Supporting information for

«DFT Study of Molecular and Electronic Structure of Y, La and Lu Complexes with Porphyrazine and tetrakis(1,2,5-thiadiazole)porphyrazine»

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Content

Cartesian coordinates of YClPz optimized B3LYP/pcseg-2 level of theory:

N	0.000000000000	1.993336000000	-0.255275000000
N	1.993336000000	0.000000000000	-0.255275000000
N	0.000000000000	-1.993336000000	-0.255275000000
N	-1.993336000000	0.000000000000	-0.255275000000
N	2.371598000000	2.371598000000	-0.544869000000
N	2.371598000000	-2.371598000000	-0.544869000000
N	-2.371598000000	-2.371598000000	-0.544869000000
N	-2.371598000000	2.371598000000	-0.544869000000
C	1.104829000000	2.768875000000	-0.485831000000
C	2.768875000000	-1.104829000000	-0.485831000000
C	-1.104829000000	-2.768875000000	-0.485831000000
C	2.768875000000	1.104829000000	-0.485831000000
C	1.104829000000	-2.768875000000	-0.485831000000
C	-2.768875000000	-1.104829000000	-0.485831000000
C	-1.104829000000	2.768875000000	-0.485831000000
C	-2.768875000000	1.104829000000	-0.485831000000
C	0.677262000000	4.124663000000	-0.789624000000
C	4.124663000000	-0.677262000000	-0.789624000000
C	-0.677262000000	-4.124663000000	-0.789624000000
C	4.124663000000	0.677262000000	-0.789624000000
C	0.677262000000	-4.124663000000	-0.789624000000
C	-4.124663000000	-0.677262000000	-0.789624000000
C	-0.677262000000	4.124663000000	-0.789624000000
C	-4.124663000000	0.677262000000	-0.789624000000
H	1.353490000000	4.932188000000	-1.013263000000
H	4.932188000000	-1.353490000000	-1.013263000000
H	-1.353490000000	-4.932188000000	-1.013263000000
H	4.932188000000	1.353490000000	-1.013263000000
H	1.353490000000	-4.932188000000	-1.013263000000
H	-4.932188000000	-1.353490000000	-1.013263000000
H	-1.353490000000	4.932188000000	-1.013263000000
H	-4.932188000000	1.353490000000	-1.013263000000
Y	0.000000000000	0.000000000000	0.872219000000
Cl	0.000000000000	0.000000000000	3.395025000000

Cartesian coordinates of LaClPz optimized B3LYP/pcseg-2 level of theory:

N	0.000000000000	2.009718000000	-0.388711000000
N	2.009718000000	0.000000000000	-0.388711000000
N	0.000000000000	-2.009718000000	-0.388711000000
N	-2.009718000000	0.000000000000	-0.388711000000
N	2.369737000000	2.369737000000	-0.727586000000
N	2.369737000000	-2.369737000000	-0.727586000000
N	-2.369737000000	-2.369737000000	-0.727586000000
N	-2.369737000000	2.369737000000	-0.727586000000
C	1.103590000000	2.771593000000	-0.661221000000
C	2.771593000000	-1.103590000000	-0.661221000000
C	-1.103590000000	-2.771593000000	-0.661221000000
C	2.771593000000	1.103590000000	-0.661221000000
C	1.103590000000	-2.771593000000	-0.661221000000
C	-2.771593000000	-1.103590000000	-0.661221000000
C	-1.103590000000	2.771593000000	-0.661221000000
C	-2.771593000000	1.103590000000	-0.661221000000
C	0.677092000000	4.115201000000	-1.022975000000

C	4.115201000000	-0.677092000000	-1.022975000000
C	-0.677092000000	-4.115201000000	-1.022975000000
C	4.115201000000	0.677092000000	-1.022975000000
C	0.677092000000	-4.115201000000	-1.022975000000
C	-4.115201000000	-0.677092000000	-1.022975000000
C	-0.677092000000	4.115201000000	-1.022975000000
C	-4.115201000000	0.677092000000	-1.022975000000
H	1.353375000000	4.909759000000	-1.289221000000
H	4.909759000000	-1.353375000000	-1.289221000000
H	-1.353375000000	-4.909759000000	-1.289221000000
H	4.909759000000	1.353375000000	-1.289221000000
H	1.353375000000	-4.909759000000	-1.289221000000
H	-4.909759000000	-1.353375000000	-1.289221000000
H	-1.353375000000	4.909759000000	-1.289221000000
H	-4.909759000000	1.353375000000	-1.289221000000
La	0.000000000000	0.000000000000	1.031468000000
Cl	0.000000000000	0.000000000000	3.742224000000

Cartesian coordinates of LuClPz optimized B3LYP/pcseg-2 level of theory:

N	0.000000000000	1.990100000000	-0.354695000000
N	1.990100000000	0.000000000000	-0.354695000000
N	0.000000000000	-1.990100000000	-0.354695000000
N	-1.990100000000	0.000000000000	-0.354695000000
N	2.372115000000	2.372115000000	-0.632046000000
N	2.372115000000	-2.372115000000	-0.632046000000
N	-2.372115000000	-2.372115000000	-0.632046000000
N	-2.372115000000	2.372115000000	-0.632046000000
C	1.105186000000	2.768593000000	-0.574884000000
C	2.768593000000	-1.105186000000	-0.574884000000
C	-1.105186000000	-2.768593000000	-0.574884000000
C	2.768593000000	1.105186000000	-0.574884000000
C	1.105186000000	-2.768593000000	-0.574884000000
C	-2.768593000000	-1.105186000000	-0.574884000000
C	-1.105186000000	2.768593000000	-0.574884000000
C	-2.768593000000	1.105186000000	-0.574884000000
C	0.677306000000	4.126877000000	-0.865184000000
C	4.126877000000	-0.677306000000	-0.865184000000
C	-0.677306000000	-4.126877000000	-0.865184000000
C	4.126877000000	0.677306000000	-0.865184000000
C	0.677306000000	-4.126877000000	-0.865184000000
C	-4.126877000000	-0.677306000000	-0.865184000000
C	-0.677306000000	4.126877000000	-0.865184000000
C	-4.126877000000	0.677306000000	-0.865184000000
H	1.353440000000	4.937114000000	-1.078960000000
H	4.937114000000	-1.353440000000	-1.078960000000
H	-1.353440000000	-4.937114000000	-1.078960000000
H	4.937114000000	1.353440000000	-1.078960000000
H	1.353440000000	-4.937114000000	-1.078960000000
H	-4.937114000000	-1.353440000000	-1.078960000000
H	-1.353440000000	4.937114000000	-1.078960000000
H	-4.937114000000	1.353440000000	-1.078960000000
Lu	0.000000000000	0.000000000000	0.716089000000
Cl	0.000000000000	0.000000000000	3.208314000000

Cartesian coordinates of YClTTDPz optimized B3LYP/pcseg-2 level of theory:

N	0.000000000000	2.051700000000	0.058178000000
N	-2.051700000000	0.000000000000	0.058178000000
N	0.000000000000	-2.051700000000	0.058178000000
N	2.051700000000	0.000000000000	0.058178000000
N	-2.390747000000	2.390747000000	-0.156747000000
N	-2.390747000000	-2.390747000000	-0.156747000000
N	2.390747000000	-2.390747000000	-0.156747000000
N	2.390747000000	2.390747000000	-0.156747000000
C	1.139914000000	2.806802000000	-0.117198000000
C	-2.806802000000	1.139914000000	-0.117198000000
C	-1.139914000000	-2.806802000000	-0.117198000000
C	-2.806802000000	-1.139914000000	-0.117198000000
C	1.139914000000	-2.806802000000	-0.117198000000
C	2.806802000000	1.139914000000	-0.117198000000
C	-1.139914000000	2.806802000000	-0.117198000000
C	2.806802000000	-1.139914000000	-0.117198000000
C	-0.710892000000	4.181178000000	-0.346152000000
C	-4.181178000000	-0.710892000000	-0.346152000000
C	0.710892000000	-4.181178000000	-0.346152000000
C	-4.181178000000	0.710892000000	-0.346152000000
C	-0.710892000000	-4.181178000000	-0.346152000000
C	4.181178000000	-0.710892000000	-0.346152000000
C	0.710892000000	4.181178000000	-0.346152000000
C	4.181178000000	0.710892000000	-0.346152000000
N	1.261767000000	5.355725000000	-0.570618000000
N	-5.355725000000	1.261767000000	-0.570618000000
N	-1.261767000000	-5.355725000000	-0.570618000000
N	-5.355725000000	-1.261767000000	-0.570618000000
N	1.261767000000	-5.355725000000	-0.570618000000
N	5.355725000000	1.261767000000	-0.570618000000
N	-1.261767000000	5.355725000000	-0.570618000000
N	5.355725000000	-1.261767000000	-0.570618000000
S	0.000000000000	6.389954000000	-0.759840000000
S	-6.389954000000	0.000000000000	-0.759840000000
S	0.000000000000	-6.389954000000	-0.759840000000
S	6.389954000000	0.000000000000	-0.759840000000
Y	0.000000000000	0.000000000000	1.127579000000
Cl	0.000000000000	0.000000000000	3.624089000000

Cartesian coordinates of LaClTTDPz optimized B3LYP/pcseg-2 level of theory:

N	0.000000000000	2.068301000000	0.011564000000
N	-2.068301000000	0.000000000000	0.011564000000
N	0.000000000000	-2.068301000000	0.011564000000
N	2.068301000000	0.000000000000	0.011564000000
N	-2.389442000000	2.389442000000	-0.251569000000
N	-2.389442000000	-2.389442000000	-0.251569000000
N	2.389442000000	-2.389442000000	-0.251569000000
N	2.389442000000	2.389442000000	-0.251569000000
C	1.139075000000	2.810705000000	-0.206125000000
C	-2.810705000000	1.139075000000	-0.206125000000
C	-1.139075000000	-2.810705000000	-0.206125000000
C	-2.810705000000	-1.139075000000	-0.206125000000

C	1.139075000000	-2.810705000000	-0.206125000000
C	2.810705000000	1.139075000000	-0.206125000000
C	-1.139075000000	2.810705000000	-0.206125000000
C	2.810705000000	-1.139075000000	-0.206125000000
C	-0.711225000000	4.176340000000	-0.493377000000
C	-4.176340000000	-0.711225000000	-0.493377000000
C	0.711225000000	-4.176340000000	-0.493377000000
C	-4.176340000000	0.711225000000	-0.493377000000
C	-0.711225000000	-4.176340000000	-0.493377000000
C	4.176340000000	-0.711225000000	-0.493377000000
C	0.711225000000	4.176340000000	-0.493377000000
C	4.176340000000	0.711225000000	-0.493377000000
N	1.261874000000	5.338538000000	-0.773498000000
N	-5.338538000000	1.261874000000	-0.773498000000
N	-1.261874000000	-5.338538000000	-0.773498000000
N	-5.338538000000	-1.261874000000	-0.773498000000
N	1.261874000000	-5.338538000000	-0.773498000000
N	5.338538000000	1.261874000000	-0.773498000000
N	-1.261874000000	5.338538000000	-0.773498000000
N	5.338538000000	-1.261874000000	-0.773498000000
S	0.000000000000	6.363860000000	-1.010597000000
S	-6.363860000000	0.000000000000	-1.010597000000
S	0.000000000000	-6.363860000000	-1.010597000000
S	6.363860000000	0.000000000000	-1.010597000000
La	0.000000000000	0.000000000000	1.388401000000
Cl	0.000000000000	0.000000000000	4.067734000000

Cartesian coordinates of LuClTTDPz optimized B3LYP/pcseg-2 level of theory:

N	0.000000000000	2.048312000000	-0.045052000000
N	-2.048312000000	0.000000000000	-0.045052000000
N	0.000000000000	-2.048312000000	-0.045052000000
N	2.048312000000	0.000000000000	-0.045052000000
N	-2.391057000000	2.391057000000	-0.248271000000
N	-2.391057000000	-2.391057000000	-0.248271000000
N	2.391057000000	-2.391057000000	-0.248271000000
N	2.391057000000	2.391057000000	-0.248271000000
C	1.140162000000	2.806151000000	-0.210129000000
C	-2.806151000000	1.140162000000	-0.210129000000
C	-1.140162000000	-2.806151000000	-0.210129000000
C	-2.806151000000	-1.140162000000	-0.210129000000
C	1.140162000000	-2.806151000000	-0.210129000000
C	2.806151000000	1.140162000000	-0.210129000000
C	-1.140162000000	2.806151000000	-0.210129000000
C	2.806151000000	-1.140162000000	-0.210129000000
C	-0.710843000000	4.182099000000	-0.426204000000
C	-4.182099000000	-0.710843000000	-0.426204000000
C	0.710843000000	-4.182099000000	-0.426204000000
C	-4.182099000000	0.710843000000	-0.426204000000
C	-0.710843000000	-4.182099000000	-0.426204000000
C	4.182099000000	-0.710843000000	-0.426204000000
C	0.710843000000	4.182099000000	-0.426204000000
C	4.182099000000	0.710843000000	-0.426204000000
N	1.261746000000	5.358993000000	-0.638377000000
N	-5.358993000000	1.261746000000	-0.638377000000
N	-1.261746000000	-5.358993000000	-0.638377000000

N	-5.358993000000	-1.261746000000	-0.638377000000
N	1.261746000000	-5.358993000000	-0.638377000000
N	5.358993000000	1.261746000000	-0.638377000000
N	-1.261746000000	5.358993000000	-0.638377000000
N	5.358993000000	-1.261746000000	-0.638377000000
S	0.000000000000	6.394917000000	-0.817002000000
S	-6.394917000000	0.000000000000	-0.817002000000
S	0.000000000000	-6.394917000000	-0.817002000000
S	6.394917000000	0.000000000000	-0.817002000000
Lu	0.000000000000	0.000000000000	0.964277000000
Cl	0.000000000000	0.000000000000	3.431209000000

Table S1. Bond lengths and topological parameters of ρ(r) in bond critical points of the MClPz.

Interaction	r_e (Å)	ρ (a.u.)	$\nabla^2\rho$ (a.u.)	λ_1	λ_2	λ_3	ε	G_b(a.u.)	V_b(a.u.)	H_b(a.u.)	q(A|B)	δ(A|B)
YClPz												
***r*(N$_m$-C$_\alpha$)**	1.329	0.357	-1.263	-0.865	-0.751	0.353	0.151	0.227	-0.771	0.543	0.560	1.243
***r*(N$_p$-C$_\alpha$)**	1.370	0.331	-1.056	-0.771	-0.681	0.396	0.132	0.175	-0.614	0.439	0.421	1.131
***r*(Np-Y)**	2.291	0.069	0.205	-0.098	-0.083	0.385	0.180	0.062	-0.073	0.011	0.348	0.349
***r*(La–Cl)**	2.523	0.060	0.170	-0.058	-0.058	0.286	0.000	0.053	-0.064	0.011	0.779	0.536
***r*(C–H)**	1.077	0.297	-1.228	-0.838	-0.828	0.438	0.012	0.041	-0.389	0.348	0.038	0.964
***r*(C$_\beta$–C$_\beta$)**	1.355	0.341	-0.993	-0.766	-0.612	0.385	0.252	0.130	-0.508	0.378	0.000	1.594
***r*(C$_\alpha$–C$_\beta$)**	1.454	0.288	-0.774	-0.621	-0.545	0.391	0.140	0.080	-0.353	0.273	0.054	1.068
LaClPz												
***r*(N$_m$-C$_\alpha$)**	1.330	0.355	-1.254	-0.861	-0.747	0.353	0.151	0.226	-0.766	0.540	0.562	1.242
***r*(N$_p$-C$_\alpha$)**	1.369	0.332	-1.059	-0.774	-0.683	0.398	0.133	0.175	-0.616	0.440	0.412	1.137
***r*(N$_p$-La)**	2.461	0.063	0.160	-0.078	-0.066	0.304	0.182	0.049	-0.059	0.010	0.356	0.366
***r*(La–Cl)**	2.711	0.054	0.135	-0.045	-0.045	0.225	0.000	0.042	-0.050	0.008	0.793	0.564
***r*(C–H)**	1.077	0.297	-1.226	-0.837	-0.827	0.438	0.013	0.041	-0.388	0.347	0.036	0.964
***r*(C$_\beta$–C$_\beta$)**	1.354	0.341	-0.993	-0.766	-0.612	0.385	0.253	0.130	-0.509	0.378	0.000	1.597
***r*(C$_\alpha$–C$_\beta$)**	1.456	0.287	-0.768	-0.617	-0.542	0.391	0.140	0.079	-0.351	0.271	0.050	1.065
LuClPz												
***r*(N$_m$-C$_\alpha$)**	1.329	0.357	-1.265	-0.866	-0.752	0.353	0.151	0.228	-0.772	0.544	0.560	1.244
***r*(N$_p$-C$_\alpha$)**	1.370	0.330	-1.055	-0.771	-0.681	0.397	0.132	0.175	-0.614	0.439	0.423	1.128
***r*(Np-Lu)**	2.260	0.075	0.235	-0.108	-0.093	0.436	0.158	0.060	-0.071	0.011	0.340	0.357
***r*(La–Cl)**	2.493	0.065	0.187	-0.065	-0.065	0.316	0.000	0.051	-0.063	0.012	0.763	0.552
***r*(C–H)**	1.077	0.297	-1.228	-0.838	-0.828	0.438	0.012	0.041	-0.389	0.348	0.038	0.964
***r*(C$_\beta$–C$_\beta$)**	1.355	0.341	-0.992	-0.765	-0.612	0.385	0.251	0.130	-0.508	0.378	0.000	1.593
***r*(C$_\alpha$–C$_\beta$)**	1.454	0.289	-0.775	-0.621	-0.545	0.392	0.140	0.080	-0.354	0.274	0.055	1.069

Table S2. Bond lengths and topological parameters of ρ(r) in bond critical points of the MClTTDPz.

Interaction	r_e (Å)	ρ (a.u.)	$\nabla^2\rho$ (a.u.)	λ_1	λ_2	λ_3	ε	G_b(a.u.)	V_b(a.u.)	H_b(a.u.)	q(A|B)	δ(A|B)
YClTTDPz												
***r*(N$_m$-C$_\alpha$)**	1.319	0.361	-1.176	-0.840	-0.724	0.388	0.160	0.295	-0.883	0.589	0.522	1.259
***r*(N$_t$–C$_\beta$)**	1.317	0.361	-1.176	-0.840	-0.724	0.388	0.160	0.295	-0.883	0.589	0.522	1.350
***r*(N$_p$-C$_\alpha$)**	1.379	0.323	-1.000	-0.747	-0.652	0.399	0.147	0.172	-0.593	0.422	0.405	1.130
***r*(Np-La)**	2.313	0.066	0.193	-0.092	-0.079	0.364	0.173	0.058	-0.068	0.010	0.354	0.337
***r*(Y–Cl)**	2.497	0.064	0.176	-0.063	-0.063	0.301	0.000	0.057	-0.070	0.013	0.757	0.574
***r*(C$_\beta$–C$_\beta$)**	1.422	0.312	-0.866	-0.691	-0.589	0.414	0.174	0.096	-0.408	0.312	0.000	1.093
***r*(C$_\alpha$–C$_\beta$)**	1.458	0.286	-0.768	-0.619	-0.540	0.391	0.145	0.076	-0.344	0.268	0.004	1.008
***r*(N$_t$-S)**	1.643	0.235	-0.342	-0.375	-0.277	0.310	0.355	0.180	-0.445	0.265	0.615	1.308
LaClTTDPz												
***r*(N$_m$-C$_\alpha$)**	1.320	0.361	-1.277	-0.877	-0.749	0.350	0.171	0.242	-0.804	0.561	0.562	1.258
***r*(N$_t$–C$_\beta$)**	1.316	0.361	-1.176	-0.841	-0.724	0.389	0.161	0.296	-0.886	0.590	0.526	1.352
***r*(N$_p$-C$_\alpha$)**	1.377	0.324	-1.006	-0.751	-0.654	0.400	0.148	0.173	-0.597	0.424	0.395	1.137
***r*(Np-La)**	2.486	0.061	0.152	-0.074	-0.063	0.289	0.179	0.047	-0.056	0.009	0.362	0.353
***r*(La–Cl)**	2.680	0.058	0.140	-0.049	-0.049	0.238	0.000	0.045	-0.055	0.010	0.770	0.606
***r*(C$_\beta$–C$_\beta$)**	1.423	0.311	-0.864	-0.690	-0.588	0.414	0.174	0.095	-0.407	0.311	0.000	1.092
***r*(C$_\alpha$–C$_\beta$)**	1.460	0.284	-0.762	-0.615	-0.537	0.390	0.145	0.075	-0.342	0.266	0.001	1.006
***r*(N$_t$-S)**	1.644	0.235	-0.344	-0.375	-0.276	0.307	0.355	0.179	-0.443	0.264	0.611	1.307
LuClTTDPz												
***r*(N$_m$-C$_\alpha$)**	1.319	0.363	-1.289	-0.884	-0.755	0.350	0.170	0.245	-0.811	0.567	0.562	1.260
***r*(N$_t$–C$_\beta$)**	1.317	0.361	-1.176	-0.840	-0.724	0.387	0.160	0.294	-0.883	0.588	0.521	1.349
***r*(N$_p$-C$_\alpha$)**	1.379	0.323	-0.998	-0.747	-0.651	0.400	0.147	0.171	-0.592	0.421	0.406	1.128
***r*(N$_p$-Lu)**	2.284	0.072	0.221	-0.102	-0.088	0.411	0.152	0.056	-0.066	0.010	0.347	0.346
***r*(La–Cl)**	2.468	0.069	0.195	-0.070	-0.070	0.334	0.000	0.054	-0.068	0.014	0.740	0.588
***r*(C$_\beta$–C$_\beta$)**	1.422	0.312	-0.866	-0.691	-0.589	0.414	0.174	0.096	-0.408	0.312	0.000	1.093
***r*(C$_\alpha$–C$_\beta$)**	1.458	0.286	-0.770	-0.620	-0.541	0.391	0.145	0.076	-0.344	0.268	0.005	1.008
***r*(N$_t$-S)**	1.643	0.235	-0.342	-0.376	-0.277	0.310	0.355	0.180	-0.445	0.265	0.615	1.308

Table S3. Charge on atoms in MClPz and MClTTDPz

YClPz

Name	C_β	C_α	H	N_p	N_m	Y	Cl	On ligand
q(A)	+0.0166	+0.928	+0.038	-1.191	-1.121	+2.171	-0.779	-1.391

LaClPz

Name	C_β	C_α	H	N_p	N_m	La	Cl	On ligand
q(A)	+0.14	+0.92	+0.36	-1.179	-1.123	+2.21	-0.793	-1.423

LuClPz

Name	C_β	C_α	H	N_p	N_m	Lu	Cl	On ligand
q(A)	+0.017	+0.929	+0.038	-1.187	-1.121	+2.125	-0.763	-1.362

YClTTDPz

Name	C_β	C_α	N_p	N_m	Y	Cl	S	N_t	On ligand
q(A)	+0.526	+0.963	-1.164	-1.124	+2.173	-0.757	+1.23	-1.137	-1.416

LaClTTDPz

Name	C_β	C_α	N_p	N_m	La	Cl	S	N_t	On ligand
q(A)	+0.525	+0.958	-1.153	-1.125	+2.218	-0.77	+1.223	-1.137	-1.447

LuClTTDPz

Name	C_β	C_α	N_p	N_m	Lu	Cl	S	N_t	On ligand
q(A)	+0.526	+0.963	-1.16	-1.123	+2.127	-0.74	+1.231	-1.137	-1.386