Supporting information for

«DFT Study of molecular and electronic structure of Ca(II) and Zn(II) complexes with porphyrazine and tetrakis(1,2,5-thiadiazole)porphyrazine»

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Contents:

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

N	-0.092626000000	2.001736000000	0.182671000000
N	-2.001736000000	-0.092626000000	0.182671000000
N	0.092626000000	-2.001736000000	0.182671000000
N	2.001736000000	0.092626000000	0.182671000000
N	2.259202000000	2.478426000000	-0.123037000000
N	-2.478426000000	2.259202000000	-0.123037000000
N	-2.259202000000	-2.478426000000	-0.123037000000
N	2.478426000000	-2.259202000000	-0.123037000000
C	0.972044000000	2.817835000000	-0.063189000000
C	-2.817835000000	0.972044000000	-0.063189000000
C	-0.972044000000	-2.817835000000	-0.063189000000
C	2.716027000000	1.228113000000	-0.063189000000
C	-1.228113000000	2.716027000000	-0.063189000000
C	-2.716027000000	-1.228113000000	-0.063189000000
C	1.228113000000	-2.716027000000	-0.063189000000
C	2.817835000000	-0.972044000000	-0.063189000000
C	0.485706000000	4.153000000000	-0.391589000000
C	-4.153000000000	0.485706000000	-0.391589000000
C	-0.485706000000	-4.153000000000	-0.391589000000
C	4.090399000000	0.867152000000	-0.391589000000
C	-0.867152000000	4.090399000000	-0.391589000000
C	-4.090399000000	-0.867152000000	-0.391589000000
C	0.867152000000	-4.090399000000	-0.391589000000
C	4.153000000000	-0.485706000000	-0.391589000000
H	1.123852000000	4.985879000000	-0.634781000000
H	-4.985879000000	1.123852000000	-0.634781000000
H	-1.123852000000	-4.985879000000	-0.634781000000
H	4.860788000000	1.579486000000	-0.634781000000
H	-1.579486000000	4.860788000000	-0.634781000000
H	4.860788000000	-1.579486000000	-0.634781000000
H	1.579486000000	-4.860788000000	-0.634781000000
H	4.985879000000	-1.123852000000	-0.634781000000
Ca	0.000000000000	0.000000000000	1.261894000000

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

N	-0.974056000000	1.815121000000	0.364154000000
N	-1.815121000000	-0.974056000000	0.364154000000
N	0.974056000000	-1.815121000000	0.364154000000
N	1.815121000000	0.974056000000	0.364154000000
N	-3.236805000000	0.976045000000	0.143599000000
N	-0.976045000000	-3.236805000000	0.143599000000
N	3.236805000000	-0.976045000000	0.143599000000
N	0.976045000000	3.236805000000	0.143599000000
C	-2.329072000000	1.936326000000	0.181263000000
C	-1.936326000000	-2.329072000000	0.181263000000
C	2.329072000000	-1.936326000000	0.181263000000
C	3.011259000000	0.325973000000	0.181263000000
C	-0.325973000000	3.011259000000	0.181263000000
C	-3.011259000000	-0.325973000000	0.181263000000
C	0.325973000000	-3.011259000000	0.181263000000
C	1.936326000000	2.329072000000	0.181263000000
C	-2.606418000000	3.351210000000	-0.060310000000
C	-3.351210000000	-2.606418000000	-0.060310000000
C	2.606418000000	-3.351210000000	-0.060310000000
C	4.024552000000	1.351670000000	-0.060310000000

C	-1.351670000000	4.024552000000	-0.060310000000
C	-4.024552000000	-1.351670000000	-0.060310000000
C	1.351670000000	-4.024552000000	-0.060310000000
C	3.351210000000	2.606418000000	-0.060310000000
N	-3.645851000000	4.123839000000	-0.291749000000
N	-4.123839000000	-3.645851000000	-0.291749000000
N	3.645851000000	-4.123839000000	-0.291749000000
N	5.317836000000	1.420879000000	-0.291749000000
N	-1.420879000000	5.317836000000	-0.291749000000
N	-5.317836000000	-1.420879000000	-0.291749000000
N	1.420879000000	-5.317836000000	-0.291749000000
N	4.123839000000	3.645851000000	-0.291749000000
S	-3.023204000000	5.633637000000	-0.490092000000
S	-5.633637000000	-3.023204000000	-0.490092000000
S	3.023204000000	-5.633637000000	-0.490092000000
S	5.633637000000	3.023204000000	-0.490092000000
Ca	0.000000000000	0.000000000000	1.384053000000

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

N	0.000000000000	1.978859000000	0.000000000000
N	-1.978859000000	0.000000000000	0.000000000000
N	0.000000000000	-1.978859000000	0.000000000000
N	1.978859000000	0.000000000000	0.000000000000
N	2.379067000000	2.379067000000	0.000000000000
N	-2.379067000000	2.379067000000	0.000000000000
N	-2.379067000000	-2.379067000000	0.000000000000
N	2.379067000000	-2.379067000000	0.000000000000
C	1.108009000000	2.772569000000	0.000000000000
C	-2.772569000000	1.108009000000	0.000000000000
C	-1.108009000000	-2.772569000000	0.000000000000
C	2.772569000000	1.108009000000	0.000000000000
C	-1.108009000000	2.772569000000	0.000000000000
C	-2.772569000000	-1.108009000000	0.000000000000
C	1.108009000000	-2.772569000000	0.000000000000
C	2.772569000000	-1.108009000000	0.000000000000
C	0.677767000000	4.164526000000	0.000000000000
C	-4.164526000000	0.677767000000	0.000000000000
C	-0.677767000000	-4.164526000000	0.000000000000
C	4.164526000000	0.677767000000	0.000000000000
C	-0.677767000000	4.164526000000	0.000000000000
C	-4.164526000000	-0.677767000000	0.000000000000
C	0.677767000000	-4.164526000000	0.000000000000
C	4.164526000000	-0.677767000000	0.000000000000
H	1.351226000000	5.004849000000	0.000000000000
H	-5.004849000000	1.351226000000	0.000000000000
H	-1.351226000000	-5.004849000000	0.000000000000
H	5.004849000000	1.351226000000	0.000000000000
H	-1.351226000000	5.004849000000	0.000000000000
H	-5.004849000000	-1.351226000000	0.000000000000
H	1.351226000000	-5.004849000000	0.000000000000
H	5.004849000000	-1.351226000000	0.000000000000
Zn	0.000000000000	0.000000000000	0.000000000000

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

N	0.000000000000	2.024496000000	0.000000000000
N	-2.024496000000	0.000000000000	0.000000000000
N	0.000000000000	-2.024496000000	0.000000000000
N	2.024496000000	0.000000000000	0.000000000000
N	-2.391263000000	2.391263000000	0.000000000000
N	-2.391263000000	-2.391263000000	0.000000000000
N	2.391263000000	-2.391263000000	0.000000000000
N	2.391263000000	2.391263000000	0.000000000000
C	-1.137996000000	2.796116000000	0.000000000000
C	-2.796116000000	-1.137996000000	0.000000000000
C	1.137996000000	-2.796116000000	0.000000000000
C	2.796116000000	-1.137996000000	0.000000000000
C	1.137996000000	2.796116000000	0.000000000000
C	-2.796116000000	1.137996000000	0.000000000000
C	-1.137996000000	-2.796116000000	0.000000000000
C	2.796116000000	1.137996000000	0.000000000000
C	-0.710604000000	4.190394000000	0.000000000000
C	-4.190394000000	-0.710604000000	0.000000000000
C	0.710604000000	-4.190394000000	0.000000000000
C	4.190394000000	-0.710604000000	0.000000000000
C	0.710604000000	4.190394000000	0.000000000000
C	-4.190394000000	0.710604000000	0.000000000000
C	-0.710604000000	-4.190394000000	0.000000000000
C	4.190394000000	0.710604000000	0.000000000000
N	-1.262118000000	5.385704000000	0.000000000000
N	-5.385704000000	-1.262118000000	0.000000000000
N	1.262118000000	-5.385704000000	0.000000000000
N	5.385704000000	-1.262118000000	0.000000000000
N	1.262118000000	5.385704000000	0.000000000000
N	-5.385704000000	1.262118000000	0.000000000000
N	-1.262118000000	-5.385704000000	0.000000000000
N	5.385704000000	1.262118000000	0.000000000000
S	0.000000000000	6.438480000000	0.000000000000
S	-6.438480000000	0.000000000000	0.000000000000
S	0.000000000000	-6.438480000000	0.000000000000
S	6.438480000000	0.000000000000	0.000000000000
Zn	0.000000000000	0.000000000000	0.000000000000

Bond lengths and topological parameters of ρ(r) in bond critical points of the CaPz:

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.)	δ(A|B)
N_m-$C_{\alpha 1,2}$	1,332	0,354	-1,245	-0,856	-0,743	0,354	0,152	0,222	-0,756	0,534	1,240
N_p-$C_{\alpha 1,2}$	1,364	0,336	-1,085	-0,789	-0,695	0,398	0,135	0,178	-0,627	0,449	1,156
N_p–Ca	2,276	0,054	0,219	-0,075	-0,066	0,360	0,139	0,055	-0,055	0,000	0,270
$C_{\alpha 1,2}$-$C_{\beta 1,2}$	1,458	0,286	-0,759	-0,612	-0,538	0,391	0,139	0,078	-0,346	0,268	1,061
$C_{\beta 1,2}$-H	1,077	0,296	-1,215	-0,832	-0,821	0,437	0,014	0,042	-0,388	0,346	0,967
$C_{\beta 1}$-$C_{\beta 2}$	1,354	0,341	-0,990	-0,765	-0,609	0,384	0,256	0,130	-0,508	0,378	1,604

Bond lengths and topological parameters of ρ(r) in bond critical points of the ZnPz:

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,)	δ(A|B)
N_m-$C_{\alpha 1,2}$	1,331	0,356	-1,258	-0,863	-0,748	0,353	0,153	0,225	-0,764	0,539	1,243
N_p-$C_{\alpha 1,2}$	1,363	0,336	-1,100	-0,792	-0,696	0,387	0,138	0,184	-0,642	0,459	1,130
N_p–Zn	1,979	0,094	0,394	-0,131	-0,124	0,649	0,061	0,122	-0,146	0,024	0,464
$C_{\alpha 1,2}$-$C_{\beta 1,2}$	1,457	0,286	-0,764	-0,615	-0,540	0,391	0,138	0,079	-0,348	0,270	1,064
$C_{\beta 1,2}$-H	1,077	0,296	-1,222	-0,835	-0,824	0,437	0,013	0,041	-0,388	0,347	0,966
$C_{\beta 1}$-$C_{\beta 2}$	1,355	0,340	-0,986	-0,763	-0,607	0,385	0,256	0,130	-0,506	0,376	1,603

Bond lengths and topological parameters of ρ(r) in bond critical points of the CaTTDPz:

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,)	δ(A|B)
N_m-$C_{\alpha 1,2}$	1,322	0,360	-1,272	-0,875	-0,747	0,350	0,172	0,239	-0,796	0,557	1,256
N_p-$C_{\alpha 1,2}$	1,373	0,328	-1,030	-0,765	-0,665	0,400	0,150	0,175	-0,608	0,433	1,153
N_p–Ca	2,299	0,052	0,207	-0,071	-0,062	0,340	0,135	0,052	-0,052	0,000	0,262
$C_{\alpha 1,2}$-$C_{\beta 1,2}$	1,462	0,283	-0,756	-0,611	-0,535	0,390	0,143	0,075	-0,339	0,264	1,002
$C_{\beta 1,2}$–$N_{25\text{-}32}$	1,316	0,361	-1,172	-0,841	-0,724	0,393	0,161	0,299	-0,891	0,592	1,355
$C_{\beta 1}$-$C_{\beta 2}$	1,424	0,310	-0,860	-0,687	-0,586	0,414	0,172	0,095	-0,405	0,310	1,089
$N_{25\text{-}32}$–$S_{33\text{-}36}$	1,645	0,234	-0,347	-0,373	-0,275	0,301	0,354	0,176	-0,438	0,263	1,304

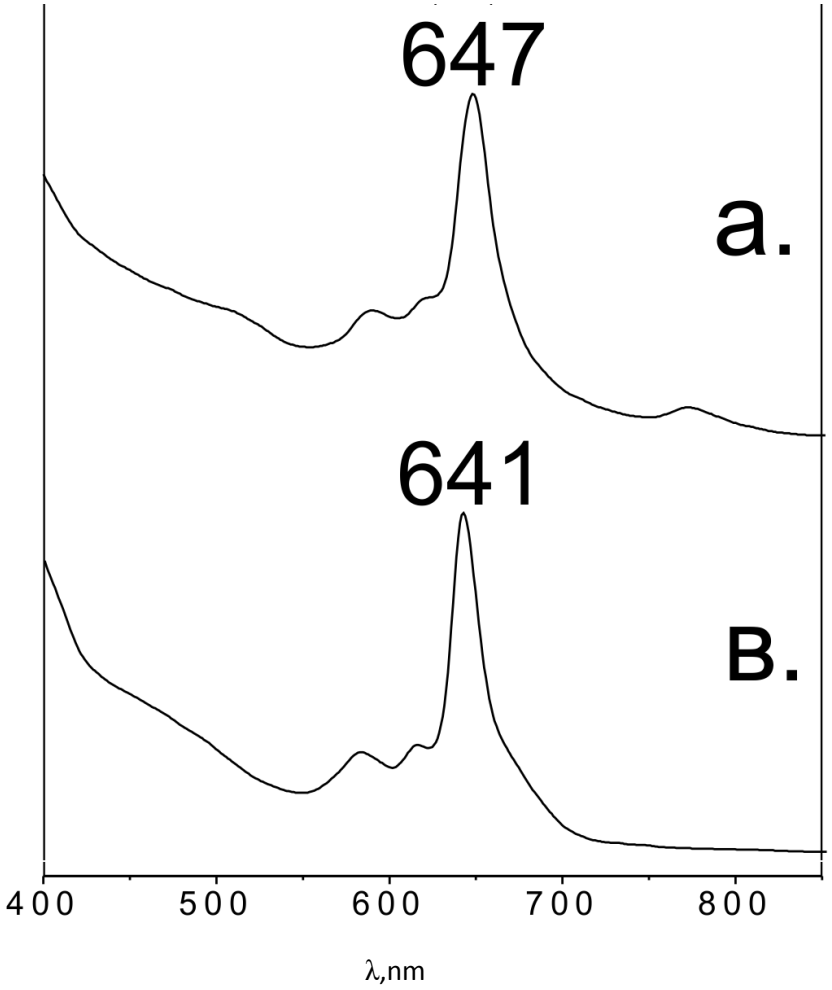
Bond lengths and topological parameters of ρ(r) in bond critical points of the ZnTTDPz:

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.)	δ(A|B)
N_m-$C_{\alpha 1,2}$	1,317	0,365	-1,303	-0,893	-0,761	0,350	0,173	0,247	-0,819	0,573	1,258
N_p-$C_{\alpha 1,2}$	1,375	0,326	-1,025	-0,760	-0,659	0,394	0,155	0,177	-0,610	0,433	1,127
N_p–Zn	2,024	0,085	0,339	-0,116	-0,109	0,564	0,059	0,105	-0,124	0,020	0,446
$C_{\alpha 1,2}$-$C_{\beta 1,2}$	1,458	0,285	-0,768	-0,618	-0,540	0,390	0,144	0,076	-0,343	0,268	1,006
$C_{\beta 1,2}$–N_{25-32}	1,316	0,361	-1,173	-0,839	-0,723	0,389	0,161	0,296	-0,885	0,589	1,352
$C_{\beta 1}$-$C_{\beta 2}$	1,421	0,312	-0,868	-0,692	-0,590	0,414	0,173	0,096	-0,409	0,313	1,093
N_{25-32}–S_{33-36}	1,643	0,365	-1,303	-0,893	-0,761	0,350	0,173	0,247	-0,819	0,573	1,258

Charge on atoms in CaPz, ZnPz, CaTTDPz and ZnTTDPz molecules:

Name	N_{1-4}	N_{5-8}	C_{17-24}	H_{25-32}	C_{9--16}	Ca_{33}	Zn_{33}
q(A) CaPz	-1,169	-1,127	+0,003	+0,025	+0,924	+1,564	-
q(A) ZnPz	-1,160	-1,119	0,010	0,032	0,940	-	1,255

	N_{1-4}	N_{25-32}	N_{5-8}	C_{17-24}	C_{9--16}	S_{33-36}	Ca_{37}	Zn_{37}
q(A) CaTTDPz	-1,143	-1,142	-1,127	+0,521	+0,960	+1,197	+1,580	-
q(A) ZnTTDPz	-1,123	-1,138	-1,128	0,523	0,975	1,215	-	1,258



Electronic absorption spectra of the CaTTDPz in pyridine (a), in acetone (в).