1.53314900	-1.62383500	2.72402500
C	2.83587300	-1.92900700	3.19704000
H	3.09756800	-2.48447800	4.08612900
C	3.71870300	-1.34357000	2.27024900
C	1.54598100	-1.63942700	-2.71731800
C	2.85146300	-1.95543100	-3.17596300
H	3.11870100	-2.52109400	-4.05690200
C	3.72842100	-1.36473400	-2.24714900
B	-3.48776100	0.00033700	-0.00337500
H	-4.69354900	-0.00408100	-0.00540500
B	3.48797000	-0.00063700	0.00384500
H	4.69381100	0.00300400	0.00584300
H	4.83216700	2.58399900	-0.00026600
H	0.62838700	3.71834800	-0.01986300

H	4.79894800	-1.31919800	2.24489600
H	0.57123200	-1.87824600	3.14950300
H	4.80849200	-1.34529200	-2.21165900
H	0.58669500	-1.89476300	-3.14807500
H	-0.62679500	-3.71815800	0.01755800
H	-4.83091500	-2.58511700	0.00137400
H	-4.79956900	1.31449200	-2.24585200
H	-0.57242800	1.87907600	-3.14970800
H	-4.80881500	1.34619200	2.21139600
H	-0.58703700	1.89651700	3.14776100
Dy	-0.00021000	0.00042600	0.00037700

Tm(Tp)2

N	3.17003100	0.54246900	1.29721300
N	1.79105800	0.81347100	1.61201100
N	3.16977100	0.65956500	-1.23849400
N	1.79070300	1.00955900	-1.49390200
N	3.02999800	-1.64053600	-0.06810500
N	1.65568400	-1.94124300	-0.11749500
N	-3.17018800	-0.65925800	-1.23831000
N	-1.79133000	-1.01022800	-1.49371100
N	-3.17044900	-0.54131700	1.29741100
N	-1.79169200	-0.81313500	1.61239300
N	-3.02888400	1.64116100	-0.06864700
N	-1.65435100	1.94089000	-0.11809500
C	1.81071900	1.58766100	2.73889300
C	3.14428000	1.83174800	3.17227700
H	3.46972000	2.40192800	4.03061300
C	3.97915600	1.16156600	2.23101400
C	1.83008500	1.88123000	-2.56266400

C	3.16355800	2.10466300	-2.99668900
H	3.48878400	2.73301600	-3.81641700
C	3.97867600	1.31676500	-2.13381500
C	1.56968500	-3.30191800	-0.15604000
C	2.86422500	-3.89703300	-0.14571000
H	3.11010900	-4.94891400	-0.16465000
C	3.75641500	-2.80852900	-0.08720900
C	-1.83132800	-1.88226100	-2.56219100
C	-3.16498300	-2.10499400	-2.99603700
H	-3.49065200	-2.73343300	-3.81553100
C	-3.97956500	-1.31626500	-2.13335700
C	-1.81196800	-1.58690700	2.73957700
C	-3.14570800	-1.82995900	3.17296700
H	-3.47159200	-2.39962900	4.03149600
C	-3.98004500	-1.15956000	2.23139800
C	-1.56736900	3.30149400	-0.15717500
C	-2.86148800	3.89753700	-0.14708900
H	-3.10661900	4.94959300	-0.16647400
C	-3.75446600	2.80967200	-0.08788000
B	3.60315300	-0.18151700	-0.00979500
H	4.80906500	-0.26339800	-0.00981600
B	-3.60302800	0.18254100	-0.00986300
H	-4.80888500	0.26522200	-0.00991100
H	-5.05480400	-1.19767200	-2.11207100
H	-0.90582000	-2.28664700	-2.94945700
H	-5.05525700	-1.08057100	2.17023600
H	-0.88657800	-1.93216400	3.18633400
H	-4.83503900	2.78773200	-0.05806500
H	-0.59609200	3.77938100	-0.19668400
H	0.88505300	1.93246200	3.18544000
H	5.05443500	1.08327500	2.16994700

H	5.05398300	1.19887400	-2.11257500
H	0.90429900	2.28488300	-2.94996600
H	4.83697300	-2.78581300	-0.05758000
H	0.59875900	-3.78052600	-0.19531100
Tm	-0.00003200	-0.00075300	-0.00954700

Yb(Tp)2

Yb	0.00053600	0.00159300	0.01182600
N	3.08088900	1.48929600	-0.05563500
N	1.72750500	1.86101600	-0.09163400
N	3.08225200	-0.78936000	-1.26423600
N	1.71885500	-1.01589800	-1.55534000
N	3.08372900	-0.69414900	1.31003100
N	1.73070300	-0.84649000	1.65931300
N	-3.07836600	-1.48702600	-0.08694800
N	-1.72455700	-1.85597000	-0.13079500
N	-3.08347700	0.66639700	1.32371900
N	-1.74066400	0.81224000	1.67601900
N	-3.08188400	0.81550900	-1.24713900
N	-1.72868800	1.04891500	-1.53323700
C	1.71280800	3.22590000	-0.13805200
C	3.03588800	3.75186100	-0.13305200
H	3.33654600	4.78982100	-0.16281500
C	3.86950900	2.61840600	-0.08455400
C	1.70343200	-1.72788600	-2.72307900
C	3.02628000	-1.97405000	-3.18303800
H	3.31654400	-2.51476700	-4.07669200
C	3.86043700	-1.37361200	-2.23822300
C	1.72671500	-1.50186600	2.85354300
C	3.05010500	-1.77749300	3.29642400

H	3.35147100	-2.27628400	4.20934000
C	3.88306000	-1.24818500	2.29152400
C	-1.70821900	-3.21905800	-0.20618500
C	-3.03068500	-3.74656100	-0.21236900
H	-3.33011000	-4.78368900	-0.26410900
C	-3.86566200	-2.61586300	-0.13980100
C	-1.72740300	1.44143700	2.88385800
C	-3.05107500	1.70602900	3.34260000
H	-3.36300000	2.18461500	4.25586100
C	-3.88341500	1.18816000	2.31664700
C	-1.70390200	1.78474700	-2.68567100
C	-3.02700700	2.03934100	-3.15046300
H	-3.32778400	2.59780900	-4.02253700
C	-3.86061000	1.40901300	-2.20868700
B	3.56338700	0.00291500	-0.00019600
H	4.77084400	0.00543400	-0.01080000
B	-3.56232000	-0.00317500	-0.00043400
H	-4.76981400	-0.00661100	-0.01110500
H	-4.94367200	-2.53725700	-0.11918500
H	-0.76291600	-3.74562500	-0.25191500
H	-4.96124300	1.16640000	2.23706700
H	-0.78294600	1.67286800	3.37265800
H	-4.93852800	1.34536200	-2.15164800
H	-0.75884100	2.08677100	-3.11709700
H	0.76815400	3.75480500	-0.17264900
H	4.94742400	2.53794900	-0.06560600
H	4.93839800	-1.31202600	-2.17975400
H	0.75810300	-2.02047000	-3.15081700
H	4.96093500	-1.22581100	2.21228300
H	0.78197600	-1.74280000	3.32752500

Lu(Tp)2

N	-2.91130000	-1.50390000	-0.09990000
N	-1.54340000	-1.81890000	-0.11210000
N	-2.91730000	0.79080000	-1.23150000
N	-1.53470000	0.98430000	-1.47970000
N	-2.91990000	0.62630000	1.31250000
N	-1.53550000	0.78690000	1.58420000
N	2.91200000	1.50260000	0.10010000
N	1.54430000	1.81810000	0.11580000
N	2.91850000	-0.79250000	1.23020000
N	1.53580000	-0.98360000	1.47880000
N	2.91910000	-0.62660000	-1.31380000
N	1.53470000	-0.78680000	-1.58480000
C	-1.45880000	-3.18140000	-0.19220000
C	-2.75480000	-3.75790000	-0.22950000
H	-3.01050000	-4.80530000	-0.29150000
C	-3.64070000	-2.66130000	-0.17000000
C	-1.45910000	1.79280000	-2.59510000
C	-2.75760000	2.12990000	-3.05640000
H	-3.01220000	2.74590000	-3.90690000
C	-3.64890000	1.48190000	-2.17960000
C	-1.46180000	1.44140000	2.79850000
C	-2.76110000	1.71090000	3.30030000
H	-3.01620000	2.20850000	4.22510000
C	-3.65260000	1.18480000	2.34620000
C	1.46040000	3.18060000	0.19800000
C	2.75680000	3.75640000	0.23420000
H	3.01300000	4.80360000	0.29750000
C	3.64200000	2.65960000	0.17040000

C	1.45870000	-1.79170000	2.59430000
C	2.75690000	-2.13120000	3.05520000
H	3.01060000	-2.74750000	3.90570000
C	3.64920000	-1.48500000	2.17810000
C	1.46020000	-1.43820000	-2.80060000
C	2.75910000	-1.70630000	-3.30410000
H	3.01360000	-2.20170000	-4.23020000
C	3.65120000	-1.18200000	-2.34930000
B	-3.42870000	-0.01270000	-0.00430000
H	-4.63390000	-0.03010000	-0.00840000
B	3.42910000	0.01140000	0.00310000
H	4.63440000	0.02860000	0.00610000
H	4.72240000	2.62900000	0.17080000
H	0.49220000	3.66270000	0.22590000
H	4.72970000	-1.46210000	2.16330000
H	0.49280000	-2.07400000	2.99160000
H	4.73170000	-1.15880000	-2.33310000
H	0.49490000	-1.66850000	-3.23180000
H	-0.49040000	-3.66320000	-0.21710000
H	-4.72110000	-2.63110000	-0.17240000
H	-4.72940000	1.45740000	-2.16490000
H	-0.49350000	2.07720000	-2.99180000
H	-4.73310000	1.16110000	2.32930000
H	-0.49680000	1.67200000	3.23020000
Lu	-0.00010000	0.00010000	0.00030000

The Cartesian coordinates of the optimized geometries in solvent phase (B3LYP/ CEP-121G level)

La(Tp)2 : DMSO

N	3.11857400	1.46106400	-0.43644800
N	1.81369700	1.83823600	-0.08559100
N	2.75028100	-0.88173400	-1.42630500
N	1.35759100	-1.10350900	-1.26330300
N	3.55625800	-0.61432400	0.99260300
N	2.36333100	-0.68076000	1.73645500
N	-3.11866600	-1.46097700	-0.43656600
N	-1.81380900	-1.83820900	-0.08570500
N	-3.55623600	0.61440600	0.99252200
N	-2.36330800	0.68076000	1.73637800
N	-2.75022600	0.88181100	-1.42637700
N	-1.35754800	1.10348800	-1.26337300
C	1.78069500	3.20399900	-0.15775900
C	3.04660700	3.72025200	-0.55180700
H	3.32443800	4.75419600	-0.69446900
C	3.86282800	2.58346000	-0.71661400
C	0.98595000	-1.90727400	-2.32466800
C	2.10606300	-2.22313700	-3.14142700
H	2.11658300	-2.83731700	-4.03106500
C	3.20030900	-1.56566800	-2.54928300
C	2.69522000	-1.28123800	2.92882700
C	4.07797100	-1.61418500	2.95856900
H	4.62349300	-2.09331200	3.75900900
C	4.58853400	-1.17907900	1.71939700
C	-1.78087600	-3.20397300	-0.15784700
C	-3.04681900	-3.72017100	-0.55187200
H	-3.32470400	-4.75410300	-0.69451300
C	-3.86298400	-2.58334200	-0.71669400
C	-2.69517800	1.28118400	2.92878100
C	-4.07791700	1.61418100	2.95853800
H	-4.62342200	2.09328600	3.75900300

C	-4.58849300	1.17916800	1.71934100
C	-0.98584300	1.90724200	-2.32469000
C	-2.10592300	2.22318400	-3.14147200
H	-2.11639800	2.83737500	-4.03110000
C	-3.20020200	1.56575400	-2.54934600
B	3.60327200	-0.03305800	-0.45124300
H	4.74922900	-0.04773500	-0.83016600
B	-3.60328700	0.03315500	-0.45131800
H	-4.74923400	0.04791900	-0.83025700
H	-4.90050300	-2.50006700	-1.00833100
H	-0.86615100	-3.73513300	0.07008800
H	-5.59045700	1.22282600	1.31608000
H	-1.93475300	1.44643000	3.68120000
H	-4.24054100	1.52485200	-2.84012300
H	0.04420400	2.22012700	-2.42468200
H	0.86594600	3.73511700	0.07017800
H	4.90035000	2.50023200	-1.00825300
H	4.24065000	-1.52471300	-2.84004800
H	-0.04407600	-2.22022700	-2.42467900
H	5.59050200	-1.22267300	1.31613900
H	1.93479800	-1.44655600	3.68123400
La	0.00001600	-0.00008600	0.68943300

La(Tp)2 : chloroform

N	3.12294800	1.45594200	-0.41032100
N	1.81156400	1.84007600	-0.09140200
N	2.78629400	-0.88774800	-1.40462100
N	1.38990700	-1.09369100	-1.29845200
N	3.51430300	-0.61743400	1.04387800
N	2.30161300	-0.69969100	1.75609100
N	-3.12335200	-1.45615300	-0.40885800
N	-1.81200500	-1.84029500	-0.08981500

N	-3.51405300	0.61876200	1.04337200
N	-2.30126000	0.70147300	1.75539700
N	-2.78616300	0.88649600	-1.40542200
N	-1.38972900	1.09219100	-1.29953700
C	1.77721500	3.20322400	-0.20368600
C	3.04815600	3.71069500	-0.59096500
H	3.32642300	4.74072200	-0.75850800
C	3.86874400	2.57152200	-0.71013900
C	1.04750200	-1.88215900	-2.37561200
C	2.19292700	-2.20325900	-3.15469700
H	2.23002900	-2.80809000	-4.04960000
C	3.26977700	-1.56273700	-2.51510800
C	2.61395500	-1.28208200	2.96382500
C	4.00047300	-1.58899200	3.03354400
H	4.53278800	-2.05087000	3.85267000
C	4.53571500	-1.15649400	1.80483300
C	-1.77802800	-3.20356900	-0.20068700
C	-3.04917600	-3.71110900	-0.58719200
H	-3.32774400	-4.74123700	-0.75361600
C	-3.86948800	-2.57184600	-0.70739500
C	-2.61338200	1.28516500	2.96258200
C	-3.99981900	1.59247500	3.03209500
H	-4.53195200	2.05531900	3.85079600
C	-4.53527800	1.15886000	1.80387400
C	-1.04721000	1.87962400	-2.37740400
C	-2.19261400	2.20033600	-3.15667900
H	-2.22963800	2.80439700	-4.05210400
C	-3.26956900	1.56062700	-2.51644700
B	3.60667400	-0.03837400	-0.39856700
H	4.76413000	-0.05519600	-0.73912100
B	-3.60669500	0.03830600	-0.39847100
H	-4.76417100	0.05509000	-0.73896100
H	-4.91153400	-2.48267600	-0.98038000

H	-0.85808100	-3.73840300	-0.00419200
H	-5.54819800	1.18768900	1.42794700
H	-1.83753300	1.45954700	3.69726100
H	-4.32051400	1.52837100	-2.76699400
H	-0.01709100	2.17597000	-2.51956800
H	0.85716300	3.73801900	-0.00758000
H	4.91076500	2.48234200	-0.98321600
H	4.32069600	-1.53044800	-2.76576400
H	0.01744200	-2.17888500	-2.51743300
H	5.54860900	-1.18545600	1.42884900
H	1.83820400	-1.45589700	3.69874000
La	0.00000800	-0.00002000	0.63693600

La(Tp)2 : butanal

N	3.11941300	1.45985200	-0.42882700
N	1.81290000	1.83919600	-0.08601600
N	2.76073500	-0.88341400	-1.41993800
N	1.36696100	-1.10064900	-1.27349700
N	3.54379900	-0.61487400	1.00780200
N	2.34490600	-0.68592500	1.74251000
N	-3.11943600	-1.45983200	-0.42889100
N	-1.81293700	-1.83920500	-0.08605800
N	-3.54380200	0.61489100	1.00775700
N	-2.34491500	0.68592700	1.74247800
N	-2.76070000	0.88344000	-1.41996700
N	-1.36692500	1.10063900	-1.27351000
C	1.77909200	3.20426000	-0.17109800
C	3.04594100	3.71782000	-0.56504600
H	3.32352100	4.75060400	-0.71619800
C	3.86354600	2.58021100	-0.71647300
C	1.00367600	-1.90004000	-2.33926400
C	2.13122400	-2.21727800	-3.14529400
H	2.14944000	-2.82870600	-4.03655800

C	3.22048800	-1.56441200	-2.53939300
C	2.67137500	-1.28125100	2.93947900
C	4.05528100	-1.60701000	2.98058200
H	4.59705200	-2.08133900	3.78637900
C	4.57305900	-1.17260400	1.74443100
C	-1.77915000	-3.20426700	-0.17116600
C	-3.04599800	-3.71779800	-0.56515400
H	-3.32359200	-4.75057500	-0.71633300
C	-3.86358100	-2.58017300	-0.71657400
C	-2.67138900	1.28125400	2.93944500
C	-4.05529200	1.60702800	2.98053400
H	-4.59706500	2.08136200	3.78632700
C	-4.57306400	1.17263100	1.74437700
C	-1.00361300	1.90004200	-2.33925700
C	-2.13114600	2.21732100	-3.14529100
H	-2.14934100	2.82876600	-4.03654400
C	-3.22042900	1.56446700	-2.53941200
B	3.60420400	-0.03427200	-0.43558600
H	4.75360700	-0.04945200	-0.80336100
B	-3.60419900	0.03430000	-0.43563400
H	-4.75359700	0.04950500	-0.80342500
H	-4.90211000	-2.49507600	-1.00399100
H	-0.86297500	-3.73667500	0.04798200
H	-5.57827200	1.21211100	1.34895100
H	-1.90657900	1.44890000	3.68696600
H	-4.26398000	1.52587000	-2.81861300
H	0.02661400	2.20827900	-2.45142700
H	0.86290300	3.73664800	0.04804100
H	4.90208200	2.49513700	-1.00386800
H	4.26404000	-1.52578700	-2.81858600
H	-0.02654400	-2.20829500	-2.45145100
H	5.57827200	-1.21206900	1.34901500
H	1.90655800	-1.44891100	3.68699100

La	-0.00000300	-0.00003400	0.67432200

La(Tp)2 : formamide

N	3.11821900	1.46183200	-0.43846000
N	1.81406500	1.83829200	-0.08435000
N	2.74719300	-0.88061900	-1.42833000
N	1.35501600	-1.10383300	-1.26009700
N	3.55984400	-0.61415400	0.98792300
N	2.36871800	-0.68009700	1.73445100
N	-3.11828900	-1.46175200	-0.43857400
N	-1.81415000	-1.83822700	-0.08443900
N	-3.55983500	0.61421900	0.98783500
N	-2.36870700	0.68011800	1.73435800
N	-2.74716500	0.88068500	-1.42841400
N	-1.35501500	1.10383400	-1.26018300
C	1.78104000	3.20420000	-0.15316200
C	3.04630000	3.72129900	-0.54840600
H	3.32393100	4.75557000	-0.68911900
C	3.86215000	2.58483500	-0.71730300
C	0.98061400	-1.90869300	-2.32013700
C	2.09828000	-2.22392800	-3.14045100
H	2.10631400	-2.83866000	-4.02977000
C	3.19406200	-1.56507400	-2.55257400
C	2.70248600	-1.28262600	2.92515100
C	4.08491600	-1.61745700	2.95119800
H	4.63167800	-2.09832900	3.74975200
C	4.59317400	-1.18128900	1.71139400
C	-1.78115000	-3.20413600	-0.15321500
C	-3.04641700	-3.72122100	-0.54846000

H	-3.32406500	-4.75548800	-0.68916000
C	-3.86224200	-2.58474600	-0.71739900
C	-2.70247500	1.28253900	2.92510500
C	-4.08491200	1.61734200	2.95119500
H	-4.63167500	2.09813700	3.74979500
C	-4.59316900	1.18127500	1.71136000
C	-0.98055800	1.90865100	-2.32018900
C	-2.09819100	2.22392700	-3.14054000
H	-2.10618800	2.83864000	-4.02986900
C	-3.19399100	1.56510400	-2.55266300
B	3.60298600	-0.03225800	-0.45570600
H	4.74789500	-0.04661900	-0.83795200
B	-3.60301200	0.03233100	-0.45578300
H	-4.74791300	0.04675900	-0.83804300
H	-4.89924500	-2.50209300	-1.01105700
H	-0.86696700	-3.73483900	0.07790100
H	-5.59410800	1.22569600	1.30562000
H	-1.94346900	1.44771100	3.67895100
H	-4.23329800	1.52342200	-2.84704300
H	0.04938200	2.22308600	-2.41625200
H	0.86684800	3.73489200	0.07794300
H	4.89916100	2.50219500	-1.01093800
H	4.23337200	-1.52336600	-2.84694200
H	-0.04930600	-2.22319100	-2.41621300
H	5.59411000	-1.22568800	1.30564700
H	1.94348200	-1.44785800	3.67898500
La	0.00002500	-0.00004300	0.69434700

La(Tp)2 : toluene

N	3.12978100	1.47899900	-0.39095100
N	1.80059900	1.85364700	-0.14237500
N	2.88644200	-0.89408700	-1.34875500
N	1.49231900	-1.13104200	-1.30996800

N	3.47855100	-0.56285400	1.12763700
N	2.23467400	-0.66566100	1.78054600
N	-3.12978200	-1.47898700	-0.39101200
N	-1.80060400	-1.85363900	-0.14242300
N	-3.47856700	0.56284300	1.12760100
N	-2.23469700	0.66563600	1.78052600
N	-2.88642500	0.89410800	-1.34878000
N	-1.49230100	1.13104800	-1.30997600
C	1.75002900	3.21107500	-0.30802000
C	3.02772000	3.72408600	-0.66140400
H	3.29739000	4.75155700	-0.85620500
C	3.86958500	2.59506500	-0.70213600
C	1.22469800	-1.95390900	-2.38166400
C	2.41495600	-2.26095800	-3.09592000
H	2.51206800	-2.88263600	-3.97449700
C	3.44116400	-1.57769600	-2.41938600
C	2.49861800	-1.24148800	3.00227000
C	3.88507000	-1.52210700	3.14059200
H	4.38561000	-1.97105400	3.98633100
C	4.47078500	-1.07838000	1.93986800
C	-1.75003200	-3.21106500	-0.30808600
C	-3.02772100	-3.72407200	-0.66148300
H	-3.29739200	-4.75154100	-0.85629100
C	-3.86958000	-2.59504700	-0.70223400
C	-2.49865000	1.24147200	3.00224300
C	-3.88510800	1.52207000	3.14056300
H	-4.38565500	1.97101100	3.98630000
C	-4.47081500	1.07832300	1.93984300
C	-1.22466900	1.95398000	-2.38162000
C	-2.41490700	2.26099300	-3.09592600
H	-2.51200300	2.88268500	-3.97449500
C	-3.44111800	1.57767100	-2.41945600
B	3.63537100	-0.00718600	-0.31975300

H	4.80943300	-0.00879800	-0.59764000
B	-3.63537100	0.00719700	-0.31980000
H	-4.80943000	0.00881500	-0.59770100
H	-4.92352300	-2.51314500	-0.92727100
H	-0.81477000	-3.73775700	-0.17058000
H	-5.50156200	1.08477400	1.61495700
H	-1.69271900	1.42217200	3.70238500
H	-4.50196400	1.52223300	-2.61867000
H	-0.20924500	2.27361300	-2.57270900
H	0.81476400	3.73776400	-0.17052100
H	4.92353300	2.51316800	-0.92715100
H	4.50202200	-1.52229500	-2.61855100
H	0.20926900	-2.27349500	-2.57280800
H	5.50153200	-1.08485200	1.61498100
H	1.69268200	-1.42217300	3.70241200
La	-0.00000200	-0.00000500	0.52338100

La(Tp)2 : water

N	3.11836200	1.46170000	-0.43785800
N	1.81401600	1.83834000	-0.08461900
N	2.74821400	-0.88086700	-1.42766500
N	1.35589800	-1.10372200	-1.26092100
N	3.55878800	-0.61409500	0.98938800
N	2.36710100	-0.68031600	1.73505600
N	-3.11842700	-1.46162600	-0.43797200
N	-1.81409700	-1.83829800	-0.08471200
N	-3.55877700	0.61416400	0.98929300
N	-2.36709300	0.68032700	1.73496800
N	-2.74818600	0.88093500	-1.42775400
N	-1.35588900	1.10371500	-1.26102200
C	1.78090200	3.20419300	-0.15459500
C	3.04627600	3.72106500	-0.54972100
H	3.32387900	4.75523900	-0.69118400

C	3.86229000	2.58453100	-0.71732700
C	0.98231600	-1.90831200	-2.32133400
C	2.10070400	-2.22373100	-3.14059300
H	2.10947500	-2.83831300	-4.02999700
C	3.19601200	-1.56517600	-2.55152900
C	2.70027800	-1.28234400	2.92620800
C	4.08280800	-1.61660400	2.95336300
H	4.62917500	-2.09702800	3.75245500
C	4.59179000	-1.18061200	1.71381300
C	-1.78102600	-3.20415200	-0.15465100
C	-3.04641500	-3.72099500	-0.54977000
H	-3.32404900	-4.75516300	-0.69121200
C	-3.86239100	-2.58444100	-0.71741600
C	-2.70027000	1.28227700	2.92615400
C	-4.08280200	1.61653300	2.95333500
H	-4.62916900	2.09690000	3.75246000
C	-4.59178200	1.18062700	1.71375600
C	-0.98226600	1.90829200	-2.32139100
C	-2.10063100	2.22377300	-3.14066100
H	-2.10937600	2.83836200	-4.03005900
C	-3.19595400	1.56524400	-2.55160000
B	3.60314100	-0.03239100	-0.45429200
H	4.74837600	-0.04683200	-0.83551300
B	-3.60315900	0.03246500	-0.45437500
H	-4.74838600	0.04696200	-0.83561000
H	-4.89951900	-2.50162000	-1.01058100
H	-0.86669400	-3.73498000	0.07559200
H	-5.59303100	1.22476700	1.30876200
H	-1.94082000	1.44756300	3.67953300
H	-4.23556700	1.52376100	-2.84491400
H	0.04768800	2.22234900	-2.41856800
H	0.86655400	3.73499800	0.07563700
H	4.89942400	2.50173600	-1.01047800

H	4.23562300	-1.52365100	-2.84484800
H	-0.04762000	-2.22242500	-2.41852000
H	5.59304100	-1.22472200	1.30882000
H	1.94082600	-1.44768800	3.67957300
La	0.00003200	-0.00005900	0.69285100

Lu(tp)2 : DMSO

N	-3.08810400	-1.08410100	-0.83751700
N	-1.75334100	-1.37275700	-1.16929100
N	-2.92936600	1.42664700	-0.41378800
N	-1.56109600	1.65275400	-0.65162900
N	-2.81983700	-0.20883400	1.54314400
N	-1.42466900	-0.33267200	1.71388700
N	2.79533700	1.28622200	0.92024800
N	1.40177300	1.50541700	0.92708500
N	2.93097300	-1.26381200	0.80312000
N	1.56565900	-1.61285000	0.79927800
N	3.06347500	0.12163900	-1.33230800
N	1.68181600	0.07143800	-1.75940700
C	-1.79180800	-2.43378400	-2.03329600
C	-3.13355100	-2.83987800	-2.26433000
H	-3.47991200	-3.64416700	-2.89596800
C	-3.91928900	-1.96075500	-1.49146100
C	-1.46219500	2.92910600	-1.13606700
C	-2.74421500	3.53645300	-1.21104500
H	-2.98311600	4.53277100	-1.55193900
C	-3.64204900	2.55331300	-0.74812800
C	-1.22540500	-0.57135300	3.04998700
C	-2.46554700	-0.60414100	3.74443900
H	-2.62489400	-0.77214700	4.79942300
C	-3.44602800	-0.37251200	2.76033700
C	1.20020800	2.68098200	1.60912100
C	2.43823400	3.22786100	2.03530800

H	2.59868000	4.14040000	2.59077900
C	3.41899300	2.31850900	1.58315200
C	1.48529400	-2.86858800	1.35106800
C	2.77704600	-3.33870100	1.70380300
H	3.03279200	-4.28589900	2.15578000
C	3.65975800	-2.29713500	1.34396700
C	1.72926700	0.13906600	-3.16621000
C	3.06981100	0.22806100	-3.61708700
H	3.40375700	0.29222100	-4.64493300
C	3.88960800	0.21668300	-2.46883300
B	-3.45940600	0.06922000	0.15175200
H	-4.65519900	0.12600700	0.26286600
B	3.44543100	0.07646800	0.14330900
H	4.64309500	0.13298700	0.27630000
H	4.49450900	2.33595200	1.68964700
H	0.19785100	3.06220900	1.74853000
H	4.73404500	-2.22412400	1.43905100
H	0.52514400	-3.35522900	1.45820000
H	4.96502900	0.26449700	-2.36500000
H	0.81004400	0.11882100	-3.73819000
H	-0.87401600	-2.84086500	-2.43584800
H	-4.99139100	-1.90242500	-1.36809200
H	-4.71695000	2.58005800	-0.63897300
H	-0.49503300	3.33585700	-1.39821800
H	-4.52238100	-0.31540600	2.84016600
H	-0.22287300	-0.70576400	3.43241100
Lu	0.03047300	-0.08714000	-0.18590700

Lu(Tp)2 : water

N	3.08880100	1.09212500	-0.82550100
N	1.75400600	1.38629000	-1.15186200
N	2.92784400	-1.42240300	-0.42958100

N	1.55947500	-1.64338200	-0.67132200
N	2.82080000	0.19178400	1.54577500
N	1.42603800	0.31458600	1.71874100
N	-2.79251700	-1.29753400	0.90939800
N	-1.39867400	-1.51400500	0.91491900
N	-2.93410000	1.25344700	0.81322600
N	-1.56940400	1.60543800	0.81328200
N	-3.06223100	-0.11482600	-1.33346000
N	-1.67987100	-0.05676800	-1.75939700
C	1.79266300	2.45449700	-2.00685400
C	3.13469500	2.85986000	-2.23737900
H	3.48131300	3.66898900	-2.86263900
C	3.92032900	1.97262700	-1.47373200
C	1.45893600	-2.91417700	-1.16973900
C	2.73995700	-3.52298400	-1.24991200
H	2.97751400	-4.51586900	-1.60159600
C	3.63900000	-2.54657400	-0.77527500
C	1.22772500	0.54011800	3.05702900
C	2.46834600	0.56587600	3.75094300
H	2.62850800	0.72360400	4.80737200
C	3.44794600	0.34339000	2.76383800
C	-1.19470300	-2.69352800	1.58908400
C	-2.43163100	-3.24574900	2.01155400
H	-2.59031400	-4.16244400	2.56062700
C	-3.41411200	-2.33509500	1.56562800
C	-1.49237300	2.85812600	1.37275900
C	-2.78557900	3.32332500	1.72663500
H	-3.04388600	4.26723700	2.18402000
C	-3.66574000	2.28211100	1.35941800
C	-1.72663100	-0.11156100	-3.16724600
C	-3.06672000	-0.19978600	-3.61950600
H	-3.39983100	-0.25593200	-4.64813200
C	-3.88751200	-0.20133100	-2.47182900

B	3.45957100	-0.07207500	0.15091300
H	4.65527300	-0.13136100	0.26112100
B	-3.44508500	-0.08249100	0.14190100
H	-4.64269800	-0.14294700	0.27419100
H	-4.48959200	-2.35534300	1.67198400
H	-0.19160800	-3.07387000	1.72561500
H	-4.74000300	2.20637900	1.45263700
H	-0.53331000	3.34590000	1.48438900
H	-4.96288500	-0.25333400	-2.36930500
H	-0.80719400	-0.08355600	-3.73857400
H	0.87475000	2.86715600	-2.40339500
H	4.99257300	1.91121000	-1.35309200
H	4.71374800	-2.57629500	-0.66538800
H	0.49143100	-3.31633100	-1.43761700
H	4.52432400	0.28507100	2.84229700
H	0.22547900	0.67097900	3.44145200
Lu	-0.03105300	0.09233000	-0.18383200

Lu(Tp)2 : formamide

N	2.88323700	1.40927500	-0.55784900
N	1.50286900	1.59050700	-0.76647600
N	3.08223800	-1.12765900	-0.79080000
N	1.74614500	-1.46077700	-1.05169800
N	2.87535300	-0.07090700	1.52395100
N	1.49125900	-0.21180500	1.75483300
N	-2.99324100	-1.22859000	0.77836200
N	-1.63390500	-1.61182200	0.83076100
N	-2.79778800	1.32059400	0.87305800
N	-1.39888800	1.50831500	0.93381800
N	-3.00779600	0.13696800	-1.37376400
N	-1.61344500	0.03461100	-1.75222300
C	1.36290100	2.81735200	-1.34653400

C	2.63002600	3.44010500	-1.51798600
H	2.83145700	4.41068700	-1.94440200
C	3.56019300	2.51877100	-1.00761700
C	1.77499700	-2.58708300	-1.83118100
C	3.11372800	-2.98367000	-2.07983200
H	3.45831000	-3.82620300	-2.66100500
C	3.91095100	-2.03503700	-1.40892100
C	1.34385600	-0.35047300	3.11539600
C	2.60878200	-0.29714200	3.76151100
H	2.81064500	-0.37947100	4.81922300
C	3.54715200	-0.12591800	2.72396900
C	-1.60990700	-2.86522600	1.39754800
C	-2.92281800	-3.29686600	1.70192500
H	-3.22017200	-4.23438500	2.15264500
C	-3.76516500	-2.23947700	1.30249200
C	-1.19606900	2.68579900	1.60806300
C	-2.43703800	3.26823100	1.97832600
H	-2.59862500	4.18907500	2.51772900
C	-3.42052500	2.37325100	1.50200900
C	-1.61058100	0.08712100	-3.16313300
C	-2.92879000	0.21249600	-3.65861600
H	-3.22367100	0.27635200	-4.69944000
C	-3.79011900	0.24317800	-2.54276600
B	3.46541200	0.10949400	0.08944400
H	4.65909000	0.19823700	0.15423000
B	-3.44597900	0.11739400	0.08510100
H	-4.64787700	0.20609400	0.17272500
H	-4.84132000	-2.13860900	1.35459700
H	-0.66551500	-3.37340700	1.54654200
H	-4.50003900	2.41731900	1.56691700
H	-0.19170100	3.04662300	1.77592400
H	-4.86291400	0.32582000	-2.47393500
H	-0.67061300	0.02622200	-3.70424900

H	0.37847400	3.18489300	-1.60801700
H	4.63904100	2.57369700	-0.93934100
H	4.98710300	-1.94722600	-1.32741400
H	0.85337700	-3.04097100	-2.16900400
H	4.62459000	-0.03354600	2.76200400
H	0.35996200	-0.47609800	3.54462200
Lu	-0.03181000	-0.13736600	-0.10894100

Lu(tp)2 : Butanal

N	2.93808800	1.38992100	0.57072200
N	1.56463600	1.70032000	0.64621500
N	2.94687600	-0.21948100	-1.40700500
N	1.53772200	-0.25130100	-1.72175700
N	2.93011400	-1.13825500	0.97252200
N	1.55350500	-1.39806200	1.13377600
N	-2.95519400	-1.23909400	-0.80205300
N	-1.58309100	-1.48280300	-0.98658700
N	-2.94366100	-0.08672700	1.47513000
N	-1.56315100	-0.08784100	1.77304600
N	-2.96132200	1.30882100	-0.65918300
N	-1.58883400	1.58937700	-0.80808100
C	1.48680800	3.00121900	1.08051500
C	2.78505400	3.53777100	1.27959700
H	3.04268500	4.53126800	1.61625800
C	3.67181200	2.49030200	0.94891200
C	1.47462600	-0.49579300	-3.10321000
C	2.77720400	-0.61904000	-3.64948000
H	3.03077000	-0.80713400	-4.68465300
C	3.68164900	-0.44619900	-2.58204400
C	1.46042300	-2.51391500	1.93055900
C	2.75353400	-2.98254900	2.28004600
H	3.00103000	-3.83635700	2.89375600

C	3.65148200	-2.08813000	1.65822000
C	-1.49067400	-2.63440300	-1.71981300
C	-2.78437100	-3.14438400	-2.01096700
H	-3.03238700	-4.03385000	-2.57062000
C	-3.67910900	-2.23255600	-1.41412100
C	-1.47052400	-0.15953900	3.14244900
C	-2.76359700	-0.20204600	3.73063100
H	-3.00640900	-0.25922200	4.78162100
C	-3.66505100	-0.15496300	2.64941600
C	-1.51322000	2.81472800	-1.41814400
C	-2.81280300	3.33415900	-1.66027000
H	-3.07046100	4.27403900	-2.12549200
C	-3.69794100	2.35326000	-1.16938500
B	3.45199700	0.00499600	0.01826900
H	4.65746900	0.00505800	0.04542400
B	-3.47015800	-0.00548400	0.01392900
H	-4.67287300	-0.01060600	0.01892600
H	-4.75958200	-2.22526100	-1.38812400
H	-0.52092200	-3.02533500	-1.99620900
H	-4.74569400	-0.16670600	2.63385100
H	-0.50028900	-0.17556800	3.62027000
H	-4.77825900	2.32735300	-1.15276300
H	-0.54888700	3.24739100	-1.64763500
H	0.52229800	3.46992400	1.22231700
H	4.75208200	2.45590400	0.95941100
H	4.76264000	-0.46267200	-2.55982300
H	0.51326600	-0.56097900	-3.59624200
H	4.73210800	-2.06415900	1.66091400
H	0.49050600	-2.91086500	2.19854200
Lu	0.02676200	0.00688100	-0.01740000

Lu(tp)2 : chloroform

N	-2.92943200	1.51204100	0.07682000

N	-1.55845100	1.81889500	0.08654700
N	-2.94167700	-0.76523800	1.23972300
N	-1.55884900	-0.95946300	1.48664000
N	-2.93992500	-0.63703500	-1.30425700
N	-1.55349000	-0.80454800	-1.56836300
N	2.92973200	-1.51164900	-0.07777100
N	1.55879000	-1.81864900	-0.08793900
N	2.94171800	0.76644900	-1.23904800
N	1.55891300	0.96046300	-1.48608800
N	2.93977700	0.63639500	1.30487100
N	1.55337800	0.80346000	1.56896100
C	-1.46724100	3.18271500	0.14870700
C	-2.76094200	3.76681500	0.17727700
H	-3.01073000	4.81621500	0.22517500
C	-3.65381600	2.67508500	0.13100400
C	-1.48223800	-1.76073600	2.60775400
C	-2.78152700	-2.09181700	3.07442300
H	-3.03566600	-2.70158600	3.92955300
C	-3.67427400	-1.44821300	2.19413300
C	-1.47749300	-1.48557100	-2.76962800
C	-2.77678000	-1.76381000	-3.26946000
H	-3.02988000	-2.28081100	-4.18415200
C	-3.67182800	-1.21702300	-2.32871200
C	1.46775000	-3.18243100	-0.15109700
C	2.76152700	-3.76634400	-0.18028000
H	3.01143600	-4.81567200	-0.22911000
C	3.65426700	-2.67456600	-0.13280900
C	1.48228900	1.76232100	-2.60673300
C	2.78157300	2.09392500	-3.07307300
H	3.03569400	2.70419900	-3.92784500
C	3.67431200	1.45005100	-2.19299000
C	1.47709100	1.48309100	2.77090900
C	2.77627200	1.76088500	3.27129400

H	3.02919700	2.27687300	4.18659900
C	3.67147300	1.21522100	2.33003600
B	-3.45135900	0.02515900	0.00097500
H	-4.65562400	0.04215600	0.00311300
B	3.45143000	-0.02480200	-0.00085200
H	4.65568900	-0.04156300	-0.00288400
H	4.73487300	-2.65208000	-0.13501100
H	0.49848900	-3.66218300	-0.17119300
H	4.75481100	1.42421100	-2.18077300
H	0.51709700	2.04948300	-3.00217700
H	4.75205700	1.19113900	2.31744900
H	0.51179600	1.72756000	3.19397200
H	-0.49792000	3.66236400	0.16836000
H	-4.73442400	2.65272400	0.13337100
H	-4.75477000	-1.42215000	2.18207800
H	-0.51705200	-2.04791100	3.00320400
H	-4.75240800	-1.19281200	-2.31599800
H	-0.51229300	-1.73059400	-3.19259300
Lu	-0.00009300	-0.00009600	-0.00009800

Lu(Tp)2 : toluene

N	-2.91426700	1.52045400	0.00156300
N	-1.54414500	1.81950500	0.00097000
N	-2.94496100	-0.70308100	1.27246200
N	-1.56212400	-0.89557800	1.53090000
N	-2.93404300	-0.69394000	-1.27235700
N	-1.54837800	-0.88222800	-1.53686100
N	2.93455500	-1.50017300	-0.14269700
N	1.56446200	-1.81932500	-0.16244700
N	2.92507500	0.82436800	-1.21166600
N	1.54228300	1.01678000	-1.45031000
N	2.93383300	0.59298500	1.33306300
N	1.54816500	0.74084500	1.59743100

C	-1.44456300	3.18336200	-0.00067500
C	-2.73884800	3.77571000	-0.00385100
H	-2.98009800	4.83490600	-0.00886300
C	-3.63983900	2.69239000	0.00238000
C	-1.48580900	-1.63021100	2.69673800
C	-2.78488900	-1.92905000	3.18468300
H	-3.04903200	-2.49387700	4.06329500
C	-3.67728200	-1.33085200	2.27062200
C	-1.48292400	-1.61436700	-2.69691800
C	-2.78210400	-1.92320300	-3.18575500
H	-3.03569000	-2.48120500	-4.06968100
C	-3.66608800	-1.32481100	-2.26534900
C	1.48499200	-3.18314300	-0.28180000
C	2.77933200	-3.75536100	-0.33912500
H	3.04067300	-4.79449800	-0.43498100
C	3.66022800	-2.65201400	-0.24435000
C	1.46610100	1.87237000	-2.53545300
C	2.76523500	2.23183800	-2.98281800
H	3.00948000	2.87742200	-3.82086300
C	3.65751800	1.55305300	-2.12906900
C	1.46232900	1.37168300	2.83813500
C	2.76136900	1.62011400	3.34760400
H	3.01469000	2.09717500	4.29213200
C	3.66559700	1.12281200	2.38679500
B	-3.44492900	0.03194700	0.00128900
H	-4.64948700	0.05909700	-0.00656600
B	3.44500100	-0.01171700	-0.00113100
H	4.64955900	-0.01864000	-0.01313500
H	4.74078700	-2.62740500	-0.24617700
H	0.51594900	-3.66354200	-0.33075300
H	4.73798800	1.53745000	-2.11597700
H	0.50084900	2.16603600	-2.92334300
H	4.74612400	1.09824900	2.37347500

H	0.49702100	1.58587400	3.27137300
H	-0.47547200	3.66368100	-0.01213000
H	-4.72039900	2.66787400	0.00428400
H	-4.75775200	-1.29504100	2.25779100
H	-0.52051600	-1.90372000	3.10464200
H	-4.74661000	-1.30016900	-2.25181300
H	-0.51774100	-1.88912100	-3.11012000
Lu	-0.00008400	-0.01011100	-0.00020400

Yb(Tp)2: butanal

Yb	0.01010700	-0.11843800	-0.05885800
N	-3.09551500	1.47144000	0.44769300
N	-1.71886700	1.74815000	0.52410800
N	-3.20084400	-1.02511900	1.03850900
N	-1.85325800	-1.34080900	1.27163800
N	-3.21640100	-0.28642800	-1.41332800
N	-1.87006000	-0.43073600	-1.79082200
N	3.23382500	-1.36499300	-0.41630700
N	1.89678800	-1.78316300	-0.53778800
N	3.12281300	1.14205900	-0.99538900
N	1.75571100	1.34742800	-1.24864800
N	3.11635400	0.39154400	1.46942400
N	1.75000200	0.40962700	1.80288100
C	-1.62349400	3.05492300	0.91877500
C	-2.91393200	3.63572700	1.10196500
H	-3.14626200	4.64513900	1.40541200
C	-3.81779900	2.59652600	0.79928900
C	-1.84440800	-2.33687800	2.20477200
C	-3.18344700	-2.68353600	2.58966100
H	-3.49315000	-3.42957800	3.30302700
C	-4.00022100	-1.82079800	1.82893500

C	-1.87580400	-0.74075800	-3.12002100
C	-3.20663800	-0.81272800	-3.61789500
H	-3.52967000	-1.04314800	-4.62233700
C	-4.01961500	-0.52620000	-2.50685900
C	1.93987200	-3.09041900	-0.93065700
C	3.28967300	-3.53027600	-1.06688700
H	3.64082200	-4.51265200	-1.36384500
C	4.07480500	-2.41255300	-0.72414700
C	1.69862300	2.34241400	-2.18298700
C	3.00833900	2.78994800	-2.54337900
H	3.27939100	3.55427400	-3.24721200
C	3.88364000	2.00249500	-1.76135000
C	1.69566000	0.70780600	3.12923400
C	3.00644000	0.89405300	3.66832300
H	3.26940700	1.13747200	4.68876300
C	3.87948200	0.67177800	2.58380200
B	-3.66021700	0.07684000	0.03659000
H	-4.86671100	0.12858000	0.06200100
B	3.64026700	0.08074500	0.02973800
H	4.84674400	0.13417200	0.05157500
H	5.15349900	-2.29003800	-0.69647700
H	1.02127000	-3.62918100	-1.10037200
H	4.96234100	1.98532500	-1.70196100
H	0.73977700	2.69483800	-2.54311600
H	4.95811300	0.70461100	2.52944700
H	0.73781200	0.78578300	3.61723100
H	-0.64547000	3.50754400	1.05285200
H	-4.89643900	2.58432400	0.79038400
H	-5.07902400	-1.73779400	1.79570400
H	-0.91487000	-2.74995300	2.54647700
H	-5.09825800	-0.46534800	-2.42160200
H	-0.93797800	-0.90377900	-3.64480800

Yb(Tp)2 : chloroform

Yb	-0.00346800	0.07039800	-0.00904600
N	3.12207400	-1.40766100	-0.60748200
N	1.74500100	-1.73282200	-0.65894600
N	3.20089200	0.16497100	1.43778500
N	1.86754700	0.21811100	1.83190600
N	3.17877600	1.14926300	-0.95128400
N	1.82071300	1.46214100	-1.17253100
N	-3.18718300	1.35786400	0.56140600
N	-1.82961000	1.73226700	0.65437700
N	-3.17917100	-0.24497700	-1.44836400
N	-1.82666400	-0.27925700	-1.84432400
N	-3.13424700	-1.19688000	0.93996000
N	-1.76620200	-1.47538800	1.14312100
C	1.68573500	-2.99579200	-1.16650300
C	2.99404700	-3.51152400	-1.43791700
H	3.25345000	-4.48224100	-1.84553800
C	3.87054000	-2.46608800	-1.06491200
C	1.87362200	0.39238700	3.18854700
C	3.20838200	0.46864800	3.69043700
H	3.51941900	0.61781400	4.71312300
C	4.03243000	0.32114600	2.54259600
C	1.80212200	2.57405800	-1.96299100
C	3.14120000	2.98452800	-2.27096400
H	3.44118100	3.84206200	-2.86689100
C	3.96770800	2.06449900	-1.61753700
C	-1.82929400	3.00807100	1.13971500
C	-3.15733900	3.48626700	1.35830800
H	-3.47590300	4.44742500	1.73135600
C	-3.99475100	2.40091700	0.97733400
C	-1.81456600	-0.51747400	-3.17792200
C	-3.12983500	-0.64693200	-3.69251000

H	-3.44226300	-0.83883500	-4.71412500
C	-3.97222500	-0.46522300	-2.56299800
C	-1.73672600	-2.52917400	1.99680700
C	-3.04514700	-2.95551500	2.36055300
H	-3.32417900	-3.75860200	3.02867100
C	-3.90226300	-2.07172100	1.66755300
B	3.65250100	-0.03493900	-0.04346800
H	4.85904400	-0.05879300	-0.08680800
B	-3.65864400	-0.02943000	0.01937400
H	-4.86503500	-0.05648800	0.02342600
H	-5.07345300	2.31736900	0.96857000
H	-0.88933900	3.53719900	1.29574800
H	-5.05998000	-0.48395700	-2.49056400
H	-0.86157600	-0.60575500	-3.70890700
H	-4.99105300	-2.01716400	1.64212300
H	-0.77691800	-2.94288600	2.31032800
H	0.71625000	-3.46619700	-1.31723300
H	4.94910600	-2.40731200	-1.08916500
H	5.10041100	0.29360000	2.43350500
H	0.93970900	0.48142100	3.72643800
H	5.04673300	2.01158300	-1.56846000
H	0.86252000	3.00386300	-2.26687400

Yb(Tp)2 : DMSO

Yb	0.00047800	-0.00321600	0.38344900
N	-3.35783200	0.57634400	1.16463900
N	-2.08164700	0.71045700	1.73253500
N	-3.08153800	-1.46305300	-0.37114100
N	-1.73403900	-1.81611400	-0.20100100
N	-2.89966400	0.90909300	-1.34056400
N	-1.51631000	1.14995200	-1.36005700
N	2.89848200	-0.88562200	-1.35815900

N	1.51527200	-1.12697000	-1.37671700
N	3.08421500	1.46735500	-0.34599300
N	1.73588000	1.81730900	-0.17602400
N	3.35870300	-0.59951100	1.15243500
N	2.08259500	-0.73548400	1.72008800
C	-2.28040600	1.23140800	2.97885800
C	-3.66803500	1.43876300	3.23245500
H	-4.12614100	1.83604800	4.12651400
C	-4.31392500	1.01048600	2.05764200
C	-1.68211800	-3.17247000	-0.34758500
C	-2.97586300	-3.70947400	-0.61195900
H	-3.24339300	-4.74359900	-0.77347200
C	-3.83210500	-2.59248400	-0.61827400
C	-1.29566800	1.96557900	-2.43205900
C	-2.51349100	2.26097900	-3.11197600
H	-2.65021900	2.87767300	-3.98837700
C	-3.50381200	1.57242200	-2.38720600
C	1.28996000	-1.91772200	-2.46631500
C	2.50479200	-2.19645000	-3.15849600
H	2.63792600	-2.79281800	-4.04940000
C	3.49811900	-1.52419600	-2.42254200
C	1.68555800	3.17656400	-0.29355900
C	2.98106400	3.71845600	-0.53876100
H	3.24993100	4.75570700	-0.67619000
C	3.83678600	2.60138100	-0.56434900
C	2.27989200	-1.28012900	2.95649000
C	3.66653000	-1.50153300	3.20363400
H	4.12349500	-1.91802900	4.08949100
C	4.31331800	-1.05637100	2.03558600
B	-3.59096800	0.00916500	-0.27064300
H	-4.77798300	0.01082600	-0.48675500
B	3.59238400	-0.00681500	-0.27250400
H	4.77931700	-0.00619300	-0.48909300

H	4.56571100	-1.45826500	-2.57898800
H	0.28396200	-2.24304700	-2.69475800
H	4.90456400	2.53729500	-0.72007400
H	0.73843500	3.69133000	-0.19934800
H	5.36295600	-1.03355000	1.77816900
H	1.43240800	-1.48353900	3.59825000
H	-1.43319700	1.42898000	3.62280400
H	-5.36383800	0.98524200	1.80161900
H	-4.89904500	-2.52562700	-0.77851000
H	-0.73517200	-3.68863300	-0.25936100
H	-4.57216100	1.51077400	-2.54015000
H	-0.29049400	2.29526100	-2.65787700

Yb(Tp)2 : formamide

Yb	0.00001800	-0.00085800	-0.00097800
N	-3.17212500	0.08179700	-1.47966100
N	-1.81519800	0.10530200	-1.83740900
N	-3.17227900	1.23916800	0.81337700
N	-1.81547300	1.54049900	1.00782800
N	-3.16914300	-1.32587200	0.66860100
N	-1.81152000	-1.64433800	0.82768600
N	3.17097100	-0.07914300	1.48069600
N	1.81375800	-0.10271200	1.83738300
N	3.17378000	-1.23948200	-0.81087100
N	1.81733300	-1.54208900	-1.00583000
N	3.16879900	1.32570400	-0.66937300
N	1.81108200	1.64296700	-0.83010000
C	-1.78953400	0.18186200	-3.20033000
C	-3.11002900	0.20890700	-3.73726100
H	-3.40206500	0.26680800	-4.77572900
C	-3.95431100	0.14345900	-2.61314600
C	-1.78976500	2.68246500	1.75566100

C	-3.11029600	3.13139400	2.05134100
H	-3.40228900	4.00139600	2.62135000
C	-3.95451500	2.18832000	1.43598800
C	-1.78347800	-2.86293600	1.44274700
C	-3.10295300	-3.34453800	1.68708900
H	-3.39304000	-4.27347300	2.15611200
C	-3.94926400	-2.34029200	1.18111600
C	1.78702100	-0.17765400	3.20037400
C	3.10709200	-0.20343400	3.73840500
H	3.39831600	-0.25989400	4.77718100
C	3.95225900	-0.13898800	2.61489700
C	1.79297500	-2.68484200	-1.75251600
C	3.11403900	-3.13313100	-2.04676800
H	3.40706600	-4.00355600	-2.61559800
C	3.95714000	-2.18876300	-1.43185700
C	1.78273000	2.86082800	-1.44660000
C	3.10207500	3.34301800	-1.69048200
H	3.39191600	4.27157100	-2.16041200
C	3.94865100	2.33996400	-1.18261000
B	-3.65747600	-0.00213700	0.00121700
H	-4.86388300	-0.00401700	0.00215800
B	3.65748400	0.00317700	0.00011600
H	4.86389100	0.00586800	0.00014000
H	5.03102300	-0.13206800	2.54615900
H	0.83836800	-0.20944500	3.72032100
H	5.03577700	-2.12842800	-1.39431700
H	0.84523900	-3.12280600	-2.03763100
H	5.02748700	2.27965500	-1.15187800
H	0.83341800	3.32435500	-1.68166900
H	-0.84128900	0.21388400	-3.72100700
H	-5.03302300	0.13696400	-2.54353600
H	-5.03322300	2.12881100	1.39913700
H	-0.84150800	3.11939700	2.04062600

H	-5.02808300	-2.27921800	1.15132900
H	-0.83428900	-3.32739400	1.67647500

Yb(Tp)2 : toluene

Yb	0.00000600	0.00023200	0.00012900
N	3.12813300	0.79489700	-1.25414900
N	1.77284600	0.99262600	-1.55999900
N	3.12688800	-1.48553100	-0.06668400
N	1.77145000	-1.84968600	-0.07901800
N	3.13188400	0.68397600	1.31437900
N	1.77752200	0.85577600	1.63917900
N	-3.12834500	-0.79837600	1.25171100
N	-1.77309600	-0.99682300	1.55721300
N	-3.12721900	1.48519300	0.07028900
N	-1.77187300	1.84962300	0.08447800
N	-3.13136700	-0.68077400	-1.31644100
N	-1.77686800	-0.85117900	-1.64144400
C	1.75204800	1.72848500	-2.70942400
C	3.07358700	2.01380200	-3.15869000
H	3.36956300	2.57332600	-4.03400200
C	3.91311000	1.40380000	-2.20864700
C	1.75088800	-3.21318900	-0.13759000
C	3.07248100	-3.74468600	-0.16383500
H	3.36850200	-4.78254500	-0.20918400
C	3.91182800	-2.61650600	-0.11768000
C	1.75982700	1.48709800	2.84910500
C	3.08269800	1.73078100	3.31884700
H	3.38104200	2.21071200	4.23944200
C	3.91954400	1.20647900	2.31671200
C	-1.75239500	-1.73539900	2.70487800
C	-3.07397600	-2.02144000	3.15357700

H	-3.37002500	-2.58276600	4.02770900
C	-3.91340900	-1.40987400	2.20446300
C	-1.75166100	3.21298400	0.14654000
C	-3.07339300	3.74407800	0.17395800
H	-3.36967700	4.78172900	0.22224200
C	-3.91245600	2.61587100	0.12359400
C	-1.75870400	-1.47968400	-2.85283700
C	-3.08139000	-1.72299100	-3.32327900
H	-3.37937800	-2.20097500	-4.24500200
C	-3.91862900	-1.20134600	-2.32008800
B	3.61236800	-0.00302900	-0.00266700
H	4.81913400	-0.00522600	-0.00459200
B	-3.61238100	0.00277400	0.00221100
H	-4.81914900	0.00471900	0.00373600
H	-4.99173600	-1.36848000	2.14252600
H	-0.80589300	-2.02032400	3.14575600
H	-4.99075800	2.54103800	0.12192400
H	-0.80541800	3.73794800	0.16842600
H	-4.99680000	-1.16514900	-2.25247100
H	-0.81311100	-1.72254200	-3.32003400
H	0.80550600	2.01242100	-3.15085200
H	4.99144200	1.36228900	-2.14688200
H	4.99014800	-2.54191400	-0.11703200
H	0.80451300	-3.73799000	-0.15755800
H	4.99768600	1.16961300	2.24902000
H	0.81441400	1.73150600	3.31586000

Yb(Tp)2 : water

N	-3.21781400	0.31471300	-1.41069600
N	-1.87145900	0.46437000	-1.78219400
N	-3.15831100	1.07152000	1.04470800

N	-1.80018300	1.31311200	1.29110700
N	-3.14864900	-1.43794100	0.46652400
N	-1.78124200	-1.77823000	0.50960500
N	3.13919000	-0.21801000	1.48924500
N	1.78316300	-0.21904600	1.82172700
N	3.17760000	-1.18912800	-0.88818500
N	1.81929600	-1.48012500	-1.10423700
N	3.18809500	1.35921200	-0.53413300
N	1.84055200	1.69954400	-0.71544000
C	-1.87549900	0.73812400	-3.11537800
C	-3.20598000	0.76869500	-3.62527900
H	-3.51782100	0.96349500	-4.64887500
C	-4.02031400	0.50424700	-2.51793500
C	-1.75955800	2.34061000	2.18616800
C	-3.06815000	2.76728300	2.53335600
H	-3.35645700	3.55709900	3.21985800
C	-3.92646800	1.94532900	1.78355700
C	-1.73586500	-3.08456800	0.92622700
C	-3.04633100	-3.58903300	1.15245000
H	-3.32849100	-4.57874300	1.48151500
C	-3.91061000	-2.51652200	0.84992300
C	1.71843600	-0.42554700	3.16443000
C	3.02940400	-0.56658200	3.72304600
H	3.30218600	-0.74334900	4.75601600
C	3.90271700	-0.42945800	2.61542200
C	1.79799100	-2.55552400	-1.95178600
C	3.12630900	-2.96142100	-2.30092700
H	3.41409900	-3.77964900	-2.93955200
C	3.96518800	-2.07122300	-1.59969100
C	1.83464500	2.97698400	-1.21890700
C	3.16489700	3.47211800	-1.36484700

H	3.46664800	4.44272000	-1.73174200
C	3.98961200	2.41885000	-0.92548700
B	-3.65818400	-0.02134300	0.04979900
H	-4.86461500	-0.03308300	0.07533600
B	3.65821300	-0.01847700	0.02894300
H	4.86463900	-0.02658000	0.04235600
H	4.98134600	-0.46256200	2.56648100
H	0.76054900	-0.47386700	3.66742900
H	5.04416500	-2.00153900	-1.56697300
H	0.84755600	-2.97271500	-2.27377600
H	5.06836400	2.35143400	-0.85765200
H	0.88627100	3.46053300	-1.43706200
H	-0.93714200	0.89495900	-3.64779000
H	-5.09900800	0.42800800	-2.42985500
H	-5.00541100	1.91549700	1.73016500
H	-0.79937900	2.70864300	2.53788800
H	-4.98933800	-2.44897500	0.88116800
H	-0.78769000	-3.57785100	1.03627600
Yb	-0.00006900	0.02973600	-0.03910300