Supporting Information

Electronic and steric effects controlling monomer-dimer self-assembly in 6*H*-1,4-diazepinoporphyrazines: experimental and theoretical study

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Mass spectra

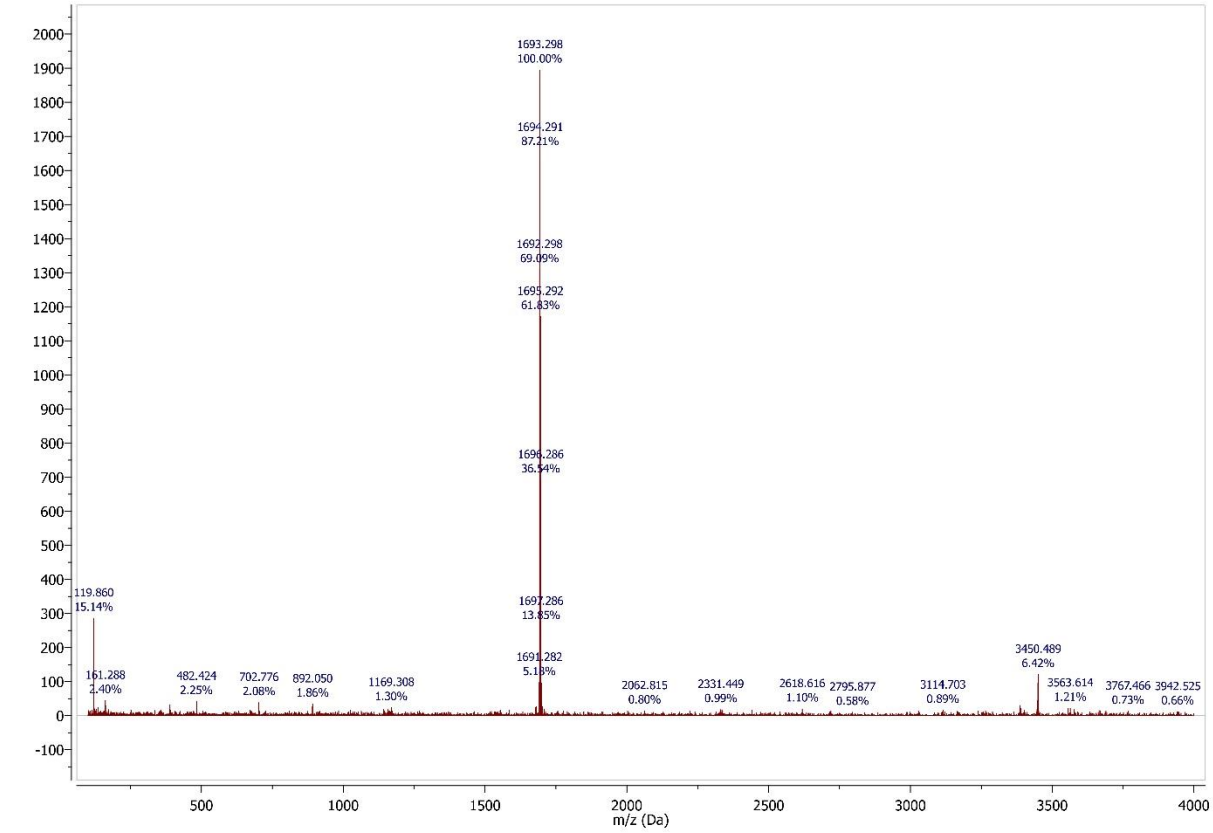

Fig. S1 MALDI-TOF mass spectrum of $^{t\text{Bu}}\text{Ph}_8\text{Dz}_4\text{PzNi}$.

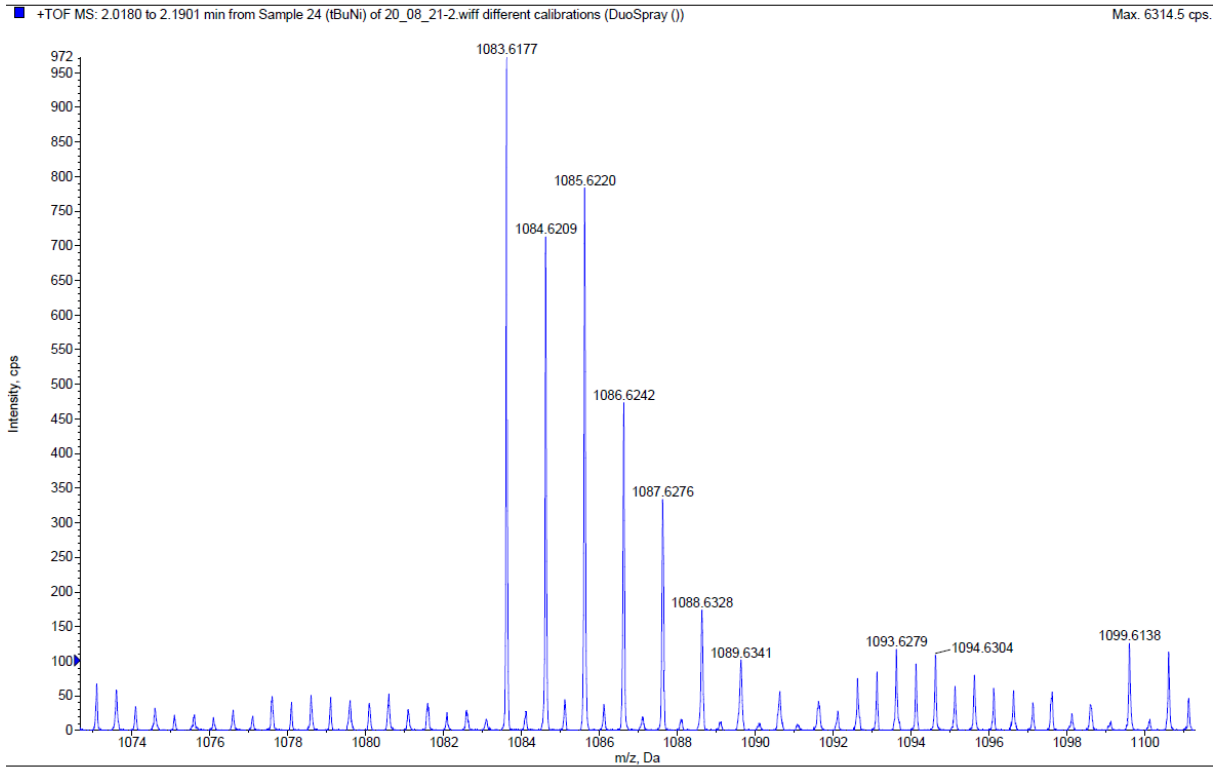

Fig. S2 High-resolution ESI-TOF mass spectrum of $t\text{Bu}_8\text{Dz}_4\text{PzNi}$.

NMR spectra

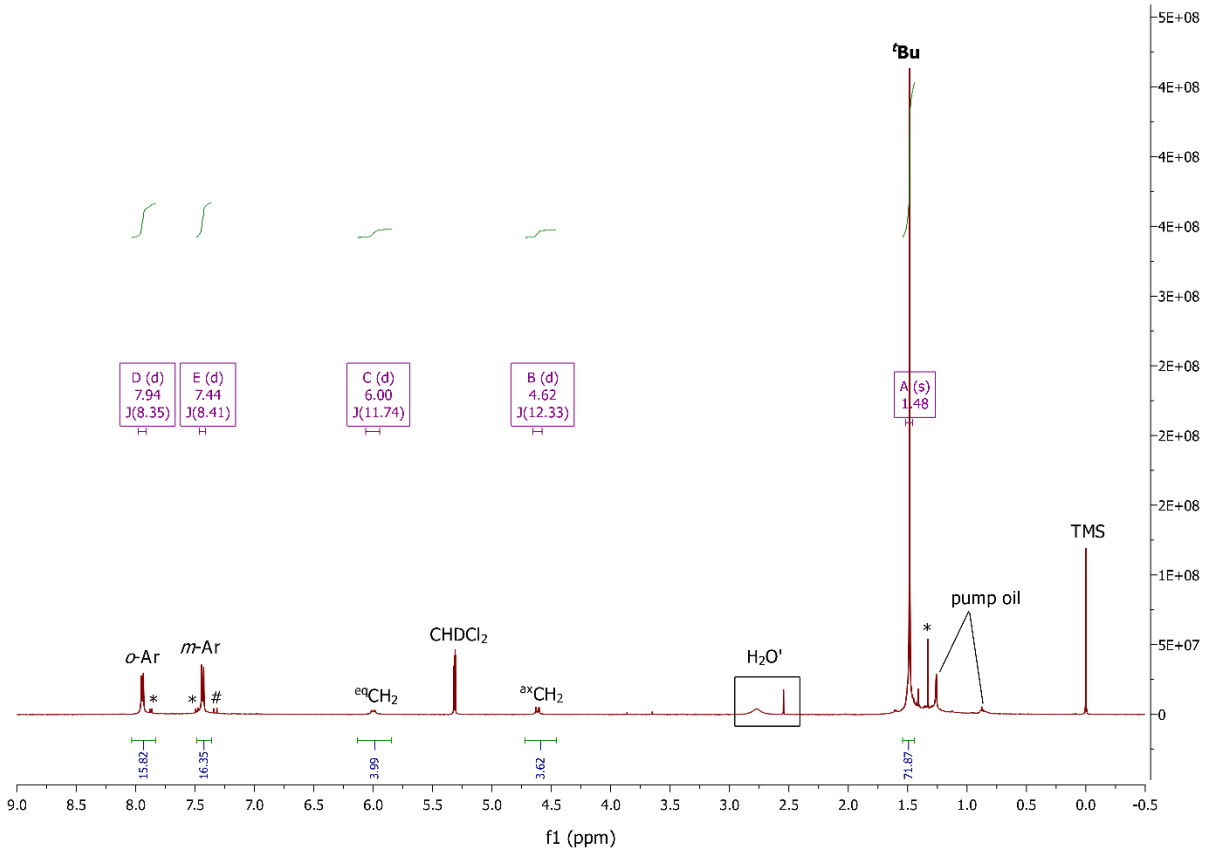

Fig. S3 ^{1}H NMR spectrum of $^{tBu}Ph_8Dz_4PzNi$ (CD_2Cl_2, 298 K). * ^{1}H NMR signals of the isomer of $^{tBu}Ph_8Dz_4PzNi$ resulting from imine-enamine tautomerization of 6*H*-1,4-diazepine heterocycle or that of the aggregated form of $^{tBu}Ph_8Dz_4PzNi$ dimer. # ^{1}H NMR signals of the trace impurities of chloroform (7.32 ppm) and benzene (7.35 ppm).[1] H_2O' designates the signals of water molecules included into the structure of $^{tBu}Ph_8Dz_4PzNi$ *via* HO–H···N^{Dz} hydrogen bonds.[2]

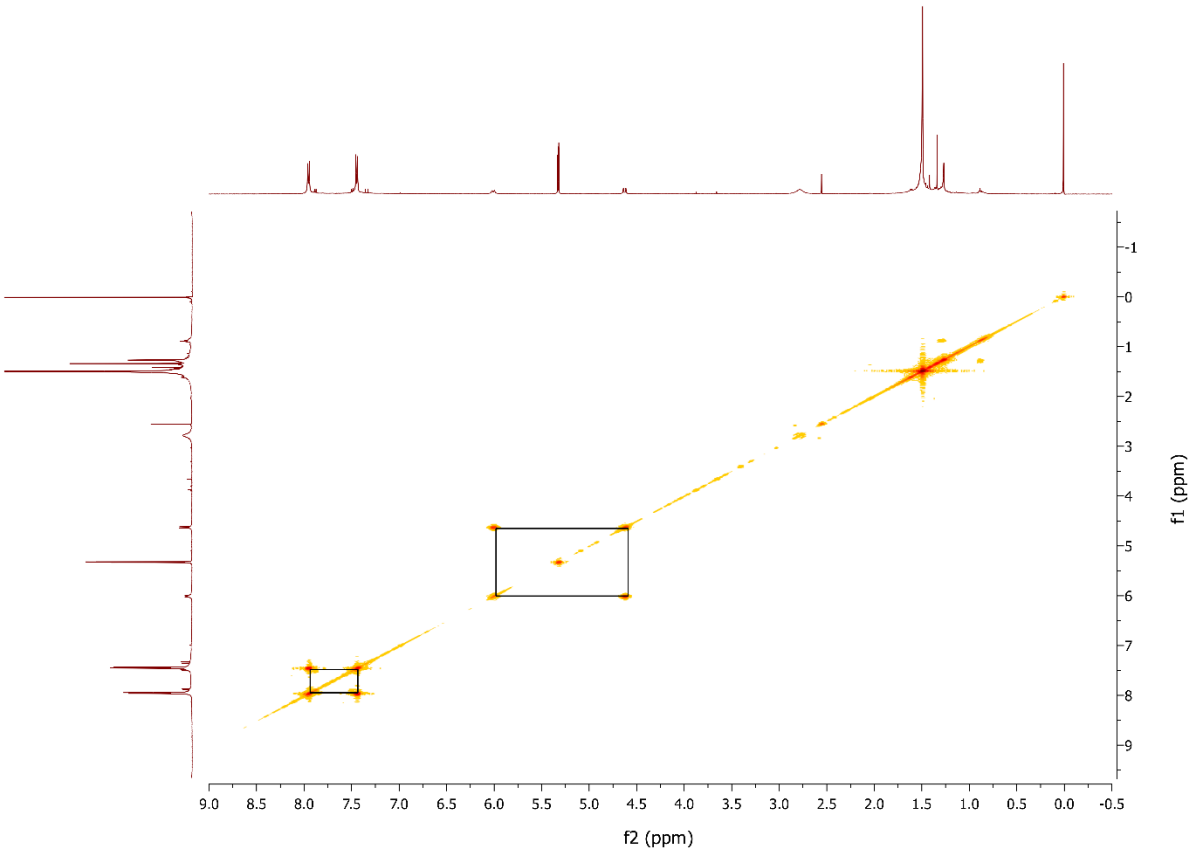

Fig. S4 ^{1}H-^{1}H COSY spectrum of $^{t\text{Bu}}Ph_8Dz_4PzNi$ (CD_2Cl_2, 298 K).

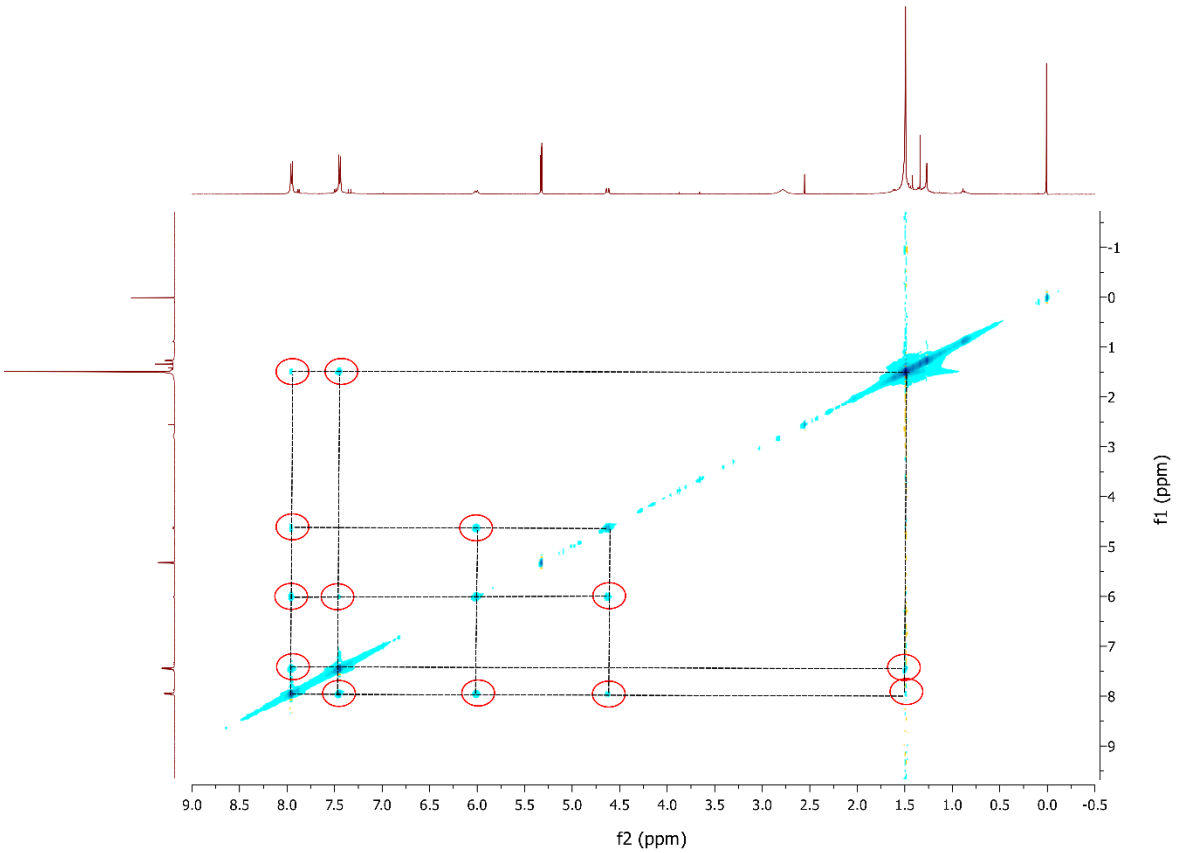

Fig. S5 ^{1}H-^{1}H NOESY spectrum of $^{t\text{Bu}}Ph_8Dz_4PzNi$ (CD_2Cl_2, 298 K).

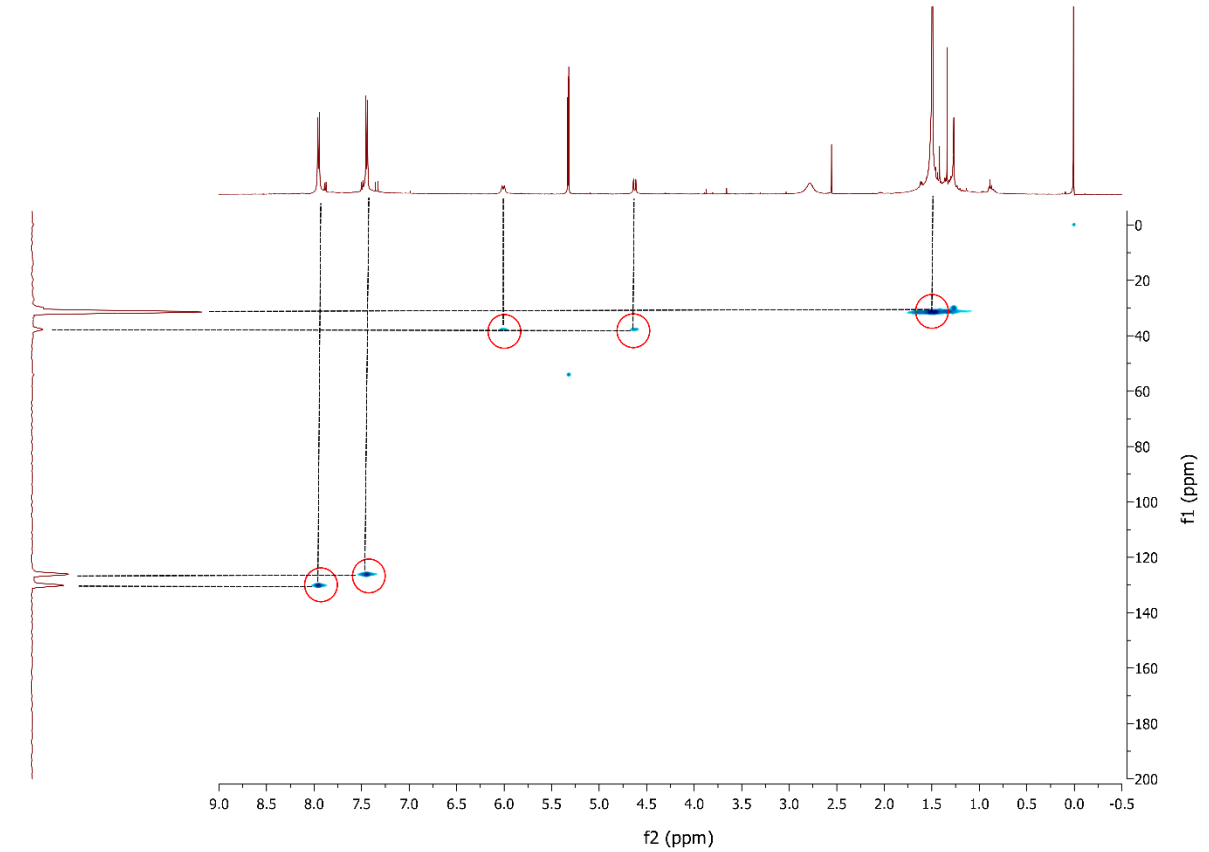

Fig. S6 ^{1}H-^{13}C HMQC spectrum of $^{t\text{Bu}}Ph_8Dz_4PzNi$ (CD_2Cl_2, 298 K).

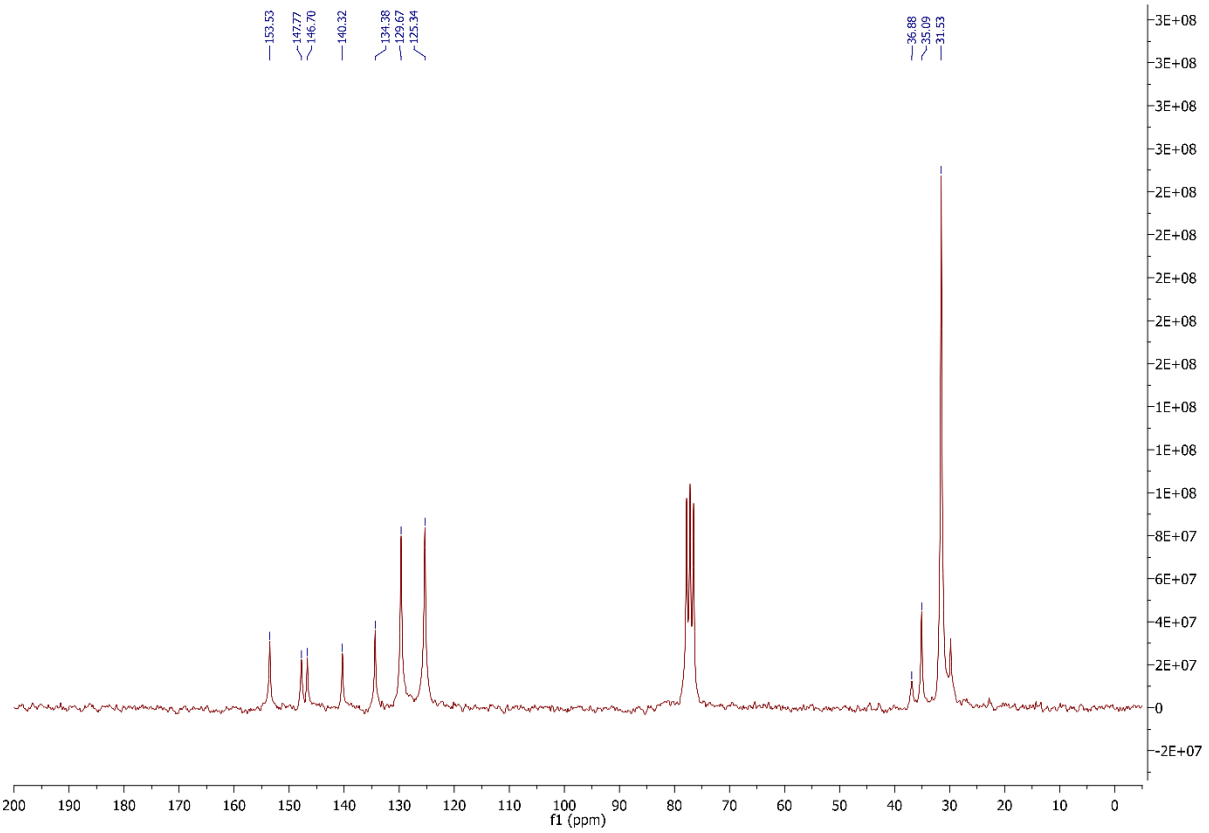

Fig. S7 ^{13}C NMR spectrum of $^{t\text{Bu}}Ph_8Dz_4PzNi$ ($CDCl_3$, 298 K).

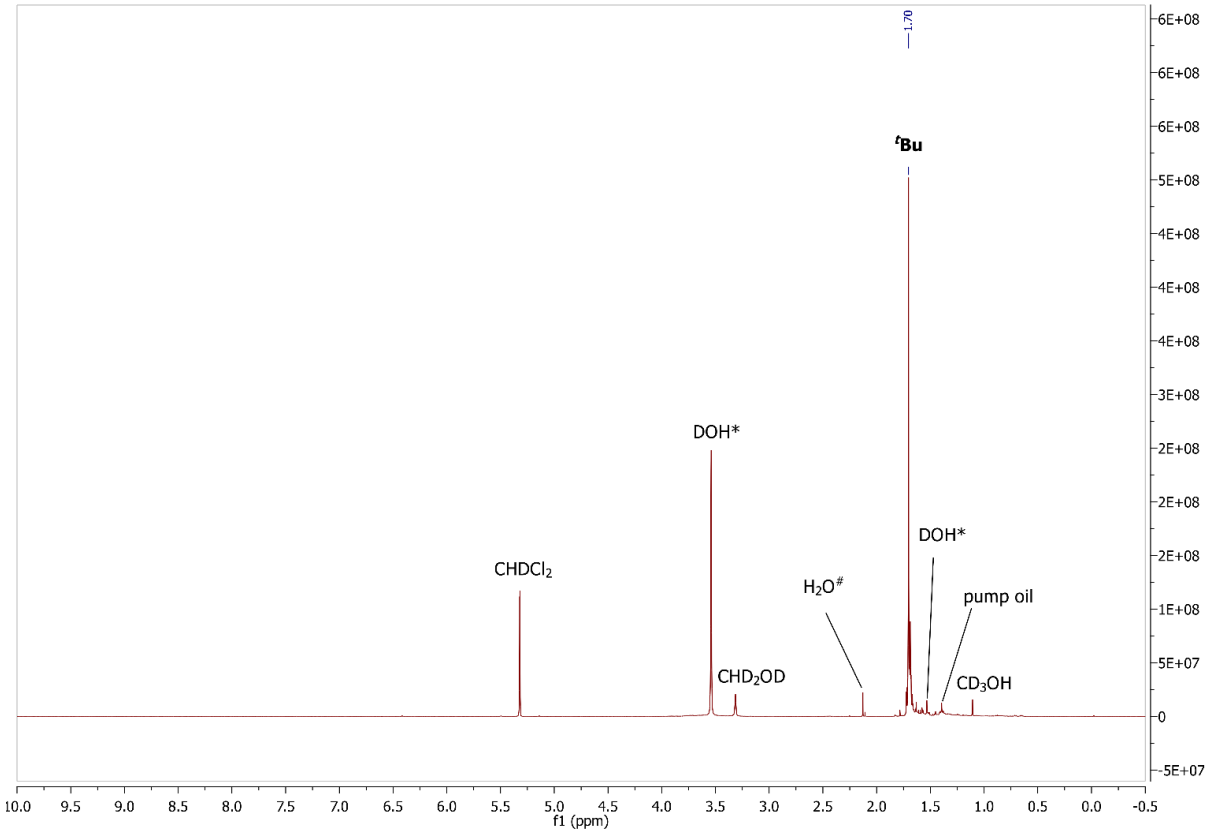

Fig. S7a ^{1}H NMR spectrum of *t*Bu$_8$Dz$_4$PzNi (CD_2Cl_2, 298 K). DOH* designates the signals of water surrounded by different solvation shells (CD_3OD or CD_2Cl_2). $H_2O^{\#}$ designates the signals of water molecules included into the structure of *t*Bu$_8$Dz$_4$PzNi *via* HO–H···N^{Dz} hydrogen bonds.[2]

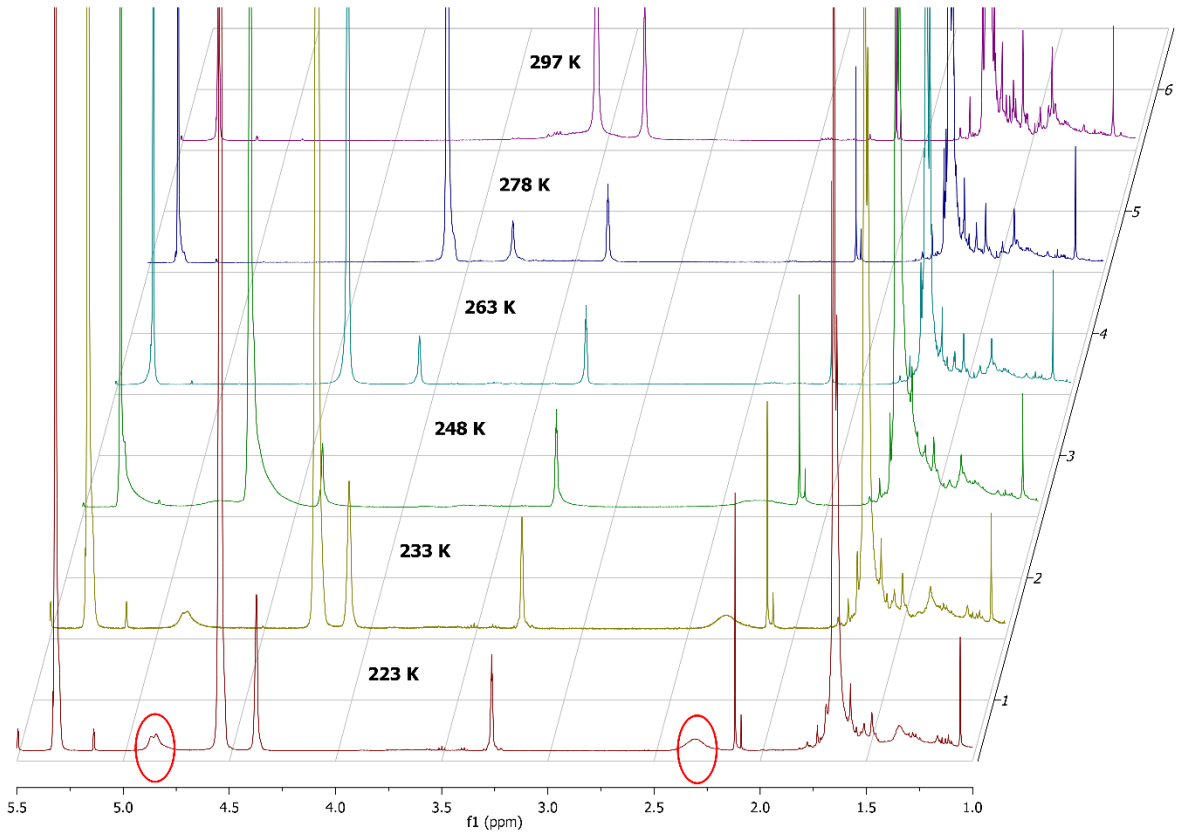

Fig. S8 Temperature dependence of the ^{1}H NMR spectra of *t*Bu$_8$Dz$_4$PzNi (CD_2Cl_2).

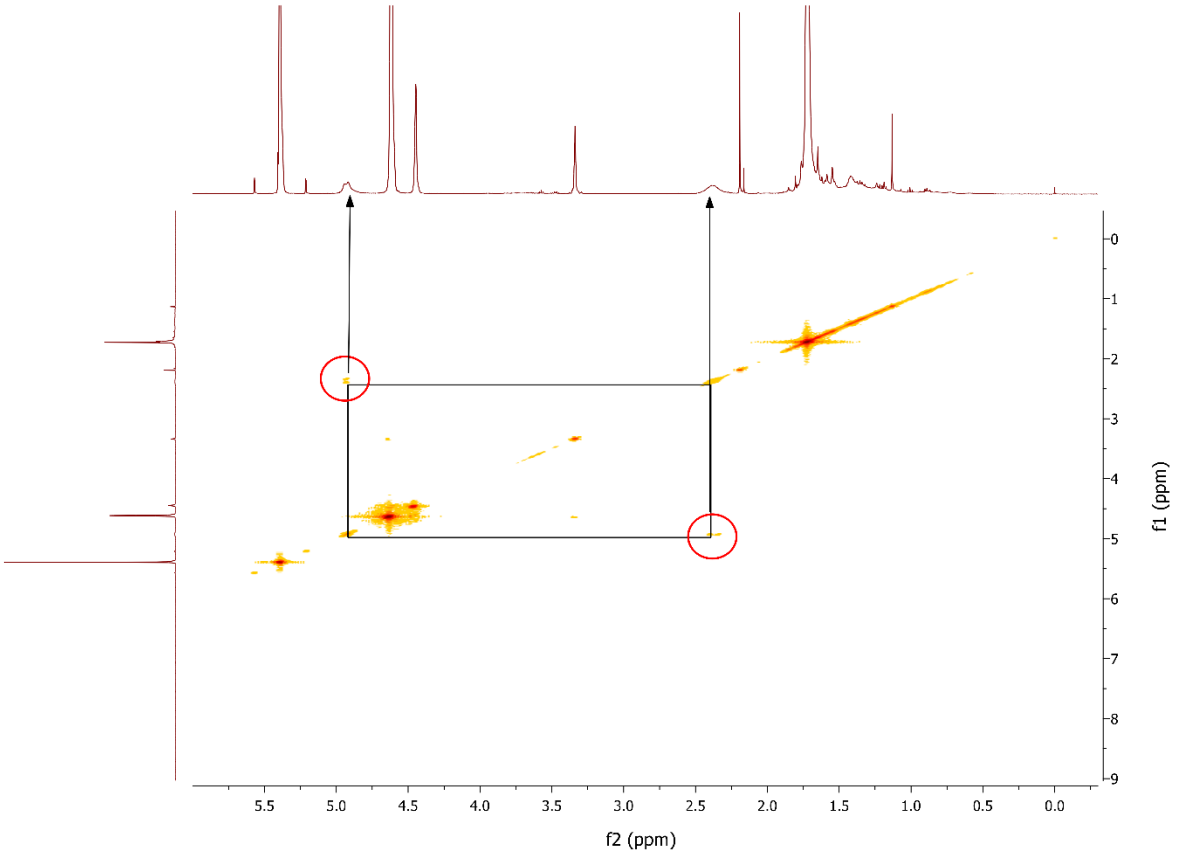

Fig. S9 ^{1}H-^{1}H COSY spectrum of *t*Bu$_8$Dz$_4$PzNi (CD_2Cl_2, 223 K).

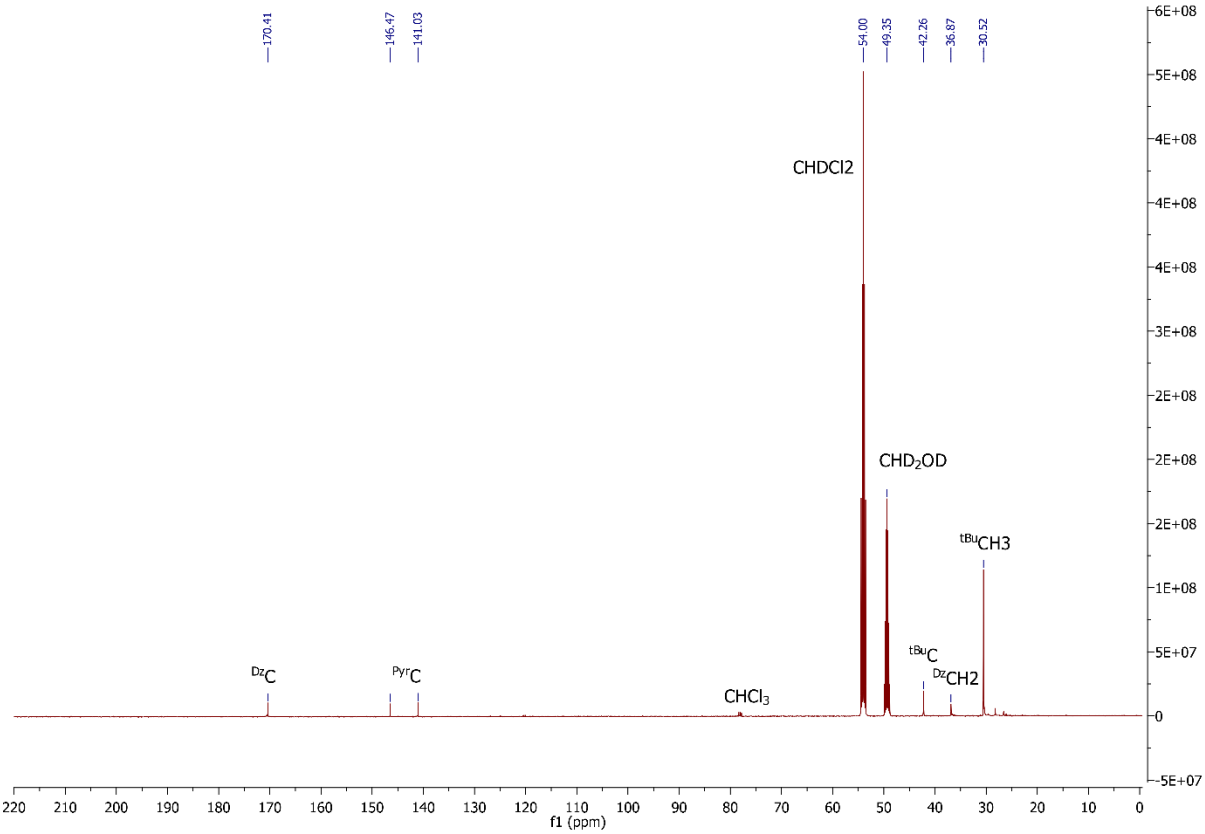

Fig. S10 ^{13}C NMR spectrum of *t*Bu$_8$Dz$_4$PzNi (CD_2Cl_2, 298 K).

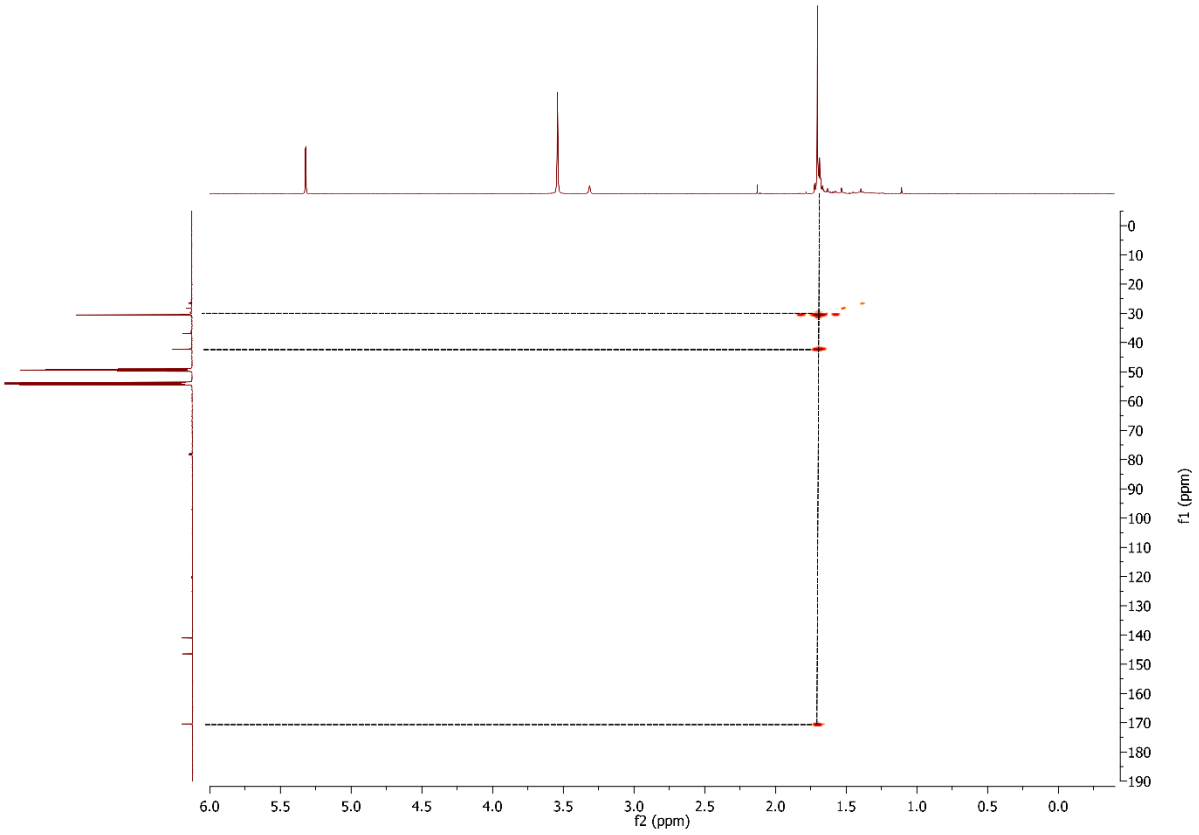

Fig. S11 ^{1}H-^{13}C HMBC spectrum of *t*Bu$_8$Dz$_4$PzNi (CD_2Cl_2, 298 K).

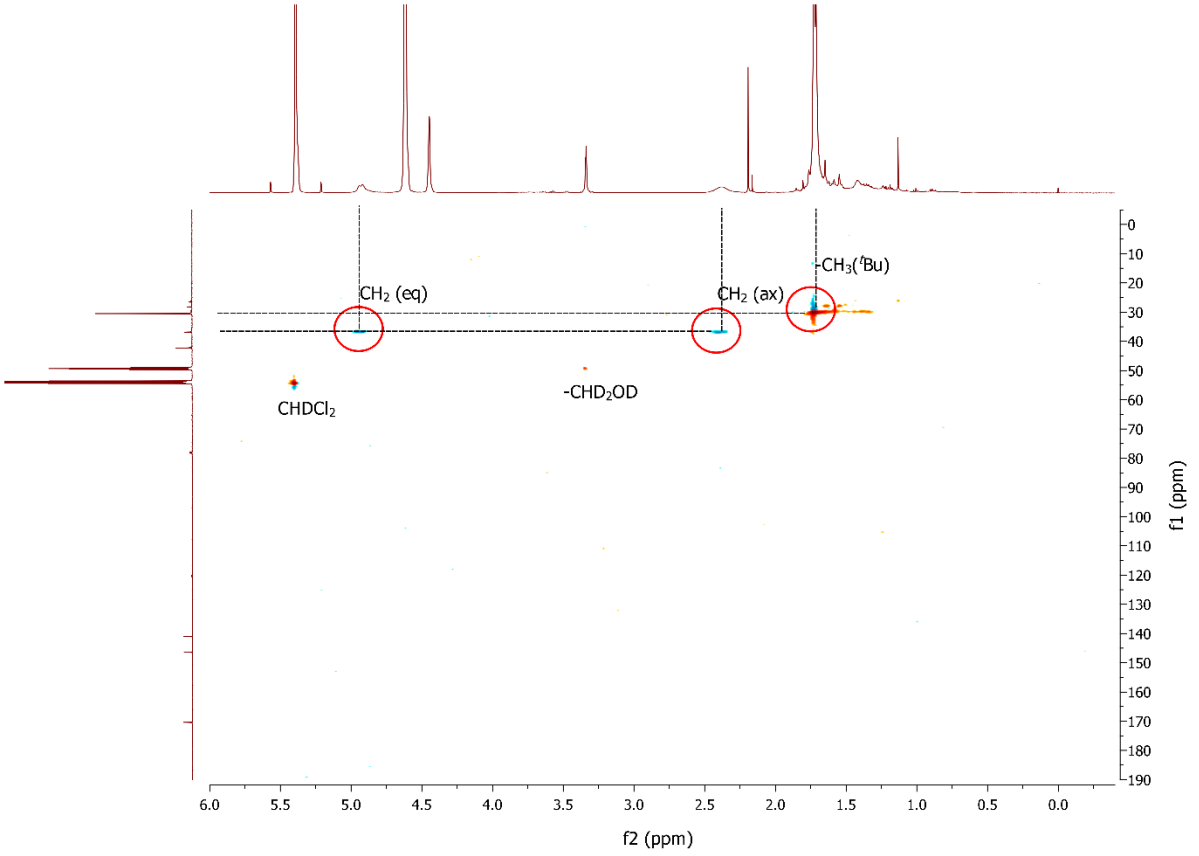

Fig. S12 ^{1}H-^{13}C HSQC spectrum of *t*Bu$_8$Dz$_4$PzNi (CD_2Cl_2, 223 K).

Table S1 Chemical shifts (δ) and temperature dependence of the diastereotopic proton resonances of 1,4-diazepine rings in 6*H*-1,4-diazepinoporphyrazines

Compd	Solvent	Temp., K	δ, ppm			References	Form of compd in solution[b]
			H^{eq}	Coalescence	H^{ax}		
tBu$_2$Dz(CN)$_2$	$CDCl_3$	273	4.6 (d)		1.6 (d)	3	
	pyridine-d_5	363		3.36 (br s)			
tBu$_8$Dz$_4$PzMg	CD_2Cl_2	223	4.9 (d)		2.3 (d)	3	monomer
	pyridine-d_5	363		3.7 (br s)			
tBu$_8$Dz$_4$PzNi	CD_2Cl_2	223	4.9 (br d)		2.4 (br s)	tw	monomer
	CD_2Cl_2	273		No signal (T_c[a])			
$^{t\text{Bu}}$Ph$_2$Dz(CN)$_2$	$CDCl_3$	293	5.73 (d)		1.96 (d)	4	
	pyridine-d_5	363		No signal (T_c)			
[$^{t\text{Bu}}$Ph$_8$Dz$_4$PzH$_2$]$_2$	CD_2Cl_2	293	6.10 (d)	No coalescence	4.70 (d)	2,5	dimer
[$^{t\text{Bu}}$Ph$_8$Dz$_4$PzMg]$_2$	DMSO-d_6	293	5.93 (d)	No coalescence	5.01 (d)	4	dimer
$^{t\text{Bu}}$Ph$_8$Dz$_4$PzMg	DMSO-d_6	293		No signal (T_c)		4	monomer
	DMF-d_7	393		4.50 (br, s)			
[$^{t\text{Bu}}$Ph$_8$Dz$_4$PzNi]$_2$	CD_2Cl_2	293	6.0 (d)	No coalescence	4.62 (d)	tw	dimer
[$^{t\text{Bu}}$Ph$_8$Dz$_4$Pz]$_2$La	CD_2Cl_2	293	6.05	No coalescence	4.69	2	double-decker
[$^{t\text{Bu}}$Ph$_8$Dz$_4$Pz]$_2$Ce	CD_2Cl_2	293	6.18 (br s)	No coalescence	5.13 (d)	2	double-decker
[$^{t\text{Bu}}$Ph$_8$Dz$_4$Pz]$_2$Lu	CD_2Cl_2	293	6.02 (br s)	No coalescence	5.13 (br s)	2	double-decker
[$^{t\text{Bu}}$Ph$_8$Dz$_4$Pz]La[Bu$_8$Pc]	CD_2Cl_2	293	6.41 (br s)	No coalescence	4.03 (br s)	6	double-decker
[$^{t\text{Bu}}$Ph$_8$Dz$_4$Pz]Lu[Bu$_8$Pc]	CD_2Cl_2	293	6.61 (br s)	No coalescence	5.19 (br s)	6	double-decker
Ph$_2$Dz(CN)$_2$	$CDCl_3$	293	5.74		1.98	7	
	DMSO-d_6	343		No signal (T_c)			
Ph$_2$DzBz$_3$PzMg	THF-d_8	210	6.45		2.55	8	monomer
	DMSO-d_6	363		4.42 (br, s)			
[Ph$_8$Dz$_4$PzMg]$_2$	DMSO-d_6	373	5.99 (d)	No coalescence	5.06 (d)	7	dimer
[Ph$_8$Dz$_4$PzZn]$_2$	DMSO-d_6	373	5.99 (d)	No coalescence	5.03 (d)	7	dimer
$^{\text{MeO}}$Ph$_2$Dz(CN)$_2$	DMSO-d_6	293	6.10 (d)		2.21 (d)	9	
[$^{\text{MeO}}$Ph$_8$Dz$_4$PzMg]$_2$	pyridine-d_5	293	6.86 (d)	No coalescence	6.07 (d)	9	dimer
$^{\text{MeO}}$Ph$_2$DzBz$_3$PzMg	DMSO-d_6	293		4.59 (br, s)		9	monomer
$^{(\text{BnO})2\text{BnO}}Ph_2$Dz(CN)$_2$	DMSO-d_6	293	5.99		2.21	10	
[$^{(\text{BnO})2\text{BnO}}Ph_8Dz_4$PzMg]$_2$	DMSO-d_6	293	5.96	No coalescence	5.13	10	dimer
$^{\text{Br}}$Styr$_2$Dz(CN)$_2$	DMSO-d_6	293	5.33 (br s)		2.10 (br s)	11	
[$^{\text{Br}}$Styr$_8$Dz$_4$PzMg]$_2$	DMSO-d_6	293	6.11 (br s)	No coalescence	4.77 (br s)	12	dimer
$^{\text{MeO}}$Styr$_2$Dz(CN)$_2$	DMSO-d_6	293	5.34 (br s)		2.02 (br s)	13	
[$^{\text{MeO}}$Styr$_8$Dz$_4$PzMg]$_2$	DMSO-d_6	293	5.69 (br s)	No coalescence	4.92 (d)	12	dimer
$^{(\text{MeO})3}$Styr(Ph)Dz(CN)$_2$	DMSO-d_6	293	5.75 (br s)		2.21 (br s)	14	
$^{(\text{MeO})3}$Styr(Ph)DzBz$_3$PzMg	pyridine-d_5	293		No signal (T_c)		14	monomer
$^{(\text{MeO})3}$Styr$_2$Dz(CN)$_2$	$CHCl_3$	293	4.96 (br s)		1.83 (br s)	15	
[$^{(\text{MeO})3}$Styr$_8$Dz$_4$PzMg]$_2$	pyridine-d_5	333	6.72 (d)	No coalescence	6.07 (d)	15	dimer

[a] T_c – coalescence temperature. [b] It is defined based on the character of the NMR signals of diastereotopic CH_2 protons.

X-ray structure analysis of $^{tBu}Ph_8Dz_4PzNi$: Bruker AXS SMART 1000, CCD-detector λ(MoKa) = 0.71073Å, graphite monochromator, ω-scanning, $2\theta_{max}$= 50°. T=150.

The structure was solved by direct method and refined by full-matrix least squares method for F^2 with anisotropic parameters for all non-hydrogen atoms. All calculations were performed with the use of the SHELXTL PLUS program packages [1-4].

1. SMART (control) and SAINT (integration) Software, Version 5.0, Bruker AXS Inc., Madison, WI, 1997.
2. SAINT: Area-Detector Integration Sofware. Bruker: Madison, 603 Wisconsin, USA, 2012.
3. Sheldrick G.M. SADABS. Program for scaling and Correction of Area Detector Data, University of Göttingen, 1997.
4. Sheldrick G.M.// Acta Crystallogr. C. 2015. V. 71. P. 3. doi.org/10.1107/S2053229614024218

Special details: Very weak crystals, no reflections are observed at 2θ>46°. The 16 tert-butyl substituents are completely disordered.

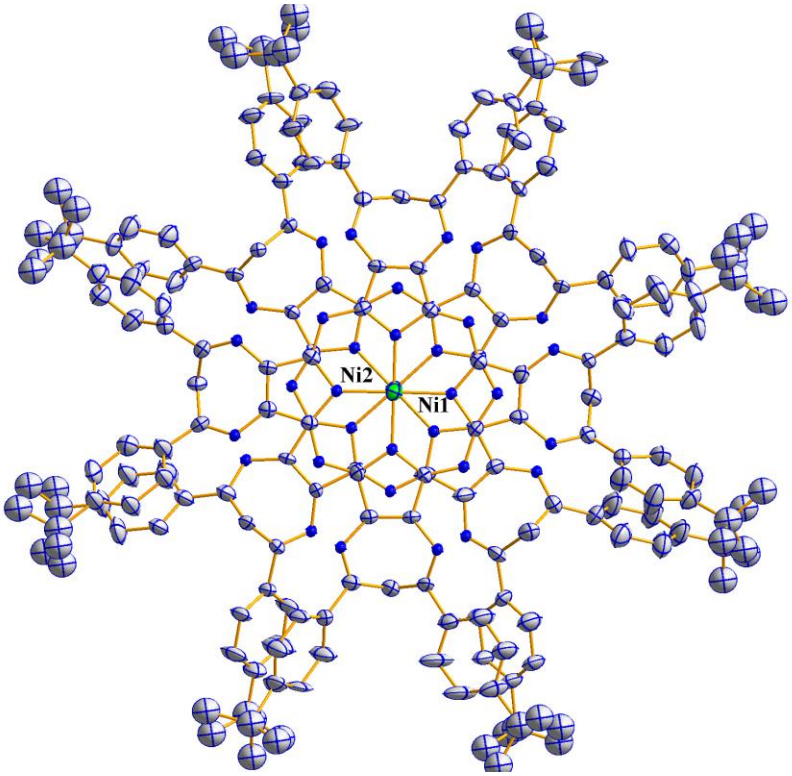

Fig. S13 Molecular structure of $^{tBu}Ph_8Dz_4PzNi$ (50% ellipsoids).

Table S2 Crystal data and structure refinement for $^{tBu}Ph_8Dz_4PzNi$

CCDC	2106082
Empirical formula	$C_{108}H_{112}N_{16}Ni$
Formula weight	1692.84
Temperature	150(2) K
Wavelength	0.71073
Crystal system	Triclinic
Space group	P-1

Unit cell dimensions	a = 14.534(2) Å	α= 92.735(2)°.
	b = 25.961(4) Å	b= 97.846(2)°.
	c = 32.780(5) Å	g = 102.021(2)°.
Volume	11947(3) $Å^3$	
Z	4	
Density (calculated)	0.941 Mg/m^3	
Absorption coefficient	0.207 mm^{-1}	
F(000)	3600	
Crystal size	0.14 x 0.12 x 0.10 mm^3	
Theta range for data collection	2.20 to 25.00°.	
Index ranges	-17<=h<=17, -30<=k<=30, -38<=l<=38	
Reflections collected	97571	
Independent reflections	41984 [R(int) = 0.2063]	
Completeness to theta = 25.00°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	41984 / 46 / 1888	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.1267, wR2 = 0.2819	
R indices (all data)	R1 = 0.3015, wR2 = 0.3479	
Largest diff. peak and hole	0.840 and -0.715 e.$Å^{-3}$	

Table S3 Bond lengths [Å] and angles [°] for $^{t\mathrm{Bu}}Ph_8Dz_4PzNi$

Ni(1)-N(5)	1.858(7)	Ni(1)-N(1)	1.876(7)
Ni(1)-N(7)	1.880(7)	Ni(1)-N(3)	1.888(7)
Ni(2)-N(21)	1.878(7)	Ni(2)-N(19)	1.881(6)
Ni(2)-N(23)	1.889(7)	Ni(2)-N(17)	1.890(7)
N(1)-C(84)	1.381(10)	N(1)-C(1)	1.406(9)
N(2)-C(1)	1.302(10)	N(2)-C(2)	1.305(10)
N(3)-C(2)	1.355(9)	N(3)-C(29)	1.383(10)
N(4)-C(29)	1.303(9)	N(4)-C(30)	1.316(9)
N(5)-C(30)	1.377(10)	N(5)-C(56)	1.378(10)
N(6)-C(57)	1.332(10)	N(6)-C(56)	1.340(10)
N(7)-C(57)	1.377(9)	N(7)-C(83)	1.392(10)
N(8)-C(83)	1.311(10)	N(8)-C(84)	1.342(10)
N(9)-C(86)	1.287(10)	N(9)-C(85)	1.352(10)
N(10)-C(98)	1.303(10)	N(10)-C(109)	1.372(10)
N(11)-C(4)	1.314(10)	N(11)-C(3)	1.373(10)
N(12)-C(16)	1.286(10)	N(12)-C(28)	1.360(10)
N(13)-C(32)	1.283(10)	N(13)-C(31)	1.365(10)
N(14)-C(44)	1.275(10)	N(14)-C(55)	1.364(10)
N(15)-C(59)	1.310(10)	N(15)-C(58)	1.355(10)
N(16)-C(71)	1.298(10)	N(16)-C(82)	1.379(10)
N(17)-C(136)	1.350(10)	N(17)-C(110)	1.390(9)
N(18)-C(137)	1.334(9)	N(18)-C(136)	1.347(10)
N(19)-C(137)	1.349(10)	N(19)-C(163)	1.423(11)
N(20)-C(163)	1.280(12)	N(20)-C(164)	1.299(9)
N(21)-C(190)	1.346(9)	N(21)-C(164)	1.399(9)
N(22)-C(190)	1.327(9)	N(22)-C(191)	1.335(9)
N(23)-C(191)	1.346(9)	N(23)-C(216)	1.396(9)
N(24)-C(216)	1.285(9)	N(24)-C(110)	1.296(9)
N(25)-C(112)	1.295(10)	N(25)-C(111)	1.381(10)
N(26)-C(124)	1.305(10)	N(26)-C(135)	1.362(10)
N(27)-C(139)	1.329(12)	N(27)-C(138)	1.370(11)
N(28)-C(151)	1.276(12)	N(28)-C(162)	1.364(11)
N(29)-C(166)	1.274(10)	N(29)-C(165)	1.371(9)
N(30)-C(178)	1.299(11)	N(30)-C(189)	1.377(10)
N(31)-C(193)	1.319(10)	N(31)-C(192)	1.338(10)
N(32)-C(205)	1.311(10)	N(32)-C(215)	1.391(9)
C(1)-C(109)	1.451(11)	C(2)-C(3)	1.447(11)
C(3)-C(28)	1.384(11)	C(4)-C(15)	1.486(13)
C(4)-C(5)	1.508(13)	C(5)-C(6)	1.339(13)
C(5)-C(14)	1.377(13)	C(6)-C(7)	1.393(14)
C(7)-C(8)	1.333(14)	C(8)-C(13)	1.357(15)
C(8)-C(9)	1.542(17)	C(13)-C(14)	1.398(15)
C(15)-C(16)	1.526(12)	C(16)-C(17)	1.478(12)
C(17)-C(27)	1.370(13)	C(17)-C(18)	1.416(13)
C(18)-C(19)	1.375(14)	C(19)-C(20)	1.352(15)
C(20)-C(26)	1.372(15)	C(20)-C(21)	1.610(18)
C(22)-C(214)	1.382(12)	C(22)-C(209)	1.390(14)
C(26)-C(27)	1.339(14)	C(28)-C(29)	1.485(11)
C(30)-C(31)	1.431(11)	C(31)-C(55)	1.375(11)
C(32)-C(33)	1.464(14)	C(32)-C(43)	1.600(13)
C(33)-C(34)	1.291(14)	C(33)-C(42)	1.371(14)
C(34)-C(35)	1.424(14)	C(35)-C(36)	1.306(13)
C(36)-C(41)	1.291(15)	C(36)-C(37)	1.516(17)
C(41)-C(42)	1.436(14)	C(43)-C(44)	1.567(12)
C(44)-C(45)	1.493(13)	C(45)-C(54)	1.344(12)
C(45)-C(46)	1.378(13)	C(46)-C(47)	1.393(14)
C(47)-C(48)	1.391(14)	C(48)-C(53)	1.392(14)
C(48)-C(49)	1.533(17)	C(53)-C(54)	1.364(14)
C(55)-C(56)	1.466(11)	C(57)-C(58)	1.465(11)
C(58)-C(82)	1.351(11)	C(59)-C(60)	1.482(12)
C(59)-C(70)	1.526(12)	C(60)-C(61)	1.370(13)
C(60)-C(69)	1.375(12)	C(61)-C(62)	1.363(12)
C(62)-C(63)	1.327(13)	C(63)-C(68)	1.387(13)
C(63)-C(64)	1.580(17)	C(68)-C(69)	1.415(13)
C(70)-C(71)	1.486(11)	C(71)-C(72)	1.471(12)
C(72)-C(73)	1.343(12)	C(72)-C(81)	1.363(12)
C(73)-C(74)	1.405(13)	C(74)-C(75)	1.307(13)
C(75)-C(80)	1.343(14)	C(75)-C(76)	1.556(17)
C(80)-C(81)	1.419(13)	C(82)-C(83)	1.439(11)
C(84)-C(85)	1.438(11)	C(85)-C(109)	1.404(11)
C(86)-C(87)	1.483(12)	C(86)-C(97)	1.484(11)
C(87)-C(88)	1.344(13)	C(87)-C(96)	1.391(12)
C(88)-C(89)	1.388(14)	C(89)-C(90)	1.359(16)
C(90)-C(95)	1.362(16)	C(90)-C(91)	1.498(18)
C(95)-C(96)	1.369(14)	C(97)-C(98)	1.542(12)
C(98)-C(99)	1.418(12)	C(99)-C(108)	1.343(13)
C(99)-C(100)	1.393(13)	C(100)-C(101)	1.384(13)
C(101)-C(102)	1.387(14)	C(102)-C(107)	1.349(14)
C(102)-C(103)	1.535(17)	C(107)-C(108)	1.348(14)
C(110)-C(111)	1.480(11)	C(111)-C(135)	1.349(11)
C(112)-C(123)	1.489(12)	C(112)-C(113)	1.510(12)
C(113)-C(114)	1.336(12)	C(113)-C(122)	1.378(12)
C(114)-C(115)	1.399(12)	C(115)-C(116)	1.358(14)
C(116)-C(121)	1.380(13)	C(116)-C(117)	1.537(13)
C(117)-C(18A)	1.496(16)	C(117)-C(19A)	1.496(15)
C(117)-C(20A)	1.496(16)	C(117)-C(119)	1.574(16)
C(117)-C(118)	1.574(16)	C(117)-C(120)	1.574(16)
C(121)-C(122)	1.429(13)	C(123)-C(124)	1.533(12)
C(124)-C(125)	1.475(12)	C(125)-C(134)	1.360(12)
C(125)-C(126)	1.367(13)	C(126)-C(127)	1.400(14)
C(127)-C(128)	1.355(13)	C(128)-C(133)	1.373(14)
C(128)-C(129)	1.577(18)	C(133)-C(134)	1.358(13)
C(135)-C(136)	1.441(11)	C(137)-C(138)	1.446(11)

C(138)-C(162)	1.361(13)	C(139)-C(140)	1.470(13)
C(139)-C(150)	1.580(14)	C(140)-C(141)	1.272(14)
C(140)-C(149)	1.388(14)	C(141)-C(142)	1.432(15)
C(142)-C(143)	1.367(16)	C(143)-C(148)	1.342(15)
C(143)-C(144)	1.563(18)	C(148)-C(149)	1.423(15)
C(150)-C(151)	1.597(14)	C(151)-C(152)	1.482(12)
C(152)-C(153)	1.331(12)	C(152)-C(161)	1.3693(10)
C(153)-C(154)	1.399(13)	C(154)-C(155)	1.306(14)
C(155)-C(160)	1.305(13)	C(155)-C(156)	1.590(17)
C(160)-C(161)	1.398(12)	C(162)-C(163)	1.432(14)
C(164)-C(165)	1.480(11)	C(165)-C(189)	1.389(10)
C(166)-C(167)	1.506(11)	C(166)-C(177)	1.521(12)
C(167)-C(168)	1.367(13)	C(167)-C(176)	1.370(12)
C(168)-C(169)	1.355(13)	C(169)-C(170)	1.375(15)
C(170)-C(175)	1.354(14)	C(170)-C(171)	1.526(17)
C(175)-C(176)	1.403(13)	C(177)-C(178)	1.494(12)
C(178)-C(179)	1.468(13)	C(179)-C(180)	1.320(12)
C(179)-C(188)	1.331(14)	C(180)-C(181)	1.406(13)
C(181)-C(182)	1.360(15)	C(182)-C(187)	1.328(15)
C(182)-C(183)	1.512(17)	C(187)-C(188)	1.390(14)
C(189)-C(190)	1.430(10)	C(191)-C(192)	1.465(11)
C(192)-C(215)	1.376(11)	C(193)-C(194)	1.483(12)
C(193)-C(204)	1.483(11)	C(194)-C(195)	1.355(13)
C(194)-C(203)	1.363(13)	C(195)-C(196)	1.344(14)
C(196)-C(197)	1.358(15)	C(197)-C(202)	1.333(15)
C(197)-C(198)	1.561(18)	C(202)-C(203)	1.368(14)
C(204)-C(205)	1.494(12)	C(205)-C(206)	1.497(12)
C(206)-C(207)	1.358(12)	C(206)-C(214)	1.406(13)
C(207)-C(208)	1.404(12)	C(208)-C(209)	1.338(14)
C(209)-C(210)	1.564(17)	C(215)-C(216)	1.440(10)
C(9)-C(12)	1.514(10)	C(9)-C(11)	1.514(10)
C(9)-C(10)	1.514(11)	C(9)-C(10A)	1.56(3)
C(21)-C(23A)	1.43(3)	C(21)-C(24)	1.526(11)
C(21)-C(23)	1.526(11)	C(21)-C(25)	1.527(11)
C(37)-C(40)	1.480(9)	C(37)-C(38)	1.480(9)
C(37)-C(39)	1.480(9)	C(49)-C(50)	1.505(9)
C(49)-C(52)	1.506(9)	C(49)-C(51)	1.507(9)
C(64)-C(67)	1.441(17)	C(64)-C(66)	1.496(18)
C(64)-C(65)	1.588(18)	C(76)-C(77)	1.441(17)
C(76)-C(79)	1.465(17)	C(76)-C(78)	1.476(18)
C(91)-C(92A)	1.40(3)	C(91)-C(93A)	1.44(3)
C(91)-C(94)	1.535(17)	C(91)-C(93)	1.535(17)
C(91)-C(92)	1.535(17)	C(91)-C(94A)	1.57(3)
C(103)-C(104)	1.480(9)	C(103)-C(106)	1.481(9)
C(103)-C(105)	1.481(9)	C(129)-C(130)	1.496(9)
C(129)-C(132)	1.498(9)	C(129)-C(131)	1.498(9)
C(144)-C(145)	1.480(8)	C(144)-C(146)	1.480(8)
C(144)-C(147)	1.481(8)	C(156)-C(159)	1.437(18)
C(156)-C(157)	1.448(18)	C(156)-C(158)	1.473(17)
C(171)-C(172)	1.451(9)	C(171)-C(174)	1.451(9)
C(171)-C(173)	1.452(9)	C(183)-C(184)	1.517(9)
C(183)-C(186)	1.517(9)	C(183)-C(185)	1.517(9)
C(198)-C(201)	1.503(9)	C(198)-C(199)	1.504(9)
C(198)-C(200)	1.504(9)	C(210)-C(03A)	1.456(18)
C(210)-C(02A)	1.456(18)	C(210)-C(01A)	1.457(18)
C(210)-C(213)	1.510(18)	C(210)-C(211)	1.511(18)
C(210)-C(212)	1.511(18)		

N(5)-Ni(1)-N(1)	178.8(3)	N(5)-Ni(1)-N(7)	90.4(3)
N(1)-Ni(1)-N(7)	89.9(3)	N(5)-Ni(1)-N(3)	89.6(3)
N(1)-Ni(1)-N(3)	90.0(3)	N(7)-Ni(1)-N(3)	177.5(3)
N(21)-Ni(2)-N(19)	90.9(3)	N(21)-Ni(2)-N(23)	88.8(3)
N(19)-Ni(2)-N(23)	178.5(3)	N(21)-Ni(2)-N(17)	178.0(3)
N(19)-Ni(2)-N(17)	89.7(3)	N(23)-Ni(2)-N(17)	90.5(3)
C(84)-N(1)-C(1)	105.2(7)	C(84)-N(1)-Ni(1)	128.6(6)
C(1)-N(1)-Ni(1)	126.1(6)	C(1)-N(2)-C(2)	120.0(7)
C(2)-N(3)-C(29)	106.7(7)	C(2)-N(3)-Ni(1)	127.0(6)
C(29)-N(3)-Ni(1)	126.2(6)	C(29)-N(4)-C(30)	120.2(7)
C(30)-N(5)-C(56)	103.9(7)	C(30)-N(5)-Ni(1)	128.6(5)
C(56)-N(5)-Ni(1)	127.4(6)	C(57)-N(6)-C(56)	119.0(7)
C(57)-N(7)-C(83)	105.0(7)	C(57)-N(7)-Ni(1)	127.5(6)
C(83)-N(7)-Ni(1)	127.4(6)	C(83)-N(8)-C(84)	121.6(8)
C(86)-N(9)-C(85)	119.0(8)	C(98)-N(10)-C(109)	121.4(8)
C(4)-N(11)-C(3)	116.4(8)	C(16)-N(12)-C(28)	118.3(8)
C(32)-N(13)-C(31)	120.2(8)	C(44)-N(14)-C(55)	116.3(8)
C(59)-N(15)-C(58)	117.9(8)	C(71)-N(16)-C(82)	117.6(8)
C(136)-N(17)-C(110)	106.8(7)	C(136)-N(17)-Ni(2)	128.0(6)
C(110)-N(17)-Ni(2)	125.1(6)	C(137)-N(18)-C(136)	119.7(7)
C(137)-N(19)-C(163)	105.9(8)	C(137)-N(19)-Ni(2)	127.7(5)
C(163)-N(19)-Ni(2)	126.4(7)	C(163)-N(20)-C(164)	121.5(8)
C(190)-N(21)-C(164)	105.2(7)	C(190)-N(21)-Ni(2)	129.6(5)
C(164)-N(21)-Ni(2)	125.2(6)	C(190)-N(22)-C(191)	121.2(7)
C(191)-N(23)-C(216)	105.8(7)	C(191)-N(23)-Ni(2)	128.0(5)
C(216)-N(23)-Ni(2)	126.2(6)	C(216)-N(24)-C(110)	120.5(7)
C(112)-N(25)-C(111)	116.9(8)	C(124)-N(26)-C(135)	118.7(7)
C(139)-N(27)-C(138)	116.3(8)	C(151)-N(28)-C(162)	117.6(8)
C(166)-N(29)-C(165)	116.6(7)	C(178)-N(30)-C(189)	117.2(8)
C(193)-N(31)-C(192)	117.2(8)	C(205)-N(32)-C(215)	116.5(7)
N(2)-C(1)-N(1)	127.9(8)	N(2)-C(1)-C(109)	123.0(8)
N(1)-C(1)-C(109)	108.9(8)	N(2)-C(2)-N(3)	128.9(8)
N(2)-C(2)-C(3)	119.5(8)	N(3)-C(2)-C(3)	111.6(7)
N(11)-C(3)-C(28)	128.3(8)	N(11)-C(3)-C(2)	123.8(8)
C(28)-C(3)-C(2)	106.6(8)	N(11)-C(4)-C(15)	121.7(8)
N(11)-C(4)-C(5)	116.2(9)	C(15)-C(4)-C(5)	122.1(9)
C(6)-C(5)-C(14)	116.9(11)	C(6)-C(5)-C(4)	121.1(10)

C(14)-C(5)-C(4)	122.0(11)	C(5)-C(6)-C(7)	123.0(12)
C(8)-C(7)-C(6)	121.6(12)	C(7)-C(8)-C(13)	115.7(10)
C(7)-C(8)-C(9)	121.3(12)	C(13)-C(8)-C(9)	122.7(12)
C(8)-C(13)-C(14)	124.0(11)	C(5)-C(14)-C(13)	118.6(12)
C(4)-C(15)-C(16)	106.8(9)	N(12)-C(16)-C(17)	118.3(9)
N(12)-C(16)-C(15)	120.3(9)	C(17)-C(16)-C(15)	121.4(9)
C(27)-C(17)-C(18)	115.7(10)	C(27)-C(17)-C(16)	120.8(10)
C(18)-C(17)-C(16)	123.5(11)	C(19)-C(18)-C(17)	121.5(11)
C(20)-C(19)-C(18)	120.2(11)	C(19)-C(20)-C(26)	118.1(11)
C(19)-C(20)-C(21)	118.9(12)	C(26)-C(20)-C(21)	122.7(13)
C(214)-C(22)-C(209)	122.3(11)	C(27)-C(26)-C(20)	122.7(12)
C(26)-C(27)-C(17)	121.5(10)	N(12)-C(28)-C(3)	132.2(8)
N(12)-C(28)-C(29)	122.1(8)	C(3)-C(28)-C(29)	105.6(8)
N(4)-C(29)-N(3)	128.3(8)	N(4)-C(29)-C(28)	121.9(8)
N(3)-C(29)-C(28)	109.4(8)	N(4)-C(30)-N(5)	126.7(8)
N(4)-C(30)-C(31)	121.5(8)	N(5)-C(30)-C(31)	111.8(7)
N(13)-C(31)-C(55)	128.7(9)	N(13)-C(31)-C(30)	123.4(8)
C(55)-C(31)-C(30)	107.8(8)	N(13)-C(32)-C(33)	120.0(9)
N(13)-C(32)-C(43)	119.5(8)	C(33)-C(32)-C(43)	120.5(9)
C(34)-C(33)-C(42)	116.5(12)	C(34)-C(33)-C(32)	119.5(11)
C(42)-C(33)-C(32)	123.7(12)	C(33)-C(34)-C(35)	120.2(12)
C(36)-C(35)-C(34)	125.1(11)	C(41)-C(36)-C(35)	114.4(12)
C(41)-C(36)-C(37)	120.1(12)	C(35)-C(36)-C(37)	125.1(12)
C(36)-C(41)-C(42)	123.2(12)	C(33)-C(42)-C(41)	119.9(11)
C(44)-C(43)-C(32)	102.8(8)	N(14)-C(44)-C(45)	118.6(10)
N(14)-C(44)-C(43)	122.3(8)	C(45)-C(44)-C(43)	119.0(9)
C(54)-C(45)-C(46)	117.2(10)	C(54)-C(45)-C(44)	122.0(10)
C(46)-C(45)-C(44)	120.7(11)	C(45)-C(46)-C(47)	118.0(11)
C(48)-C(47)-C(46)	125.5(11)	C(47)-C(48)-C(53)	113.4(10)
C(47)-C(48)-C(49)	122.7(12)	C(53)-C(48)-C(49)	123.8(12)
C(54)-C(53)-C(48)	120.8(12)	C(45)-C(54)-C(53)	124.9(11)
N(14)-C(55)-C(31)	131.1(9)	N(14)-C(55)-C(56)	124.1(8)
C(31)-C(55)-C(56)	104.1(8)	N(6)-C(56)-N(5)	128.2(8)
N(6)-C(56)-C(55)	119.4(8)	N(5)-C(56)-C(55)	112.4(8)
N(6)-C(57)-N(7)	127.3(8)	N(6)-C(57)-C(58)	122.2(8)
N(7)-C(57)-C(58)	110.5(8)	C(82)-C(58)-N(15)	130.8(8)
C(82)-C(58)-C(57)	106.3(7)	N(15)-C(58)-C(57)	122.4(8)
N(15)-C(59)-C(60)	119.9(9)	N(15)-C(59)-C(70)	118.7(7)
C(60)-C(59)-C(70)	121.3(9)	C(61)-C(60)-C(69)	118.7(9)
C(61)-C(60)-C(59)	120.1(9)	C(69)-C(60)-C(59)	121.2(10)
C(62)-C(61)-C(60)	121.8(11)	C(63)-C(62)-C(61)	122.3(11)
C(62)-C(63)-C(68)	117.0(9)	C(62)-C(63)-C(64)	121.3(12)
C(68)-C(63)-C(64)	121.6(11)	C(63)-C(68)-C(69)	122.3(10)
C(60)-C(69)-C(68)	117.7(11)	C(71)-C(70)-C(59)	107.9(8)
N(16)-C(71)-C(72)	118.6(9)	N(16)-C(71)-C(70)	119.5(8)
C(72)-C(71)-C(70)	121.8(8)	C(73)-C(72)-C(81)	116.3(9)
C(73)-C(72)-C(71)	124.8(10)	C(81)-C(72)-C(71)	118.9(9)
C(72)-C(73)-C(74)	120.5(10)	C(75)-C(74)-C(73)	123.8(11)
C(74)-C(75)-C(80)	117.2(10)	C(74)-C(75)-C(76)	121.0(12)
C(80)-C(75)-C(76)	121.9(13)	C(75)-C(80)-C(81)	120.4(11)
C(72)-C(81)-C(80)	121.7(10)	C(58)-C(82)-N(16)	130.3(8)
C(58)-C(82)-C(83)	107.5(8)	N(16)-C(82)-C(83)	121.7(8)
N(8)-C(83)-N(7)	126.9(8)	N(8)-C(83)-C(82)	122.3(8)
N(7)-C(83)-C(82)	110.6(8)	N(8)-C(84)-N(1)	125.4(8)
N(8)-C(84)-C(85)	121.4(8)	N(1)-C(84)-C(85)	113.1(8)
N(9)-C(85)-C(109)	130.2(8)	N(9)-C(85)-C(84)	125.0(8)
C(109)-C(85)-C(84)	104.1(8)	N(9)-C(86)-C(87)	116.5(9)
N(9)-C(86)-C(97)	120.1(8)	C(87)-C(86)-C(97)	122.8(9)
C(88)-C(87)-C(96)	117.5(10)	C(88)-C(87)-C(86)	121.3(10)
C(96)-C(87)-C(86)	121.1(10)	C(87)-C(88)-C(89)	121.1(12)
C(90)-C(89)-C(88)	122.4(12)	C(89)-C(90)-C(95)	115.4(11)
C(89)-C(90)-C(91)	121.8(15)	C(95)-C(90)-C(91)	122.8(14)
C(90)-C(95)-C(96)	123.9(12)	C(95)-C(96)-C(87)	119.4(11)
C(86)-C(97)-C(98)	108.2(8)	N(10)-C(98)-C(99)	120.5(9)
N(10)-C(98)-C(97)	115.9(8)	C(99)-C(98)-C(97)	123.5(9)
C(108)-C(99)-C(100)	115.9(10)	C(108)-C(99)-C(98)	122.0(11)
C(100)-C(99)-C(98)	122.0(12)	C(101)-C(100)-C(99)	121.1(11)
C(100)-C(101)-C(102)	120.6(11)	C(107)-C(102)-C(101)	116.5(11)
C(107)-C(102)-C(103)	121.8(13)	C(101)-C(102)-C(103)	121.5(12)
C(102)-C(107)-C(108)	122.6(12)	C(99)-C(108)-C(107)	123.2(12)
N(10)-C(109)-C(85)	126.7(8)	N(10)-C(109)-C(1)	123.7(8)
C(85)-C(109)-C(1)	108.5(8)	N(24)-C(110)-N(17)	129.4(8)
N(24)-C(110)-C(111	122.7(8)	N(17)-C(110)-C(111)	107.8(8)
C(135)-C(111)-N(25)	131.0(8)	C(135)-C(111)-C(110)	107.2(8)
N(25)-C(111)-C(110)	121.2(8)	N(25)-C(112)-C(123)	121.7(8)
N(25)-C(112)-C(113)	116.2(9)	C(123)-C(112)-C(113)	122.0(9)
C(114)-C(113)-C(122)	119.1(9)	C(114)-C(113)-C(112)	119.9(9)
C(122)-C(113)-C(112)	121.0(10)	C(113)-C(114)-C(115)	120.6(10)
C(116)-C(115)-C(114)	121.5(11)	C(115)-C(116)-C(121)	119.6(10)
C(115)-C(116)-C(117)	121.5(12)	C(121)-C(116)-C(117)	118.9(11)
C(18A)-C(117)-C(19A)	108.5(16)	C(18A)-C(117)-C(20A)	112.8(17)
C(19A)-C(117)-C(20A)	103.3(17)	C(18A)-C(117)-C(116)	107.3(12)
C(19A)-C(117)-C(116)	114.1(13)	C(20A)-C(117)-C(116)	110.9(12)
C(116)-C(117)-C(119)	108.9(11)	C(116)-C(117)-C(118)	111.2(12)
C(119)-C(117)-C(118)	107.9(16)	C(116)-C(117)-C(120)	108.9(12)
C(119)-C(117)-C(120)	106.7(16)	C(118)-C(117)-C(120)	113.1(16)
C(116)-C(121)-C(122)	117.7(10)	C(113)-C(122)-C(121)	121.3(11)
C(112)-C(123)-C(124)	107.9(8)	N(26)-C(124)-C(125)	119.5(9)
N(26)-C(124)-C(123)	120.1(8)	C(125)-C(124)-C(123)	120.3(8)
C(134)-C(125)-C(126)	117.4(9)	C(134)-C(125)-C(124)	119.4(10)
C(126)-C(125)-C(124)	123.0(10)	C(125)-C(126)-C(127)	119.5(11)
C(128)-C(127)-C(126)	121.4(10)	C(127)-C(128)-C(133)	118.3(10)
C(127)-C(128)-C(129)	119.8(11)	C(133)-C(128)-C(129)	121.7(11)
C(134)-C(133)-C(128)	119.8(11)	C(133)-C(134)-C(125)	123.1(11)
C(111)-C(135)-N(26)	129.9(8)	C(111)-C(135)-C(136)	106.7(8)
N(26)-C(135)-C(136)	122.8(8)	N(18)-C(136)-N(17)	126.9(8)
N(18)-C(136)-C(135)	121.6(8)	N(17)-C(136)-C(135)	111.3(7)

N(18)-C(137)-N(19)	127.9(7)	N(18)-C(137)-C(138)	120.5(8)
N(19)-C(137)-C(138)	111.6(8)	C(162)-C(138)-N(27)	130.1(9)
C(162)-C(138)-C(137)	105.7(9)	N(27)-C(138)-C(137)	123.6(9)
N(27)-C(139)-C(140)	117.5(11)	N(27)-C(139)-C(150)	121.5(9)
C(140)-C(139)-C(150)	121.0(10)	C(141)-C(140)-C(149)	116.3(11)
C(141)-C(140)-C(139)	124.4(12)	C(149)-C(140)-C(139)	119.2(12)
C(140)-C(141)-C(142)	125.2(13)	C(143)-C(142)-C(141)	120.0(13)
C(148)-C(143)-C(142)	114.8(12)	C(148)-C(143)-C(144)	123.3(12)
C(142)-C(143)-C(144)	121.5(13)	C(143)-C(148)-C(149)	123.8(13)
C(140)-C(149)-C(148)	119.4(13)	C(139)-C(150)-C(151)	101.8(9)
N(28)-C(151)-C(152)	120.5(9)	N(28)-C(151)-C(150)	123.1(8)
C(152)-C(151)-C(150)	116.3(10)	C(153)-C(152)-C(161)	118.1(10)
C(153)-C(152)-C(151)	126.0(10)	C(161)-C(152)-C(151)	115.7(9)
C(152)-C(153)-C(154)	120.1(11)	C(155)-C(154)-C(153)	123.9(11)
C(160)-C(155)-C(154)	114.1(11)	C(160)-C(155)-C(156)	124.0(12)
C(154)-C(155)-C(156)	121.7(12)	C(155)-C(160)-C(161)	126.9(11)
C(152)-C(161)-C(160)	116.4(9)	C(138)-C(162)-N(28)	130.0(10)
C(138)-C(162)-C(163)	108.8(9)	N(28)-C(162)-C(163)	121.0(10)
N(20)-C(163)-N(19)	126.9(9)	N(20)-C(163)-C(162)	125.1(10)
N(19)-C(163)-C(162)	108.0(10)	N(20)-C(164)-N(21)	129.0(8)
N(20)-C(164)-C(165)	121.0(7)	N(21)-C(164)-C(165)	109.8(8)
N(29)-C(165)-C(189)	131.0(7)	N(29)-C(165)-C(164)	122.9(7)
C(189)-C(165)-C(164)	105.3(7)	N(29)-C(166)-C(167)	119.0(8)
N(29)-C(166)-C(177)	120.5(7)	C(167)-C(166)-C(177)	120.5(8)
C(168)-C(167)-C(176)	118.6(9)	C(168)-C(167)-C(166)	118.5(9)
C(176)-C(167)-C(166)	122.8(10)	C(169)-C(168)-C(167)	121.1(10)
C(168)-C(169)-C(170)	121.8(11)	C(175)-C(170)-C(169)	117.5(10)
C(175)-C(170)-C(171)	118.0(12)	C(169)-C(170)-C(171)	124.5(13)
C(170)-C(175)-C(176)	121.5(11)	C(167)-C(176)-C(175)	119.4(11)
C(178)-C(177)-C(166)	106.4(9)	N(30)-C(178)-C(179)	117.3(9)
N(30)-C(178)-C(177)	119.2(9)	C(179)-C(178)-C(177)	123.5(9)
C(180)-C(179)-C(188)	113.9(10)	C(180)-C(179)-C(178)	124.7(10)
C(188)-C(179)-C(178)	121.4(10)	C(179)-C(180)-C(181)	123.2(11)
C(182)-C(181)-C(180)	121.9(12)	C(187)-C(182)-C(181)	114.4(11)
C(187)-C(182)-C(183)	124.1(13)	C(181)-C(182)-C(183)	121.4(12)
C(182)-C(187)-C(188)	122.1(12)	C(179)-C(188)-C(187)	124.4(12)
N(30)-C(189)-C(165)	129.1(7)	N(30)-C(189)-C(190)	123.7(7)
C(165)-C(189)-C(190)	106.3(8)	N(22)-C(190)-N(21)	125.6(7)
N(22)-C(190)-C(189)	121.0(8)	N(21)-C(190)-C(189)	113.4(7)
N(22)-C(191)-N(23)	126.8(8)	N(22)-C(191)-C(192)	120.5(8)
N(23)-C(191)-C(192)	112.8(7)	N(31)-C(192)-C(215)	132.0(8)
N(31)-C(192)-C(191)	123.9(8)	C(215)-C(192)-C(191)	103.4(8)
N(31)-C(193)-C(194)	116.9(9)	N(31)-C(193)-C(204)	118.7(8)
C(194)-C(193)-C(204)	124.3(9)	C(195)-C(194)-C(203)	116.3(11)
C(195)-C(194)-C(193)	121.8(10)	C(203)-C(194)-C(193)	121.9(11)
C(196)-C(195)-C(194)	121.6(12)	C(195)-C(196)-C(197)	123.0(13)
C(202)-C(197)-C(196)	115.0(11)	C(202)-C(197)-C(198)	122.3(13)
C(196)-C(197)-C(198)	122.6(13)	C(197)-C(202)-C(203)	123.5(13)
C(194)-C(203)-C(202)	120.4(12)	C(193)-C(204)-C(205)	108.0(8)
N(32)-C(205)-C(204)	120.8(7)	N(32)-C(205)-C(206)	117.3(8)
C(204)-C(205)-C(206)	121.8(8)	C(207)-C(206)-C(214)	118.0(9)
C(207)-C(206)-C(205)	123.0(10)	C(214)-C(206)-C(205)	118.9(9)
C(206)-C(207)-C(208)	121.3(10)	C(209)-C(208)-C(207)	121.4(10)
C(208)-C(209)-C(22)	117.7(9)	C(208)-C(209)-C(210)	123.6(12)
C(22)-C(209)-C(210)	118.8(12)	C(22)-C(214)-C(206)	119.1(10)
C(192)-C(215)-N(32)	128.0(8)	C(192)-C(215)-C(216)	109.1(8)
N(32)-C(215)-C(216)	122.1(8)	N(24)-C(216)-N(23)	128.2(7)
N(24)-C(216)-C(215)	122.9(8)	N(23)-C(216)-C(215)	108.9(7)
C(12)-C(9)-C(11)	107.3(12)	C(12)-C(9)-C(10)	95.7(15)
C(11)-C(9)-C(10)	117.1(18)	C(12)-C(9)-C(8)	111.4(12)
C(11)-C(9)-C(8)	112.2(12)	C(10)-C(9)-C(8)	111.8(18)
C(12)-C(9)-C(10A)	119.9(17)	C(11)-C(9)-C(10A)	100.0(16)
C(8)-C(9)-C(10A)	105.6(17)	C(24)-C(21)-C(23)	134.9(17)
C(23A)-C(21)-C(25)	132.7(18)	C(24)-C(21)-C(25)	97.9(12)
C(23)-C(21)-C(25)	104.0(14)	C(23A)-C(21)-C(20)	115.4(16)
C(24)-C(21)-C(20)	102.3(11)	C(23)-C(21)-C(20)	106.0(15)
C(25)-C(21)-C(20)	110.5(13)	C(40)-C(37)-C(38)	105.0(12)
C(40)-C(37)-C(39)	112.0(12)	C(38)-C(37)-C(39)	106.0(12)
C(40)-C(37)-C(36)	113.6(11)	C(38)-C(37)-C(36)	110.2(12)
C(39)-C(37)-C(36)	109.7(12)	C(50)-C(49)-C(52)	110.1(12)
C(50)-C(49)-C(51)	111.1(12)	C(52)-C(49)-C(51)	106.1(12)
C(50)-C(49)-C(48)	111.0(11)	C(52)-C(49)-C(48)	107.6(11)
C(51)-C(49)-C(48)	110.8(11)	C(67)-C(64)-C(66)	114.5(15)
C(67)-C(64)-C(63)	108.9(13)	C(66)-C(64)-C(63)	109.1(13)
C(67)-C(64)-C(65)	105.9(13)	C(66)-C(64)-C(65)	107.7(13)
C(63)-C(64)-C(65)	110.7(13)	C(77)-C(76)-C(79)	107.2(14)
C(77)-C(76)-C(78)	103.3(14)	C(79)-C(76)-C(78)	112.2(14)
C(77)-C(76)-C(75)	117.2(14)	C(79)-C(76)-C(75)	109.7(13)
C(78)-C(76)-C(75)	107.1(13)	C(92A)-C(91)-C(93A)	107(2)
C(92A)-C(91)-C(90)	112.2(19)	C(93A)-C(91)-C(90)	108.0(18)
C(90)-C(91)-C(94)	115.9(17)	C(90)-C(91)-C(93)	112.8(17)
C(94)-C(91)-C(93)	115(2)	C(90)-C(91)-C(92)	106.4(17)
C(94)-C(91)-C(92)	111(2)	C(93)-C(91)-C(92)	93.0(18)
C(92A)-C(91)-C(94A)	111(2)	C(93A)-C(91)-C(94A)	107.7(19)
C(90)-C(91)-C(94A)	111.1(18)	C(104)-C(103)-C(106)	103.0(12)
C(104)-C(103)-C(105)	110.4(13)	C(106)-C(103)-C(105)	108.3(13)
C(104)-C(103)-C(102)	106.6(11)	C(106)-C(103)-C(102)	110.0(12)
C(105)-C(103)-C(102)	117.6(12)	C(130)-C(129)-C(132)	111.1(13)
C(130)-C(129)-C(131)	110.7(12)	C(132)-C(129)-C(131)	101.5(12)
C(130)-C(129)-C(128)	110.2(11)	C(132)-C(129)-C(128)	109.1(11)
C(131)-C(129)-C(128)	114.0(12)	C(145)-C(144)-C(146)	110.3(12)
C(145)-C(144)-C(147)	112.9(12)	C(146)-C(144)-C(147)	107.7(12)
C(145)-C(144)-C(143)	110.8(11)	C(146)-C(144)-C(143)	106.7(12)
C(147)-C(144)-C(143)	108.2(12)	C(159)-C(156)-C(157)	111.4(15)
C(159)-C(156)-C(158)	103.8(15)	C(157)-C(156)-C(158)	117.2(15)
C(159)-C(156)-C(155)	106.7(13)	C(157)-C(156)-C(155)	105.6(13)
C(158)-C(156)-C(155)	111.9(13)	C(172)-C(171)-C(174)	117.2(14)

C(172)-C(171)-C(173)	100.3(12)	C(174)-C(171)-C(173)	102.1(12)
C(172)-C(171)-C(170)	109.8(12)	C(174)-C(171)-C(170)	116.8(12)
C(173)-C(171)-C(170)	108.5(12)	C(182)-C(183)-C(184)	110.4(12)
C(182)-C(183)-C(186)	110.7(12)	C(184)-C(183)-C(186)	107.6(12)
C(182)-C(183)-C(185)	113.0(11)	C(184)-C(183)-C(185)	107.3(12)
C(186)-C(183)-C(185)	107.7(11)	C(201)-C(198)-C(199)	109.3(12)
C(201)-C(198)-C(200)	105.0(12)	C(199)-C(198)-C(200)	109.5(12)
C(201)-C(198)-C(197)	112.0(11)	C(199)-C(198)-C(197)	110.1(11)
C(200)-C(198)-C(197)	110.9(12)	C(03A)-C(210)-C(02A)	107(2)
C(03A)-C(210)-C(01A)	111(2)	C(02A)-C(210)-C(01A)	112(2)
C(213)-C(210)-C(211)	119(2)	C(213)-C(210)-C(212)	105.4(19)
C(211)-C(210)-C(212)	107(2)	C(03A)-C(210)-C(209)	108.1(16)
C(02A)-C(210)-C(209)	113.3(18)	C(01A)-C(210)-C(209)	105.2(16)
C(213)-C(210)-C(209)	106.0(16)	C(211)-C(210)-C(209)	110.6(17)
C(212)-C(210)-C(209)	108.3(16)		

UV-vis and TD-DFT study

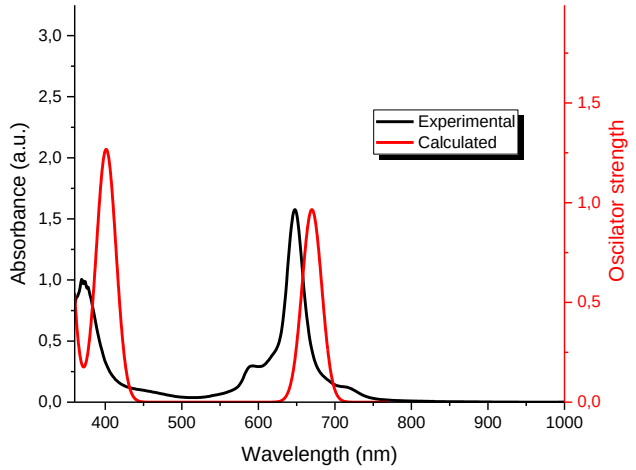

Fig. S14 Calculated (TD-DFT) and experimental (pyridine solution) spectra of the *t*Bu$_8$Dz$_4$PzMg monomer.

DFT calculation details

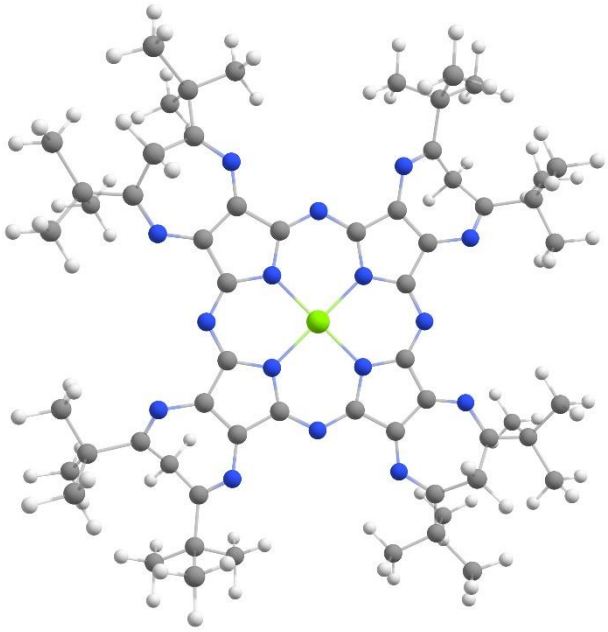

Table S4 Optimized geometry of *t*Bu$_8$Dz$_4$PzMg (monomer)

CARTESIAN COORDINATES (ANGSTROEM)

C	2.448165000000	-3.507067000000	-0.049951000000	C	3.506486000000	2.447956000000	0.059678000000
C	3.458646000000	-2.514518000000	-0.040182000000	C	2.514146000000	3.458645000000	0.047744000000
C	2.769682000000	-1.211655000000	0.002142000000	C	1.211112000000	2.769791000000	0.007612000000
C	1.157999000000	-2.794544000000	-0.009879000000	C	2.793727000000	1.157889000000	0.021984000000
C	-3.507089000000	-2.448811000000	0.058723000000	C	3.654585000000	-5.476531000000	-0.355536000000
C	-2.514749000000	-3.459529000000	0.048817000000	C	4.665413000000	-4.743703000000	-1.239848000000
C	-1.211635000000	-2.770700000000	0.009777000000	C	5.410908000000	-3.744222000000	-0.363213000000
C	-2.794246000000	-1.158818000000	0.021003000000	H	5.342712000000	-5.435342000000	-1.767420000000
C	-2.448454000000	3.506124000000	-0.053504000000	H	4.080957000000	-4.159879000000	-1.991566000000
C	-3.459033000000	2.513631000000	-0.042576000000	N	-1.436225000000	-1.408650000000	0.023573000000
C	-2.770141000000	1.210679000000	-0.000184000000	N	-0.033068000000	-3.400576000000	-0.003629000000
C	-1.158354000000	2.793550000000	-0.013459000000	N	-1.408114000000	1.435461000000	-0.013099000000

N	-3.400141000000	0.032223000000	0.013971000000
N	1.435701000000	1.407778000000	0.022717000000
N	3.399614000000	-0.033151000000	0.015822000000
N	0.032609000000	3.399676000000	-0.007219000000
N	2.598525000000	-4.853688000000	0.074816000000
N	4.802066000000	-2.683880000000	0.080355000000
N	1.407666000000	-1.436444000000	-0.010104000000
C	-3.654566000000	5.475876000000	-0.358666000000
C	-4.667465000000	4.743027000000	-1.240545000000
C	-5.411365000000	3.744152000000	-0.361743000000
H	-5.345744000000	5.434665000000	-1.766891000000
H	-4.084921000000	4.158586000000	-1.993251000000
N	-2.598214000000	4.852777000000	0.070598000000
N	-4.802131000000	2.683415000000	0.080287000000
Mg	-0.000110000000	-0.000503000000	0.006973000000
C	3.745438000000	5.411453000000	0.362312000000
C	4.744603000000	4.669145000000	1.242100000000
C	5.476754000000	3.654231000000	0.362018000000
H	5.436562000000	5.348416000000	1.766759000000
H	4.160354000000	4.088311000000	1.996283000000
N	2.684176000000	4.801535000000	-0.077572000000
N	4.853153000000	2.597215000000	-0.064976000000
C	-5.477944000000	-3.654723000000	0.358765000000
C	-4.747193000000	-4.669090000000	1.240656000000
C	-3.746819000000	-5.412031000000	0.362854000000
H	-5.439991000000	-5.347966000000	1.764726000000
H	-4.163992000000	-4.087817000000	1.995311000000
N	-4.853549000000	-2.598086000000	-0.067980000000
N	-2.684800000000	-4.802524000000	-0.075829000000
C	-3.865897000000	-6.906755000000	0.009749000000
C	6.907691000000	-3.861445000000	-0.017980000000
C	3.847267000000	-6.938342000000	0.080598000000
C	-6.906991000000	3.862620000000	-0.012131000000
C	-3.844831000000	6.938473000000	0.076070000000
C	3.864240000000	6.906175000000	0.009098000000
C	6.939319000000	3.842854000000	-0.073608000000
C	-6.940090000000	-3.843081000000	-0.078341000000
C	2.457163000000	-7.594795000000	0.247339000000
H	1.830114000000	-7.019061000000	0.957088000000
H	1.914405000000	-7.625966000000	-0.722993000000
H	2.574741000000	-8.637417000000	0.618786000000
C	-2.667503000000	-7.605980000000	0.707058000000
H	-1.711959000000	-7.151345000000	0.371262000000
H	-2.730860000000	-7.499963000000	1.813405000000
H	-2.664489000000	-8.692549000000	0.463366000000
C	7.600506000000	-2.659722000000	-0.716087000000
H	7.486883000000	-2.719683000000	-1.821861000000
H	7.146636000000	-1.705992000000	-0.374162000000
H	8.688733000000	-2.655808000000	-0.479919000000
C	-7.603407000000	2.662449000000	-0.709292000000
H	-7.494124000000	2.723892000000	-1.815426000000
H	-7.149051000000	1.707848000000	-0.370440000000
H	-8.690695000000	2.659083000000	-0.468828000000
C	-2.453589000000	7.594789000000	0.234269000000
H	-1.822558000000	7.019230000000	0.940618000000
H	-1.916755000000	7.625214000000	-0.739386000000
H	-2.568700000000	8.637689000000	0.605710000000
C	2.664910000000	7.604839000000	0.705425000000
H	1.709900000000	7.149636000000	0.368869000000
H	2.727440000000	7.498927000000	1.811828000000
H	2.661461000000	8.691393000000	0.461660000000
C	7.595183000000	2.450862000000	-0.227293000000
H	7.625517000000	1.917375000000	0.748204000000
H	7.019291000000	1.817623000000	-0.931396000000
H	8.638083000000	2.564364000000	-0.599225000000
C	-7.595166000000	-2.450960000000	-0.234201000000
H	-7.626352000000	-1.916288000000	0.740620000000
H	-7.018221000000	-1.818800000000	-0.938414000000
H	-8.637697000000	-2.564428000000	-0.607181000000
C	-3.728865000000	-7.074099000000	-1.520982000000
H	-3.704858000000	-8.153009000000	-1.794311000000
H	-4.582366000000	-6.600058000000	-2.054847000000
H	-2.793455000000	-6.591223000000	-1.873306000000
C	7.083054000000	-3.727935000000	1.512088000000
H	6.614535000000	-4.584290000000	2.046225000000
H	8.163351000000	-3.701461000000	1.779665000000
H	6.599361000000	-2.794905000000	1.869588000000
C	4.566068000000	-6.936861000000	1.453543000000
H	5.566816000000	-6.456760000000	1.392589000000
H	3.965671000000	-6.379746000000	2.204799000000
H	4.707558000000	-7.980040000000	1.817117000000
C	-7.077836000000	3.727829000000	1.518371000000
H	-6.606105000000	4.582807000000	2.051913000000
H	-8.157348000000	3.703015000000	1.789232000000
H	-6.594672000000	2.793593000000	1.873407000000
C	-4.556502000000	6.939216000000	1.452691000000
H	-5.557424000000	6.458713000000	1.397564000000
H	-3.952152000000	6.383416000000	2.201751000000
H	-4.696371000000	7.982965000000	1.815246000000
C	3.728333000000	7.073357000000	-1.521734000000
H	3.703443000000	8.152232000000	-1.795107000000
H	4.582794000000	6.600208000000	-2.054860000000
H	2.793718000000	6.589522000000	-1.874833000000
C	6.939902000000	4.550146000000	-1.452503000000
H	6.383614000000	3.943697000000	-2.199501000000
H	6.459807000000	5.551428000000	-1.400298000000
H	7.983589000000	4.688499000000	-1.815821000000
C	-6.939671000000	-4.551603000000	-1.456577000000
H	-6.382322000000	-3.946091000000	-2.203541000000
H	-6.460183000000	-5.553095000000	-1.403088000000
H	-7.983069000000	-4.689685000000	-1.820812000000
C	-5.172831000000	-7.559684000000	0.490738000000
H	-5.179152000000	-8.633908000000	0.202151000000
H	-5.284354000000	-7.516198000000	1.596717000000
H	-6.069509000000	-7.090123000000	0.032077000000
C	7.560661000000	-5.165684000000	-0.506233000000
H	7.510765000000	-5.274384000000	-1.612229000000
H	8.636647000000	-5.170149000000	-0.224256000000
H	7.096170000000	-6.064843000000	-0.047167000000
C	-7.559951000000	5.168167000000	-0.496779000000
H	-7.513828000000	5.278045000000	-1.602815000000
H	-8.634912000000	5.173784000000	-0.210942000000
H	-7.092530000000	6.066086000000	-0.038318000000
C	5.170472000000	7.559746000000	0.491035000000
H	5.176418000000	8.633953000000	0.202382000000
H	5.281215000000	7.516411000000	1.597096000000
H	6.067736000000	7.090646000000	0.033028000000
C	-7.757681000000	-4.667371000000	0.937637000000
H	-7.424965000000	-5.725526000000	1.001385000000
H	-7.704491000000	-4.223753000000	1.957038000000
H	-8.827515000000	-4.679786000000	0.632862000000
C	4.664926000000	-7.755428000000	-0.941202000000
H	4.213390000000	-7.703503000000	-1.957190000000
H	5.722122000000	-7.421287000000	-1.013367000000
H	4.681216000000	-8.825054000000	-0.635866000000
C	-4.667446000000	7.754164000000	-0.942792000000
H	-4.221396000000	7.700202000000	-1.961095000000
H	-5.725148000000	7.420415000000	-1.008648000000
H	-4.681540000000	8.824336000000	-0.639275000000
C	7.755486000000	4.668528000000	0.942398000000
H	7.422357000000	5.726646000000	1.004516000000
H	7.701353000000	4.226094000000	1.962260000000

H 8.825646000000 4.680958000000 0.638780000000

Table S5 TD-DFT calculated UV-Vis spectrum of *t*Bu$_8$Dz$_4$PzMg (monomer)

state	eV	nm	fL	fV	Rl	RV			
0	1.851	670.0	0.482592	0.851625	29.643740	39.263723	0.70 (139-> 140)	0.24 (139-> 141)	0.02 (138-> 141)
1	1.851	669.9	0.482763	0.851834	-29.391594	-38.937041	0.70 (139-> 141)	0.24 (139-> 140)	0.02 (138-> 140)
2	2.906	426.7	0.000396	0.000946	-1.371706	-2.034510	0.83 (137-> 141)	0.03 (134-> 140)	0.03 (134-> 141)
3	2.906	426.6	0.000393	0.000918	1.400589	2.061209	0.83 (137-> 140)	0.03 (134-> 141)	0.03 (134-> 140)
4	2.939	421.8	0.000000	0.000000	0.095571	-0.069935	0.42 (135-> 140)	0.42 (136-> 141)	0.05 (136-> 140)
5	2.950	420.3	0.000011	0.000018	0.025506	0.032006	0.33 (135-> 141)	0.33 (136-> 140)	0.15 (136-> 141)
6	3.091	401.2	0.633192	0.672879	170.149042	175.384927	0.74 (138-> 140)	0.06 (134-> 140)	0.05 (138-> 141)
7	3.091	401.1	0.633320	0.672793	-170.174084	-175.401039	0.74 (138-> 141)	0.06 (134-> 141)	0.05 (137-> 140)
8	3.101	399.8	0.000874	0.000800	0.029563	0.027533	0.33 (136-> 141)	0.33 (135-> 140)	0.14 (136-> 140)
9	3.164	391.9	0.000001	0.000001	-0.010852	-0.010790	0.44 (135-> 141)	0.44 (136-> 140)	0.05 (136-> 141)
10	3.336	371.7	0.001538	0.001659	-0.002587	-0.002688	0.94 (139-> 142)	0.01 (135-> 140)	0.01 (136-> 141)
11	3.476	356.7	0.002539	0.003452	-13.336334	-14.988002	0.91 (130-> 140)	0.02 (134-> 141)	0.01 (123-> 140)
12	3.476	356.7	0.002670	0.003615	13.734937	15.422047	0.91 (130-> 141)	0.02 (134-> 140)	0.01 (123-> 141)
13	3.647	339.9	0.894280	0.936963	-0.094576	-0.106366	0.71 (134-> 140)	0.07 (138-> 140)	0.07 (134-> 141)
14	3.648	339.9	0.894985	0.937472	-0.405722	-0.410218	0.71 (134-> 141)	0.07 (138-> 141)	0.07 (134-> 140)
15	3.687	336.2	0.000015	0.000016	0.004294	0.020645	0.40 (132-> 141)	0.39 (131-> 140)	0.05 (129-> 142)
16	3.708	334.4	0.000018	0.000026	0.001678	0.002032	0.32 (131-> 140)	0.31 (132-> 141)	0.10 (131-> 141)
17	3.748	330.8	0.001084	0.001234	-3.870946	-3.360235	0.55 (133-> 141)	0.16 (129-> 141)	0.15 (133-> 140)
18	3.749	330.7	0.001058	0.001274	3.786467	3.267691	0.55 (133-> 140)	0.16 (129-> 140)	0.15 (133-> 141)
19	3.764	329.4	0.010109	0.010676	-0.018524	-0.018870	0.15 (131-> 141)	0.15 (132-> 140)	0.09 (125-> 140)
20	3.918	316.4	0.000000	0.000000	-0.001688	-0.001464	0.30 (132-> 140)	0.30 (131-> 141)	0.10 (128-> 141)
21	4.054	305.8	0.000000	0.000000	-0.016326	0.034607	0.27 (128-> 140)	0.27 (127-> 141)	0.14 (125-> 141)
22	4.130	300.2	0.051093	0.048182	-0.496365	-0.477330	0.66 (129-> 140)	0.16 (133-> 140)	0.04 (133-> 141)
23	4.130	300.2	0.050653	0.047767	0.557120	0.536401	0.66 (129-> 141)	0.16 (133-> 141)	0.04 (133-> 140)
24	4.153	298.6	0.000008	0.000011	-0.002715	-0.003365	0.16 (125-> 141)	0.16 (124-> 140)	0.12 (128-> 140)
25	4.236	292.7	0.002101	0.002072	0.100016	0.099326	0.19 (132-> 140)	0.19 (131-> 141)	0.11 (127-> 140)
26	4.322	286.9	0.000002	0.000002	-0.007531	-0.006362	0.25 (128-> 141)	0.25 (127-> 140)	0.15 (131-> 141)
27	4.326	286.6	0.024601	0.018184	55.249318	47.405252	0.77 (139-> 143)	0.10 (139-> 144)	0.01 (126-> 141)
28	4.326	286.6	0.024509	0.018091	-55.115955	-47.261059	0.77 (139-> 144)	0.10 (139-> 143)	0.01 (126-> 140)
29	4.345	285.3	0.000018	0.000029	-0.002483	-0.002165	0.87 (139-> 146)	0.03 (138-> 142)	0.01 (132-> 141)
30	4.391	282.4	0.000001	0.000001	-0.054605	-0.049642	0.75 (139-> 145)	0.06 (124-> 141)	0.06 (125-> 140)
31	4.510	274.9	0.000000	0.000000	-0.126518	-0.141649	0.82 (139-> 147)	0.06 (137-> 142)	0.01 (132-> 141)
32	4.549	272.6	0.005573	0.006040	-0.640909	-0.667223	0.20 (124-> 141)	0.20 (125-> 140)	0.10 (127-> 140)
33	4.582	270.6	0.000001	0.000001	0.761979	0.720860	0.27 (124-> 140)	0.26 (125-> 141)	0.15 (128-> 140)
34	4.615	268.6	0.000005	0.000005	-0.007305	-0.016921	0.25 (125-> 140)	0.24 (124-> 141)	0.19 (139-> 145)
35	4.623	268.2	0.047018	0.042598	-1.687049	-1.661780	0.53 (126-> 141)	0.11 (126-> 140)	0.10 (123-> 141)
36	4.623	268.2	0.047786	0.043344	1.447512	1.432777	0.53 (126-> 140)	0.11 (126-> 141)	0.10 (123-> 140)
37	4.663	265.9	0.000794	0.000835	0.153110	0.156933	0.33 (138-> 142)	0.09 (127-> 141)	0.09 (128-> 140)
38	4.691	264.3	0.318267	0.305142	162.694903	159.115675	0.22 (135-> 142)	0.08 (123-> 140)	0.07 (136-> 142)
39	4.691	264.3	0.317291	0.304031	-161.490318	-157.916451	0.22 (136-> 142)	0.08 (123-> 141)	0.07 (135-> 142)
40	4.692	264.3	0.001281	0.001225	-0.580171	-0.568330	0.99 (139-> 150)	0.00 (139-> 153)	0.00 (123-> 150)
41	4.705	263.5	0.000005	0.000005	-0.002793	-0.209071	0.64 (137-> 142)	0.13 (139-> 147)	0.03 (138-> 145)
42	4.792	258.7	0.055633	0.054103	57.336277	56.383023	0.46 (122-> 140)	0.19 (122-> 141)	0.03 (136-> 142)
43	4.792	258.7	0.055442	0.053951	-58.019827	-57.074724	0.46 (122-> 141)	0.19 (122-> 140)	0.03 (135-> 142)
44	4.848	255.7	0.067869	0.071972	-0.384475	-0.396057	0.25 (138-> 146)	0.16 (137-> 147)	0.09 (136-> 144)
45	4.868	254.7	0.003369	0.002923	-15.061573	-13.712743	0.69 (139-> 148)	0.05 (136-> 142)	0.04 (139-> 149)
46	4.868	254.7	0.003563	0.003091	15.643729	14.223579	0.68 (139-> 149)	0.05 (135-> 142)	0.04 (139-> 148)
47	4.883	253.9	0.017148	0.014150	28.086315	25.945912	0.11 (119-> 140)	0.08 (136-> 147)	0.07 (135-> 142)
48	4.883	253.9	0.017284	0.014243	-28.595434	-26.411261	0.12 (119-> 141)	0.08 (135-> 147)	0.07 (138-> 143)
49	4.912	252.4	0.000006	0.000006	-0.047517	-0.047714	0.18 (137-> 146)	0.15 (138-> 147)	0.06 (136-> 143)
50	4.936	251.2	0.000074	0.000069	-0.015909	-0.015427	0.35 (138-> 142)	0.11 (124-> 140)	0.11 (125-> 141)
51	5.001	247.9	0.053274	0.046599	-22.946440	-21.488995	0.32 (119-> 141)	0.21 (119-> 140)	0.14 (123-> 140)
52	5.002	247.9	0.055347	0.048367	24.441268	22.873333	0.33 (119-> 140)	0.21 (119-> 141)	0.12 (123-> 141)
53	5.012	247.4	0.013350	0.011464	-7.739725	-7.261637	0.28 (123-> 140)	0.19 (123-> 141)	0.15 (126-> 140)
54	5.012	247.4	0.012919	0.011066	6.347663	5.960237	0.28 (123-> 141)	0.18 (123-> 140)	0.15 (126-> 141)
55	5.069	244.6	0.000026	0.000030	0.015507	0.016760	0.40 (134-> 142)	0.17 (138-> 142)	0.14 (137-> 145)
56	5.139	241.2	0.000001	0.000001	-0.178316	-0.220565	0.22 (137-> 142)	0.21 (138-> 145)	0.07 (135-> 143)
57	5.217	237.7	0.025992	0.026783	25.823925	25.646085	0.16 (135-> 142)	0.12 (136-> 145)	0.10 (138-> 144)
58	5.217	237.7	0.025883	0.026715	-25.589786	-25.407649	0.16 (136-> 142)	0.12 (135-> 145)	0.10 (138-> 143)
59	5.272	235.2	0.000000	0.000000	-0.231087	-0.279063	0.36 (121-> 140)	0.35 (120-> 141)	0.05 (127-> 141)
60	5.316	233.2	0.000006	0.000008	-0.001406	-0.001687	0.52 (134-> 142)	0.13 (137-> 145)	0.06 (133-> 142)

61	5.330	232.6	0.003655	0.004483	0.049957	0.055341	0.26 (121-> 141)	0.26 (120-> 140)	0.15 (120-> 141)
62	5.425	228.5	0.000001	0.000001	0.011028	0.009808	0.36 (120-> 140)	0.36 (121-> 141)	0.04 (129-> 146)
63	5.529	224.2	0.000212	0.000029	0.012989	0.004981	0.57 (139-> 151)	0.24 (130-> 142)	0.01 (128-> 143)
64	5.550	223.4	0.000000	0.000000	0.032402	0.030867	0.94 (139-> 152)	0.01 (138-> 145)	0.01 (139-> 147)
65	5.581	222.2	0.001909	0.001696	-0.020781	-0.019606	0.51 (130-> 142)	0.20 (139-> 151)	0.04 (120-> 141)
66	5.598	221.5	0.000055	0.000026	-0.006897	-0.004720	0.15 (121-> 140)	0.15 (120-> 141)	0.13 (121-> 141)
67	5.620	220.6	0.000114	0.000063	0.005842	0.004581	0.44 (133-> 142)	0.09 (137-> 145)	0.05 (120-> 141)
68	5.643	219.7	0.006364	0.006647	0.566084	0.640094	0.41 (118-> 141)	0.14 (117-> 141)	0.06 (132-> 146)
69	5.643	219.7	0.006643	0.006896	-0.751632	-0.817748	0.41 (118-> 140)	0.14 (117-> 140)	0.06 (131-> 146)
70	5.673	218.6	0.160765	0.140047	-31.646250	-29.820946	0.51 (132-> 142)	0.08 (137-> 143)	0.05 (129-> 143)
71	5.673	218.5	0.160966	0.140150	32.019436	30.174868	0.51 (131-> 142)	0.08 (137-> 144)	0.05 (129-> 144)
72	5.717	216.9	0.000005	0.000005	-0.010908	-0.009394	0.38 (129-> 142)	0.11 (138-> 145)	0.07 (133-> 145)
73	5.776	214.6	0.000385	0.000109	0.017963	-0.010542	0.12 (133-> 146)	0.11 (115-> 141)	0.11 (116-> 140)
74	5.819	213.1	0.000078	0.000068	-0.001685	-0.001546	0.11 (119-> 142)	0.11 (109-> 141)	0.11 (108-> 140)
75	5.848	212.0	0.000016	0.000014	-0.005862	-0.004945	0.22 (116-> 140)	0.21 (115-> 141)	0.12 (126-> 142)
76	5.857	211.7	0.255428	0.212252	8.475877	7.707928	0.26 (138-> 143)	0.18 (138-> 144)	0.11 (137-> 143)
77	5.857	211.7	0.255393	0.212118	-7.754232	-7.042711	0.26 (138-> 144)	0.18 (138-> 143)	0.12 (137-> 144)
78	5.915	209.6	0.000439	0.000558	0.015297	0.017200	0.42 (138-> 146)	0.23 (137-> 147)	0.10 (134-> 146)
79	5.943	208.6	0.022877	0.017801	8.852098	7.881797	0.36 (128-> 142)	0.10 (118-> 141)	0.07 (130-> 143)
80	5.943	208.6	0.023490	0.018291	-8.819640	-7.854027	0.36 (127-> 142)	0.10 (118-> 140)	0.07 (130-> 144)
81	5.994	206.8	0.000000	0.000000	-0.074012	-0.078044	0.35 (138-> 145)	0.28 (134-> 145)	0.08 (135-> 144)

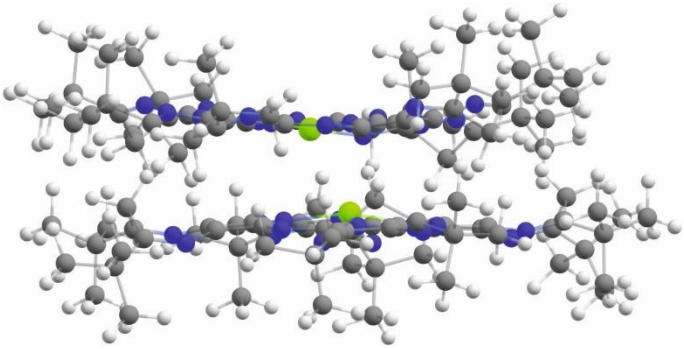

Table S6 Optimized geometry of [*t*Bu$_8$Dz$_4$PzMg]$_2$ (dimer)

CARTESIAN COORDINATES (ANGSTROEM)

C	-3.751206000000	-0.314037000000	-1.395852000000	H	-7.439276000000	0.425110000000	-0.342371000000
C	-3.773017000000	1.096396000000	-1.520823000000	H	-5.738175000000	0.539375000000	0.229447000000
C	-2.362844000000	1.541944000000	-1.493376000000	H	0.551421000000	-7.448850000000	-0.393847000000
C	-2.338361000000	-0.702302000000	-1.308903000000	H	0.661729000000	-5.747538000000	0.178463000000
C	1.146290000000	-3.775541000000	-1.582703000000	N	0.461587000000	-1.561334000000	-1.357159000000
C	-0.260544000000	-3.769949000000	-1.424802000000	N	-1.936791000000	-1.973341000000	-1.276570000000
C	-0.662358000000	-2.360817000000	-1.331121000000	N	2.448511000000	0.436204000000	-1.741659000000
C	1.575828000000	-2.360840000000	-1.564702000000	N	2.835467000000	-1.965910000000	-1.750377000000
C	4.642402000000	1.143702000000	-1.962468000000	N	0.422895000000	2.442492000000	-1.701324000000
C	4.634935000000	-0.274732000000	-1.995273000000	N	-1.980658000000	2.809788000000	-1.647651000000
C	3.232538000000	-0.690167000000	-1.824965000000	N	2.820093000000	2.836360000000	-1.872550000000
C	3.232041000000	1.562956000000	-1.857189000000	N	-1.154088000000	5.654926000000	-2.160663000000
C	-0.305287000000	4.632158000000	-1.870275000000	N	1.954548000000	5.684361000000	-2.126751000000
C	1.113575000000	4.642739000000	-1.894991000000	N	-4.758483000000	-1.211709000000	-1.536253000000
C	1.542494000000	3.233860000000	-1.828012000000	N	-4.833505000000	1.857983000000	-1.899331000000
C	-0.709603000000	3.222416000000	-1.732300000000	N	1.913988000000	-4.824508000000	-1.980316000000
C	-0.846889000000	6.896924000000	-1.934887000000	N	-1.148510000000	-4.788574000000	-1.542903000000
C	0.364254000000	7.218487000000	-1.059696000000	N	-1.550991000000	0.430808000000	-1.308762000000
C	1.630059000000	6.915469000000	-1.852347000000	C	6.916180000000	1.660797000000	-1.940912000000
C	-6.006058000000	-0.928307000000	-1.305350000000	C	7.232779000000	0.357375000000	-1.208512000000
C	-6.386843000000	0.400927000000	-0.666564000000	C	6.895949000000	-0.807313000000	-2.132780000000
C	-6.065880000000	1.498732000000	-1.677350000000	H	8.270555000000	0.323848000000	-0.837161000000
C	1.581715000000	-6.061803000000	-1.747575000000	H	6.531906000000	0.285725000000	-0.342883000000
C	0.508597000000	-6.396428000000	-0.714714000000	N	5.680373000000	1.994650000000	-2.178352000000
C	-0.841347000000	-6.031549000000	-1.317893000000	N	5.650002000000	-1.107355000000	-2.347179000000
H	0.342818000000	8.249384000000	-0.668240000000	Mg	0.497174000000	0.484156000000	-1.238559000000
H	0.328488000000	6.503940000000	-0.203410000000	C	-2.913449000000	-3.879893000000	2.199824000000

C	-3.914499000000	-2.874489000000	2.166514000000
C	-3.217540000000	-1.592520000000	1.964890000000
C	-1.623151000000	-3.193859000000	1.995179000000
C	3.033945000000	-2.900938000000	1.574018000000
C	2.049250000000	-3.905081000000	1.740346000000
C	0.743374000000	-3.207782000000	1.789699000000
C	2.320978000000	-1.623029000000	1.497461000000
C	2.020118000000	3.013365000000	1.438116000000
C	3.025956000000	2.014505000000	1.400874000000
C	2.334226000000	0.727345000000	1.258867000000
C	0.733150000000	2.328279000000	1.295166000000
C	-3.904829000000	2.085019000000	1.702368000000
C	-2.887890000000	3.061438000000	1.575253000000
C	-1.615750000000	2.338080000000	1.531354000000
C	-3.218079000000	0.773621000000	1.771335000000
C	-5.827386000000	3.395967000000	1.578012000000
C	-5.164718000000	4.356177000000	0.595175000000
C	-4.035009000000	5.073117000000	1.324808000000
C	-4.154381000000	-5.842561000000	2.419489000000
C	-5.281043000000	-5.258946000000	1.576665000000
C	-5.902767000000	-4.084759000000	2.331392000000
C	5.031016000000	-4.081111000000	1.368128000000
C	4.301503000000	-5.224692000000	0.671215000000
C	3.334509000000	-5.848784000000	1.670723000000
H	-4.697392000000	3.750385000000	-0.217713000000
H	-5.884297000000	5.057992000000	0.145068000000
H	-4.815749000000	-4.842283000000	0.652649000000
H	-6.030016000000	-6.015536000000	1.289547000000
H	3.701962000000	-4.773043000000	-0.154800000000
H	4.996518000000	-5.963143000000	0.242306000000
N	0.968872000000	-1.855069000000	1.617993000000
N	-0.436430000000	-3.813959000000	1.955423000000
N	0.963950000000	0.963334000000	1.082698000000
N	2.942500000000	-0.448389000000	1.359642000000
N	-1.859550000000	0.989022000000	1.642566000000
N	-3.833458000000	-0.403510000000	1.910673000000
N	-0.434156000000	2.947604000000	1.413299000000
N	-5.224055000000	2.300744000000	1.947070000000
N	-2.969888000000	4.412790000000	1.661906000000
N	-3.043680000000	-5.182021000000	2.571577000000
N	-5.234929000000	-2.979218000000	2.477539000000
N	4.384979000000	-2.996242000000	1.667291000000
N	2.250399000000	-5.218657000000	2.027250000000
N	-1.867762000000	-1.845068000000	1.846447000000
C	4.999168000000	3.261156000000	1.559261000000
C	4.383188000000	4.440447000000	0.805525000000
C	3.254945000000	4.980364000000	1.681695000000
H	5.129256000000	5.213616000000	0.557396000000
H	3.941028000000	4.054290000000	-0.145701000000
N	4.345122000000	2.145314000000	1.700585000000
N	2.149799000000	4.309871000000	1.819447000000
Mg	-0.477313000000	-0.462733000000	1.444439000000
C	-7.322084000000	-4.145435000000	2.919884000000
C	2.314174000000	-7.119566000000	-2.600204000000
C	-1.918003000000	-7.074878000000	-1.673000000000
C	2.616521000000	7.994335000000	-2.345602000000
C	-1.720796000000	7.980863000000	-2.585078000000
C	-7.131710000000	2.208532000000	-2.538916000000
C	-7.038928000000	-2.003061000000	-1.697394000000
C	7.946695000000	-1.680138000000	-2.842926000000
C	8.012082000000	2.626186000000	-2.428813000000
C	6.521447000000	-4.134689000000	1.743631000000
C	3.541785000000	-7.236453000000	2.310923000000
C	-4.066969000000	6.568996000000	1.683112000000
C	-7.216096000000	3.635366000000	2.203128000000
C	-4.233296000000	-7.217254000000	3.112422000000
C	3.314750000000	6.316198000000	2.454078000000
C	6.381065000000	3.337222000000	2.240573000000
C	8.441874000000	2.225266000000	-3.861216000000
H	9.180231000000	2.957989000000	-4.259030000000
H	8.918648000000	1.222722000000	-3.877644000000
H	7.564933000000	2.204226000000	-4.543906000000
C	-7.282688000000	-4.865482000000	4.289827000000
H	-8.295444000000	-4.857830000000	4.752749000000
H	-6.965936000000	-5.924812000000	4.190945000000
H	-6.578581000000	-4.355482000000	4.982641000000
C	2.152650000000	-6.728714000000	-4.089143000000
H	2.698672000000	-7.447090000000	-4.741378000000
H	1.079780000000	-6.733888000000	-4.385218000000
H	2.549224000000	-5.706506000000	-4.262102000000
C	-1.994353000000	-7.198804000000	-3.213584000000
H	-1.032909000000	-7.560937000000	-3.641334000000
H	-2.793795000000	-7.916268000000	-3.507720000000
H	-2.219676000000	-6.209268000000	-3.666010000000
C	2.719261000000	7.911919000000	-3.887926000000
H	1.753179000000	8.163361000000	-4.374936000000
H	3.491533000000	8.620616000000	-4.263594000000
H	2.999161000000	6.881487000000	-4.193152000000
C	-1.059252000000	8.421888000000	-3.915130000000
H	-1.719857000000	9.143935000000	-4.446405000000
H	-0.083337000000	8.921711000000	-3.740976000000
H	-0.887798000000	7.547869000000	-4.580084000000
C	-6.746555000000	2.014735000000	-4.026265000000
H	-6.741573000000	0.936485000000	-4.300023000000
H	-7.473045000000	2.539594000000	-4.686912000000
H	-5.729321000000	2.418180000000	-4.212786000000
C	-7.246920000000	-1.965251000000	-3.230826000000
H	-7.931837000000	-2.783875000000	-3.548789000000
H	-7.693154000000	-1.001613000000	-3.560716000000
H	-6.275230000000	-2.092411000000	-3.754860000000
C	7.773954000000	-1.509688000000	-4.371981000000
H	7.960207000000	-0.461971000000	-4.690621000000
H	8.484849000000	-2.170442000000	-4.917781000000
H	6.737448000000	-1.776500000000	-4.669050000000
C	6.633638000000	-4.505697000000	3.243071000000
H	6.197180000000	-5.508272000000	3.445764000000
H	7.701576000000	-4.525622000000	3.558600000000
H	6.092895000000	-3.762934000000	3.868316000000
C	3.469707000000	-7.081823000000	3.848882000000
H	3.547100000000	-8.075827000000	4.344412000000
H	4.296740000000	-6.439915000000	4.225377000000
H	2.509623000000	-6.606359000000	4.139361000000
C	-4.501478000000	6.717281000000	3.161635000000
H	-4.478719000000	7.788479000000	3.465657000000
H	-5.534473000000	6.338578000000	3.322115000000
H	-3.818161000000	6.145886000000	3.826196000000
C	-7.066622000000	3.607542000000	3.743475000000
H	-6.415457000000	4.436806000000	4.097888000000
H	-8.061051000000	3.711310000000	4.233372000000
H	-6.604357000000	2.650139000000	4.062964000000
C	-4.141638000000	-7.000044000000	4.642747000000
H	-4.993458000000	-6.395845000000	5.021172000000
H	-4.147012000000	-7.979182000000	5.172900000000
H	-3.202393000000	-6.462617000000	4.893159000000
C	2.994943000000	6.040944000000	3.942878000000
H	3.768958000000	5.392985000000	4.409427000000
H	2.952589000000	6.996467000000	4.512594000000
H	2.017039000000	5.523230000000	4.031749000000
C	6.153961000000	3.605060000000	3.749385000000
H	7.129067000000	3.626898000000	4.286662000000
H	5.647492000000	4.579237000000	3.920616000000
H	5.521882000000	2.805882000000	4.192832000000

C	9.245972000000	2.613721000000	-1.500317000000
H	9.796243000000	1.648733000000	-1.539915000000
H	9.958450000000	3.410008000000	-1.809734000000
H	8.960651000000	2.805173000000	-0.442722000000
C	-8.289337000000	-4.888719000000	1.970937000000
H	-8.046768000000	-5.969832000000	1.877179000000
H	-9.328301000000	-4.819388000000	2.362674000000
H	-8.277705000000	-4.441997000000	0.952534000000
C	1.798581000000	-8.552755000000	-2.396416000000
H	0.738833000000	-8.656446000000	-2.710059000000
H	2.397209000000	-9.254572000000	-3.017865000000
H	1.884124000000	-8.889810000000	-1.340254000000
C	-1.657306000000	-8.454104000000	-1.038714000000
H	-1.516209000000	-8.375640000000	0.060604000000
H	-2.530345000000	-9.119283000000	-1.220102000000
H	-0.765725000000	-8.959025000000	-1.463777000000
C	2.229475000000	9.418908000000	-1.911722000000
H	2.987828000000	10.143572000000	-2.282001000000
H	1.245506000000	9.732900000000	-2.323041000000
H	2.188319000000	9.517546000000	-0.804133000000
C	-1.896230000000	9.213426000000	-1.672061000000
H	-0.938243000000	9.748068000000	-1.491854000000
H	-2.589099000000	9.938967000000	-2.152909000000
H	-2.326564000000	8.934341000000	-0.686563000000
C	-8.561321000000	1.691167000000	-2.312959000000
H	-9.269877000000	2.267654000000	-2.947557000000
H	-8.663320000000	0.621884000000	-2.592507000000
H	-8.891643000000	1.806951000000	-1.257850000000
C	-8.386687000000	-1.832212000000	-0.970631000000
H	-8.927038000000	-0.909680000000	-1.268689000000
H	-9.050254000000	-2.692965000000	-1.208054000000
H	-8.247919000000	-1.809961000000	0.132606000000
C	9.389493000000	-1.348719000000	-2.423912000000
H	10.098422000000	-2.025520000000	-2.949904000000
H	9.677943000000	-0.306011000000	-2.678584000000
H	9.540494000000	-1.491926000000	-1.330848000000
C	7.306301000000	-5.153106000000	0.893551000000
H	8.395046000000	-5.056108000000	1.100269000000
H	7.022110000000	-6.202316000000	1.119840000000
H	7.151897000000	-4.982368000000	-0.193405000000
C	4.867879000000	-7.911779000000	1.923556000000
H	5.747925000000	-7.330773000000	2.271985000000
H	4.926240000000	-8.915276000000	2.399619000000
H	4.962163000000	-8.060736000000	0.825335000000
C	-5.016848000000	7.373101000000	0.774424000000
H	-6.082961000000	7.100500000000	0.924828000000
H	-4.920886000000	8.458943000000	0.996626000000
H	-4.769679000000	7.227023000000	-0.299619000000
C	-7.872477000000	4.958092000000	1.773511000000
H	-8.873931000000	5.048511000000	2.249040000000
H	-7.276998000000	5.840398000000	2.090712000000
H	-8.022462000000	5.018477000000	0.673120000000
C	-5.505968000000	-8.007048000000	2.758230000000
H	-5.486396000000	-8.995148000000	3.268807000000
H	-6.434852000000	-7.488908000000	3.080520000000
H	-5.579043000000	-8.199225000000	1.664716000000
C	4.662158000000	7.046679000000	2.340059000000
H	4.612566000000	8.008323000000	2.896885000000
H	5.493262000000	6.455705000000	2.778509000000
H	4.925499000000	7.285999000000	1.286792000000
C	7.292240000000	4.426816000000	1.644470000000
H	6.925176000000	5.454811000000	1.843964000000
H	8.308554000000	4.349313000000	2.090113000000
H	7.397979000000	4.308647000000	0.544588000000
C	-3.267802000000	-6.535026000000	-1.137675000000
H	-3.234362000000	-6.460812000000	-0.029690000000
H	-3.467631000000	-5.520559000000	-1.538653000000
H	-4.096131000000	-7.222131000000	-1.422664000000
C	-7.836353000000	-2.706947000000	3.144771000000
H	-7.169381000000	-2.146749000000	3.829848000000
H	-7.864918000000	-2.140169000000	2.189346000000
H	-8.863229000000	-2.737910000000	3.572745000000
C	3.815550000000	-7.075354000000	-2.224950000000
H	3.970439000000	-7.418075000000	-1.178514000000
H	4.393941000000	-7.750154000000	-2.895542000000
H	4.213356000000	-6.043795000000	-2.322269000000
C	4.006910000000	7.648232000000	-1.751316000000
H	3.995176000000	7.719332000000	-0.641808000000
H	4.295641000000	6.612778000000	-2.027603000000
H	4.773443000000	8.359100000000	-2.133873000000
C	-3.105443000000	7.378129000000	-2.909260000000
H	-3.594352000000	6.986875000000	-1.991382000000
H	-3.759844000000	8.157688000000	-3.359376000000
H	-3.014179000000	6.526112000000	-3.612072000000
C	-7.089505000000	3.718987000000	-2.204713000000
H	-7.416784000000	3.900127000000	-1.158139000000
H	-6.060760000000	4.115837000000	-2.327718000000
H	-7.775757000000	4.276688000000	-2.881079000000
C	-6.448041000000	-3.377348000000	-1.302801000000
H	-6.312496000000	-3.423836000000	-0.201799000000
H	-7.139672000000	-4.194065000000	-1.608805000000
H	-5.454887000000	-3.532645000000	-1.770685000000
C	7.651182000000	-3.156017000000	-2.476154000000
H	7.846154000000	-3.335619000000	-1.397956000000
H	6.588336000000	-3.401086000000	-2.682424000000
H	8.309581000000	-3.835013000000	-3.063408000000
C	7.426513000000	4.055596000000	-2.481507000000
H	7.084957000000	4.382767000000	-1.475566000000
H	8.202129000000	4.768055000000	-2.841086000000
H	6.544227000000	4.099883000000	-3.150384000000
C	7.118829000000	-2.721876000000	1.530049000000
H	8.194138000000	-2.716864000000	1.817813000000
H	7.033905000000	-2.415062000000	0.464653000000
H	6.569142000000	-1.969256000000	2.130230000000
C	2.369931000000	-8.137058000000	1.843729000000
H	1.397082000000	-7.658705000000	2.081851000000
H	2.416500000000	-8.312255000000	0.746187000000
H	2.423093000000	-9.126446000000	2.351436000000
C	-2.628916000000	7.118964000000	1.523288000000
H	-1.919715000000	6.566285000000	2.171513000000
H	-2.281336000000	6.990438000000	0.475361000000
H	-2.604299000000	8.201845000000	1.779634000000
C	-8.126574000000	2.459153000000	1.769731000000
H	-9.121576000000	2.543700000000	2.261874000000
H	-8.285451000000	2.466579000000	0.669268000000
H	-7.664093000000	1.489809000000	2.049320000000
C	-3.001983000000	-8.041063000000	2.657548000000
H	-2.949209000000	-8.994204000000	3.230212000000
H	-3.074421000000	-8.292000000000	1.577450000000
H	-2.069889000000	-7.460364000000	2.818948000000
C	2.201679000000	7.223402000000	1.872835000000
H	2.165331000000	8.186735000000	2.429909000000
H	2.393087000000	7.447602000000	0.801974000000
H	1.216408000000	6.719011000000	1.953239000000
C	7.085774000000	1.970491000000	2.085410000000
H	6.432165000000	1.145403000000	2.433677000000
H	7.331537000000	1.782500000000	1.019717000000
H	8.035153000000	1.965793000000	2.666029000000

Table S7 TD-DFT calculated UV-Vis spectrum of [*t*Bu$_8$Dz$_4$PzMg]$_2$ (dimer)

state	eV	nm	fL	fV	Rl	RV			
0	1.441	860.7	0.012451	0.031443	-27.389298	-43.806555	0.72 (279-> 280)	0.25 (278-> 280)	0.01 (279-> 282)
1	1.491	831.4	0.007143	0.011189	-0.739969	0.113609	0.75 (279-> 281)	0.13 (279-> 283)	0.08 (278-> 281)
2	1.560	794.6	0.009794	0.023475	-1.388010	-2.791637	0.71 (279-> 282)	0.22 (278-> 282)	0.03 (279-> 283)
3	1.597	776.5	0.024552	0.037118	-9.358047	-14.028312	0.48 (279-> 283)	0.22 (278-> 281)	0.16 (278-> 283)
4	1.694	731.8	0.045949	0.094944	60.036593	86.370702	0.53 (278-> 280)	0.17 (278-> 282)	0.15 (279-> 280)
5	1.769	700.7	0.051333	0.106181	31.067373	44.252005	0.46 (278-> 281)	0.38 (278-> 283)	0.08 (279-> 281)
6	1.907	650.3	0.645964	1.165400	-31.005358	-41.716621	0.34 (278-> 283)	0.25 (279-> 283)	0.16 (278-> 281)
7	1.927	643.4	0.624664	1.117100	-10.140934	-13.222023	0.50 (278-> 282)	0.13 (279-> 282)	0.13 (278-> 280)
8	2.622	472.8	0.000441	0.000853	-21.466690	-23.945547	0.86 (277-> 280)	0.05 (276-> 280)	0.01 (277-> 281)
9	2.669	464.5	0.001188	0.001676	17.821898	20.691045	0.77 (276-> 280)	0.07 (277-> 280)	0.02 (275-> 280)
10	2.776	446.6	0.001381	0.001680	1.046582	1.090027	0.56 (277-> 283)	0.19 (277-> 281)	0.10 (276-> 282)
11	2.798	443.1	0.002254	0.001645	13.795709	14.607507	0.40 (277-> 282)	0.16 (276-> 282)	0.15 (276-> 283)
12	2.840	436.6	0.001783	0.001915	7.401693	8.180677	0.50 (277-> 281)	0.20 (277-> 283)	0.09 (275-> 280)
13	2.856	434.2	0.011618	0.013628	-1.624596	-1.863052	0.33 (275-> 281)	0.27 (272-> 281)	0.12 (276-> 281)
14	2.869	432.1	0.044908	0.052735	-96.823448	-103.669467	0.41 (275-> 280)	0.14 (272-> 280)	0.11 (277-> 281)
15	2.884	429.9	0.010115	0.011483	81.174600	85.626501	0.28 (274-> 282)	0.12 (275-> 280)	0.12 (276-> 281)
16	2.913	425.6	0.006137	0.008376	7.495387	9.119425	0.18 (276-> 282)	0.14 (274-> 283)	0.14 (273-> 283)
17	2.915	425.4	0.002730	0.004068	-6.753616	-7.854504	0.47 (276-> 281)	0.16 (276-> 283)	0.08 (272-> 281)
18	2.956	419.4	0.007543	0.008337	45.425167	46.708890	0.24 (277-> 282)	0.21 (274-> 282)	0.16 (276-> 283)
19	2.975	416.7	0.063642	0.071803	20.397732	20.760307	0.25 (273-> 281)	0.18 (273-> 280)	0.05 (274-> 282)
20	2.988	415.0	0.088411	0.095101	-119.290980	-120.211226	0.24 (273-> 281)	0.17 (273-> 280)	0.10 (276-> 283)
21	3.018	410.8	0.104480	0.110009	0.577725	0.101453	0.22 (276-> 282)	0.15 (274-> 283)	0.15 (276-> 283)
22	3.041	407.8	0.009094	0.011867	11.746711	11.135185	0.27 (275-> 282)	0.22 (273-> 282)	0.13 (274-> 283)
23	3.064	404.7	0.089700	0.104955	42.546477	46.627704	0.28 (275-> 283)	0.16 (273-> 283)	0.09 (274-> 283)
24	3.069	404.0	0.100619	0.107789	-51.754085	-52.510795	0.14 (275-> 283)	0.12 (275-> 281)	0.11 (272-> 281)
25	3.079	402.7	0.017373	0.018365	32.272984	32.936467	0.53 (270-> 280)	0.12 (275-> 283)	0.12 (274-> 280)
26	3.088	401.5	0.224804	0.232402	33.556506	34.571217	0.23 (271-> 280)	0.21 (272-> 280)	0.10 (275-> 282)
27	3.112	398.5	0.171462	0.182270	-37.704180	-38.373020	0.15 (272-> 282)	0.13 (271-> 280)	0.13 (274-> 281)
28	3.135	395.4	0.153462	0.159484	5.120332	5.104330	0.42 (271-> 281)	0.11 (275-> 281)	0.11 (272-> 283)
29	3.171	391.0	0.003469	0.004032	-0.757422	-0.707920	0.32 (279-> 284)	0.17 (271-> 280)	0.10 (273-> 280)
30	3.176	390.4	0.039687	0.041474	-17.413913	-18.043705	0.33 (274-> 281)	0.24 (279-> 284)	0.08 (273-> 281)
31	3.192	388.4	0.047241	0.051015	17.077715	17.951142	0.34 (274-> 280)	0.11 (270-> 280)	0.09 (274-> 283)
32	3.224	384.5	0.001973	0.001722	-5.316359	-6.286676	0.21 (279-> 285)	0.15 (271-> 283)	0.14 (274-> 280)
33	3.226	384.3	0.065228	0.071793	-13.033289	-14.148225	0.16 (279-> 285)	0.12 (279-> 284)	0.11 (271-> 282)
34	3.228	384.1	0.016754	0.018285	-34.739903	-35.423317	0.16 (272-> 282)	0.09 (271-> 280)	0.09 (272-> 280)
35	3.239	382.8	0.020203	0.022353	12.310771	13.035728	0.26 (279-> 285)	0.19 (272-> 280)	0.08 (279-> 284)
36	3.279	378.2	0.006678	0.007533	21.170283	21.532391	0.29 (278-> 284)	0.28 (270-> 281)	0.12 (269-> 280)
37	3.284	377.5	0.012020	0.013927	-10.965451	-11.782330	0.21 (271-> 281)	0.16 (279-> 285)	0.13 (272-> 281)
38	3.328	372.5	0.009522	0.009685	-8.624776	-6.441875	0.25 (270-> 282)	0.14 (269-> 283)	0.14 (278-> 284)
39	3.336	371.6	0.018958	0.019996	99.981255	101.517933	0.34 (270-> 283)	0.16 (269-> 283)	0.09 (278-> 284)
40	3.357	369.3	0.124428	0.133869	65.968617	70.664809	0.33 (270-> 281)	0.15 (269-> 280)	0.12 (278-> 285)
41	3.375	367.4	0.170031	0.185413	-92.807020	-99.063376	0.37 (278-> 285)	0.16 (269-> 280)	0.09 (270-> 283)
42	3.381	366.7	0.115289	0.125814	-5.865688	-5.004123	0.17 (278-> 284)	0.16 (270-> 282)	0.14 (278-> 285)
43	3.409	363.7	0.046101	0.051317	-33.640485	-35.093972	0.33 (271-> 282)	0.14 (270-> 283)	0.14 (273-> 282)
44	3.422	362.3	0.333420	0.357225	58.131505	60.318675	0.30 (270-> 282)	0.17 (269-> 281)	0.10 (270-> 283)
45	3.457	358.6	0.184603	0.203432	-9.351188	-9.842304	0.20 (271-> 283)	0.09 (269-> 281)	0.09 (278-> 285)
46	3.475	356.8	0.073605	0.079683	0.976911	1.163120	0.36 (260-> 280)	0.30 (262-> 280)	0.05 (259-> 280)
47	3.488	355.4	0.428951	0.467533	-3.048385	-3.344621	0.19 (269-> 282)	0.17 (263-> 282)	0.13 (271-> 282)
48	3.506	353.7	0.129147	0.138950	-146.086120	-151.041622	0.13 (269-> 282)	0.12 (263-> 282)	0.12 (263-> 283)
49	3.517	352.5	0.134834	0.144633	129.573172	134.245506	0.22 (263-> 283)	0.13 (269-> 282)	0.11 (265-> 283)
50	3.548	349.5	0.042726	0.043744	-7.882464	-9.056662	0.40 (260-> 281)	0.17 (262-> 281)	0.14 (267-> 280)
51	3.579	346.5	0.781435	0.835734	-7.587370	-7.972012	0.23 (269-> 283)	0.13 (268-> 282)	0.10 (269-> 281)
52	3.589	345.5	0.014827	0.015038	-6.326723	-6.232982	0.37 (267-> 280)	0.11 (260-> 281)	0.08 (265-> 280)
53	3.612	343.3	0.004284	0.004554	3.903890	4.423935	0.23 (262-> 280)	0.21 (260-> 280)	0.08 (268-> 282)
54	3.624	342.1	0.053233	0.056512	53.541120	55.577533	0.25 (268-> 283)	0.20 (268-> 282)	0.06 (269-> 282)
55	3.638	340.8	0.102051	0.108750	-59.101142	-61.171944	0.27 (268-> 283)	0.23 (268-> 282)	0.09 (269-> 283)
56	3.652	339.5	0.047803	0.050352	-0.641423	-0.779391	0.32 (266-> 282)	0.14 (267-> 281)	0.07 (264-> 283)
57	3.659	338.8	0.049354	0.054604	9.196919	9.729769	0.23 (267-> 281)	0.16 (264-> 281)	0.12 (266-> 282)
58	3.681	336.8	0.036378	0.039276	-6.171968	-6.450025	0.38 (266-> 283)	0.14 (263-> 282)	0.07 (264-> 282)
59	3.708	334.3	0.038008	0.039840	-1.759439	-1.813041	0.55 (261-> 281)	0.08 (267-> 281)	0.07 (264-> 281)
60	3.765	329.3	0.037054	0.038841	-12.909578	-13.193216	0.13 (265-> 280)	0.12 (266-> 283)	0.09 (257-> 282)
61	3.782	327.9	0.015382	0.016218	-1.829499	-1.898739	0.17 (261-> 280)	0.09 (254-> 280)	0.05 (256-> 281)
62	3.830	323.7	0.354601	0.367188	-162.728467	-164.218516	0.22 (265-> 280)	0.15 (265-> 281)	0.08 (267-> 280)

63	3.840	322.9	0.241632	0.251806	72.419662	72.987585	0.29 (265-> 281)	0.13 (265-> 280)	0.09 (267-> 281)
64	3.860	321.2	0.009870	0.009835	-3.269114	-3.380285	0.62 (268-> 280)	0.13 (262-> 280)	0.04 (266-> 280)
65	3.879	319.6	0.001283	0.001174	1.780569	1.741208	0.47 (263-> 280)	0.13 (264-> 280)	0.08 (265-> 280)
66	3.900	317.9	0.026671	0.027356	-11.661599	-11.703747	0.18 (261-> 280)	0.13 (262-> 281)	0.09 (256-> 281)
67	3.907	317.3	0.187337	0.190264	20.726487	20.704412	0.17 (267-> 283)	0.12 (266-> 282)	0.09 (264-> 283)
68	3.936	315.0	0.457454	0.467791	25.673083	26.031409	0.31 (267-> 282)	0.27 (265-> 282)	0.04 (263-> 282)
69	3.952	313.8	0.150820	0.154722	32.877408	33.468696	0.24 (263-> 281)	0.16 (265-> 283)	0.14 (279-> 286)
70	3.957	313.3	0.018201	0.018415	-15.313353	-16.049425	0.63 (279-> 286)	0.05 (268-> 281)	0.04 (267-> 281)
71	3.964	312.7	0.004055	0.003863	5.432381	5.682570	0.53 (268-> 281)	0.07 (262-> 281)	0.06 (264-> 280)
72	3.987	311.0	0.227147	0.228071	-10.420091	-10.425261	0.15 (263-> 281)	0.11 (264-> 281)	0.10 (263-> 283)
73	4.024	308.1	0.051148	0.050100	-1.590889	-1.617043	0.18 (256-> 280)	0.13 (279-> 287)	0.05 (258-> 280)
74	4.029	307.7	0.045860	0.045038	-5.466651	-5.487623	0.19 (256-> 280)	0.19 (279-> 287)	0.05 (258-> 280)
75	4.038	307.0	0.003792	0.003960	10.663414	10.602552	0.13 (264-> 280)	0.10 (279-> 287)	0.09 (259-> 280)
76	4.071	304.5	0.012113	0.010054	-2.847769	-3.083212	0.29 (279-> 287)	0.19 (258-> 280)	0.10 (259-> 280)
77	4.076	304.2	0.038690	0.035592	6.751823	6.505229	0.10 (257-> 282)	0.08 (261-> 280)	0.08 (259-> 282)
78	4.083	303.6	0.018549	0.019278	5.954472	6.188773	0.40 (278-> 286)	0.09 (258-> 281)	0.06 (259-> 281)
79	4.091	303.0	0.008813	0.008120	-5.995832	-5.753240	0.28 (259-> 282)	0.11 (258-> 280)	0.05 (268-> 281)
80	4.106	302.0	0.015033	0.015856	5.135367	5.114513	0.31 (279-> 288)	0.18 (259-> 283)	0.04 (261-> 283)
81	4.116	301.2	0.037276	0.037863	6.411129	6.365332	0.23 (279-> 288)	0.08 (259-> 281)	0.07 (259-> 283)
82	4.126	300.5	0.002471	0.002399	2.025341	2.016581	0.20 (260-> 283)	0.08 (262-> 283)	0.07 (265-> 282)
83	4.132	300.1	0.017814	0.019128	-0.861029	-1.045898	0.49 (260-> 282)	0.11 (262-> 282)	0.05 (278-> 286)
84	4.144	299.2	0.006249	0.008783	2.631655	3.072789	0.24 (278-> 286)	0.14 (279-> 288)	0.07 (259-> 283)
85	4.156	298.3	0.002038	0.002355	-3.667794	-3.201741	0.28 (260-> 283)	0.09 (261-> 282)	0.07 (265-> 282)
86	4.161	298.0	0.014725	0.015479	-11.189075	-11.148164	0.07 (254-> 281)	0.07 (265-> 283)	0.05 (261-> 283)
87	4.170	297.3	0.010159	0.009248	5.619463	5.344731	0.10 (257-> 283)	0.07 (264-> 281)	0.06 (258-> 281)
88	4.173	297.1	0.000776	0.000530	0.562611	0.423665	0.26 (266-> 280)	0.13 (264-> 281)	0.05 (268-> 280)
89	4.180	296.6	0.007224	0.007366	13.857769	13.352403	0.29 (278-> 287)	0.12 (261-> 282)	0.08 (279-> 290)
90	4.188	296.0	0.009588	0.009388	-2.650350	-2.547330	0.17 (266-> 280)	0.07 (264-> 281)	0.06 (254-> 280)
91	4.190	295.9	0.005872	0.005514	1.011799	1.012497	0.16 (266-> 280)	0.10 (254-> 280)	0.07 (261-> 280)
92	4.206	294.8	0.000655	0.000538	-2.010152	-1.994109	0.21 (261-> 283)	0.14 (265-> 283)	0.10 (267-> 283)
93	4.214	294.2	0.014400	0.016837	4.225010	4.555750	0.27 (279-> 289)	0.15 (266-> 281)	0.08 (279-> 290)
94	4.230	293.1	0.004852	0.005558	4.693656	4.885943	0.42 (266-> 281)	0.21 (279-> 289)	0.04 (268-> 281)
95	4.241	292.4	0.002983	0.002773	-0.855369	-1.334704	0.62 (278-> 288)	0.08 (278-> 291)	0.06 (279-> 291)
96	4.242	292.3	0.000206	0.000209	1.927586	1.619617	0.13 (278-> 287)	0.11 (279-> 289)	0.10 (266-> 283)
97	4.260	291.0	0.007995	0.008787	11.231083	11.193832	0.20 (256-> 281)	0.08 (262-> 281)	0.07 (262-> 283)
98	4.285	289.3	0.006408	0.006033	-2.112765	-2.094198	0.36 (262-> 283)	0.08 (256-> 281)	0.07 (279-> 292)
99	4.296	288.6	0.001879	0.001700	-3.374675	-3.315483	0.55 (279-> 292)	0.12 (279-> 293)	0.06 (262-> 283)
100	4.308	287.8	0.004276	0.004343	4.879079	4.660815	0.16 (255-> 282)	0.12 (257-> 283)	0.12 (253-> 282)
101	4.311	287.6	0.005747	0.005458	4.612910	4.957530	0.23 (279-> 293)	0.16 (279-> 290)	0.12 (278-> 289)
102	4.323	286.8	0.024030	0.018403	-5.569290	-4.533980	0.43 (279-> 291)	0.14 (278-> 288)	0.09 (279-> 290)
103	4.331	286.3	0.000470	0.000422	1.818375	1.695536	0.44 (262-> 282)	0.07 (260-> 282)	0.06 (262-> 283)
104	4.368	283.9	0.002431	0.002258	-0.936940	-0.872954	0.26 (264-> 282)	0.17 (261-> 282)	0.16 (258-> 282)
105	4.381	283.0	0.003368	0.003913	2.674314	2.870257	0.10 (258-> 283)	0.09 (261-> 283)	0.09 (264-> 283)
106	4.387	282.6	0.008100	0.008569	1.414901	1.147683	0.11 (258-> 283)	0.08 (278-> 290)	0.08 (264-> 283)
107	4.393	282.2	0.005391	0.004937	-39.388692	-37.618272	0.12 (278-> 290)	0.10 (259-> 280)	0.08 (279-> 294)
108	4.396	282.0	0.002987	0.002537	25.130128	23.640176	0.18 (278-> 291)	0.08 (278-> 290)	0.07 (259-> 281)
109	4.414	280.9	0.004635	0.004934	3.334781	3.554571	0.14 (259-> 281)	0.13 (278-> 291)	0.11 (279-> 294)
110	4.427	280.1	0.015214	0.013801	17.428330	16.443705	0.17 (278-> 292)	0.11 (279-> 290)	0.10 (279-> 292)
111	4.435	279.6	0.147064	0.136296	7.700748	7.247282	0.29 (278-> 292)	0.07 (278-> 293)	0.06 (277-> 284)
112	4.464	277.7	0.064146	0.063943	186.993627	182.977357	0.30 (277-> 284)	0.06 (277-> 286)	0.05 (254-> 280)
113	4.473	277.2	0.007025	0.006713	-18.295685	-17.872385	0.17 (254-> 280)	0.11 (248-> 280)	0.10 (277-> 284)
114	4.485	276.4	0.043234	0.043168	8.096033	8.945714	0.36 (276-> 284)	0.09 (277-> 284)	0.05 (279-> 295)
115	4.488	276.3	0.080205	0.078958	-194.459039	-191.888573	0.32 (277-> 285)	0.06 (277-> 284)	0.05 (277-> 286)
116	4.514	274.7	0.033103	0.030811	37.467639	36.673071	0.17 (279-> 294)	0.06 (275-> 284)	0.05 (277-> 285)
117	4.531	273.6	0.011204	0.011636	-16.814949	-16.966983	0.08 (279-> 294)	0.08 (278-> 291)	0.05 (255-> 282)
118	4.535	273.4	0.006645	0.005623	-7.190912	-6.215597	0.21 (278-> 293)	0.06 (278-> 287)	0.05 (276-> 285)
119	4.538	273.2	0.004448	0.004542	4.132885	4.016543	0.13 (257-> 280)	0.12 (258-> 282)	0.05 (251-> 280)
120	4.546	272.7	0.008634	0.008573	6.224313	6.287716	0.16 (257-> 280)	0.13 (258-> 282)	0.06 (251-> 280)
121	4.550	272.5	0.019812	0.020468	-20.145536	-20.499672	0.08 (258-> 283)	0.07 (258-> 282)	0.05 (257-> 280)
122	4.552	272.4	0.015649	0.016185	25.535586	25.767297	0.09 (276-> 285)	0.06 (257-> 280)	0.06 (255-> 280)
123	4.554	272.2	0.019837	0.019981	-8.076440	-8.315300	0.13 (257-> 281)	0.10 (276-> 285)	0.05 (263-> 281)
124	4.560	271.9	0.002994	0.002895	-3.183932	-2.969573	0.30 (253-> 280)	0.24 (255-> 280)	0.11 (257-> 281)
125	4.566	271.5	0.016707	0.015996	-1.427226	-1.604552	0.11 (255-> 282)	0.10 (278-> 289)	0.06 (253-> 282)
126	4.572	271.2	0.006542	0.005874	3.406471	3.417561	0.12 (278-> 289)	0.07 (255-> 282)	0.06 (258-> 283)
127	4.583	270.5	0.020395	0.020716	-15.628580	-15.965751	0.09 (246-> 280)	0.07 (278-> 291)	0.05 (278-> 293)
128	4.585	270.4	0.041807	0.040740	12.295668	12.366065	0.15 (278-> 290)	0.09 (278-> 293)	0.05 (278-> 289)

129	4.591	270.0	0.044059	0.044167	-26.486414	-26.016596	0.11 (255-> 283)	0.09 (278-> 290)	0.09 (251-> 282)
130	4.592	270.0	0.009643	0.009627	2.711164	2.416251	0.10 (255-> 282)	0.09 (251-> 283)	0.08 (246-> 280)
131	4.599	269.6	0.130425	0.123315	-63.830520	-61.935696	0.16 (275-> 284)	0.07 (251-> 283)	0.06 (258-> 283)
132	4.603	269.3	0.026382	0.024576	23.519322	22.822124	0.33 (250-> 281)	0.08 (278-> 293)	0.04 (256-> 283)
133	4.610	269.0	0.008054	0.007278	22.681760	21.571282	0.23 (279-> 295)	0.12 (275-> 284)	0.09 (278-> 294)
134	4.634	267.6	0.022647	0.019612	-44.346324	-39.980124	0.08 (275-> 284)	0.07 (276-> 284)	0.06 (256-> 282)
135	4.637	267.4	0.006630	0.005578	21.052092	18.127428	0.12 (251-> 282)	0.11 (252-> 282)	0.05 (251-> 283)
136	4.653	266.4	0.115474	0.113695	-10.661987	-10.514993	0.15 (256-> 282)	0.09 (279-> 297)	0.06 (246-> 280)
137	4.663	265.9	0.077154	0.075502	-5.205533	-6.473610	0.18 (274-> 285)	0.08 (252-> 283)	0.04 (256-> 283)
138	4.668	265.6	0.038371	0.038201	32.362561	33.303752	0.13 (256-> 282)	0.09 (279-> 297)	0.08 (252-> 283)
139	4.677	265.1	0.012376	0.011778	17.637510	17.148499	0.21 (256-> 283)	0.12 (252-> 282)	0.04 (256-> 282)
140	4.679	265.0	0.045625	0.045381	-46.435920	-45.325199	0.08 (279-> 297)	0.05 (273-> 285)	0.04 (254-> 281)
141	4.685	264.6	0.024780	0.024854	45.308309	45.609966	0.28 (275-> 285)	0.06 (274-> 285)	0.05 (252-> 282)
142	4.693	264.2	0.017213	0.017866	-10.260246	-12.023418	0.12 (275-> 285)	0.12 (256-> 282)	0.06 (273-> 285)
143	4.705	263.5	0.100708	0.095277	-120.325784	-117.592129	0.05 (254-> 281)	0.04 (274-> 285)	0.04 (277-> 284)
144	4.709	263.3	0.008899	0.007968	11.215361	9.438536	0.25 (255-> 281)	0.19 (253-> 281)	0.07 (275-> 285)
145	4.716	262.9	0.016098	0.016074	38.651992	36.675279	0.06 (255-> 281)	0.05 (248-> 280)	0.05 (254-> 282)
146	4.724	262.5	0.103335	0.101019	-113.847334	-111.863093	0.05 (279-> 296)	0.05 (256-> 282)	0.05 (248-> 280)
147	4.729	262.2	0.072341	0.069399	84.921824	83.019154	0.16 (248-> 280)	0.06 (252-> 280)	0.05 (251-> 280)
148	4.731	262.1	0.029230	0.028101	-4.853052	-4.820752	0.09 (250-> 280)	0.07 (254-> 283)	0.05 (248-> 283)
149	4.738	261.7	0.059906	0.056392	17.764536	16.757783	0.10 (276-> 285)	0.07 (248-> 282)	0.06 (254-> 282)
150	4.750	261.0	0.006791	0.007081	-8.603220	-8.521310	0.33 (279-> 296)	0.07 (279-> 297)	0.06 (276-> 285)

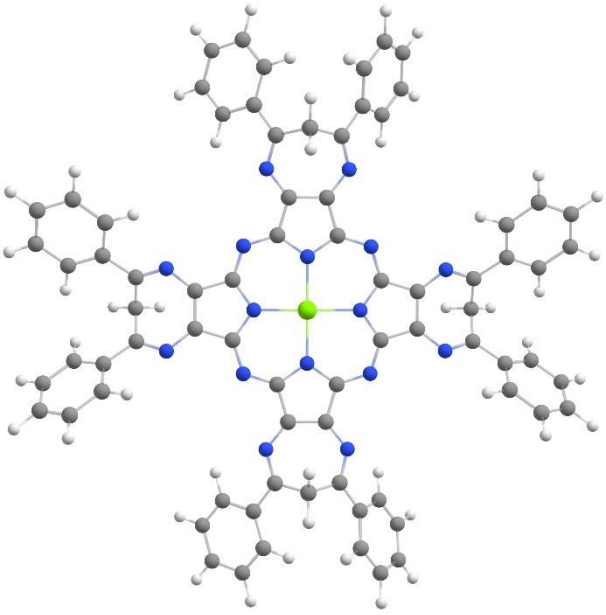

Table S8 Optimized geometry of Ph_8Dz_4PzMg (monomer)

CARTESIAN COORDINATES (ANGSTROEM)

C	19.110497000000	-18.074711000000	1.281694000000	C	23.983388000000	-14.495478000000	1.029912000000
C	20.526019000000	-18.052955000000	1.109632000000	C	23.964534000000	-13.070071000000	1.059162000000
C	20.931932000000	-16.637089000000	1.183992000000	C	22.545574000000	-12.674327000000	1.136622000000
C	22.897598000000	-21.319637000000	1.892128000000	C	18.235648000000	-22.829147000000	1.104744000000
C	18.688092000000	-16.672620000000	1.455107000000	C	22.576677000000	-14.934585000000	1.091709000000
C	15.593497000000	-13.212138000000	2.071065000000	C	18.609944000000	-20.321605000000	0.964047000000
C	15.616437000000	-14.637762000000	2.043278000000	C	19.691910000000	-20.427337000000	-0.102629000000
C	17.010096000000	-15.028686000000	1.761934000000	C	21.014118000000	-20.277887000000	0.633935000000
C	16.791035000000	-21.314299000000	2.349438000000	C	21.887846000000	-21.440244000000	0.904325000000
C	16.974615000000	-12.768974000000	1.804486000000	C	17.883898000000	-21.507134000000	1.464847000000
C	16.071433000000	-22.407019000000	2.842684000000	C	21.779224000000	-22.662616000000	0.199598000000
C	20.401977000000	-9.620987000000	1.273938000000	C	22.641625000000	-23.733172000000	0.481015000000
C	18.986374000000	-9.647502000000	1.442381000000	C	23.627598000000	-23.603406000000	1.473193000000
C	18.605017000000	-11.066997000000	1.562885000000	C	23.754537000000	-22.388765000000	2.174156000000
C	16.433151000000	-23.718924000000	2.478382000000	H	22.985691000000	-20.359009000000	2.422723000000
C	20.849609000000	-11.026542000000	1.294864000000	H	16.528463000000	-20.280786000000	2.623654000000
C	17.520081000000	-23.924078000000	1.612908000000	H	15.219312000000	-22.238005000000	3.522030000000

H	15.868171000000	-24.580206000000	2.872175000000
H	17.817457000000	-24.947094000000	1.329079000000
H	19.092548000000	-23.017566000000	0.442782000000
H	19.615653000000	-21.359089000000	-0.689664000000
H	19.576444000000	-19.559101000000	-0.792025000000
H	21.039011000000	-22.778280000000	-0.607546000000
H	22.544902000000	-24.674755000000	-0.084384000000
H	24.300890000000	-24.447207000000	1.698186000000
H	24.530397000000	-22.277870000000	2.949858000000
N	17.776358000000	-13.884798000000	1.665788000000
N	17.422474000000	-16.294508000000	1.653446000000
N	19.741459000000	-11.839389000000	1.431910000000
N	17.350849000000	-11.488585000000	1.744192000000
N	21.771963000000	-13.817355000000	1.189314000000
N	22.194544000000	-16.214177000000	1.076488000000
N	22.124172000000	-11.407281000000	1.172886000000
N	18.314106000000	-19.150955000000	1.471941000000
N	21.381970000000	-19.103094000000	1.084772000000
N	19.800996000000	-15.862671000000	1.352367000000
C	16.542769000000	-6.526474000000	2.590658000000
C	22.672865000000	-6.317314000000	2.188871000000
C	23.496072000000	-5.234374000000	2.515171000000
C	23.334273000000	-3.998074000000	1.860875000000
C	22.347678000000	-3.860050000000	0.870408000000
C	21.518939000000	-4.944519000000	0.544720000000
C	20.824700000000	-7.365871000000	0.884684000000
C	19.500813000000	-7.227647000000	0.148703000000
C	18.417903000000	-7.406722000000	1.204583000000
C	17.648702000000	-6.264768000000	1.740757000000
C	21.662598000000	-6.189226000000	1.202603000000
C	17.971466000000	-4.919228000000	1.447057000000
C	17.215172000000	-3.867637000000	1.986756000000
C	16.115534000000	-4.140372000000	2.816866000000
C	15.782413000000	-5.476409000000	3.114579000000
H	16.302565000000	-7.577892000000	2.812272000000
H	22.788902000000	-7.294694000000	2.682138000000
H	24.272914000000	-5.351710000000	3.288918000000
H	23.981223000000	-3.143694000000	2.120576000000
H	22.224372000000	-2.900886000000	0.340860000000
H	20.778114000000	-4.820460000000	-0.260630000000
H	19.398289000000	-6.276722000000	-0.402761000000
H	19.413861000000	-8.071965000000	-0.573869000000
H	18.838187000000	-4.679050000000	0.815321000000
H	17.490493000000	-2.825321000000	1.755757000000
H	15.518156000000	-3.312989000000	3.234830000000
H	14.920043000000	-5.698506000000	3.765069000000
N	21.225984000000	-8.545480000000	1.291958000000
N	18.156966000000	-8.603648000000	1.668062000000
Mg	19.771998000000	-13.850764000000	1.407943000000
C	28.729110000000	-15.340888000000	0.640052000000
C	29.755521000000	-16.106383000000	0.065914000000
C	29.451768000000	-17.284433000000	-0.635910000000
C	28.108772000000	-17.688075000000	-0.770270000000
C	27.082306000000	-16.920304000000	-0.211667000000
C	27.065018000000	-10.789630000000	-0.391607000000
C	28.075612000000	-9.965818000000	-0.898715000000
C	29.373268000000	-10.018238000000	-0.354479000000
C	29.646076000000	-10.895244000000	0.708449000000
C	26.225487000000	-12.534723000000	1.179749000000
C	26.491960000000	-13.775357000000	2.017952000000
C	26.259507000000	-14.959980000000	1.088909000000
C	28.634253000000	-11.724755000000	1.215271000000
C	27.328711000000	-11.691426000000	0.669963000000
C	27.376693000000	-15.734573000000	0.510334000000
H	28.991811000000	-14.413034000000	1.167316000000
H	30.260036000000	-17.888262000000	-1.081121000000
H	27.862344000000	-18.611843000000	-1.319876000000
H	26.025722000000	-17.214998000000	-0.306891000000
H	26.041797000000	-10.757485000000	-0.796604000000
H	27.852993000000	-9.274806000000	-1.728709000000
H	30.170650000000	-9.371507000000	-0.756805000000
H	30.654762000000	-10.931533000000	1.152133000000
H	28.864224000000	-12.378779000000	2.070899000000
H	27.494892000000	-13.789967000000	2.479190000000
H	25.725376000000	-13.823078000000	2.825720000000
H	30.802466000000	-15.776274000000	0.168425000000
N	24.996047000000	-12.215520000000	0.855917000000
N	25.035553000000	-15.305914000000	0.775852000000
C	10.953716000000	-15.654611000000	2.841705000000
C	9.844132000000	-16.456425000000	2.533301000000
C	10.002944000000	-17.616435000000	1.757662000000
C	11.281974000000	-17.965427000000	1.281305000000
C	12.387481000000	-17.161257000000	1.575079000000
C	12.157301000000	-11.047277000000	1.421852000000
C	11.025627000000	-10.262561000000	1.175646000000
C	9.899977000000	-10.357932000000	2.016262000000
C	9.922948000000	-11.237956000000	3.110961000000
C	13.412539000000	-12.753057000000	2.738513000000
C	13.402185000000	-13.995464000000	3.615266000000
C	13.440974000000	-15.178173000000	2.656736000000
C	11.056260000000	-12.027787000000	3.356938000000
C	12.189682000000	-11.951934000000	2.513036000000
C	12.242734000000	-15.992664000000	2.367180000000
H	10.799840000000	-14.743150000000	3.436249000000
H	9.130870000000	-18.248726000000	1.521532000000
H	11.414632000000	-18.874928000000	0.671872000000
H	13.395476000000	-17.412725000000	1.210385000000
H	13.050646000000	-10.981664000000	0.781792000000
H	11.016844000000	-9.568653000000	0.318695000000
H	9.006408000000	-9.742414000000	1.819748000000
H	9.052645000000	-11.308030000000	3.784223000000
H	11.062104000000	-12.684141000000	4.241099000000
H	12.543316000000	-14.039077000000	4.307621000000
H	14.343469000000	-14.010020000000	4.212176000000
H	8.846071000000	-16.169294000000	2.903416000000
N	14.514915000000	-12.393832000000	2.126643000000
N	14.562385000000	-15.485119000000	2.053072000000

Table S9 TD-DFT calculated UV-Vis spectrum of Ph_8Dz_4PzMg (monomer)

state	eV	nm	fL	fV	Rl	RV			
0	1.749	708.8	0.631576	1.033558	-50.892183	-67.390659	0.50 (144-> 146)	0.45 (144-> 145)	0.01 (143-> 145)
1	1.750	708.3	0.633928	1.036832	45.090694	59.948631	0.50 (144-> 145)	0.45 (144-> 146)	0.01 (143-> 146)
2	2.666	465.0	0.004123	0.003906	4.541309	4.231671	0.90 (142-> 146)	0.03 (139-> 146)	0.02 (140-> 147)
3	2.677	463.1	0.017363	0.018183	2.283274	3.527082	0.68 (142-> 145)	0.19 (143-> 145)	0.03 (139-> 145)
4	2.694	460.2	0.004544	0.004766	-8.594657	-8.792910	0.40 (140-> 146)	0.40 (141-> 145)	0.05 (140-> 145)
5	2.718	456.2	0.005925	0.005907	0.193601	-0.127576	0.41 (140-> 146)	0.39 (141-> 145)	0.06 (141-> 146)
6	2.837	437.1	1.041598	1.103907	-10.608096	2.748124	0.69 (143-> 145)	0.22 (142-> 145)	0.02 (138-> 145)
7	2.847	435.4	0.877451	0.918276	-0.722348	-7.891433	0.78 (143-> 146)	0.05 (144-> 147)	0.04 (140-> 145)
8	2.849	435.1	0.167950	0.175966	16.889866	-0.415193	0.51 (144-> 147)	0.14 (141-> 146)	0.13 (140-> 145)

9	2.878	430.9	0.019406	0.019934	-3.538843	0.880400	0.40 (144-> 147)	0.24 (141-> 146)	0.24 (140-> 145)
10	2.914	425.5	0.016295	0.016716	-0.158974	0.153872	0.43 (140-> 145)	0.41 (141-> 146)	0.05 (140-> 146)
11	3.421	362.4	0.443935	0.442732	29.985465	26.373616	0.49 (144-> 149)	0.17 (139-> 146)	0.13 (139-> 145)
12	3.422	362.3	0.445717	0.445637	-23.324134	-22.806811	0.48 (144-> 150)	0.17 (139-> 145)	0.14 (139-> 146)
13	3.458	358.6	0.083540	0.081322	122.941831	120.382200	0.40 (134-> 146)	0.15 (126-> 146)	0.09 (134-> 145)
14	3.459	358.4	0.085860	0.083739	-127.190040	-125.402933	0.42 (134-> 145)	0.15 (126-> 145)	0.10 (134-> 146)
15	3.531	351.1	0.005242	0.004819	1.990986	1.751335	0.86 (144-> 148)	0.01 (138-> 146)	0.01 (139-> 146)
16	3.533	350.9	0.000673	0.000708	-1.294044	-1.369292	0.36 (144-> 151)	0.10 (137-> 145)	0.10 (136-> 146)
17	3.541	350.2	0.058975	0.058270	-7.126928	-6.025245	0.32 (138-> 145)	0.13 (139-> 145)	0.09 (144-> 150)
18	3.542	350.1	0.061541	0.060878	6.686892	4.609446	0.30 (138-> 146)	0.13 (139-> 146)	0.09 (144-> 149)
19	3.568	347.5	0.001873	0.002131	-2.761721	-3.481021	0.15 (136-> 146)	0.14 (137-> 145)	0.14 (137-> 146)
20	3.666	338.2	0.086535	0.093979	-42.662721	-45.284693	0.31 (144-> 151)	0.13 (144-> 149)	0.08 (139-> 146)
21	3.668	338.0	0.156654	0.173880	81.123534	86.455326	0.24 (144-> 150)	0.19 (139-> 145)	0.18 (138-> 145)
22	3.671	337.7	0.083908	0.094128	-38.908473	-43.028053	0.24 (144-> 151)	0.12 (144-> 149)	0.11 (139-> 146)
23	3.722	333.1	0.007123	0.007645	1.113743	0.813968	0.17 (120-> 146)	0.17 (121-> 145)	0.11 (136-> 145)
24	3.741	331.4	0.000061	0.000086	0.630649	0.481941	0.68 (144-> 152)	0.04 (142-> 147)	0.03 (137-> 145)
25	3.832	323.6	0.000987	0.000998	8.347888	6.546732	0.33 (142-> 147)	0.17 (144-> 152)	0.12 (143-> 148)
26	3.841	322.8	0.061816	0.061211	16.177988	15.152840	0.13 (136-> 145)	0.13 (137-> 146)	0.12 (137-> 145)
27	3.852	321.8	0.788793	0.786938	-108.551356	-104.779742	0.22 (140-> 147)	0.13 (143-> 149)	0.13 (141-> 148)
28	3.855	321.6	0.754962	0.751235	89.748711	85.931094	0.18 (141-> 147)	0.11 (140-> 148)	0.10 (142-> 149)
29	3.871	320.3	0.000796	0.000797	1.475445	1.492942	0.34 (143-> 147)	0.15 (142-> 148)	0.09 (141-> 150)
30	3.952	313.8	0.293301	0.280319	-85.170109	-83.468011	0.35 (144-> 153)	0.09 (141-> 151)	0.06 (140-> 152)
31	3.957	313.4	0.247995	0.234687	64.450430	59.446423	0.28 (144-> 154)	0.10 (140-> 151)	0.07 (141-> 152)
32	3.968	312.5	0.014426	0.014951	15.253057	15.543521	0.14 (143-> 151)	0.10 (142-> 152)	0.06 (140-> 153)
33	3.982	311.4	0.010692	0.010976	15.681125	15.857023	0.42 (144-> 154)	0.04 (135-> 145)	0.04 (132-> 145)
34	3.986	311.1	0.002502	0.002803	-7.980240	-8.835275	0.33 (144-> 153)	0.07 (135-> 146)	0.06 (135-> 145)
35	4.020	308.4	0.008946	0.008163	-5.623277	-5.217895	0.14 (142-> 151)	0.11 (143-> 152)	0.06 (120-> 146)
36	4.060	305.3	0.000040	0.000040	0.897050	1.313627	0.29 (120-> 145)	0.29 (121-> 146)	0.04 (120-> 146)
37	4.121	300.9	0.000072	0.000026	-0.198744	-0.035122	0.14 (135-> 146)	0.08 (144-> 154)	0.08 (132-> 146)
38	4.122	300.8	0.000255	0.000097	0.457991	-0.061871	0.13 (135-> 145)	0.09 (144-> 153)	0.07 (132-> 145)
39	4.137	299.7	0.000070	0.000063	0.115538	0.077465	0.30 (120-> 145)	0.30 (121-> 146)	0.05 (120-> 146)
40	4.208	294.7	0.001380	0.001176	0.197846	0.270793	0.13 (120-> 146)	0.12 (121-> 145)	0.12 (136-> 145)
41	4.300	288.4	0.001355	0.001188	-0.572228	-0.514745	0.21 (121-> 145)	0.20 (120-> 146)	0.06 (137-> 146)
42	4.313	287.5	0.011153	0.007419	-0.265869	1.886306	0.17 (133-> 146)	0.16 (133-> 145)	0.13 (132-> 145)
43	4.354	284.8	0.000957	0.000775	0.950721	0.836153	0.47 (143-> 147)	0.24 (142-> 148)	0.05 (141-> 150)
44	4.361	284.3	0.004568	0.003735	-5.913137	-5.309050	0.13 (133-> 145)	0.09 (133-> 146)	0.09 (119-> 145)
45	4.366	284.0	0.002097	0.001942	-4.878374	-4.523697	0.43 (142-> 147)	0.20 (143-> 148)	0.04 (140-> 150)
46	4.409	281.2	0.080670	0.066438	45.044040	40.323149	0.38 (141-> 147)	0.12 (140-> 148)	0.09 (131-> 146)
47	4.410	281.2	0.070673	0.057839	-34.818797	-33.244182	0.39 (140-> 147)	0.12 (141-> 148)	0.09 (131-> 145)
48	4.449	278.7	0.202842	0.173602	250.267773	227.341104	0.10 (131-> 145)	0.09 (141-> 147)	0.09 (131-> 146)
49	4.454	278.4	0.219240	0.187812	-255.866159	-236.509604	0.14 (131-> 146)	0.13 (131-> 145)	0.08 (140-> 147)
50	4.480	276.8	0.007376	0.006373	8.392831	8.134270	0.09 (132-> 145)	0.09 (133-> 146)	0.08 (132-> 146)
51	4.524	274.1	0.015928	0.014118	-9.610315	-11.290670	0.51 (130-> 145)	0.10 (129-> 145)	0.07 (130-> 147)
52	4.527	273.9	0.018373	0.016218	-27.651368	-18.978015	0.52 (129-> 146)	0.08 (129-> 147)	0.06 (130-> 146)
53	4.540	273.1	0.034434	0.029807	48.324679	45.455313	0.26 (128-> 145)	0.11 (127-> 146)	0.09 (127-> 145)
54	4.540	273.1	0.002233	0.002019	-10.400124	-9.858562	0.34 (127-> 146)	0.12 (127-> 145)	0.10 (128-> 145)
55	4.583	270.5	0.001170	0.000968	-3.402374	-1.686208	0.18 (133-> 145)	0.17 (133-> 146)	0.13 (132-> 145)
56	4.585	270.4	0.002553	0.002116	3.285112	2.894496	0.16 (118-> 145)	0.16 (119-> 146)	0.07 (119-> 145)
57	4.609	269.0	0.004100	0.003207	4.392654	3.907592	0.15 (119-> 146)	0.14 (118-> 145)	0.08 (116-> 147)
58	4.631	267.7	0.072313	0.061379	18.665723	12.122150	0.24 (131-> 145)	0.16 (126-> 145)	0.10 (134-> 145)
59	4.632	267.6	0.072754	0.062946	-33.320524	-27.331509	0.26 (131-> 146)	0.16 (126-> 146)	0.08 (134-> 146)
60	4.656	266.3	0.003317	0.003177	-7.233068	-8.028087	0.23 (125-> 145)	0.10 (125-> 146)	0.08 (124-> 145)
61	4.660	266.1	0.021845	0.019748	37.273405	36.367373	0.11 (124-> 146)	0.11 (125-> 146)	0.08 (122-> 146)
62	4.676	265.1	0.002785	0.002412	2.088929	2.228711	0.25 (123-> 145)	0.17 (124-> 145)	0.09 (122-> 145)
63	4.679	265.0	0.005488	0.004780	-32.297474	-30.311061	0.21 (123-> 146)	0.15 (122-> 146)	0.15 (124-> 146)
64	4.692	264.2	0.000009	0.000005	0.042048	0.031677	0.99 (144-> 164)	0.00 (126-> 164)	0.00 (112-> 164)
65	4.730	262.1	0.002999	0.002360	-4.931800	-4.190611	0.13 (119-> 145)	0.13 (118-> 146)	0.08 (133-> 145)
66	4.731	262.1	0.002243	0.001793	-7.549575	-6.688539	0.26 (111-> 146)	0.12 (116-> 145)	0.10 (111-> 145)
67	4.733	262.0	0.000606	0.000521	3.259972	2.523826	0.24 (111-> 145)	0.10 (116-> 146)	0.10 (116-> 145)
68	4.734	261.9	0.004320	0.003698	-31.944537	-29.420965	0.11 (116-> 146)	0.08 (111-> 145)	0.07 (111-> 146)
69	4.738	261.7	0.003918	0.003451	40.021213	37.710933	0.18 (116-> 146)	0.12 (116-> 145)	0.06 (111-> 146)
70	4.778	259.5	0.002429	0.002066	4.689797	4.471019	0.14 (139-> 147)	0.14 (118-> 146)	0.14 (119-> 145)
71	4.797	258.5	0.002949	0.003381	-1.258984	0.111047	0.67 (144-> 159)	0.07 (144-> 163)	0.03 (138-> 151)
72	4.834	256.5	0.157841	0.133641	30.199185	22.888896	0.24 (143-> 150)	0.11 (142-> 149)	0.10 (141-> 152)
73	4.835	256.5	0.166216	0.141006	-30.364556	-25.360783	0.19 (142-> 150)	0.16 (143-> 149)	0.11 (142-> 149)
74	4.846	255.8	0.011110	0.009415	-5.589053	-2.992437	0.37 (130-> 146)	0.19 (139-> 147)	0.07 (129-> 146)

75	4.848	255.8	0.008213	0.006971	0.288017	-2.510713	0.35 (129-> 145)	0.15 (139-> 147)	0.05 (130-> 145)
76	4.856	255.3	0.003168	0.002693	2.478063	2.286467	0.28 (139-> 147)	0.18 (129-> 145)	0.13 (130-> 146)
77	4.858	255.2	0.016384	0.012925	-0.228226	-0.791907	0.07 (136-> 147)	0.06 (128-> 146)	0.06 (130-> 146)
78	4.863	254.9	0.002163	0.001487	-2.221916	-1.967043	0.12 (129-> 145)	0.12 (127-> 145)	0.09 (130-> 146)
79	4.870	254.6	0.014393	0.011864	9.891764	7.938335	0.29 (128-> 146)	0.17 (127-> 146)	0.14 (127-> 145)
80	4.872	254.5	0.010358	0.008196	0.973995	1.650107	0.29 (127-> 145)	0.16 (128-> 145)	0.10 (128-> 146)
81	4.884	253.9	0.003237	0.002614	-3.300472	-2.854335	0.18 (138-> 148)	0.12 (136-> 149)	0.12 (137-> 150)
82	4.889	253.6	0.009023	0.007623	-2.822200	-2.725764	0.24 (142-> 152)	0.14 (141-> 149)	0.12 (143-> 151)
83	4.909	252.6	0.007148	0.005988	4.093277	3.889654	0.24 (143-> 152)	0.20 (140-> 149)	0.18 (141-> 150)
84	4.924	251.8	0.002671	0.002047	4.820352	4.242024	0.13 (119-> 145)	0.13 (118-> 146)	0.12 (138-> 147)
85	4.965	249.7	0.003092	0.002628	13.552707	11.715713	0.27 (125-> 146)	0.20 (125-> 145)	0.09 (124-> 145)
86	4.974	249.3	0.008824	0.007395	-29.999747	-27.089485	0.12 (124-> 145)	0.11 (122-> 145)	0.09 (125-> 146)
87	4.980	249.0	0.002704	0.002204	7.323694	6.390426	0.19 (123-> 146)	0.18 (124-> 145)	0.17 (124-> 146)
88	4.990	248.5	0.010443	0.008691	15.097786	13.613505	0.23 (122-> 145)	0.19 (122-> 146)	0.15 (123-> 145)
89	5.039	246.0	0.047447	0.040429	-60.182778	-52.437840	0.15 (110-> 145)	0.13 (110-> 146)	0.06 (115-> 145)
90	5.043	245.9	0.020397	0.017197	-20.694772	-18.650213	0.31 (143-> 148)	0.13 (141-> 149)	0.13 (140-> 150)
91	5.043	245.8	0.058612	0.049595	72.863713	66.097274	0.16 (110-> 146)	0.15 (110-> 145)	0.05 (123-> 146)
92	5.077	244.2	0.024591	0.026317	-13.337950	-17.196896	0.16 (138-> 151)	0.07 (144-> 159)	0.06 (137-> 153)
93	5.088	243.7	0.006276	0.006221	-0.943781	-0.809775	0.24 (141-> 148)	0.15 (143-> 150)	0.12 (142-> 149)
94	5.089	243.6	0.007035	0.006955	1.083984	1.081728	0.24 (140-> 148)	0.19 (142-> 150)	0.10 (141-> 148)
95	5.103	243.0	0.020181	0.016006	25.182079	18.494259	0.44 (117-> 145)	0.08 (115-> 145)	0.06 (111-> 145)
96	5.104	242.9	0.009033	0.007205	-9.983218	-4.800167	0.45 (117-> 146)	0.09 (115-> 146)	0.06 (111-> 146)
97	5.112	242.5	0.330025	0.266948	-46.435873	-39.518165	0.08 (143-> 151)	0.08 (140-> 152)	0.08 (110-> 145)
98	5.112	242.5	0.375153	0.302433	93.766732	77.257536	0.10 (141-> 152)	0.09 (142-> 154)	0.08 (110-> 146)
99	5.116	242.3	0.101610	0.081468	-57.953184	-47.704792	0.30 (143-> 151)	0.10 (141-> 149)	0.10 (140-> 150)
100	5.125	241.9	0.010253	0.007844	5.647344	4.681896	0.34 (142-> 151)	0.17 (143-> 152)	0.14 (140-> 149)
101	5.134	241.5	0.000131	0.000153	0.471042	0.518288	0.25 (142-> 148)	0.17 (141-> 150)	0.14 (140-> 149)
102	5.152	240.6	0.004664	0.004108	-0.761239	-0.465424	0.18 (114-> 145)	0.14 (113-> 146)	0.11 (113-> 145)
103	5.161	240.3	0.000053	0.000020	-0.283885	-0.144042	0.14 (113-> 146)	0.10 (144-> 155)	0.10 (114-> 145)
104	5.165	240.1	0.002883	0.002182	-4.621032	-3.894261	0.38 (144-> 155)	0.15 (144-> 156)	0.03 (140-> 151)
105	5.169	239.9	0.003419	0.002813	2.173346	1.983248	0.51 (144-> 156)	0.13 (144-> 155)	0.03 (141-> 151)
106	5.170	239.8	0.002243	0.001628	1.280927	1.217385	0.14 (144-> 155)	0.07 (142-> 151)	0.05 (138-> 152)
107	5.171	239.8	0.000984	0.000726	0.438070	0.186800	0.28 (141-> 151)	0.09 (142-> 150)	0.09 (140-> 152)
108	5.175	239.6	0.000482	0.000361	0.511315	0.397116	0.27 (140-> 151)	0.09 (142-> 149)	0.08 (141-> 152)
109	5.180	239.4	0.001150	0.001007	0.112090	0.011618	0.35 (144-> 157)	0.20 (144-> 158)	0.04 (144-> 162)
110	5.182	239.2	0.000997	0.000880	-2.673034	-2.805384	0.42 (144-> 158)	0.23 (144-> 157)	0.02 (143-> 162)
111	5.201	238.4	0.001303	0.000770	0.575258	0.181968	0.10 (143-> 153)	0.08 (144-> 157)	0.06 (142-> 154)
112	5.202	238.3	0.000100	0.000140	0.437795	-0.330974	0.12 (143-> 154)	0.09 (142-> 153)	0.06 (144-> 163)
113	5.206	238.1	0.002329	0.001496	3.036199	1.993260	0.06 (144-> 158)	0.06 (144-> 161)	0.05 (143-> 154)
114	5.210	238.0	0.000307	0.000456	-0.326284	0.226308	0.07 (144-> 160)	0.06 (143-> 153)	0.05 (112-> 146)
115	5.215	237.7	0.002346	0.002420	-4.521084	-4.391016	0.08 (142-> 153)	0.08 (112-> 145)	0.07 (143-> 154)
116	5.217	237.7	0.003400	0.002994	2.780237	3.152031	0.11 (143-> 153)	0.05 (142-> 154)	0.04 (144-> 158)
117	5.246	236.3	0.000134	0.000094	-0.826777	-0.722333	0.25 (141-> 154)	0.23 (140-> 153)	0.07 (141-> 153)
118	5.247	236.3	0.000603	0.000400	0.631458	0.398371	0.43 (134-> 147)	0.12 (126-> 147)	0.05 (120-> 146)
119	5.258	235.8	0.107844	0.083015	-109.057869	-97.653460	0.26 (112-> 146)	0.06 (141-> 151)	0.06 (140-> 151)
120	5.259	235.8	0.113182	0.086743	119.011374	105.223932	0.27 (112-> 145)	0.06 (140-> 151)	0.06 (141-> 151)
121	5.265	235.5	0.004453	0.003259	7.897496	6.589365	0.31 (140-> 154)	0.30 (141-> 153)	0.05 (140-> 153)
122	5.267	235.4	0.014529	0.011584	-19.745721	-17.294045	0.14 (114-> 146)	0.13 (113-> 145)	0.07 (114-> 145)
123	5.313	233.4	0.000387	0.000295	0.712693	0.609403	0.12 (114-> 146)	0.12 (113-> 145)	0.07 (114-> 145)
124	5.376	230.6	0.005546	0.004983	1.446716	2.031822	0.10 (144-> 158)	0.07 (144-> 166)	0.06 (144-> 161)
125	5.376	230.6	0.002285	0.002055	-1.441984	-1.421822	0.10 (144-> 157)	0.05 (142-> 162)	0.05 (142-> 157)
126	5.379	230.5	0.001159	0.001105	3.706973	3.761406	0.09 (144-> 156)	0.04 (141-> 160)	0.04 (144-> 163)
127	5.380	230.5	0.002743	0.002454	-1.133501	-1.542640	0.09 (144-> 155)	0.06 (140-> 155)	0.04 (142-> 155)
128	5.399	229.6	0.001043	0.000810	0.507786	0.457569	0.48 (144-> 166)	0.09 (144-> 172)	0.06 (144-> 161)
129	5.419	228.8	0.000442	0.000423	-0.702408	-0.728158	0.47 (115-> 146)	0.17 (117-> 146)	0.15 (110-> 146)
130	5.420	228.7	0.000414	0.000399	-1.584775	-1.524218	0.48 (115-> 145)	0.15 (117-> 145)	0.15 (110-> 145)
131	5.431	228.3	0.006818	0.005510	-6.949735	-6.604078	0.70 (144-> 160)	0.03 (144-> 163)	0.02 (128-> 149)
132	5.437	228.0	0.003102	0.002536	-5.143013	-4.550411	0.46 (144-> 163)	0.19 (144-> 161)	0.06 (144-> 159)
133	5.447	227.6	0.000413	0.000472	-2.498698	-2.642026	0.57 (144-> 162)	0.06 (143-> 152)	0.05 (139-> 152)
134	5.453	227.4	0.013082	0.011063	20.350955	18.849680	0.45 (144-> 161)	0.19 (144-> 163)	0.07 (144-> 166)
135	5.455	227.3	0.000857	0.000590	-3.136222	-2.342227	0.24 (144-> 162)	0.13 (143-> 152)	0.12 (139-> 152)
136	5.463	227.0	0.024285	0.024302	-16.777456	-16.759396	0.45 (139-> 149)	0.13 (139-> 148)	0.05 (142-> 153)
137	5.468	226.7	0.063160	0.058950	43.216400	40.853213	0.53 (139-> 150)	0.05 (133-> 147)	0.04 (142-> 154)
138	5.484	226.1	0.003135	0.003191	-4.631709	-4.489072	0.65 (139-> 148)	0.10 (139-> 149)	0.04 (143-> 148)
139	5.497	225.6	0.179033	0.146825	54.870814	46.849619	0.13 (141-> 152)	0.09 (134-> 149)	0.05 (143-> 153)
140	5.497	225.5	0.182223	0.150588	-51.783174	-49.611278	0.11 (140-> 152)	0.06 (134-> 150)	0.06 (142-> 153)

141	5.516	224.8	0.033965	0.026838	-31.954247	-27.491516	0.18 (142-> 152)	0.13 (141-> 154)	0.12 (140-> 153)
142	5.541	223.8	0.008086	0.006613	0.998432	1.186443	0.34 (138-> 147)	0.06 (135-> 148)	0.05 (134-> 151)
143	5.548	223.5	0.099472	0.086263	19.508759	16.974166	0.11 (141-> 152)	0.08 (139-> 150)	0.07 (142-> 154)
144	5.550	223.4	0.094773	0.082012	-11.619420	-10.471310	0.11 (140-> 152)	0.09 (142-> 153)	0.08 (137-> 147)
145	5.561	222.9	0.000828	0.000572	-2.454706	-2.111454	0.35 (134-> 148)	0.09 (120-> 150)	0.08 (121-> 149)
146	5.583	222.1	0.000104	0.000056	-0.440143	-0.221209	0.29 (109-> 146)	0.28 (108-> 145)	0.04 (144-> 166)
147	5.604	221.2	0.167128	0.132079	118.704964	98.207011	0.19 (134-> 150)	0.18 (137-> 147)	0.07 (120-> 151)
148	5.607	221.1	0.167363	0.133097	-117.111025	-99.835995	0.17 (136-> 147)	0.14 (134-> 149)	0.07 (121-> 151)
149	5.630	220.2	0.028809	0.022453	-3.294734	-1.043481	0.19 (126-> 147)	0.07 (131-> 148)	0.06 (133-> 149)
150	5.646	219.6	0.000719	0.000562	1.129243	0.827798	0.31 (134-> 151)	0.08 (138-> 147)	0.06 (120-> 150)

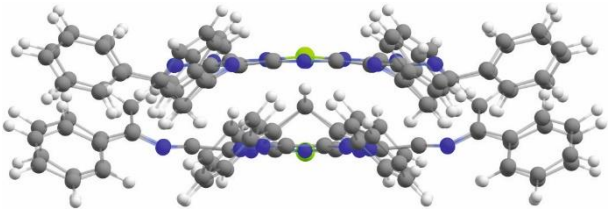

Table S10 Optimized geometry of $[Ph_8Dz_4PzMg]_2$ (dimer)

CARTESIAN COORDINATES (ANGSTROEM)

C	-4.202419000000	-0.756400000000	-1.478703000000	C	1.945278000000	7.618704000000	-1.202346000000
C	-4.217085000000	0.667515000000	-1.463943000000	C	-2.053828000000	7.597130000000	-1.357704000000
C	-2.817035000000	1.098260000000	-1.603052000000	C	-7.622558000000	1.941465000000	-1.206825000000
C	-7.567386000000	2.888557000000	-2.260569000000	C	-7.599893000000	-2.055815000000	-1.354495000000
C	-2.793774000000	-1.158386000000	-1.610314000000	C	1.824018000000	8.821680000000	-0.469923000000
C	0.753438000000	-4.204296000000	-1.478755000000	C	2.617092000000	9.934182000000	-0.783549000000
C	-0.670447000000	-4.219059000000	-1.462672000000	C	3.544267000000	9.869060000000	-1.836113000000
C	-1.101415000000	-2.819133000000	-1.602579000000	C	3.684576000000	8.673843000000	-2.566339000000
C	-7.469971000000	-3.066398000000	-2.341756000000	C	2.896031000000	7.562038000000	-2.252702000000
C	1.155131000000	-2.795663000000	-1.610894000000	C	-3.063719000000	7.466581000000	-2.345585000000
C	-8.571008000000	-3.835939000000	-2.728726000000	C	-3.832780000000	8.567453000000	-2.733991000000
C	4.201352000000	0.751260000000	-1.475196000000	C	-3.610925000000	9.828193000000	-2.147284000000
C	4.215620000000	-0.672631000000	-1.462662000000	C	-2.617818000000	9.970132000000	-1.165332000000
C	2.815638000000	-1.103059000000	-1.602453000000	C	-1.846289000000	8.866888000000	-0.773323000000
C	-9.831307000000	-3.613902000000	-2.141131000000	C	-8.825195000000	1.821237000000	-0.473701000000
C	2.792776000000	1.153536000000	-1.607418000000	C	-9.938783000000	2.611780000000	-0.789854000000
C	-9.972620000000	-2.620095000000	-1.159800000000	C	-9.875133000000	3.535296000000	-1.845711000000
C	-0.754497000000	4.199459000000	-1.478544000000	C	-8.680283000000	3.674535000000	-2.576751000000
C	0.669331000000	4.214079000000	-1.462088000000	H	-6.623129000000	2.980494000000	-2.819080000000
C	1.100289000000	2.814022000000	-1.600507000000	H	-6.475583000000	-3.221940000000	-2.787678000000
C	-8.869208000000	-1.848049000000	-0.769259000000	H	-8.450236000000	-4.615851000000	-3.499251000000
C	-1.156344000000	2.790721000000	-1.609955000000	H	-10.701317000000	-4.218958000000	-2.446318000000
C	-1.825647000000	-8.824550000000	-0.461993000000	H	-10.951582000000	-2.446503000000	-0.684243000000
C	-2.618321000000	-9.937861000000	-0.773752000000	H	-9.002634000000	-1.088442000000	0.012538000000
C	-3.543359000000	-9.875844000000	-1.828383000000	H	-1.135356000000	-8.888114000000	0.391364000000
C	-3.681934000000	-8.682911000000	-2.562652000000	H	-4.162462000000	-10.754740000000	-2.074058000000
C	-2.893898000000	-7.570230000000	-2.250780000000	H	-4.408614000000	-8.625304000000	-3.390408000000
C	-1.269111000000	6.403850000000	-0.979579000000	H	-2.985355000000	-6.627399000000	-2.811768000000
C	-0.093416000000	6.466949000000	-0.018834000000	H	3.214016000000	-6.479605000000	-2.793069000000
C	1.138588000000	6.417423000000	-0.905046000000	H	4.602963000000	-8.456098000000	-3.509229000000
C	3.058604000000	-7.473802000000	-2.346660000000	H	4.206260000000	-10.706737000000	-2.455286000000
C	3.825397000000	-8.575845000000	-2.736179000000	H	2.439164000000	-10.954708000000	-0.687532000000
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C	-6.469003000000	-0.093555000000	-0.018871000000	H	-0.126234000000	7.355699000000	0.633596000000
C	-6.420425000000	1.136811000000	-0.907422000000	H	-0.108311000000	5.556553000000	0.627324000000
C	3.603462000000	-9.835896000000	-2.148006000000	H	-7.357249000000	-0.125400000000	0.634313000000
C	2.612606000000	-9.975923000000	-1.163516000000	H	-5.558066000000	-0.107366000000	0.626534000000
C	1.267961000000	-6.408152000000	-0.977755000000	H	0.125607000000	-7.357518000000	0.637313000000
C	0.092718000000	-6.469717000000	-0.016411000000	H	0.107858000000	-5.558327000000	0.628302000000
C	-1.139191000000	-6.421693000000	-0.902827000000	H	-2.519220000000	-10.858968000000	-0.177144000000
C	1.843311000000	-8.871489000000	-0.770422000000	H	1.131965000000	8.887717000000	0.381801000000
C	2.050938000000	-7.602432000000	-1.356254000000	H	2.516562000000	10.857134000000	-0.190039000000
C	-1.945356000000	-7.623784000000	-1.198286000000	H	4.163762000000	10.747272000000	-2.083234000000

H	4.413108000000	8.613705000000	-3.392283000000
H	2.988848000000	6.617448000000	-2.810493000000
H	-3.219099000000	6.471882000000	-2.790874000000
H	-4.612176000000	8.446207000000	-3.504962000000
H	-4.215577000000	10.698066000000	-2.453658000000
H	-2.444390000000	10.949451000000	-0.690452000000
H	-1.087224000000	9.000777000000	0.008924000000
H	-8.890156000000	1.132105000000	0.380475000000
H	-10.861501000000	2.512092000000	-0.195827000000
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N	2.008908000000	0.017192000000	-1.647469000000
N	2.424746000000	-2.380458000000	-1.600323000000
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N	2.377756000000	2.423201000000	-1.596580000000
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N	1.593337000000	-5.261765000000	-1.528196000000
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C	6.419476000000	-1.143053000000	-0.908737000000
C	7.621248000000	-1.946088000000	-1.213831000000
C	7.598272000000	2.052256000000	-1.342110000000
C	8.831114000000	-1.816276000000	-0.494518000000
C	9.944380000000	-2.604710000000	-0.817211000000
C	9.872983000000	-3.536108000000	-1.865554000000
C	8.670739000000	-3.685252000000	-2.582498000000
H	6.608480000000	-3.000617000000	-2.807468000000
H	6.482673000000	3.200879000000	-2.796073000000
H	8.457633000000	4.598365000000	-3.499889000000
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H	7.354899000000	0.113466000000	0.638819000000
H	5.556049000000	0.095274000000	0.629131000000
H	8.902886000000	-1.119564000000	0.352746000000
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C	3.486970000000	-2.464396000000	1.522701000000
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C	-3.983376000000	-6.789177000000	1.321063000000
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C	-8.871379000000	5.227357000000	0.997250000000
C	-7.542958000000	4.966208000000	0.633320000000
C	-7.554613000000	-4.916863000000	0.566208000000
C	-8.909915000000	-5.112565000000	0.866195000000
C	-9.538569000000	-4.328786000000	1.846845000000
C	-8.801692000000	-3.337047000000	2.521941000000
H	-6.854411000000	-2.370067000000	2.737374000000
H	-2.488667000000	-6.815941000000	2.883804000000
H	-2.955068000000	-9.198084000000	3.560796000000
H	-4.729310000000	-10.512941000000	2.354503000000
H	-5.998611000000	-9.444654000000	0.468593000000
H	-5.524599000000	-7.107236000000	-0.194641000000
H	5.524133000000	-7.090110000000	-0.234003000000
H	4.489828000000	-10.606439000000	2.066548000000
H	2.723461000000	-9.292344000000	3.284575000000
H	2.376864000000	-6.857164000000	2.735296000000
H	6.825275000000	-2.478574000000	2.866472000000
H	9.214819000000	-2.932206000000	3.525570000000
H	10.528848000000	-4.702196000000	2.312059000000
H	9.451414000000	-5.981221000000	0.437995000000
H	7.106429000000	-5.520425000000	-0.207126000000
H	-3.920889000000	3.889715000000	-0.594603000000

H	-5.184646000000	5.169122000000	-0.633603000000	N	2.638112000000	-4.813435000000	1.523002000000
H	-3.889959000000	-3.926195000000	-0.591774000000	N	-1.414416000000	-1.425381000000	1.719586000000
H	-5.169614000000	-5.189828000000	-0.627771000000	C	3.256773000000	7.412442000000	2.365284000000
H	3.923646000000	-3.888413000000	-0.594362000000	C	7.448101000000	3.153066000000	2.236123000000
H	5.188388000000	-5.166668000000	-0.634105000000	C	8.797282000000	3.357525000000	2.541628000000
H	5.878219000000	-9.480872000000	0.301681000000	C	9.533001000000	4.350999000000	1.867783000000
H	-5.524488000000	7.091004000000	-0.226933000000	C	8.906197000000	5.128063000000	0.880630000000
H	-5.878110000000	9.481066000000	0.311872000000	C	7.553615000000	4.924671000000	0.573554000000
H	-4.485679000000	10.605577000000	2.074209000000	C	5.376591000000	3.675181000000	0.951566000000
H	-2.716025000000	9.290869000000	3.286901000000	C	4.551796000000	4.566699000000	0.039586000000
H	-2.370300000000	6.856198000000	2.734798000000	C	3.677379000000	5.385434000000	0.974811000000
H	-6.817593000000	2.488743000000	2.875220000000	C	3.982553000000	6.789796000000	1.317843000000
H	-9.202368000000	2.952465000000	3.544670000000	C	6.799809000000	3.937423000000	1.248096000000
H	-10.516314000000	4.723285000000	2.332366000000	C	4.969405000000	7.544726000000	0.644224000000
H	-9.444372000000	5.991920000000	0.448091000000	C	5.230477000000	8.872400000000	1.010990000000
H	-7.104262000000	5.520770000000	-0.207579000000	C	4.513175000000	9.472484000000	2.058053000000
H	-7.092180000000	-5.525959000000	-0.222235000000	C	3.518967000000	8.736482000000	2.730602000000
H	-9.481951000000	-5.878867000000	0.318711000000	H	2.485149000000	6.817605000000	2.877910000000
H	-10.604703000000	-4.485236000000	2.081236000000	H	6.853674000000	2.381378000000	2.748965000000
H	-9.288759000000	-2.714940000000	3.291588000000	H	9.282956000000	2.740485000000	3.316221000000
N	1.426293000000	-1.415986000000	1.721621000000	H	10.596805000000	4.514004000000	2.108240000000
N	0.010230000000	-3.397234000000	1.659765000000	H	9.477565000000	5.895363000000	0.333816000000
N	1.417280000000	1.424875000000	1.722186000000	H	7.092899000000	5.528435000000	-0.219980000000
N	3.398236000000	0.008783000000	1.661439000000	H	5.170929000000	5.188517000000	-0.628578000000
N	-1.424034000000	1.415344000000	1.720946000000	H	3.892479000000	3.923481000000	-0.590847000000
N	-3.395728000000	-0.009229000000	1.658971000000	H	5.526053000000	7.106881000000	-0.195682000000
N	-0.007701000000	3.396408000000	1.660727000000	H	5.997176000000	9.445632000000	0.465053000000
N	-4.826547000000	2.631463000000	1.538215000000	H	4.723715000000	10.515675000000	2.347141000000
N	-2.635068000000	4.812962000000	1.523729000000	H	2.948300000000	9.201186000000	3.552168000000
N	-2.631171000000	-4.827970000000	1.542422000000	N	4.814765000000	2.637325000000	1.527072000000
N	-4.812105000000	-2.636170000000	1.524580000000	N	2.632390000000	4.827542000000	1.541568000000
N	4.829038000000	-2.631050000000	1.539746000000	Mg	0.001283000000	-0.000159000000	1.830595000000

Table S11 TD-DFT calculated UV-Vis spectrum of $[Ph_8Dz_4PzMg]_2$ (dimer)

state	eV	nm	fL	fV	Rl	RV			
0	0.898	1380.4	0.000027	0.000100	13.371408	25.659816	0.98 (295-> 296)	0.01 (295-> 297)	0.00 (295-> 303)
1	0.899	1379.5	0.000029	0.000106	13.628078	26.262695	0.98 (295-> 297)	0.01 (295-> 296)	0.00 (295-> 304)
2	1.416	875.8	0.082727	0.207677	3.808623	6.035187	0.81 (295-> 298)	0.15 (294-> 296)	0.01 (294-> 297)
3	1.416	875.3	0.082952	0.207990	3.702491	5.863068	0.81 (295-> 299)	0.15 (294-> 297)	0.01 (294-> 296)
4	1.873	661.9	0.725729	1.285824	-59.413696	-79.093571	0.77 (294-> 296)	0.12 (295-> 298)	0.02 (293-> 297)
5	1.874	661.6	0.724916	1.283711	-59.205985	-78.792657	0.77 (294-> 297)	0.12 (295-> 299)	0.02 (293-> 296)
6	2.230	556.1	0.000019	0.000015	-11.940300	-10.406172	0.47 (292-> 296)	0.44 (291-> 297)	0.01 (291-> 296)
7	2.258	549.2	0.000013	0.000015	0.060197	0.066705	0.34 (292-> 297)	0.34 (291-> 296)	0.11 (291-> 297)
8	2.259	548.8	0.001621	0.001955	10.076663	10.691140	0.51 (294-> 298)	0.35 (290-> 297)	0.05 (290-> 296)
9	2.260	548.6	0.001469	0.001781	9.842043	10.514139	0.51 (294-> 299)	0.36 (290-> 296)	0.04 (290-> 297)
10	2.271	546.0	0.000085	0.000103	-0.059182	-0.066129	0.36 (291-> 297)	0.33 (292-> 296)	0.11 (291-> 296)
11	2.293	540.8	0.060485	0.072705	14.681415	16.074370	0.58 (289-> 296)	0.16 (293-> 296)	0.05 (293-> 297)
12	2.294	540.5	0.063347	0.076056	14.958323	16.375145	0.57 (289-> 297)	0.15 (293-> 297)	0.06 (293-> 296)
13	2.318	534.8	0.000149	0.000176	-0.388987	-0.422790	0.46 (291-> 296)	0.46 (292-> 297)	0.01 (291-> 297)
14	2.325	533.2	0.085548	0.102766	-131.924883	-144.445611	0.39 (288-> 297)	0.20 (289-> 296)	0.14 (293-> 296)
15	2.325	533.2	0.078023	0.093582	-125.071529	-136.822525	0.39 (288-> 296)	0.23 (289-> 297)	0.13 (293-> 297)
16	2.348	528.1	0.211709	0.258106	32.322873	35.703304	0.40 (288-> 297)	0.33 (293-> 297)	0.10 (293-> 296)
17	2.348	528.0	0.212492	0.259160	31.668995	34.997658	0.40 (288-> 296)	0.32 (293-> 296)	0.10 (293-> 297)
18	2.399	516.8	0.011425	0.014060	145.978564	162.122804	0.56 (290-> 297)	0.30 (294-> 298)	0.05 (294-> 299)
19	2.401	516.4	0.011553	0.014256	146.137929	162.569370	0.53 (290-> 296)	0.30 (294-> 299)	0.05 (294-> 298)
20	2.491	497.8	0.000002	0.000002	-0.000939	-0.001175	0.75 (295-> 300)	0.06 (287-> 297)	0.06 (286-> 296)
21	2.512	493.6	0.000001	0.000001	-0.001618	-0.001639	0.52 (295-> 301)	0.13 (287-> 296)	0.12 (286-> 297)
22	2.528	490.4	0.000179	0.000193	-0.382975	-0.396190	0.42 (286-> 296)	0.41 (287-> 297)	0.04 (292-> 298)
23	2.575	481.6	0.000162	0.000140	0.048341	0.045126	0.28 (286-> 296)	0.27 (287-> 297)	0.17 (295-> 300)
24	2.576	481.4	0.004608	0.003979	1.679382	1.560456	0.46 (286-> 297)	0.40 (287-> 296)	0.02 (295-> 302)
25	2.582	480.3	0.000010	0.000008	0.005833	0.005267	0.39 (295-> 301)	0.26 (286-> 297)	0.20 (287-> 296)
26	2.780	446.0	0.000004	0.000004	0.029825	0.033459	0.38 (292-> 298)	0.36 (291-> 299)	0.06 (291-> 298)

27	2.785	445.2	0.000007	0.000007	0.022445	0.022223	0.37 (291-> 298)	0.37 (292-> 299)	0.07 (292-> 298)
28	2.802	442.5	0.001241	0.001607	2.397536	2.865227	0.28 (292-> 299)	0.27 (291-> 298)	0.17 (291-> 299)
29	2.809	441.4	0.055385	0.060974	145.050151	152.005166	0.47 (289-> 298)	0.24 (293-> 298)	0.15 (289-> 299)
30	2.810	441.3	0.036564	0.039675	118.129203	122.912125	0.44 (289-> 299)	0.27 (293-> 299)	0.15 (289-> 298)
31	2.813	440.8	0.000326	0.000338	1.513462	1.556528	0.26 (291-> 299)	0.24 (292-> 298)	0.16 (291-> 298)
32	2.820	439.7	0.051052	0.056647	-108.446897	-114.220329	0.50 (293-> 298)	0.15 (289-> 298)	0.15 (288-> 299)
33	2.820	439.6	0.049881	0.055127	-105.685270	-111.130491	0.45 (293-> 299)	0.18 (289-> 299)	0.16 (288-> 298)
34	2.849	435.2	0.042828	0.046769	-26.628929	-27.816405	0.66 (288-> 298)	0.14 (293-> 299)	0.04 (288-> 299)
35	2.849	435.1	0.035628	0.038670	-24.065147	-25.056218	0.68 (288-> 299)	0.13 (293-> 298)	0.04 (288-> 298)
36	2.886	429.7	0.839842	0.929034	-6.607469	-6.955310	0.54 (290-> 299)	0.31 (290-> 298)	0.07 (283-> 297)
37	2.886	429.6	0.818170	0.905064	-24.095603	-25.359507	0.52 (290-> 298)	0.30 (290-> 299)	0.07 (283-> 296)
38	3.024	410.1	0.001369	0.002031	16.566223	20.180179	0.92 (295-> 302)	0.01 (287-> 296)	0.01 (286-> 297)
39	3.045	407.2	0.001168	0.001285	-14.538250	-15.240251	0.94 (295-> 303)	0.01 (276-> 297)	0.01 (294-> 298)
40	3.046	407.1	0.001295	0.001415	-15.132371	-15.821351	0.95 (295-> 304)	0.01 (276-> 296)	0.01 (294-> 299)
41	3.047	406.9	0.000139	0.000159	-26.923195	-28.871304	0.36 (287-> 299)	0.36 (286-> 298)	0.05 (295-> 308)
42	3.057	405.6	0.000038	0.000048	-0.337622	-0.381885	0.36 (287-> 298)	0.32 (286-> 299)	0.13 (295-> 305)
43	3.079	402.7	0.000002	0.000002	0.003657	0.003619	0.30 (286-> 298)	0.29 (287-> 299)	0.16 (286-> 299)
44	3.083	402.2	0.000001	0.000001	0.004628	0.005007	0.30 (286-> 299)	0.28 (287-> 298)	0.15 (287-> 299)
45	3.212	386.0	0.309846	0.303592	14.171423	14.026010	0.92 (295-> 306)	0.02 (283-> 297)	0.01 (277-> 297)
46	3.213	385.9	0.311153	0.304918	14.448284	14.303750	0.92 (295-> 307)	0.02 (283-> 296)	0.01 (277-> 296)
47	3.227	384.2	0.000551	0.000541	0.514990	0.140140	0.86 (295-> 308)	0.03 (295-> 305)	0.03 (287-> 299)
48	3.235	383.3	0.000110	0.000107	0.015703	0.012958	0.92 (295-> 309)	0.01 (295-> 338)	0.01 (294-> 301)
49	3.258	380.6	0.000057	0.000056	0.016855	0.016569	0.91 (295-> 310)	0.02 (294-> 300)	0.01 (295-> 337)
50	3.327	372.7	0.000075	0.000077	0.083370	0.085442	0.81 (295-> 305)	0.05 (287-> 298)	0.05 (286-> 299)
51	3.349	370.2	0.000002	0.000002	-0.000402	-0.000362	0.90 (294-> 300)	0.02 (295-> 310)	0.01 (286-> 299)
52	3.355	369.5	0.649089	0.679498	-36.955575	-37.806483	0.30 (283-> 297)	0.19 (295-> 313)	0.19 (283-> 296)
53	3.355	369.5	0.654198	0.684753	-36.626230	-37.462581	0.29 (283-> 296)	0.19 (295-> 312)	0.19 (283-> 297)
54	3.383	366.5	0.000001	0.000001	0.000688	0.000636	0.92 (294-> 301)	0.01 (295-> 309)	0.01 (294-> 316)
55	3.423	362.2	0.035123	0.036884	-44.875065	-45.969344	0.26 (284-> 296)	0.10 (285-> 296)	0.07 (284-> 297)
56	3.424	362.1	0.027410	0.028747	-42.869217	-43.896179	0.25 (284-> 297)	0.09 (285-> 297)	0.08 (284-> 296)
57	3.432	361.2	0.001148	0.001202	0.275459	0.302289	0.59 (295-> 311)	0.07 (271-> 296)	0.07 (270-> 297)
58	3.443	360.1	0.331952	0.342790	62.361943	63.431919	0.19 (285-> 297)	0.12 (285-> 296)	0.11 (284-> 297)
59	3.443	360.1	0.344631	0.355334	56.220973	57.121724	0.17 (285-> 296)	0.14 (285-> 297)	0.11 (284-> 296)
60	3.462	358.2	0.000006	0.000007	-0.869123	-0.947975	0.32 (279-> 296)	0.28 (278-> 297)	0.03 (256-> 296)
61	3.474	356.8	0.000015	0.000016	0.021434	0.024500	0.19 (278-> 297)	0.15 (279-> 296)	0.08 (271-> 296)
62	3.482	356.1	0.000004	0.000004	0.011885	0.008911	0.18 (278-> 296)	0.17 (279-> 297)	0.08 (271-> 297)
63	3.516	352.6	0.000099	0.000095	0.174232	0.156828	0.34 (295-> 311)	0.14 (270-> 297)	0.13 (271-> 296)
64	3.523	351.9	0.006559	0.006743	-56.460161	-57.108614	0.22 (276-> 297)	0.12 (261-> 296)	0.11 (262-> 297)
65	3.523	351.9	0.005412	0.005505	-51.898231	-52.269801	0.23 (276-> 296)	0.11 (261-> 297)	0.11 (262-> 296)
66	3.546	349.6	0.052291	0.055613	31.229123	32.192212	0.39 (262-> 296)	0.10 (261-> 297)	0.06 (261-> 296)
67	3.546	349.6	0.051451	0.054793	31.824904	32.820424	0.40 (262-> 297)	0.11 (261-> 296)	0.06 (261-> 297)
68	3.554	348.9	0.030141	0.031130	25.725901	26.040422	0.29 (261-> 296)	0.11 (276-> 296)	0.10 (276-> 297)
69	3.554	348.8	0.032006	0.032937	30.256005	30.523238	0.31 (261-> 297)	0.10 (276-> 297)	0.09 (276-> 296)
70	3.565	347.8	0.828934	0.865773	-81.803861	-83.612458	0.59 (295-> 312)	0.14 (283-> 296)	0.02 (283-> 297)
71	3.566	347.7	0.833060	0.869553	-67.764645	-69.246485	0.58 (295-> 313)	0.14 (283-> 297)	0.02 (276-> 297)
72	3.605	343.9	0.001366	0.001375	1.942504	1.910679	0.58 (295-> 314)	0.14 (276-> 296)	0.09 (276-> 297)
73	3.605	343.9	0.001950	0.001971	23.403138	23.690680	0.58 (295-> 315)	0.15 (276-> 297)	0.09 (276-> 296)
74	3.605	343.9	0.000117	0.000115	1.454012	1.399490	0.31 (279-> 297)	0.31 (278-> 296)	0.03 (246-> 296)
75	3.624	342.1	0.006148	0.006438	-13.902502	-14.233529	0.18 (281-> 297)	0.18 (282-> 296)	0.18 (271-> 297)
76	3.642	340.4	0.000074	0.000082	11.197053	14.922610	0.21 (293-> 302)	0.16 (289-> 300)	0.16 (292-> 303)
77	3.650	339.7	0.000146	0.000147	0.055249	0.054073	0.14 (278-> 296)	0.14 (279-> 297)	0.08 (270-> 296)
78	3.657	339.0	0.000066	0.000066	-0.006329	-0.001561	0.16 (278-> 297)	0.16 (279-> 296)	0.08 (271-> 296)
79	3.677	337.2	0.851452	0.869464	-121.208907	-122.478616	0.15 (292-> 302)	0.12 (293-> 303)	0.07 (291-> 300)
80	3.678	337.1	0.837580	0.855490	-115.491806	-116.726768	0.14 (291-> 302)	0.12 (293-> 304)	0.07 (292-> 300)
81	3.691	335.9	0.057388	0.058000	-21.430565	-21.573296	0.46 (277-> 296)	0.05 (293-> 303)	0.05 (291-> 300)
82	3.691	335.9	0.057512	0.057787	-21.493269	-21.548079	0.46 (277-> 297)	0.06 (293-> 304)	0.05 (292-> 300)
83	3.706	334.5	0.000159	0.000158	-0.081404	-0.087247	0.25 (293-> 300)	0.15 (289-> 302)	0.07 (290-> 301)
84	3.721	333.2	0.000170	0.000169	-0.319021	-0.314506	0.22 (293-> 301)	0.14 (288-> 302)	0.11 (290-> 300)
85	3.736	331.9	0.020224	0.020586	221.229319	222.982352	0.14 (292-> 301)	0.08 (291-> 300)	0.08 (283-> 299)
86	3.736	331.8	0.023065	0.023509	233.974398	235.984648	0.14 (291-> 301)	0.08 (283-> 298)	0.08 (292-> 300)
87	3.761	329.6	0.003523	0.002824	2.766216	2.487069	0.09 (282-> 296)	0.09 (281-> 297)	0.06 (289-> 301)
88	3.768	329.0	0.006008	0.005179	-4.381268	-4.068432	0.14 (289-> 301)	0.13 (288-> 300)	0.06 (282-> 296)
89	3.774	328.5	0.002191	0.002113	42.728060	41.913630	0.32 (283-> 298)	0.06 (280-> 297)	0.05 (277-> 298)
90	3.775	328.4	0.002523	0.002455	46.634230	45.973074	0.32 (283-> 299)	0.06 (280-> 296)	0.05 (277-> 299)
91	3.811	325.3	0.000872	0.000861	-1.679921	-1.674982	0.26 (280-> 296)	0.21 (283-> 299)	0.05 (283-> 298)
92	3.811	325.3	0.000883	0.000877	-2.278722	-2.270702	0.26 (280-> 297)	0.21 (283-> 298)	0.05 (283-> 299)

93	3.820	324.6	0.000004	0.000003	-0.012535	-0.010916	0.06 (271-> 297)	0.06 (270-> 296)	0.06 (282-> 296)
94	3.825	324.1	0.000027	0.000026	-0.395745	-0.391072	0.79 (294-> 302)	0.04 (288-> 300)	0.03 (289-> 301)
95	3.829	323.8	0.000006	0.000005	-0.009097	-0.009004	0.07 (282-> 297)	0.07 (281-> 296)	0.07 (270-> 297)
96	3.864	320.9	0.001633	0.001818	12.591824	13.212266	0.18 (263-> 296)	0.12 (266-> 296)	0.07 (263-> 297)
97	3.864	320.8	0.001208	0.001374	10.715611	11.326028	0.18 (263-> 297)	0.13 (266-> 297)	0.07 (263-> 296)
98	3.869	320.4	0.031735	0.035746	-11.694645	-12.379597	0.69 (294-> 303)	0.04 (276-> 299)	0.03 (292-> 300)
99	3.870	320.4	0.032003	0.036034	-11.782033	-12.482632	0.69 (294-> 304)	0.04 (276-> 298)	0.03 (291-> 300)
100	3.893	318.5	0.000184	0.000168	0.396187	0.376360	0.20 (281-> 296)	0.20 (282-> 297)	0.11 (271-> 296)
101	3.914	316.8	0.000017	0.000016	0.008092	0.006903	0.46 (290-> 300)	0.15 (293-> 301)	0.04 (293-> 300)
102	3.921	316.2	0.000203	0.000264	-1.388571	-1.586089	0.13 (288-> 300)	0.12 (289-> 301)	0.05 (290-> 308)
103	3.926	315.8	0.000016	0.000014	0.007835	0.007704	0.36 (290-> 301)	0.05 (282-> 297)	0.05 (281-> 296)
104	3.937	314.9	0.013591	0.013620	-0.640548	-0.630543	0.05 (293-> 300)	0.04 (289-> 303)	0.03 (288-> 304)
105	3.938	314.8	0.016940	0.016958	0.257674	0.274505	0.05 (291-> 300)	0.04 (289-> 304)	0.04 (288-> 303)
106	3.939	314.8	0.005291	0.005333	-0.454555	-0.454102	0.14 (293-> 300)	0.09 (290-> 301)	0.06 (293-> 309)
107	3.945	314.3	0.000196	0.000224	-0.260538	-0.285207	0.10 (293-> 310)	0.09 (293-> 301)	0.05 (292-> 306)
108	3.948	314.0	0.016408	0.020217	-27.213678	-30.213291	0.24 (288-> 301)	0.24 (289-> 300)	0.08 (294-> 305)
109	3.964	312.8	0.004232	0.004212	3.854541	3.740403	0.24 (280-> 296)	0.08 (294-> 306)	0.05 (293-> 307)
110	3.965	312.7	0.002973	0.003004	0.292233	0.255943	0.24 (280-> 297)	0.08 (294-> 307)	0.05 (293-> 306)
111	3.965	312.7	0.001371	0.001398	-0.310682	-0.368435	0.10 (243-> 296)	0.10 (242-> 297)	0.06 (279-> 297)
112	3.971	312.3	0.654277	0.635841	-15.410411	-15.240518	0.18 (276-> 299)	0.07 (292-> 300)	0.07 (291-> 301)
113	3.971	312.2	0.655692	0.637285	-10.522852	-10.395194	0.18 (276-> 298)	0.08 (292-> 301)	0.07 (291-> 300)
114	3.990	310.7	0.024571	0.027617	-33.431695	-35.465218	0.13 (289-> 300)	0.07 (289-> 309)	0.07 (281-> 297)
115	3.995	310.3	0.004693	0.004537	-6.876508	-7.453171	0.11 (290-> 303)	0.09 (294-> 307)	0.09 (292-> 300)
116	3.996	310.3	0.004142	0.003955	-4.495702	-5.057256	0.11 (290-> 304)	0.09 (291-> 300)	0.08 (294-> 306)
117	3.998	310.2	0.000109	0.000062	0.813717	0.554408	0.20 (294-> 308)	0.12 (293-> 305)	0.09 (292-> 306)
118	4.036	307.2	0.000411	0.000493	13.296531	14.638587	0.10 (288-> 300)	0.08 (294-> 302)	0.08 (289-> 301)
119	4.038	307.1	0.026691	0.028121	-14.051043	-14.505004	0.09 (284-> 299)	0.07 (289-> 306)	0.06 (292-> 302)
120	4.038	307.1	0.029605	0.030911	-14.334986	-14.753229	0.09 (284-> 298)	0.07 (291-> 302)	0.05 (289-> 307)
121	4.041	306.8	0.001097	0.001169	24.505577	25.609280	0.07 (289-> 301)	0.07 (288-> 300)	0.07 (286-> 306)
122	4.043	306.7	0.000141	0.000149	0.647423	0.662207	0.13 (288-> 302)	0.11 (294-> 309)	0.10 (289-> 305)
123	4.048	306.3	0.010760	0.009011	15.324063	14.793396	0.10 (285-> 298)	0.08 (280-> 297)	0.08 (285-> 299)
124	4.049	306.2	0.010899	0.009001	14.020010	13.498644	0.11 (285-> 299)	0.09 (285-> 298)	0.08 (280-> 296)
125	4.051	306.0	0.005271	0.003485	2.718005	3.298295	0.12 (284-> 298)	0.04 (285-> 299)	0.04 (276-> 298)
126	4.052	306.0	0.005519	0.003950	3.039094	3.729007	0.12 (284-> 299)	0.05 (285-> 298)	0.04 (276-> 299)
127	4.054	305.8	0.000046	0.000039	0.136691	0.128484	0.14 (289-> 302)	0.10 (290-> 310)	0.09 (288-> 305)
128	4.064	305.1	0.000006	0.000006	0.001789	0.001472	0.13 (242-> 296)	0.12 (243-> 297)	0.07 (247-> 296)
129	4.065	305.0	0.000019	0.000017	-0.001526	-0.001406	0.10 (243-> 296)	0.10 (242-> 297)	0.07 (246-> 296)
130	4.093	302.9	0.001764	0.001669	-9.876380	-9.608265	0.45 (294-> 306)	0.05 (288-> 306)	0.04 (291-> 305)
131	4.093	302.9	0.001887	0.001789	-10.249071	-9.981155	0.45 (294-> 307)	0.05 (288-> 307)	0.04 (292-> 305)
132	4.100	302.4	0.000032	0.000027	0.174915	0.122450	0.13 (294-> 308)	0.09 (279-> 298)	0.09 (278-> 299)
133	4.104	302.1	0.000012	0.000018	0.159847	-0.401546	0.13 (243-> 297)	0.12 (242-> 296)	0.12 (246-> 297)
134	4.108	301.8	0.000004	0.000004	0.001496	0.001595	0.65 (294-> 309)	0.04 (290-> 300)	0.02 (242-> 296)
135	4.110	301.6	0.001140	0.001325	0.827021	0.893340	0.61 (294-> 305)	0.06 (289-> 300)	0.04 (278-> 298)
136	4.126	300.5	0.000133	0.000126	0.084170	0.081618	0.76 (294-> 310)	0.05 (290-> 301)	0.01 (243-> 296)
137	4.129	300.3	0.000848	0.000854	0.026895	0.017109	0.49 (294-> 308)	0.10 (279-> 298)	0.10 (278-> 299)
138	4.133	300.0	0.019205	0.019019	37.377918	37.793793	0.13 (285-> 298)	0.09 (284-> 299)	0.07 (294-> 307)
139	4.133	300.0	0.013023	0.012934	27.322761	27.951091	0.13 (285-> 299)	0.09 (284-> 298)	0.07 (263-> 297)
140	4.139	299.5	0.962637	0.931299	-79.293805	-77.992353	0.28 (276-> 298)	0.06 (276-> 299)	0.04 (290-> 306)
141	4.139	299.5	0.953522	0.921595	-90.464137	-88.935152	0.27 (276-> 299)	0.06 (276-> 298)	0.05 (290-> 307)
142	4.141	299.4	0.016524	0.014097	-3.095882	-2.636630	0.12 (271-> 297)	0.12 (270-> 296)	0.10 (278-> 298)
143	4.150	298.8	0.000238	0.000229	0.014298	0.013957	0.09 (248-> 297)	0.09 (249-> 296)	0.08 (281-> 299)
144	4.151	298.7	0.000018	0.000019	-0.053390	-0.054966	0.11 (281-> 298)	0.10 (271-> 298)	0.09 (249-> 297)
145	4.155	298.4	0.000058	0.000064	-1.611810	-1.964621	0.17 (270-> 299)	0.11 (271-> 298)	0.11 (282-> 299)
146	4.174	297.0	0.000008	0.000008	-0.012767	-0.011731	0.11 (279-> 298)	0.11 (278-> 299)	0.10 (279-> 299)
147	4.182	296.5	0.000012	0.000012	0.013250	0.012956	0.13 (279-> 299)	0.13 (278-> 298)	0.12 (278-> 299)
148	4.193	295.7	0.005402	0.005432	12.300503	12.273882	0.13 (264-> 296)	0.13 (272-> 297)	0.11 (265-> 297)
149	4.194	295.6	0.005386	0.005458	12.061370	12.073567	0.13 (272-> 296)	0.13 (264-> 297)	0.11 (265-> 296)
150	4.203	295.0	0.000049	0.000031	0.120191	0.093353	0.18 (282-> 298)	0.17 (281-> 299)	0.07 (270-> 298)

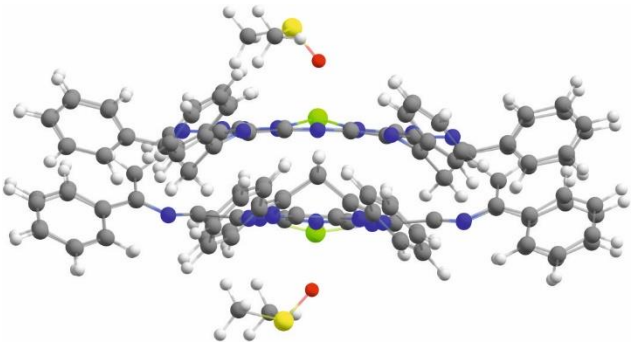

Table S12 Optimized geometry of $[Ph_8Dz_4PzMg{\cdot}DMSO]_2$ (dimer with coordinated DMSO molecule)

CARTESIAN COORDINATES (ANGSTROEM)

C	-3.751991000000	-2.313974000000	-1.523948000000	C	0.077782000000	9.376295000000	-2.456782000000
C	-4.296540000000	-1.000947000000	-1.484443000000	C	-0.241163000000	8.049453000000	-2.150563000000
C	-3.153943000000	-0.077752000000	-1.624463000000	C	-5.801617000000	5.714808000000	-2.189937000000
C	-8.236041000000	-0.186810000000	-2.253096000000	C	-6.953274000000	6.430196000000	-2.531250000000
C	-2.293614000000	-2.152247000000	-1.672077000000	C	-7.236516000000	7.657461000000	-1.901907000000
C	2.125337000000	-3.666523000000	-1.488231000000	C	-6.359477000000	8.152759000000	-0.923966000000
C	0.810386000000	-4.207548000000	-1.521509000000	C	-5.203931000000	7.436673000000	-0.579981000000
C	-0.104966000000	-3.060743000000	-1.661106000000	C	-8.997474000000	-1.684963000000	-0.495830000000
C	-5.921569000000	-5.662234000000	-2.430027000000	C	-10.327378000000	-1.370769000000	-0.808526000000
C	1.972061000000	-2.207234000000	-1.606913000000	C	-10.617613000000	-0.472019000000	-1.847686000000
C	-6.653761000000	-6.783776000000	-2.830320000000	C	-9.563479000000	0.125077000000	-2.564688000000
C	3.475779000000	2.217946000000	-1.462902000000	H	-7.395509000000	0.266538000000	-2.800789000000
C	4.024826000000	0.903215000000	-1.476567000000	H	-4.947393000000	-5.419579000000	-2.881750000000
C	2.881330000000	-0.017553000000	-1.581253000000	H	-6.256174000000	-7.444250000000	-3.619294000000
C	-7.896694000000	-7.067938000000	-2.232606000000	H	-8.476629000000	-7.951280000000	-2.548336000000
C	2.016476000000	2.058609000000	-1.564092000000	H	-9.356375000000	-6.442151000000	-0.743637000000
C	-8.391005000000	-6.221624000000	-1.227677000000	H	-8.059593000000	-4.460970000000	-0.023397000000
C	-2.403670000000	3.567159000000	-1.422896000000	H	2.280618000000	-8.764695000000	0.051102000000
C	-1.089786000000	4.110534000000	-1.411461000000	H	0.032087000000	-11.550794000000	-2.381124000000
C	-0.171455000000	2.968405000000	-1.570403000000	H	-1.134172000000	-9.626863000000	-3.508547000000
C	-7.657598000000	-5.096601000000	-0.823824000000	H	-0.567345000000	-7.261402000000	-2.846066000000
C	-2.246672000000	2.109230000000	-1.587340000000	H	5.297292000000	-4.860121000000	-2.702968000000
C	1.544696000000	-8.938113000000	-0.745539000000	H	7.437765000000	-6.083826000000	-3.226830000000
C	1.232745000000	-10.256708000000	-1.105687000000	H	7.991394000000	-8.208723000000	-1.997878000000
C	0.275321000000	-10.512500000000	-2.100101000000	H	6.415360000000	-9.074118000000	-0.244737000000
C	-0.377396000000	-9.435137000000	-2.729266000000	H	4.320418000000	-7.859479000000	0.267176000000
C	-0.067714000000	-8.119619000000	-2.371021000000	H	-2.967017000000	6.713098000000	0.729159000000
C	-3.705188000000	5.408444000000	-0.877764000000	H	-2.284369000000	5.047690000000	0.697507000000
C	-2.620626000000	5.903871000000	0.064403000000	H	-6.904583000000	-2.941417000000	0.597140000000
C	-1.472054000000	6.324783000000	-0.834901000000	H	-5.238520000000	-2.255388000000	0.593015000000
C	5.558847000000	-5.794055000000	-2.182401000000	H	2.609458000000	-6.874833000000	0.594474000000
C	6.745589000000	-6.478130000000	-2.463758000000	H	1.928333000000	-5.210786000000	0.586144000000
C	-5.598591000000	-3.625457000000	-1.028990000000	H	1.737260000000	-11.092518000000	-0.594407000000
C	-6.092725000000	-2.572388000000	-0.051972000000	H	-2.448438000000	8.611704000000	0.420696000000
C	-6.511471000000	-1.401603000000	-0.923114000000	H	-1.896455000000	10.958692000000	-0.138710000000
C	7.055931000000	-7.667753000000	-1.778056000000	H	-0.276960000000	11.478202000000	-1.987581000000
C	6.171496000000	-8.155876000000	-0.802979000000	H	0.798605000000	9.594872000000	-3.262703000000
C	3.418946000000	-5.512241000000	-0.934302000000	H	0.216311000000	7.208124000000	-2.693436000000
C	2.296421000000	-6.044092000000	-0.060361000000	H	-5.560373000000	4.752155000000	-2.666419000000
C	1.185102000000	-6.439775000000	-1.018939000000	H	-7.638795000000	6.030816000000	-3.297582000000
C	4.980743000000	-7.471494000000	-0.520987000000	H	-8.144145000000	8.223580000000	-2.170140000000
C	4.650055000000	-6.281967000000	-1.209066000000	H	-6.580349000000	9.104214000000	-0.413439000000
C	0.902592000000	-7.846509000000	-1.372856000000	H	-4.546068000000	7.837509000000	0.203047000000
C	-1.171444000000	7.742473000000	-1.125081000000	H	-8.796446000000	-2.361596000000	0.346875000000
C	-4.902878000000	6.207624000000	-1.209060000000	H	-11.144164000000	-1.824468000000	-0.224235000000
C	-7.928942000000	-1.104713000000	-1.216914000000	H	-11.664887000000	-0.229893000000	-2.094352000000
C	-6.411678000000	-4.796109000000	-1.418841000000	H	-9.782725000000	0.835670000000	-3.379394000000
C	-1.757328000000	8.811922000000	-0.410032000000	N	0.633039000000	-1.899534000000	-1.671095000000
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N	0.447808000000	-5.509083000000	-1.578504000000
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C	6.261287000000	1.299526000000	-1.007850000000
C	7.666660000000	1.024756000000	-1.374826000000
C	6.119286000000	4.721499000000	-1.370091000000
C	8.761823000000	1.627048000000	-0.715136000000
C	10.078649000000	1.334924000000	-1.097421000000
C	10.329576000000	0.436625000000	-2.146774000000
C	9.249059000000	-0.181013000000	-2.805121000000
H	7.074452000000	-0.362390000000	-2.922653000000
H	4.611874000000	5.361938000000	-2.779891000000
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H	8.104102000000	7.945312000000	-2.449057000000
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H	7.797366000000	4.382423000000	-0.011828000000
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H	5.044237000000	2.094557000000	0.582409000000
H	8.593785000000	2.305499000000	0.132782000000
H	10.916977000000	1.806418000000	-0.559516000000
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C	6.153793000000	-4.834403000000	1.372879000000
C	-6.343603000000	4.733329000000	1.369972000000
C	-7.908289000000	1.044101000000	1.348583000000
C	-4.902174000000	-6.292644000000	1.124768000000
C	-1.168506000000	-7.858181000000	1.204203000000
C	-7.567818000000	5.064811000000	0.746649000000
C	-8.261875000000	6.229450000000	1.104812000000
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C	-6.420777000000	-8.168413000000	0.719145000000
C	-7.288802000000	-7.699442000000	1.718153000000
C	-6.971665000000	-6.518633000000	2.415987000000
H	-5.527730000000	-4.896470000000	2.653222000000
H	0.295042000000	-7.304567000000	2.695676000000
H	0.862440000000	-9.683887000000	3.307045000000
H	-0.298715000000	-11.583305000000	2.133961000000
H	-1.998847000000	-11.087027000000	0.352459000000
H	-2.541708000000	-8.745576000000	-0.243469000000
H	7.826276000000	-4.478375000000	0.012519000000
H	8.203885000000	-8.000670000000	2.499066000000
H	5.962508000000	-7.512058000000	3.534582000000
H	4.663919000000	-5.479998000000	2.800013000000
H	7.147110000000	0.245230000000	2.766382000000
H	9.534150000000	0.817594000000	3.347370000000
H	11.418424000000	-0.253040000000	2.069983000000
H	10.900426000000	-1.852990000000	0.203610000000
H	8.554003000000	-2.391276000000	-0.370231000000
H	-5.252902000000	2.110514000000	-0.571359000000
H	-6.913518000000	2.806750000000	-0.559402000000
H	-2.207317000000	-5.179794000000	-0.691175000000
H	-2.890921000000	-6.843484000000	-0.728071000000
H	4.999196000000	-2.277581000000	-0.627968000000
H	6.664338000000	-2.966875000000	-0.627278000000
H	9.113835000000	-6.466350000000	0.730986000000
H	-7.980517000000	4.425340000000	-0.045350000000
H	-9.209554000000	6.473770000000	0.598060000000
H	-8.297554000000	8.001121000000	2.371116000000
H	-6.111887000000	7.443483000000	3.487112000000
H	-4.873126000000	5.347951000000	2.829531000000
H	-7.340433000000	-0.352867000000	2.897952000000
H	-9.712752000000	-0.858838000000	3.584931000000
H	-11.622453000000	0.267857000000	2.395595000000

H	-11.144496000000	1.864460000000	0.515883000000
H	-8.811080000000	2.342232000000	-0.159070000000
H	-4.591925000000	-7.845984000000	-0.381195000000
H	-6.670671000000	-9.079464000000	0.151803000000
H	-8.217074000000	-8.248784000000	1.947699000000
H	-7.650574000000	-6.139970000000	3.198545000000
N	1.743512000000	-0.839476000000	1.641388000000
N	1.181335000000	-3.206046000000	1.612749000000
N	0.659737000000	1.779611000000	1.647070000000
N	3.029508000000	1.222690000000	1.590447000000
N	-1.966468000000	0.697873000000	1.664863000000
N	-3.248495000000	-1.364782000000	1.588880000000
N	-1.407334000000	3.063951000000	1.667623000000
N	-5.576665000000	0.536562000000	1.524704000000
N	-4.380998000000	3.384676000000	1.570600000000
N	-0.706554000000	-5.526718000000	1.453699000000
N	-3.559857000000	-4.337629000000	1.412941000000
N	5.351054000000	-0.667510000000	1.449008000000
N	4.161795000000	-3.521914000000	1.533555000000
N	-0.882190000000	-1.921533000000	1.649189000000
C	0.059104000000	8.003095000000	2.462489000000
C	5.606386000000	5.643457000000	2.213679000000
C	6.788080000000	6.328337000000	2.513286000000
C	7.087461000000	7.540611000000	1.862981000000
C	6.197373000000	8.049889000000	0.904129000000
C	5.012045000000	7.364051000000	0.602785000000
C	3.463185000000	5.384114000000	0.966162000000
C	2.346959000000	5.921880000000	0.087181000000
C	1.236828000000	6.320663000000	1.045751000000
C	0.980174000000	7.727469000000	1.419641000000
C	4.692188000000	6.152404000000	1.256059000000
C	1.606919000000	8.817185000000	0.774129000000
C	1.329867000000	10.135951000000	1.161087000000
C	0.423309000000	10.393966000000	2.201458000000
C	-0.215931000000	9.318770000000	2.847894000000
H	-0.430750000000	7.146929000000	2.951120000000
H	5.352357000000	4.692193000000	2.706070000000
H	7.484945000000	5.916989000000	3.262978000000
H	8.018420000000	8.082926000000	2.098172000000
H	6.431818000000	8.987274000000	0.374241000000
H	4.346927000000	7.771321000000	-0.171012000000
H	2.668308000000	6.751625000000	-0.564907000000
H	1.975397000000	5.091501000000	-0.560746000000
H	2.297697000000	8.643288000000	-0.062096000000
H	1.820738000000	10.970298000000	0.634385000000
H	0.208564000000	11.432273000000	2.504723000000
H	-0.933316000000	9.512565000000	3.663112000000
N	3.343152000000	4.197317000000	1.514911000000
N	0.490224000000	5.392700000000	1.597093000000
Mg	-0.112095000000	-0.072668000000	2.039962000000
S	0.982276000000	0.062466000000	-5.227480000000
S	0.665491000000	0.630754000000	5.244849000000
C	2.452684000000	0.415251000000	4.906350000000
H	2.729087000000	0.883158000000	3.938933000000
H	2.633475000000	-0.678682000000	4.872884000000
H	3.015724000000	0.870574000000	5.749867000000
C	2.165461000000	1.415913000000	-4.855450000000
H	2.806185000000	1.555015000000	-5.753088000000
H	2.774865000000	1.182023000000	-3.959880000000
H	1.553491000000	2.324038000000	-4.678476000000
C	2.119008000000	-1.348056000000	-4.959818000000
H	2.872060000000	-1.340737000000	-5.777556000000
H	2.604737000000	-1.275593000000	-3.964418000000
H	1.496779000000	-2.264274000000	-5.022006000000
C	0.574982000000	2.442102000000	4.967874000000
H	1.032095000000	2.946647000000	5.846394000000
H	1.091612000000	2.718180000000	4.027100000000
H	-0.503962000000	2.690660000000	4.900314000000
O	-0.106412000000	-0.047070000000	4.088854000000
O	-0.063386000000	0.019792000000	-4.089475000000

Table S13 TD-DFT calculated UV-Vis spectrum of $[Ph_8Dz_4PzMg{\cdot}DMSO]_2$ (dimer with coordinated DMSO molecule)

state	eV	nm	fL	fV	Rl	RV			
0	0.849	1460.2	0.000040	0.000174	15.603270	32.752211	0.99 (310-> 311)	0.00 (310-> 318)	0.00 (310-> 319)
1	0.877	1413.6	0.000083	0.000409	-20.969266	-47.480744	0.99 (310-> 312)	0.00 (310-> 319)	0.00 (305-> 311)
2	1.413	877.6	0.110520	0.268374	19.172263	29.690078	0.84 (310-> 313)	0.14 (309-> 311)	0.01 (310-> 314)
3	1.436	863.3	0.114685	0.270796	-17.658717	-27.230227	0.84 (310-> 314)	0.13 (309-> 312)	0.01 (310-> 313)
4	1.893	655.0	0.845808	1.451631	-10.408390	-13.193597	0.79 (309-> 311)	0.12 (310-> 313)	0.03 (300-> 312)
5	1.914	647.8	0.818272	1.380930	13.105443	16.962608	0.79 (309-> 312)	0.12 (310-> 314)	0.03 (300-> 311)
6	2.203	562.7	0.023349	0.026286	0.466748	-0.022520	0.47 (308-> 311)	0.24 (307-> 311)	0.16 (308-> 312)
7	2.240	553.5	0.023391	0.025499	-9.795062	-10.554723	0.34 (307-> 312)	0.32 (308-> 312)	0.13 (307-> 311)
8	2.253	550.3	0.004908	0.005415	7.042830	7.635741	0.34 (307-> 311)	0.28 (307-> 312)	0.12 (308-> 311)
9	2.302	538.5	0.026372	0.028860	-21.660582	-22.309985	0.58 (306-> 311)	0.15 (306-> 312)	0.05 (309-> 313)
10	2.309	537.0	0.032677	0.038413	-30.763514	-33.296058	0.25 (308-> 312)	0.24 (308-> 311)	0.18 (307-> 312)
11	2.324	533.5	0.009494	0.010925	50.505699	54.189827	0.26 (305-> 311)	0.22 (309-> 313)	0.17 (309-> 314)
12	2.328	532.6	0.009161	0.009913	11.542132	12.867526	0.33 (309-> 313)	0.27 (305-> 311)	0.09 (309-> 314)
13	2.355	526.5	0.033700	0.038033	-14.675096	-16.005303	0.30 (306-> 312)	0.28 (304-> 311)	0.16 (309-> 314)
14	2.362	524.9	0.029091	0.033496	-1.058639	-1.162434	0.23 (306-> 312)	0.21 (303-> 311)	0.10 (304-> 311)
15	2.374	522.3	0.025601	0.028272	21.530747	22.428616	0.35 (310-> 315)	0.30 (303-> 311)	0.05 (305-> 312)
16	2.381	520.8	0.013420	0.014950	-12.797115	-12.964230	0.39 (304-> 312)	0.17 (310-> 316)	0.14 (304-> 311)
17	2.396	517.5	0.004281	0.004935	-0.255868	-0.256200	0.52 (310-> 316)	0.09 (304-> 312)	0.07 (303-> 312)
18	2.402	516.1	0.013464	0.014141	17.637323	18.059115	0.46 (310-> 315)	0.19 (303-> 311)	0.08 (304-> 311)
19	2.437	508.7	0.035465	0.039407	-26.461511	-27.892511	0.43 (303-> 312)	0.22 (305-> 312)	0.08 (310-> 316)
20	2.453	505.5	0.000254	0.000245	-15.426551	-14.855827	0.32 (309-> 314)	0.20 (305-> 311)	0.12 (305-> 312)
21	2.461	503.7	0.010035	0.011041	12.401722	10.580350	0.25 (303-> 312)	0.18 (305-> 312)	0.16 (309-> 313)
22	2.585	479.7	0.001322	0.001168	1.531251	1.505932	0.61 (302-> 311)	0.13 (302-> 312)	0.10 (301-> 311)
23	2.601	476.6	0.003490	0.003120	-1.902447	-1.383536	0.35 (301-> 311)	0.24 (302-> 311)	0.23 (302-> 312)
24	2.617	473.7	0.000206	0.000204	-4.656998	-4.439402	0.48 (302-> 312)	0.38 (301-> 311)	0.01 (310-> 315)
25	2.642	469.3	0.001928	0.001599	8.134793	8.536331	0.82 (301-> 312)	0.04 (310-> 317)	0.02 (308-> 313)
26	2.788	444.7	0.003384	0.003680	5.615207	5.863417	0.50 (307-> 313)	0.16 (307-> 314)	0.11 (310-> 317)
27	2.793	444.0	0.001063	0.001181	-4.994386	-5.292192	0.60 (308-> 313)	0.16 (308-> 314)	0.04 (307-> 313)
28	2.810	441.1	0.005148	0.005215	20.610993	20.702123	0.28 (307-> 314)	0.21 (308-> 314)	0.19 (310-> 317)
29	2.818	439.9	0.001766	0.001820	-3.346814	-3.398592	0.33 (307-> 314)	0.21 (308-> 314)	0.19 (310-> 317)
30	2.838	436.9	0.003411	0.003687	13.287501	14.021972	0.21 (308-> 314)	0.20 (310-> 317)	0.15 (306-> 313)
31	2.859	433.7	0.013862	0.014986	-2.283626	-2.413251	0.50 (306-> 313)	0.08 (310-> 317)	0.05 (308-> 314)
32	2.869	432.2	0.058734	0.061826	-26.123954	-26.186413	0.49 (306-> 314)	0.09 (305-> 313)	0.08 (304-> 313)
33	2.884	430.0	0.035744	0.037908	-6.009993	-5.220531	0.32 (304-> 313)	0.21 (305-> 313)	0.16 (306-> 314)
34	2.905	426.7	0.012729	0.013540	-30.195883	-30.955023	0.59 (310-> 318)	0.11 (304-> 314)	0.04 (306-> 314)
35	2.915	425.4	0.003134	0.003117	1.115221	1.780903	0.27 (304-> 314)	0.19 (303-> 313)	0.16 (310-> 318)
36	2.932	422.9	0.116883	0.123201	-6.280664	-8.319685	0.22 (305-> 314)	0.13 (305-> 313)	0.13 (303-> 314)
37	2.940	421.7	0.228803	0.240563	-3.761657	-3.742158	0.22 (305-> 313)	0.16 (304-> 313)	0.15 (303-> 313)
38	2.955	419.5	0.212984	0.223049	37.549805	38.980855	0.23 (305-> 314)	0.18 (304-> 314)	0.17 (303-> 313)
39	2.963	418.5	0.004930	0.005164	-15.555803	-15.564948	0.57 (310-> 319)	0.07 (303-> 313)	0.07 (304-> 314)
40	2.973	417.0	0.002081	0.002230	-4.344908	-4.891272	0.47 (303-> 314)	0.17 (310-> 319)	0.07 (304-> 314)
41	2.999	413.4	0.100195	0.100700	29.397934	29.666272	0.71 (310-> 320)	0.07 (302-> 313)	0.04 (301-> 314)
42	3.020	410.6	0.179032	0.180726	7.424026	6.625527	0.76 (310-> 321)	0.05 (310-> 323)	0.03 (303-> 314)
43	3.094	400.7	0.091617	0.091205	4.947537	4.818024	0.41 (310-> 322)	0.22 (302-> 313)	0.10 (310-> 323)
44	3.096	400.5	0.104334	0.105983	14.175174	14.475659	0.35 (310-> 323)	0.16 (310-> 322)	0.11 (302-> 314)
45	3.140	394.9	0.099512	0.103246	30.801840	31.177709	0.25 (302-> 313)	0.24 (310-> 324)	0.11 (302-> 314)
46	3.149	393.7	0.160359	0.168049	-43.592110	-44.836366	0.27 (301-> 313)	0.26 (302-> 314)	0.08 (310-> 324)
47	3.159	392.5	0.031485	0.032747	1.747935	1.688587	0.26 (310-> 324)	0.16 (302-> 314)	0.13 (310-> 323)
48	3.171	391.1	0.148007	0.148491	0.421777	0.430506	0.56 (310-> 325)	0.15 (301-> 313)	0.10 (301-> 314)
49	3.181	389.8	0.074376	0.073233	-11.140966	-10.791131	0.24 (310-> 324)	0.21 (310-> 323)	0.16 (301-> 313)
50	3.242	382.5	0.057034	0.061231	-10.290545	-10.645469	0.24 (301-> 314)	0.22 (310-> 322)	0.10 (310-> 320)
51	3.256	380.8	1.071488	1.136208	19.326464	19.901462	0.32 (300-> 311)	0.13 (310-> 327)	0.08 (310-> 328)
52	3.271	379.1	0.960139	1.021747	-64.316675	-66.360104	0.32 (300-> 312)	0.17 (310-> 328)	0.11 (310-> 327)
53	3.285	377.4	0.066020	0.070576	10.907135	11.311225	0.69 (310-> 326)	0.07 (299-> 311)	0.04 (299-> 312)
54	3.302	375.5	0.027216	0.028637	48.396056	49.666357	0.66 (309-> 315)	0.16 (299-> 311)	0.02 (310-> 326)
55	3.311	374.5	0.007540	0.007752	19.135823	19.406470	0.80 (309-> 316)	0.04 (299-> 312)	0.02 (309-> 315)
56	3.318	373.7	0.001494	0.001601	8.818945	9.382038	0.40 (299-> 311)	0.21 (309-> 315)	0.07 (298-> 311)
57	3.338	371.5	0.000130	0.000134	2.523152	3.228684	0.60 (299-> 312)	0.08 (310-> 326)	0.06 (309-> 316)
58	3.394	365.3	0.092758	0.098726	-36.750829	-37.855182	0.26 (298-> 311)	0.11 (297-> 311)	0.07 (299-> 311)
59	3.412	363.4	0.128574	0.136303	16.641878	17.053656	0.20 (297-> 311)	0.17 (297-> 312)	0.10 (298-> 311)
60	3.420	362.5	0.195221	0.206723	33.302436	34.252880	0.13 (310-> 329)	0.12 (297-> 312)	0.08 (297-> 311)

61	3.430	361.5	0.161570	0.171537	6.834690	7.247597	0.35 (298-> 312)	0.06 (284-> 312)	0.06 (297-> 312)
62	3.448	359.6	0.829962	0.890701	-58.748933	-60.833646	0.53 (310-> 327)	0.07 (300-> 311)	0.07 (300-> 312)
63	3.453	359.1	0.941666	1.003894	-175.558599	-181.278156	0.57 (310-> 328)	0.07 (300-> 311)	0.07 (300-> 312)
64	3.467	357.6	0.152959	0.162501	114.428558	118.316999	0.60 (310-> 329)	0.09 (297-> 312)	0.04 (298-> 311)
65	3.482	356.1	0.071878	0.077071	70.667399	72.934081	0.46 (310-> 330)	0.04 (294-> 311)	0.04 (296-> 311)
66	3.490	355.3	0.017852	0.019408	29.329951	30.607836	0.21 (310-> 330)	0.11 (293-> 311)	0.08 (294-> 311)
67	3.511	353.1	0.008672	0.009129	19.675752	20.470173	0.07 (296-> 311)	0.06 (310-> 330)	0.06 (289-> 311)
68	3.521	352.1	0.007564	0.008193	-37.733313	-39.891637	0.09 (284-> 311)	0.07 (284-> 312)	0.07 (295-> 312)
69	3.529	351.3	0.021589	0.023205	-42.068924	-43.370664	0.14 (285-> 311)	0.09 (279-> 311)	0.08 (282-> 311)
70	3.548	349.5	0.008152	0.008572	-17.323600	-17.906646	0.11 (294-> 312)	0.08 (285-> 312)	0.08 (279-> 312)
71	3.555	348.8	0.006461	0.006872	20.896181	21.886707	0.07 (281-> 312)	0.05 (295-> 312)	0.04 (295-> 311)
72	3.558	348.5	0.000982	0.001056	26.045597	27.118437	0.12 (284-> 312)	0.10 (284-> 311)	0.06 (281-> 312)
73	3.573	347.0	0.002058	0.002049	13.988314	13.183708	0.11 (282-> 312)	0.07 (285-> 312)	0.06 (280-> 312)
74	3.584	345.9	0.222327	0.228757	-116.858274	-119.023720	0.19 (308-> 319)	0.12 (307-> 318)	0.05 (308-> 317)
75	3.609	343.5	0.757769	0.778444	-54.853899	-55.621471	0.12 (307-> 317)	0.12 (306-> 318)	0.09 (307-> 315)
76	3.626	342.0	0.009535	0.009677	-35.845643	-36.876899	0.47 (300-> 313)	0.06 (308-> 316)	0.03 (307-> 315)
77	3.630	341.6	0.470529	0.482404	150.396952	151.842076	0.11 (308-> 315)	0.11 (306-> 317)	0.09 (308-> 319)
78	3.636	340.9	0.039281	0.039928	147.754113	148.757126	0.41 (300-> 314)	0.09 (307-> 316)	0.06 (308-> 315)
79	3.653	339.4	0.020379	0.020953	16.977105	17.332156	0.16 (295-> 311)	0.11 (293-> 311)	0.06 (294-> 312)
80	3.658	338.9	0.005558	0.005994	5.706623	5.883851	0.07 (294-> 312)	0.06 (296-> 312)	0.05 (289-> 312)
81	3.662	338.6	0.025896	0.025897	13.326877	12.951817	0.10 (308-> 316)	0.09 (304-> 317)	0.06 (306-> 316)
82	3.675	337.4	0.080660	0.080948	-112.612793	-113.123394	0.16 (303-> 317)	0.08 (300-> 314)	0.05 (306-> 315)
83	3.692	335.8	0.007933	0.008242	-0.915396	-0.913206	0.08 (294-> 312)	0.07 (296-> 312)	0.06 (289-> 312)
84	3.699	335.2	0.013408	0.013830	17.645549	17.889315	0.09 (293-> 312)	0.08 (295-> 312)	0.06 (290-> 312)
85	3.709	334.3	0.002862	0.002500	5.125808	4.448759	0.47 (309-> 317)	0.04 (307-> 316)	0.04 (293-> 312)
86	3.710	334.2	0.000323	0.000227	0.352516	0.805984	0.27 (309-> 317)	0.05 (306-> 315)	0.04 (307-> 316)
87	3.724	333.0	0.002021	0.001893	5.406055	5.702022	0.13 (300-> 314)	0.06 (302-> 317)	0.05 (307-> 315)
88	3.743	331.3	0.001225	0.001135	-4.998878	-4.681260	0.09 (301-> 317)	0.09 (303-> 316)	0.07 (304-> 315)
89	3.764	329.4	0.016295	0.017039	-16.693377	-17.071455	0.48 (291-> 311)	0.02 (266-> 311)	0.02 (294-> 312)
90	3.777	328.2	0.012931	0.012918	-3.635554	-3.600236	0.07 (296-> 312)	0.06 (308-> 323)	0.05 (296-> 311)
91	3.789	327.2	0.014510	0.014403	0.339042	1.081486	0.29 (291-> 312)	0.25 (309-> 318)	0.03 (299-> 313)
92	3.790	327.1	0.103984	0.102238	14.423050	14.018378	0.39 (309-> 318)	0.12 (299-> 313)	0.11 (299-> 314)
93	3.811	325.3	0.008339	0.008416	-11.267825	-11.729348	0.08 (307-> 323)	0.05 (296-> 311)	0.03 (308-> 325)
94	3.820	324.6	0.039968	0.040266	2.677857	2.931255	0.23 (309-> 319)	0.06 (308-> 316)	0.04 (299-> 313)
95	3.823	324.3	0.047605	0.046993	-6.753957	-6.899875	0.30 (309-> 319)	0.05 (299-> 313)	0.05 (299-> 314)
96	3.834	323.4	0.167827	0.171309	99.558978	100.517971	0.09 (305-> 315)	0.07 (308-> 315)	0.04 (305-> 316)
97	3.838	323.0	0.189021	0.192717	35.039240	35.703925	0.07 (308-> 316)	0.06 (303-> 321)	0.06 (305-> 316)
98	3.846	322.4	0.249140	0.253290	-78.042068	-78.738150	0.08 (308-> 316)	0.06 (305-> 315)	0.05 (299-> 314)
99	3.850	322.1	0.429259	0.434504	-115.635600	-116.498599	0.06 (299-> 313)	0.04 (307-> 324)	0.04 (307-> 330)
100	3.861	321.1	0.215254	0.219052	90.435555	91.170478	0.18 (307-> 315)	0.11 (304-> 316)	0.05 (299-> 314)
101	3.868	320.6	0.386708	0.395371	-58.346896	-59.023687	0.11 (305-> 316)	0.07 (299-> 313)	0.06 (309-> 319)
102	3.880	319.6	0.338115	0.345705	30.543074	31.052794	0.09 (299-> 314)	0.08 (305-> 315)	0.06 (306-> 316)
103	3.883	319.3	0.182847	0.184223	45.288251	45.443044	0.05 (306-> 315)	0.05 (307-> 316)	0.04 (303-> 316)
104	3.890	318.7	0.027685	0.028237	0.441967	0.310874	0.07 (309-> 321)	0.07 (306-> 316)	0.07 (279-> 311)
105	3.907	317.3	0.015058	0.015513	-19.063826	-19.290687	0.14 (309-> 320)	0.05 (279-> 311)	0.04 (279-> 312)
106	3.922	316.1	0.004960	0.004520	0.688318	0.129522	0.14 (309-> 320)	0.08 (309-> 321)	0.07 (308-> 322)
107	3.924	316.0	0.000956	0.000959	-11.319752	-11.995804	0.07 (279-> 312)	0.05 (306-> 316)	0.05 (306-> 315)
108	3.932	315.3	0.003238	0.003179	-0.022169	-0.038129	0.15 (309-> 320)	0.07 (296-> 311)	0.05 (308-> 325)
109	3.933	315.2	0.007597	0.006960	6.356162	6.253090	0.05 (306-> 319)	0.04 (308-> 324)	0.04 (296-> 312)
110	3.941	314.6	0.011295	0.010586	20.990555	20.174990	0.04 (305-> 316)	0.04 (279-> 312)	0.04 (304-> 320)
111	3.948	314.1	0.028229	0.026695	-13.013040	-12.636280	0.14 (309-> 321)	0.05 (309-> 320)	0.04 (304-> 319)
112	3.953	313.7	0.002608	0.002569	-15.613058	-16.045569	0.07 (305-> 319)	0.06 (305-> 318)	0.06 (302-> 317)
113	3.954	313.6	0.026009	0.024003	8.903587	9.049514	0.10 (304-> 315)	0.06 (309-> 320)	0.05 (305-> 316)
114	3.973	312.1	0.007055	0.006034	-16.462867	-15.549892	0.12 (303-> 320)	0.05 (309-> 323)	0.05 (305-> 315)
115	3.978	311.7	0.054310	0.052097	-2.754935	-2.167766	0.04 (296-> 311)	0.04 (304-> 315)	0.03 (258-> 311)
116	3.985	311.1	0.005930	0.006853	0.346948	0.494020	0.05 (308-> 322)	0.05 (307-> 324)	0.04 (296-> 311)
117	3.988	310.9	0.003367	0.004144	-3.130765	-3.458950	0.03 (303-> 320)	0.03 (309-> 321)	0.03 (308-> 319)
118	4.000	310.0	0.005565	0.005898	16.530969	18.400127	0.10 (309-> 321)	0.04 (296-> 312)	0.03 (301-> 317)
119	4.003	309.8	0.007479	0.008251	-38.197984	-40.970988	0.06 (309-> 321)	0.05 (303-> 315)	0.04 (295-> 311)
120	4.005	309.6	0.012648	0.013655	33.139251	36.461803	0.05 (296-> 312)	0.03 (294-> 312)	0.03 (295-> 312)
121	4.008	309.3	0.010080	0.010278	-9.203400	-10.086032	0.06 (309-> 321)	0.03 (291-> 312)	0.03 (309-> 326)
122	4.014	308.9	0.085293	0.090534	-23.864708	-24.564110	0.12 (309-> 319)	0.05 (301-> 315)	0.04 (299-> 314)
123	4.024	308.1	0.001669	0.001800	-2.776919	-2.494461	0.07 (296-> 312)	0.05 (295-> 311)	0.04 (309-> 325)
124	4.029	307.8	0.005107	0.005869	-3.069820	-3.258452	0.08 (295-> 312)	0.04 (303-> 317)	0.04 (309-> 324)
125	4.046	306.4	0.046370	0.046117	10.811149	10.665216	0.08 (301-> 316)	0.08 (303-> 315)	0.07 (304-> 316)
126	4.055	305.7	0.018801	0.017894	13.266786	13.080383	0.39 (309-> 322)	0.06 (309-> 320)	0.06 (309-> 325)

127	4.063	305.2	0.261027	0.261652	8.547795	8.715100	0.12 (299-> 313)	0.07 (301-> 320)	0.06 (309-> 322)
128	4.067	304.8	0.149308	0.153582	-3.304478	-3.400495	0.09 (299-> 314)	0.07 (298-> 313)	0.06 (309-> 322)
129	4.075	304.3	0.031073	0.031365	-5.750690	-5.953446	0.25 (309-> 323)	0.22 (309-> 324)	0.03 (309-> 325)
130	4.082	303.8	0.050049	0.046269	7.905681	8.064406	0.18 (297-> 313)	0.07 (298-> 314)	0.03 (309-> 323)
131	4.085	303.5	0.070130	0.068877	-61.873930	-61.495985	0.10 (309-> 323)	0.08 (309-> 324)	0.07 (292-> 311)
132	4.092	303.0	0.050113	0.047027	1.847058	1.785811	0.14 (309-> 325)	0.09 (298-> 313)	0.06 (298-> 314)
133	4.094	302.9	0.070451	0.068500	41.625985	40.512715	0.13 (292-> 311)	0.04 (309-> 324)	0.04 (262-> 311)
134	4.096	302.7	0.002516	0.002591	-1.324850	-1.042807	0.17 (292-> 311)	0.09 (309-> 323)	0.04 (260-> 311)
135	4.106	301.9	0.016048	0.015363	35.465590	34.657602	0.22 (292-> 312)	0.14 (309-> 325)	0.03 (257-> 311)
136	4.116	301.2	0.011595	0.011794	-13.329663	-13.436524	0.17 (309-> 325)	0.08 (262-> 311)	0.07 (292-> 312)
137	4.124	300.7	0.003042	0.003237	6.027210	6.205389	0.30 (309-> 324)	0.09 (257-> 312)	0.06 (262-> 312)
138	4.130	300.2	0.005763	0.005702	-1.284458	-1.216341	0.15 (297-> 314)	0.09 (292-> 312)	0.07 (298-> 313)
139	4.135	299.9	0.003691	0.003623	-5.435405	-5.274012	0.16 (258-> 312)	0.11 (261-> 312)	0.10 (309-> 325)
140	4.141	299.4	0.003018	0.002718	-8.990355	-8.735528	0.15 (298-> 314)	0.12 (297-> 313)	0.04 (309-> 325)
141	4.152	298.6	0.001121	0.001066	-2.562886	-2.664060	0.04 (304-> 315)	0.04 (297-> 314)	0.04 (259-> 311)
142	4.155	298.4	0.005740	0.005487	-2.135734	-2.049217	0.09 (305-> 315)	0.05 (309-> 323)	0.04 (308-> 315)
143	4.161	297.9	0.003779	0.003599	5.473084	5.381042	0.09 (306-> 316)	0.06 (305-> 316)	0.05 (308-> 316)
144	4.178	296.8	0.003067	0.002973	-7.518486	-7.394333	0.10 (306-> 315)	0.09 (303-> 316)	0.07 (305-> 317)
145	4.185	296.3	0.000534	0.000570	-0.419511	-0.887560	0.07 (304-> 316)	0.05 (303-> 315)	0.04 (306-> 315)
146	4.198	295.4	0.003510	0.002232	3.479124	2.764790	0.09 (293-> 313)	0.09 (289-> 311)	0.07 (289-> 312)
147	4.206	294.8	0.001651	0.001272	0.911184	0.893584	0.11 (260-> 311)	0.05 (290-> 311)	0.04 (263-> 311)
148	4.217	294.0	0.002929	0.002108	-6.026883	-4.830613	0.10 (260-> 312)	0.06 (290-> 312)	0.04 (295-> 313)
149	4.227	293.3	0.001298	0.000970	0.216184	0.740786	0.06 (293-> 313)	0.06 (294-> 314)	0.03 (295-> 314)
150	4.231	293.0	0.000968	0.000753	0.848339	0.345128	0.08 (295-> 314)	0.08 (284-> 313)	0.07 (294-> 313)

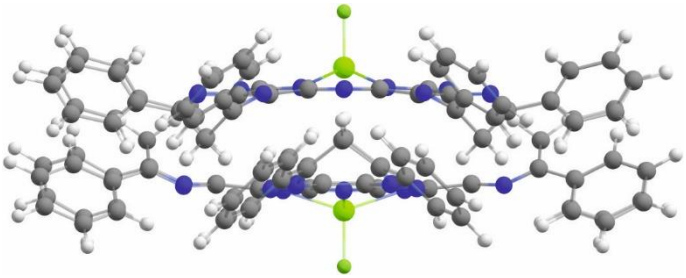

Table S14 Optimized geometry of $[Ph_8Dz_4PzMg{\cdot}F^-]_2$ (dimer with coordinated F^- anion)

CARTESIAN COORDINATES (ANGSTROEM)

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C	-4.280266000000	-0.991492000000	-1.460790000000
C	-3.133577000000	-0.074019000000	-1.616254000000
C	-8.194781000000	-0.140406000000	-2.246219000000
C	-2.279233000000	-2.140742000000	-1.652920000000
C	2.126571000000	-3.656654000000	-1.493099000000
C	0.811065000000	-4.196782000000	-1.507262000000
C	-0.100200000000	-3.046895000000	-1.661179000000
C	-5.858741000000	-5.676147000000	-2.373471000000
C	1.968402000000	-2.196488000000	-1.645959000000
C	-6.568791000000	-6.811343000000	-2.775095000000
C	3.483169000000	2.210381000000	-1.471495000000
C	4.027153000000	0.895726000000	-1.481065000000
C	2.877848000000	-0.018520000000	-1.636315000000
C	-7.825429000000	-7.099858000000	-2.208341000000
C	2.023661000000	2.048798000000	-1.621478000000
C	-8.353870000000	-6.240912000000	-1.231803000000
C	-2.383171000000	3.561363000000	-1.420550000000
C	-1.067793000000	4.102474000000	-1.423088000000
C	-0.155902000000	2.955332000000	-1.599889000000
C	-7.642174000000	-5.102240000000	-0.825991000000
C	-2.224673000000	2.104050000000	-1.596493000000
C	1.552904000000	-8.934398000000	-0.767533000000
C	1.219256000000	-10.250106000000	-1.120213000000
C	0.217775000000	-10.498607000000	-2.072359000000
C	-0.452880000000	-9.413427000000	-2.669171000000
C	-0.120421000000	-8.101076000000	-2.319737000000
C	-3.677622000000	5.408528000000	-0.870544000000
C	-2.582215000000	5.914679000000	0.050853000000
C	-1.448149000000	6.323271000000	-0.871508000000
C	5.534461000000	-5.779196000000	-2.257160000000
C	6.707923000000	-6.466977000000	-2.581662000000
C	-5.585602000000	-3.614818000000	-0.999116000000
C	-6.090020000000	-2.557297000000	-0.032902000000
C	-6.499289000000	-1.391609000000	-0.914152000000
C	7.020896000000	-7.679476000000	-1.937743000000
C	6.148383000000	-8.186783000000	-0.961585000000
C	3.419776000000	-5.510460000000	-0.963900000000
C	2.316094000000	-6.041231000000	-0.066825000000
C	1.188850000000	-6.430594000000	-1.006270000000
C	4.970479000000	-7.498777000000	-0.635883000000
C	4.639030000000	-6.284929000000	-1.279838000000
C	0.891877000000	-7.835272000000	-1.361255000000
C	-1.146795000000	7.734573000000	-1.194362000000
C	-4.887301000000	6.195498000000	-1.192887000000
C	-7.911735000000	-1.082605000000	-1.224634000000
C	-6.382705000000	-4.797399000000	-1.389991000000
C	-1.757836000000	8.824198000000	-0.532816000000
C	-1.429550000000	10.145374000000	-0.869085000000
C	-0.481538000000	10.408835000000	-1.870814000000
C	0.146133000000	9.333446000000	-2.528598000000

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C	-6.954082000000	6.389611000000	-2.496768000000
C	-7.243642000000	7.620771000000	-1.877363000000
C	-6.360817000000	8.130718000000	-0.912051000000
C	-5.197512000000	7.425664000000	-0.570091000000
C	-8.999588000000	-1.662962000000	-0.532570000000
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C	-10.586915000000	-0.402808000000	-1.882608000000
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H	-6.139296000000	-7.481951000000	-3.539176000000
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H	-8.070412000000	-4.457302000000	-0.046978000000
H	2.322801000000	-8.766635000000	-0.002071000000
H	-0.043754000000	-11.535013000000	-2.346320000000
H	-1.246454000000	-9.595534000000	-3.414205000000
H	-0.634603000000	-7.235997000000	-2.766203000000
H	5.267945000000	-4.828684000000	-2.744837000000
H	7.390688000000	-6.052622000000	-3.343302000000
H	7.947583000000	-8.222381000000	-2.190721000000
H	6.395882000000	-9.119688000000	-0.428588000000
H	4.320571000000	-7.902105000000	0.153435000000
H	-2.913367000000	6.730242000000	0.717214000000
H	-2.237847000000	5.060988000000	0.685289000000
H	-6.906401000000	-2.922096000000	0.614095000000
H	-5.238430000000	-2.235111000000	0.616163000000
H	2.640849000000	-6.873571000000	0.581902000000
H	1.959669000000	-5.205627000000	0.585273000000
H	1.740097000000	-11.090047000000	-0.631265000000
H	-2.477281000000	8.643684000000	0.277679000000
H	-1.912030000000	10.977239000000	-0.329732000000
H	-0.225933000000	11.449436000000	-2.134203000000
H	0.897173000000	9.527722000000	-3.313572000000
H	0.299306000000	7.157604000000	-2.690496000000
H	-5.540200000000	4.726496000000	-2.634487000000
H	-7.644256000000	5.973387000000	-3.250681000000
H	-8.161386000000	8.174708000000	-2.139045000000
H	-6.586856000000	9.082052000000	-0.402398000000
H	-4.534336000000	7.838563000000	0.202385000000
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H	-11.627797000000	-0.138297000000	-2.135880000000
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N	1.719632000000	0.713775000000	-1.682347000000
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C	5.861371000000	2.418449000000	-0.044853000000
C	6.257484000000	1.290039000000	-0.979219000000
C	7.664904000000	1.012474000000	-1.340288000000
C	6.121172000000	4.715056000000	-1.306504000000
C	8.759286000000	1.628539000000	-0.692033000000
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C	10.334407000000	0.405007000000	-2.089230000000
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H	8.585724000000	2.326526000000	0.138430000000
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C	0.176877000000	-9.445761000000	2.528974000000
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C	1.995661000000	2.078122000000	1.633472000000
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C	-1.477261000000	-10.255796000000	0.946895000000
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C	10.360760000000	-0.490873000000	1.868915000000
C	10.080811000000	-1.413387000000	0.848011000000
C	6.259610000000	-1.418935000000	0.893268000000
C	5.846176000000	-2.565188000000	-0.010707000000
C	5.338780000000	-3.641062000000	0.932954000000
C	8.754192000000	-1.727468000000	0.520090000000
C	7.675116000000	-1.126144000000	1.207367000000

C	6.132119000000	-4.835750000000	1.293759000000
C	-6.327155000000	4.731299000000	1.371488000000
C	-7.892829000000	1.025048000000	1.349477000000
C	-4.905952000000	-6.272621000000	1.174117000000
C	-1.154067000000	-7.845272000000	1.234276000000
C	-7.561705000000	5.066944000000	0.770747000000
C	-8.251595000000	6.228899000000	1.146859000000
C	-7.722458000000	7.084572000000	2.126074000000
C	-6.487750000000	6.768734000000	2.725344000000
C	-5.801194000000	5.608310000000	2.355269000000
C	-8.163689000000	0.088310000000	2.379861000000
C	-9.477884000000	-0.213552000000	2.750437000000
C	-10.559776000000	0.413949000000	2.103278000000
C	-10.306779000000	1.333213000000	1.072535000000
C	-8.989425000000	1.636147000000	0.699297000000
C	-5.247461000000	-7.470671000000	0.506427000000
C	-6.438872000000	-8.146671000000	0.807270000000
C	-7.314707000000	-7.643514000000	1.782605000000
C	-6.994032000000	-6.443979000000	2.446726000000
H	-5.536485000000	-4.826014000000	2.648160000000
H	0.354939000000	-7.270167000000	2.667620000000
H	0.961849000000	-9.640696000000	3.279847000000
H	-0.227834000000	-11.561493000000	2.164992000000
H	-1.990055000000	-11.087241000000	0.435452000000
H	-2.569213000000	-8.752816000000	-0.156640000000
H	7.797850000000	-4.490501000000	-0.075597000000
H	8.123113000000	-8.074157000000	2.333794000000
H	5.896754000000	-7.558894000000	3.394868000000
H	4.642059000000	-5.477634000000	2.718426000000
H	7.123099000000	0.285380000000	2.745467000000
H	9.503718000000	0.862208000000	3.349632000000
H	11.405659000000	-0.246506000000	2.125926000000
H	10.903591000000	-1.880627000000	0.282031000000
H	8.561610000000	-2.425889000000	-0.306368000000
H	-5.241129000000	2.104439000000	-0.573489000000
H	-6.904637000000	2.798456000000	-0.566908000000
H	-2.217886000000	-5.179349000000	-0.666312000000
H	-2.903510000000	-6.844891000000	-0.691040000000
H	4.993984000000	-2.228992000000	-0.651423000000
H	6.660902000000	-2.915552000000	-0.668030000000
H	9.045518000000	-6.524301000000	0.582760000000
H	-7.987448000000	4.427771000000	-0.014569000000
H	-9.202787000000	6.479043000000	0.648280000000
H	-8.267931000000	7.997544000000	2.420231000000
H	-6.054598000000	7.439617000000	3.487106000000
H	-4.834345000000	5.338896000000	2.807959000000
H	-7.301081000000	-0.390548000000	2.868704000000
H	-9.663979000000	-0.941775000000	3.558560000000
H	-11.597449000000	0.174948000000	2.392578000000
H	-11.144423000000	1.810748000000	0.537639000000
H	-8.818382000000	2.334602000000	-0.131502000000
H	-4.595616000000	-7.869047000000	-0.283707000000
H	-6.689686000000	-9.071477000000	0.261847000000
H	-8.254609000000	-8.174039000000	2.011984000000
H	-7.677681000000	-6.034167000000	3.210028000000
N	1.736940000000	-0.831827000000	1.677098000000
N	1.184179000000	-3.197122000000	1.609193000000
N	0.659881000000	1.776938000000	1.701773000000
N	3.025728000000	1.226811000000	1.613937000000
N	-1.953109000000	0.698670000000	1.703477000000
N	-3.242831000000	-1.358734000000	1.619738000000
N	-1.399764000000	3.065477000000	1.668923000000
N	-5.563445000000	0.539907000000	1.532499000000
N	-4.367930000000	3.383596000000	1.560217000000
N	-0.701333000000	-5.513224000000	1.467094000000
N	-3.553236000000	-4.327285000000	1.445669000000
N	5.343555000000	-0.662495000000	1.454618000000
N	4.156349000000	-3.511018000000	1.488499000000
N	-0.875383000000	-1.908072000000	1.676648000000
C	-0.013340000000	7.981895000000	2.373313000000
C	5.567976000000	5.653799000000	2.253407000000
C	6.735460000000	6.345913000000	2.589977000000
C	7.039881000000	7.570371000000	1.964648000000
C	6.165507000000	8.084249000000	0.993816000000
C	4.994952000000	7.390481000000	0.653860000000
C	3.455669000000	5.388825000000	0.955300000000
C	2.353621000000	5.918311000000	0.055253000000
C	1.233974000000	6.314167000000	1.001071000000
C	0.949255000000	7.719068000000	1.364627000000
C	4.670258000000	6.166508000000	1.281648000000
C	1.577230000000	8.820554000000	0.739622000000
C	1.263016000000	10.135067000000	1.113761000000
C	0.315639000000	10.380195000000	2.120510000000
C	-0.325180000000	9.293134000000	2.745762000000
H	-0.504955000000	7.115437000000	2.842222000000
H	5.308103000000	4.693880000000	2.726085000000
H	7.418948000000	5.927170000000	3.348583000000
H	7.963443000000	8.115191000000	2.224939000000
H	6.403493000000	9.029881000000	0.479094000000
H	4.343350000000	7.800671000000	-0.129967000000
H	2.680546000000	6.746365000000	-0.597609000000
H	1.993167000000	5.080990000000	-0.592244000000
H	2.299306000000	8.655721000000	-0.071422000000
H	1.756846000000	10.976725000000	0.600366000000
H	0.070670000000	11.415565000000	2.413053000000
H	-1.078346000000	9.473078000000	3.532126000000
N	3.336537000000	4.199949000000	1.500821000000
N	0.488204000000	5.385982000000	1.554682000000
Mg	-0.105416000000	-0.071256000000	2.343314000000
F	-0.097714000000	-0.088975000000	4.178748000000
F	-0.133213000000	-0.010768000000	-4.174581000000

Table S15 TD-DFT calculated UV-Vis spectrum of $[Ph_8Dz_4PzMg{\cdot}F^-]_2$ (dimer with coordinated F^- anion)

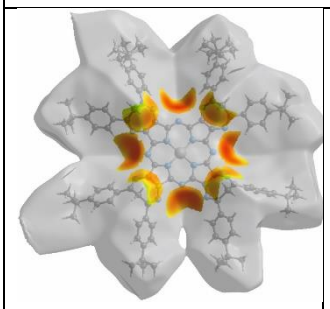
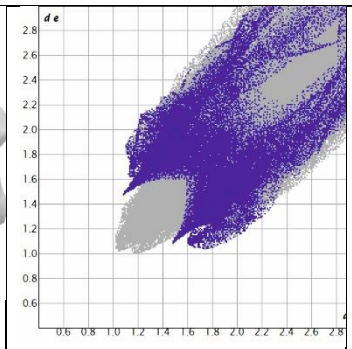
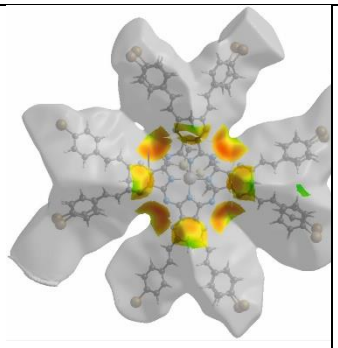
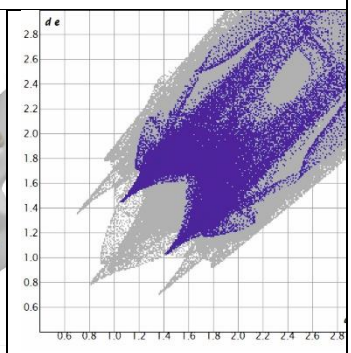
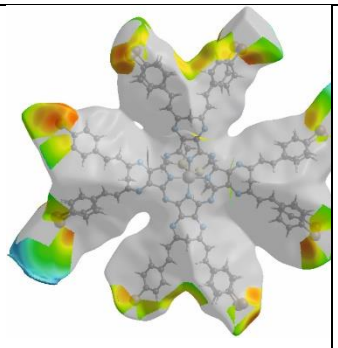
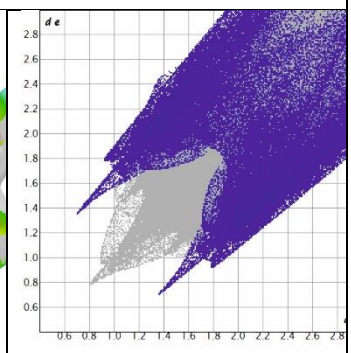
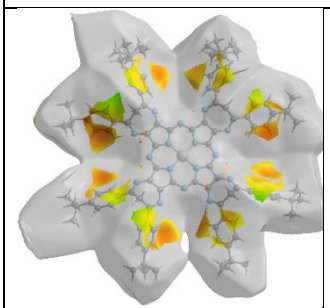
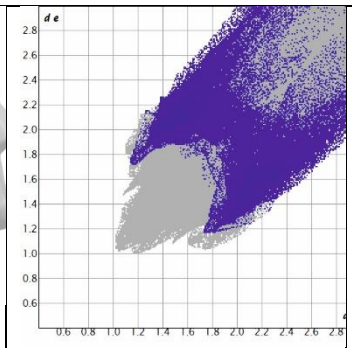
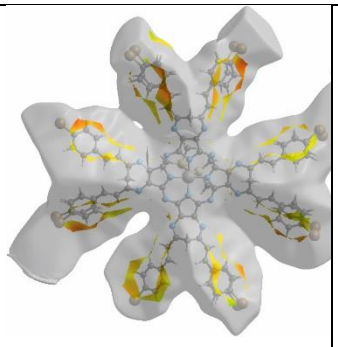
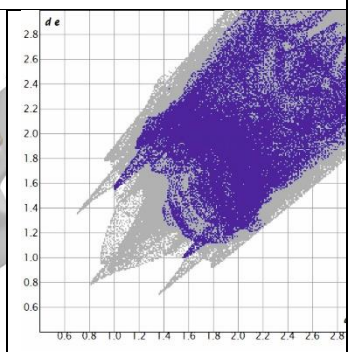
state	eV	nm	fL	fV	Rl	RV			
0	0.820	1511.1	0.000013	0.000060	-9.693832	-20.490507	0.98 (295-> 296)	0.01 (295-> 304)	0.00 (295-> 313)
1	0.833	1488.2	0.000002	0.000011	3.060513	7.312891	0.98 (295-> 297)	0.01 (295-> 305)	0.00 (295-> 312)
2	1.361	911.2	0.163923	0.370138	1.233641	1.884968	0.82 (295-> 299)	0.09 (294-> 296)	0.06 (295-> 298)
3	1.363	909.8	0.171419	0.386019	0.611214	0.890742	0.82 (295-> 298)	0.08 (294-> 297)	0.06 (295-> 299)
4	1.836	675.2	0.884979	1.442020	17.583784	22.415494	0.85 (294-> 296)	0.08 (295-> 299)	0.03 (285-> 297)
5	1.844	672.3	0.871474	1.413077	0.339015	0.441780	0.85 (294-> 297)	0.08 (295-> 298)	0.03 (285-> 296)
6	1.934	641.2	0.000587	0.000905	-0.081934	-0.091723	0.94 (295-> 300)	0.03 (295-> 301)	0.01 (295-> 332)
7	1.935	640.8	0.000131	0.000196	-0.093520	-0.097390	0.94 (295-> 301)	0.03 (295-> 300)	0.01 (295-> 333)
8	2.247	551.8	0.000018	0.000024	0.833808	1.016226	0.67 (294-> 299)	0.22 (294-> 298)	0.03 (295-> 304)
9	2.247	551.7	0.000192	0.000248	-4.122105	-4.695639	0.67 (294-> 298)	0.22 (294-> 299)	0.03 (295-> 305)

10	2.303	538.4	0.000114	0.000329	0.181984	0.356816	0.97 (295-> 302)	0.01 (287-> 296)	0.01 (286-> 297)
11	2.415	513.4	0.008899	0.008673	-5.319257	-5.196920	0.71 (291-> 296)	0.05 (285-> 296)	0.04 (289-> 296)
12	2.426	511.0	0.000628	0.000642	1.944851	2.022444	0.57 (293-> 296)	0.24 (292-> 297)	0.04 (291-> 297)
13	2.430	510.2	0.008512	0.008399	0.682618	0.909436	0.61 (291-> 297)	0.05 (285-> 297)	0.05 (288-> 296)
14	2.437	508.7	0.000065	0.000079	4.515818	4.702243	0.83 (295-> 304)	0.10 (290-> 297)	0.01 (294-> 299)
15	2.446	506.9	0.000017	0.000032	-2.111655	-3.051763	0.83 (295-> 305)	0.07 (290-> 296)	0.02 (288-> 296)
16	2.476	500.7	0.000042	0.000045	-0.101051	-0.091199	0.38 (293-> 297)	0.37 (292-> 296)	0.09 (292-> 297)
17	2.478	500.3	0.000050	0.000053	-4.587612	-4.706304	0.52 (292-> 297)	0.23 (293-> 296)	0.07 (292-> 296)
18	2.512	493.6	0.000054	0.000038	-4.948705	-4.028324	0.35 (290-> 296)	0.25 (289-> 297)	0.18 (288-> 296)
19	2.517	492.6	0.000024	0.000028	0.764829	0.785286	0.39 (292-> 296)	0.39 (293-> 297)	0.05 (295-> 303)
20	2.523	491.4	0.000066	0.000109	-5.342140	-7.082045	0.40 (289-> 296)	0.31 (288-> 297)	0.04 (290-> 297)
21	2.556	485.0	0.020048	0.022885	-12.680713	-13.534913	0.30 (289-> 297)	0.20 (288-> 296)	0.19 (295-> 306)
22	2.562	484.0	0.020125	0.022256	4.845258	5.151110	0.23 (288-> 297)	0.19 (295-> 303)	0.15 (295-> 307)
23	2.563	483.7	0.008398	0.008538	4.834392	4.726991	0.53 (295-> 303)	0.14 (288-> 297)	0.07 (289-> 296)
24	2.576	481.3	0.078940	0.078288	12.763309	12.706378	0.69 (295-> 306)	0.13 (295-> 303)	0.04 (289-> 297)
25	2.578	480.9	0.087141	0.086428	-2.634340	-2.620529	0.73 (295-> 307)	0.09 (288-> 297)	0.05 (289-> 296)
26	2.621	473.1	0.000228	0.000226	0.290851	0.281770	0.92 (295-> 308)	0.02 (292-> 297)	0.02 (293-> 296)
27	2.636	470.4	0.000067	0.000073	7.946362	8.120869	0.66 (290-> 297)	0.09 (295-> 304)	0.06 (289-> 296)
28	2.643	469.2	0.000120	0.000123	-13.335946	-13.499416	0.38 (290-> 296)	0.22 (288-> 296)	0.09 (289-> 297)
29	2.666	465.1	0.000055	0.000058	-0.180047	-0.177657	0.88 (295-> 309)	0.06 (295-> 310)	0.01 (294-> 309)
30	2.668	464.8	0.000070	0.000072	-0.185782	-0.182456	0.88 (295-> 310)	0.06 (295-> 309)	0.01 (294-> 310)
31	2.732	453.9	0.000018	0.000015	-0.126575	-0.112737	0.27 (286-> 296)	0.26 (287-> 297)	0.22 (295-> 311)
32	2.786	445.0	0.004111	0.003436	1.124198	1.030372	0.71 (287-> 296)	0.08 (293-> 298)	0.04 (292-> 299)
33	2.788	444.7	0.000088	0.000092	-0.032414	-0.034648	0.44 (286-> 296)	0.43 (287-> 297)	0.01 (290-> 300)
34	2.804	442.1	0.001064	0.000880	-0.041609	-0.036936	0.74 (286-> 297)	0.07 (287-> 296)	0.05 (292-> 299)
35	2.830	438.1	0.000000	0.000000	0.004201	0.003837	0.73 (295-> 311)	0.10 (287-> 297)	0.09 (286-> 296)
36	2.841	436.4	0.000000	0.000000	-0.002154	-0.000516	0.83 (294-> 300)	0.11 (294-> 301)	0.01 (294-> 333)
37	2.843	436.1	0.000000	0.000000	-0.007429	0.000617	0.83 (294-> 301)	0.11 (294-> 300)	0.01 (294-> 332)
38	2.878	430.9	0.000236	0.000265	8.053403	8.550847	0.60 (295-> 312)	0.14 (291-> 299)	0.05 (284-> 296)
39	2.879	430.6	0.000177	0.000204	-4.160314	-4.530653	0.61 (295-> 313)	0.11 (291-> 298)	0.05 (284-> 297)
40	2.930	423.2	0.030031	0.024437	2.246414	2.024976	0.77 (295-> 314)	0.06 (285-> 296)	0.05 (295-> 315)
41	2.931	423.0	0.033093	0.027632	-2.816774	-2.568615	0.77 (295-> 315)	0.05 (295-> 314)	0.04 (290-> 298)
42	2.940	421.7	0.000055	0.000046	-0.343938	-0.304538	0.46 (293-> 299)	0.33 (292-> 298)	0.05 (291-> 300)
43	2.948	420.6	0.000983	0.000841	-1.151067	-1.088099	0.44 (293-> 298)	0.32 (292-> 299)	0.05 (291-> 301)
44	2.950	420.3	0.064566	0.060346	17.447409	16.790750	0.44 (290-> 299)	0.12 (289-> 298)	0.09 (285-> 296)
45	2.962	418.6	0.065794	0.062380	-34.839441	-33.946033	0.28 (289-> 299)	0.22 (288-> 298)	0.15 (290-> 298)
46	2.965	418.2	0.000533	0.000452	-2.694214	-2.100712	0.31 (291-> 298)	0.13 (289-> 298)	0.11 (291-> 299)
47	2.967	417.9	0.000824	0.000545	9.363068	7.634759	0.30 (291-> 299)	0.15 (288-> 298)	0.15 (291-> 298)
48	2.987	415.0	0.000529	0.000399	6.941993	5.510194	0.24 (295-> 312)	0.22 (291-> 299)	0.12 (289-> 298)
49	2.991	414.6	0.000716	0.000569	-6.543796	-6.129869	0.22 (295-> 313)	0.20 (291-> 298)	0.15 (288-> 298)
50	2.994	414.1	0.000384	0.000366	0.208547	0.230133	0.41 (292-> 298)	0.28 (293-> 299)	0.10 (287-> 297)
51	2.999	413.4	0.004078	0.004507	1.740653	1.818950	0.39 (292-> 299)	0.29 (293-> 298)	0.11 (286-> 297)
52	3.036	408.3	0.000672	0.001192	1.477743	1.994520	0.32 (290-> 298)	0.22 (285-> 297)	0.15 (289-> 299)
53	3.042	407.6	0.001835	0.001810	1.259509	1.268905	0.25 (288-> 299)	0.25 (285-> 296)	0.19 (289-> 298)
54	3.196	388.0	0.004210	0.004704	2.664040	2.897822	0.57 (284-> 296)	0.07 (287-> 298)	0.05 (286-> 299)
55	3.198	387.7	0.001640	0.001815	-5.148923	-5.403617	0.26 (287-> 298)	0.20 (286-> 299)	0.15 (284-> 296)
56	3.204	387.0	0.003254	0.003490	-0.497166	-0.499422	0.71 (294-> 302)	0.12 (287-> 299)	0.07 (286-> 298)
57	3.207	386.7	0.004884	0.005253	-0.600090	-0.654429	0.71 (284-> 297)	0.05 (288-> 298)	0.05 (289-> 299)
58	3.252	381.2	2.169062	2.295140	15.736311	16.198773	0.39 (294-> 304)	0.25 (285-> 297)	0.13 (290-> 298)
59	3.255	381.0	0.216381	0.228569	-1.722487	-1.770333	0.53 (287-> 299)	0.12 (294-> 302)	0.03 (294-> 305)
60	3.257	380.7	0.927209	0.979066	13.827226	14.106113	0.23 (286-> 299)	0.21 (287-> 298)	0.15 (294-> 305)
61	3.259	380.4	1.158639	1.222230	4.155451	4.086866	0.19 (294-> 305)	0.19 (286-> 299)	0.11 (285-> 296)
62	3.264	379.9	0.059929	0.063349	0.124523	0.083556	0.63 (286-> 298)	0.08 (294-> 302)	0.05 (288-> 301)
63	3.399	364.7	0.001092	0.001155	-13.313986	-14.335645	0.10 (291-> 302)	0.08 (293-> 304)	0.07 (285-> 299)
64	3.401	364.6	0.001278	0.001361	31.465790	32.091529	0.17 (285-> 299)	0.11 (293-> 300)	0.10 (285-> 298)
65	3.404	364.3	0.001254	0.001331	-23.516059	-24.213617	0.12 (285-> 298)	0.08 (291-> 302)	0.06 (293-> 301)
66	3.414	363.2	0.268455	0.286470	40.229289	41.591580	0.23 (294-> 305)	0.12 (293-> 302)	0.11 (291-> 304)
67	3.414	363.1	0.606482	0.646253	-20.621845	-21.251635	0.34 (294-> 304)	0.13 (285-> 297)	0.08 (290-> 298)
68	3.427	361.8	0.025515	0.027035	-6.547244	-6.745526	0.19 (279-> 296)	0.07 (294-> 308)	0.06 (288-> 300)
69	3.433	361.2	0.443857	0.468694	-97.750856	-100.335798	0.09 (294-> 305)	0.07 (289-> 302)	0.06 (291-> 301)
70	3.435	361.0	0.717187	0.757165	-38.779208	-39.795481	0.12 (294-> 305)	0.07 (293-> 302)	0.06 (284-> 299)
71	3.436	360.9	0.064663	0.068211	-5.945774	-6.025635	0.14 (278-> 297)	0.07 (291-> 300)	0.07 (288-> 302)
72	3.438	360.6	0.761293	0.802136	139.488174	143.255098	0.18 (292-> 302)	0.08 (294-> 304)	0.08 (291-> 305)
73	3.458	358.5	0.000949	0.000856	-2.203078	-2.212820	0.93 (294-> 303)	0.01 (294-> 350)	0.01 (293-> 298)
74	3.460	358.3	0.234938	0.242988	21.134542	21.479068	0.36 (282-> 296)	0.19 (283-> 297)	0.04 (273-> 296)
75	3.462	358.2	0.211011	0.218648	-51.838255	-52.771610	0.37 (283-> 296)	0.16 (282-> 297)	0.04 (273-> 296)

76	3.489	355.3	0.004520	0.004769	39.161470	40.348387	0.34 (282-> 297)	0.15 (283-> 296)	0.08 (283-> 297)
77	3.493	354.9	0.001779	0.001899	-17.574085	-18.206592	0.30 (283-> 297)	0.18 (282-> 296)	0.08 (282-> 297)
78	3.507	353.6	0.001169	0.001213	-22.355156	-22.744862	0.71 (294-> 306)	0.04 (285-> 298)	0.02 (292-> 301)
79	3.508	353.4	0.000286	0.000316	9.663859	10.233107	0.77 (294-> 307)	0.03 (285-> 299)	0.02 (292-> 300)
80	3.527	351.5	0.000052	0.000052	-1.162714	-0.733833	0.39 (281-> 296)	0.10 (280-> 297)	0.09 (279-> 299)
81	3.541	350.1	0.000194	0.000212	0.049859	0.057744	0.23 (280-> 296)	0.20 (281-> 297)	0.06 (291-> 301)
82	3.544	349.8	0.000133	0.000145	0.993641	1.295528	0.36 (280-> 297)	0.09 (278-> 298)	0.07 (281-> 296)
83	3.549	349.4	0.000003	0.000002	0.015635	0.017531	0.79 (294-> 308)	0.03 (278-> 297)	0.02 (291-> 303)
84	3.564	347.9	0.000183	0.000175	-0.892948	-0.820530	0.27 (278-> 296)	0.18 (279-> 297)	0.04 (291-> 300)
85	3.565	347.8	0.000073	0.000079	0.245010	0.258185	0.27 (279-> 296)	0.17 (278-> 297)	0.04 (278-> 296)
86	3.571	347.2	0.001048	0.001148	-17.923030	-18.828344	0.21 (272-> 296)	0.13 (273-> 297)	0.04 (291-> 307)
87	3.571	347.2	0.000798	0.000869	14.444485	15.095491	0.17 (273-> 296)	0.10 (272-> 297)	0.06 (285-> 299)
88	3.592	345.1	0.029556	0.033732	51.728036	55.261910	0.26 (273-> 296)	0.07 (285-> 299)	0.05 (283-> 296)
89	3.593	345.0	0.027453	0.030109	-14.543474	-15.233330	0.19 (278-> 297)	0.13 (279-> 296)	0.06 (289-> 301)
90	3.594	345.0	0.056700	0.063202	-48.369111	-51.061694	0.15 (272-> 296)	0.07 (284-> 299)	0.07 (285-> 298)
91	3.596	344.7	0.156200	0.171882	-88.829479	-93.231083	0.22 (272-> 297)	0.14 (284-> 298)	0.06 (284-> 299)
92	3.597	344.7	0.143600	0.157920	77.968971	81.747442	0.22 (273-> 297)	0.14 (284-> 299)	0.05 (285-> 298)
93	3.599	344.5	0.002512	0.002831	0.782531	0.820879	0.73 (294-> 309)	0.05 (278-> 297)	0.02 (279-> 296)
94	3.601	344.3	0.001134	0.001294	-0.804153	-0.853089	0.76 (294-> 310)	0.03 (278-> 296)	0.02 (279-> 297)
95	3.608	343.7	0.005722	0.005757	-0.676714	-0.623876	0.29 (279-> 297)	0.21 (278-> 296)	0.05 (281-> 298)
96	3.611	343.4	0.307679	0.314638	-37.260780	-37.672291	0.21 (284-> 299)	0.13 (273-> 297)	0.08 (272-> 296)
97	3.612	343.3	0.348588	0.357582	65.700789	66.586002	0.24 (284-> 298)	0.12 (272-> 297)	0.05 (273-> 297)
98	3.615	343.0	0.004852	0.004960	0.965091	0.977462	0.31 (281-> 297)	0.27 (280-> 296)	0.07 (279-> 298)
99	3.653	339.4	0.002368	0.002702	1.328605	1.423437	0.10 (292-> 306)	0.08 (291-> 300)	0.07 (290-> 300)
100	3.654	339.3	0.000197	0.000214	-0.162123	-0.167649	0.08 (291-> 301)	0.07 (291-> 309)	0.07 (293-> 306)
101	3.658	339.0	0.039591	0.043619	7.158088	7.511623	0.13 (279-> 297)	0.11 (293-> 307)	0.09 (291-> 308)
102	3.677	337.2	0.000224	0.000225	-3.797221	-3.773397	0.09 (291-> 306)	0.08 (285-> 299)	0.07 (294-> 315)
103	3.677	337.2	0.000682	0.000683	-5.552699	-5.432797	0.10 (291-> 307)	0.09 (285-> 298)	0.07 (294-> 314)
104	3.680	336.9	0.001957	0.001867	-1.125453	-1.060735	0.34 (290-> 300)	0.06 (291-> 300)	0.05 (288-> 300)
105	3.683	336.6	0.000040	0.000039	-0.086221	-0.081280	0.36 (290-> 301)	0.07 (291-> 301)	0.04 (288-> 301)
106	3.695	335.6	0.001347	0.001277	-1.063973	-1.241291	0.42 (294-> 311)	0.15 (275-> 296)	0.08 (274-> 297)
107	3.706	334.5	0.001354	0.001218	0.409025	0.387451	0.38 (277-> 296)	0.12 (268-> 296)	0.07 (275-> 299)
108	3.710	334.2	0.151827	0.137556	-7.387378	-7.026429	0.17 (294-> 313)	0.07 (289-> 306)	0.05 (288-> 307)
109	3.712	334.0	0.156981	0.143369	12.804671	12.236860	0.18 (294-> 312)	0.05 (288-> 306)	0.05 (289-> 307)
110	3.715	333.7	0.003391	0.003100	0.396163	0.293533	0.11 (276-> 296)	0.11 (274-> 297)	0.09 (277-> 297)
111	3.720	333.3	0.000148	0.000134	0.311567	0.310824	0.31 (276-> 297)	0.11 (269-> 297)	0.07 (274-> 298)
112	3.747	330.9	0.000505	0.000457	1.531812	1.449799	0.19 (290-> 302)	0.14 (291-> 303)	0.12 (293-> 306)
113	3.755	330.2	0.001165	0.000956	4.100996	3.679060	0.10 (292-> 300)	0.07 (292-> 302)	0.06 (293-> 301)
114	3.757	330.0	0.000226	0.000289	1.770055	2.017492	0.10 (292-> 301)	0.09 (293-> 302)	0.07 (293-> 300)
115	3.758	329.9	0.000390	0.000384	6.971619	6.882607	0.18 (293-> 303)	0.06 (291-> 306)	0.05 (289-> 306)
116	3.760	329.7	0.000242	0.000206	0.970900	0.906316	0.06 (289-> 310)	0.05 (293-> 305)	0.05 (274-> 296)
117	3.761	329.7	0.002909	0.002910	-19.220849	-19.246234	0.19 (292-> 303)	0.10 (289-> 307)	0.06 (290-> 305)
118	3.764	329.4	0.000051	0.000058	1.146898	1.750276	0.37 (294-> 311)	0.19 (274-> 297)	0.15 (275-> 296)
119	3.767	329.1	0.000294	0.000281	-1.923787	-1.890928	0.10 (289-> 303)	0.09 (289-> 302)	0.06 (290-> 309)
120	3.770	328.9	0.001331	0.001279	0.142529	0.173422	0.10 (288-> 303)	0.09 (288-> 302)	0.06 (290-> 310)
121	3.772	328.7	0.000676	0.000718	-0.640855	-0.666193	0.14 (277-> 297)	0.13 (276-> 296)	0.11 (269-> 296)
122	3.790	327.2	0.007801	0.008063	-2.763677	-2.805751	0.30 (289-> 300)	0.26 (288-> 301)	0.03 (290-> 301)
123	3.808	325.6	0.000076	0.000082	-0.029639	-0.033195	0.78 (295-> 316)	0.09 (295-> 333)	0.02 (295-> 319)
124	3.810	325.4	0.000031	0.000031	-0.184428	-0.173167	0.18 (288-> 301)	0.16 (289-> 300)	0.09 (289-> 301)
125	3.816	324.9	0.000018	0.000013	-0.077900	-0.071442	0.73 (295-> 317)	0.09 (295-> 332)	0.08 (295-> 318)
126	3.826	324.0	0.000020	0.000023	-1.341792	-1.400698	0.09 (290-> 305)	0.07 (292-> 300)	0.07 (293-> 301)
127	3.827	324.0	0.000198	0.000244	-0.879387	-1.063096	0.11 (293-> 300)	0.10 (292-> 301)	0.09 (290-> 304)
128	3.828	323.8	0.000437	0.000463	4.165343	4.469365	0.07 (291-> 302)	0.06 (290-> 303)	0.05 (288-> 301)
129	3.851	321.9	0.001072	0.001147	-0.017705	-0.021571	0.13 (274-> 296)	0.11 (263-> 296)	0.10 (275-> 297)
130	3.854	321.7	0.069299	0.077874	4.578472	4.853874	0.21 (294-> 312)	0.13 (284-> 299)	0.08 (290-> 306)
131	3.857	321.5	0.071336	0.080741	4.769408	5.080598	0.23 (294-> 313)	0.13 (284-> 298)	0.10 (290-> 307)
132	3.862	321.0	0.000002	0.000002	0.058028	0.034443	0.66 (295-> 318)	0.17 (295-> 319)	0.09 (295-> 317)
133	3.866	320.7	0.000597	0.000722	-2.559410	-2.947561	0.69 (295-> 319)	0.17 (295-> 318)	0.03 (295-> 316)
134	3.871	320.3	0.000036	0.000047	0.062291	0.053948	0.19 (291-> 300)	0.10 (288-> 303)	0.09 (290-> 300)
135	3.872	320.2	0.000258	0.000293	-0.893688	-1.034933	0.19 (295-> 320)	0.16 (291-> 301)	0.08 (289-> 303)
136	3.873	320.2	0.001147	0.001424	-3.519399	-3.989625	0.65 (295-> 320)	0.06 (295-> 321)	0.04 (291-> 301)
137	3.876	319.9	0.000360	0.000411	1.634729	1.753835	0.82 (295-> 321)	0.07 (295-> 320)	0.02 (295-> 322)
138	3.880	319.6	0.002587	0.003099	8.888458	9.731996	0.87 (295-> 322)	0.02 (295-> 321)	0.01 (294-> 315)
139	3.887	318.9	0.009426	0.010914	-5.647310	-6.064001	0.80 (295-> 323)	0.04 (294-> 312)	0.01 (286-> 303)
140	3.904	317.6	0.000301	0.000293	0.019908	0.028487	0.13 (274-> 297)	0.12 (275-> 296)	0.10 (277-> 297)
141	3.906	317.4	0.001247	0.001314	0.189854	0.199806	0.16 (275-> 297)	0.15 (274-> 296)	0.07 (276-> 297)

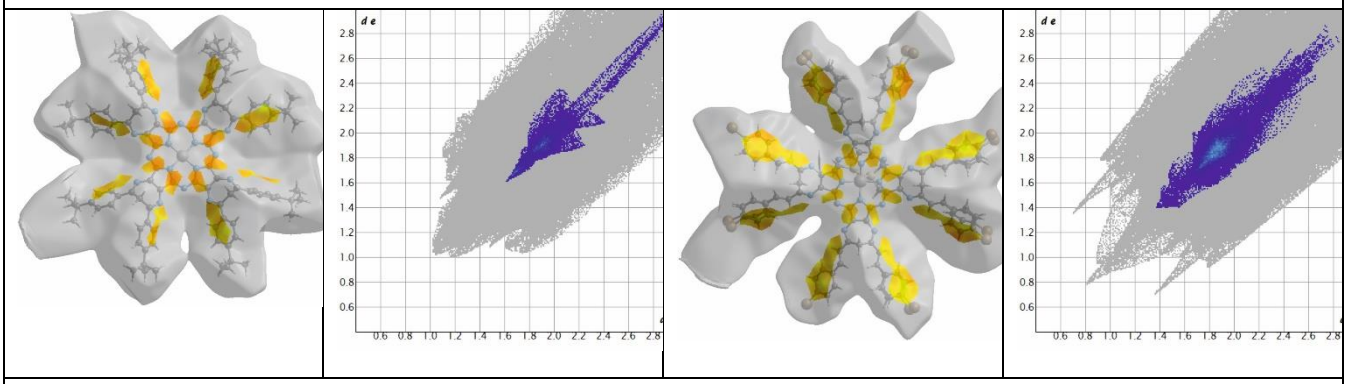
142	3.906	317.4	0.028761	0.030810	4.225671	4.367968	0.27 (294-> 312)	0.16 (294-> 313)	0.08 (295-> 323)
143	3.907	317.3	0.030101	0.032131	5.886087	6.084105	0.27 (294-> 313)	0.16 (294-> 312)	0.05 (295-> 323)
144	3.913	316.9	0.000215	0.000215	-5.528626	-5.429731	0.60 (294-> 314)	0.12 (294-> 315)	0.02 (295-> 320)
145	3.913	316.8	0.001728	0.001849	-11.418002	-11.619517	0.59 (294-> 315)	0.11 (294-> 314)	0.02 (295-> 319)
146	3.949	313.9	0.000044	0.000044	-0.010255	-0.011067	0.26 (290-> 302)	0.19 (289-> 301)	0.18 (288-> 300)
147	3.987	310.9	0.122483	0.112280	-0.077363	-0.075815	0.42 (271-> 296)	0.04 (283-> 299)	0.04 (282-> 296)
148	3.991	310.6	0.114867	0.105385	-3.329913	-3.188451	0.41 (271-> 297)	0.05 (282-> 299)	0.04 (283-> 296)
149	3.995	310.4	0.000101	0.000093	-0.084362	-0.180744	0.20 (290-> 303)	0.13 (289-> 301)	0.13 (288-> 300)
150	4.009	309.3	0.000030	0.000030	0.025172	0.063138	0.49 (295-> 324)	0.28 (295-> 333)	0.08 (295-> 316)

Table S16 Hirshfeld surface analysis and two-dimensional fingerprint plots

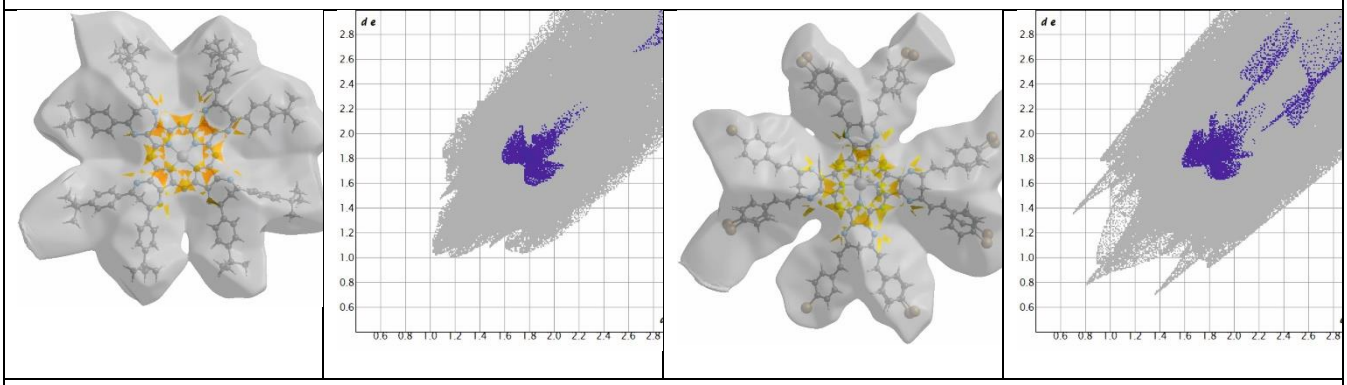
$[^{t\text{Bu}}Ph_8Dz_4PzNi]_2$		$[^{\text{Br}}Styr_8Dz_4PzMg]_2(DMSO)_2$	
Hirshfeld surfaces	2D-fingerprint plots	Hirshfeld surfaces	2D-fingerprint plots
D-H…A interactions			
$C–H^{ax}…N^{meso}$ contacts			
			
Ar–H…Br contacts			
			
C-H…π interactions			
			

π–π donor-acceptor interactions

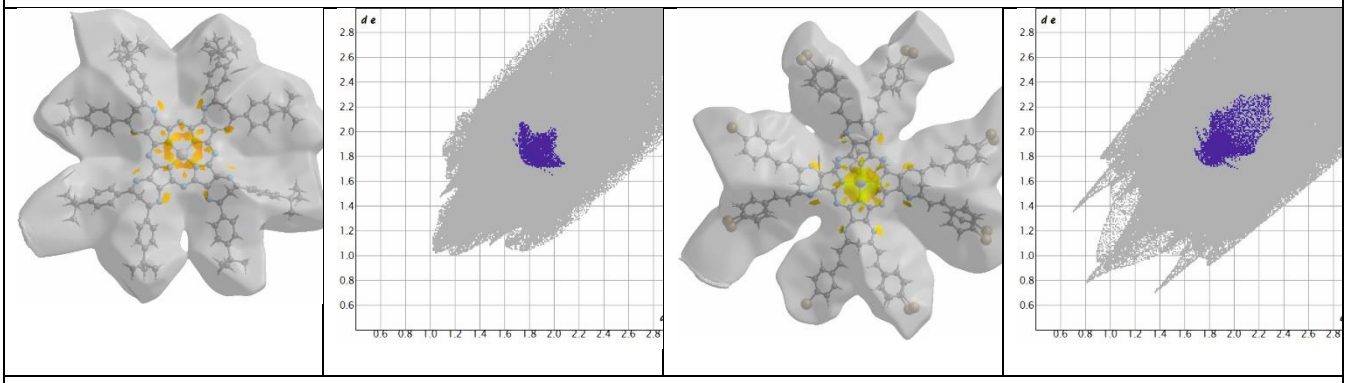
C…C contacts



C...N contacts

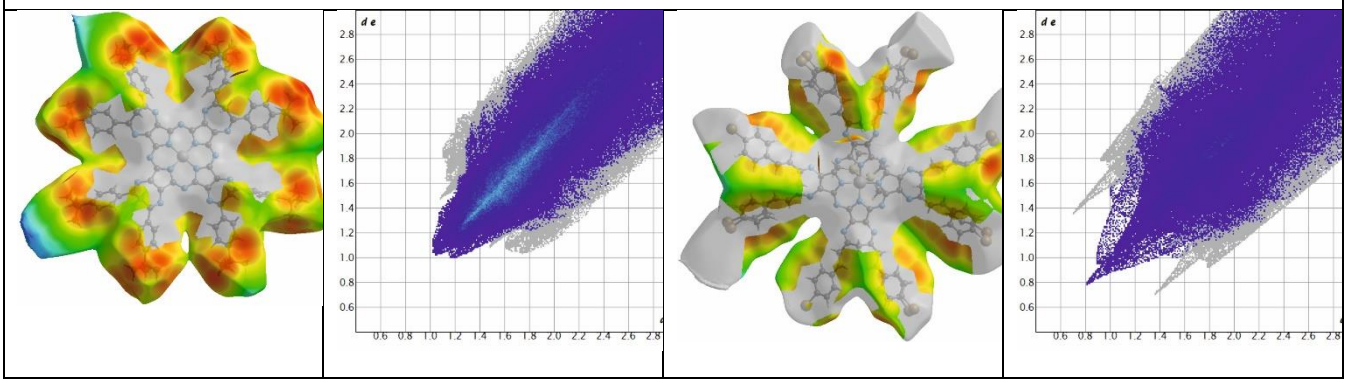


N...N contacts



repulsive interactions

H…H contacts



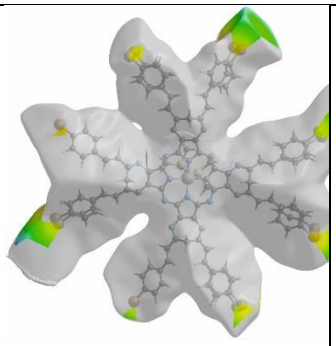
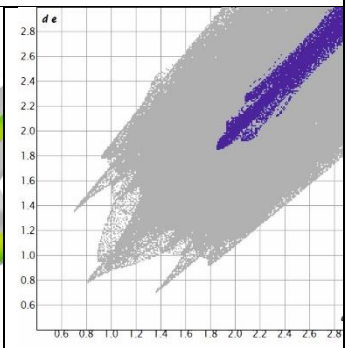
Br…Br contacts			
			

Table S17 Relative area of the surface corresponding to each kind of interactions

Contacts		Relative area, %	
		$[^{t\text{Bu}}Ph_8Dz_4PzNi]_2$	$[^{\text{Br}}Styr_8Dz_4PzMg]_2(DMSO)_2$
D-H…A interactions	C–H^{ax}…N^{meso}	9.6	6.9
	Ar–H…Br	-	26.5
C-H…π interactions	C-H…C	13	9.3
π–π donor-acceptor interactions	C…C	**3.6**	**8**
	C...N	1.3	1.5
	N...N	0.7	0.9
repulsive interactions	H…H	**71.2**	**36.8**
	Br…Br	-	5

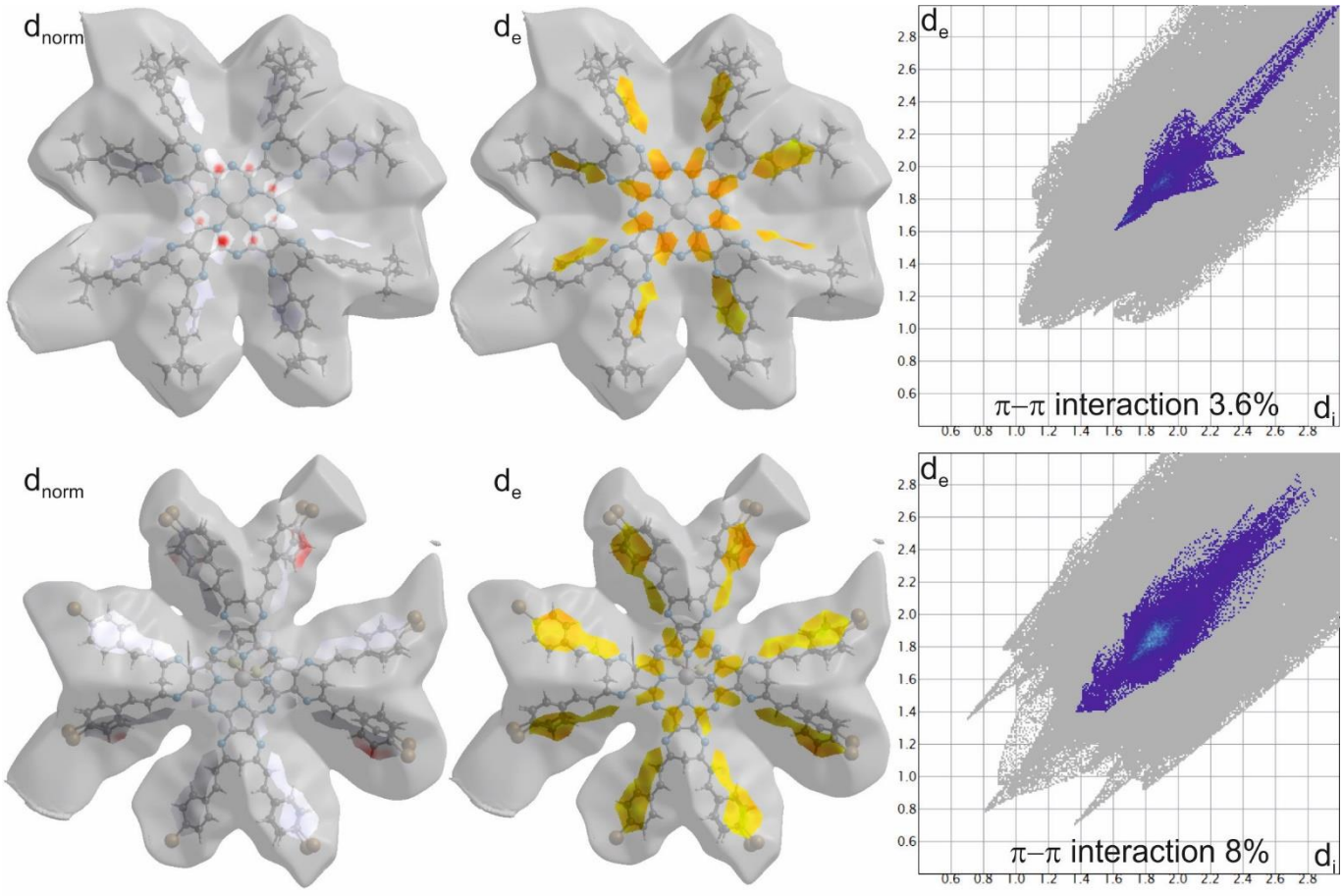


Fig. S15 Hirshfeld surfaces of $^{Br}Styr_8Dz_4PzMg\cdot DMSO$ and $^{tBu}Ph_8Dz_4PzNi$ mapped with d_{norm} and d_e for patterns associated with C…C contacts.

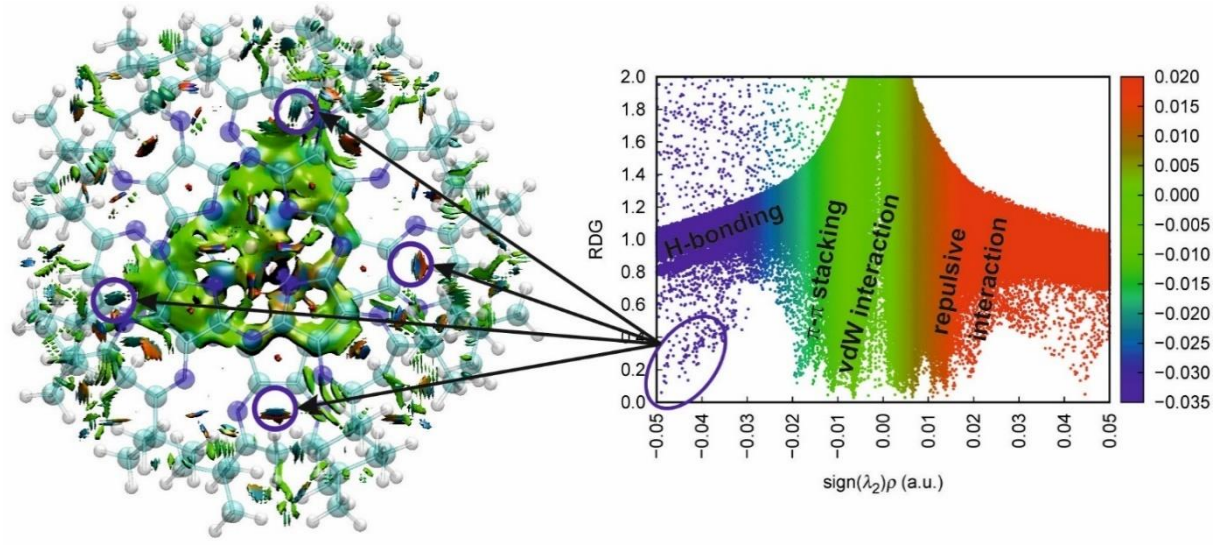


Fig. S16 The RDG isosurface map and 2D scatter plot for *t*Bu_8Dz_4PzMg dimeric complex from calculations at CAM-B3LYP def2-SV(P) def2/J level of theory.

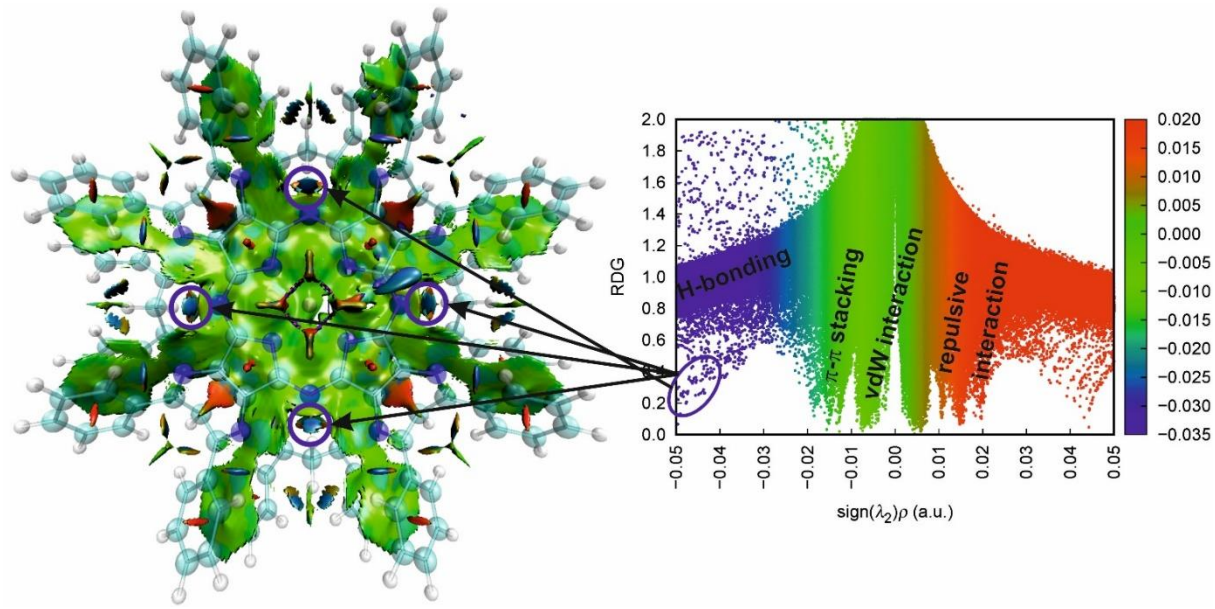


Fig. S17 The RDG isosurface map and 2D scatter plot for Ph_8Dz_4PzMg dimeric complex from calculations at CAM-B3LYP def2-SV(P) def2/J level of theory.

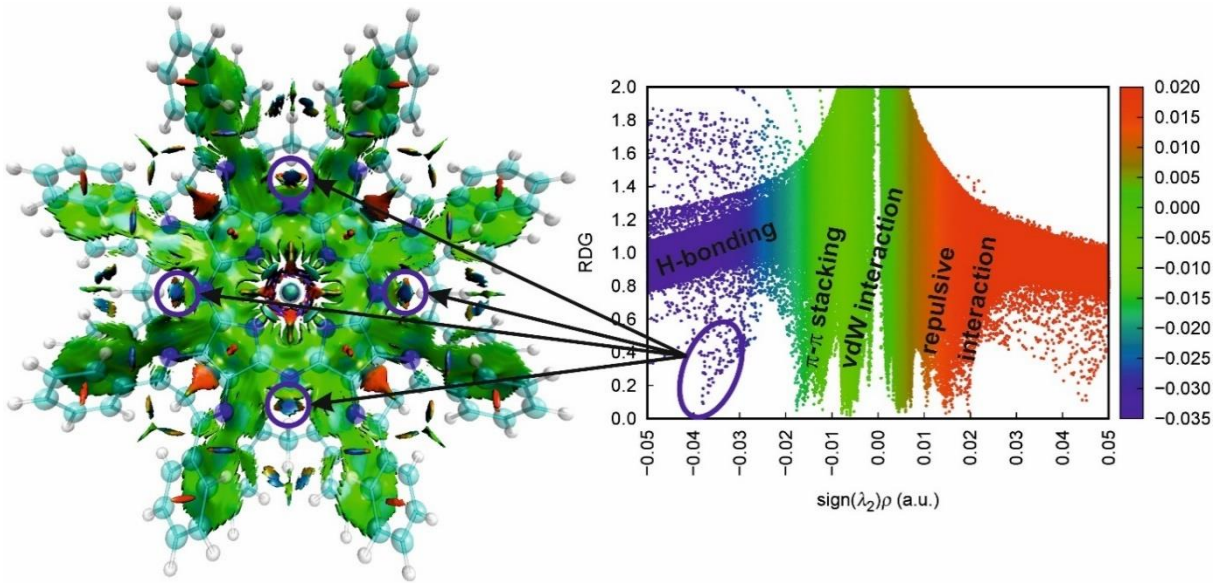


Fig. S18 The RDG isosurface map and 2D scatter plot for $Ph_8Dz_4PzMg{\cdot}F^-$ dimeric complex from calculations at CAM-B3LYP def2-SV(P) def2/J level of theory.

Table S18 NBO analysis of dimers

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

	Intermolecular interactions between 6*H*-1,4-diazepinoporphyrazine cores in dimers (kcal mol^{-1})	
dimer	C-H^{ax}···N^{meso}	C$^{\beta}$=C$^{\beta}$, C$^{\beta}$=C$^{\alpha}$, C$^{\alpha}$=N^{pyr}, C$^{\alpha}$=N^{meso}
	(LP→BD*)	(BD→BD*)
[*t*Bu$_8$Dz$_4$PzMg]$_2$	2.8	16.4
[Ph$_8$Dz$_4$PzMg]$_2$	16.9	13.8
[Ph$_8$Dz$_4$PzMg·DMSO]$_2$	16.4	18.2
[Ph$_8$Dz$_4$PzMg F$^-$]$_2$	17.9	16.6
	Intramolecular interactions in 6*H*-1,4-diazepinoporphyrazine core in dimers (kcal mol^{-1})	
	N^{pyr} with Mg^{2+}	C$^{\alpha}$=N^{pyr}, C$^{\alpha}$=N^{meso} with Mg^{2+}
	(LP→LU, RY)	(BD→LU, RY)
[Ph$_8$Dz$_4$PzMg]$_2$	143.1	64.9
[Ph$_8$Dz$_4$PzMg·DMSO]$_2$	134.0	86.5
[Ph$_8$Dz$_4$PzMg F$^-$]$_2$	105.0	53.1

Table S19 Atomic dipole corrected Hirshfeld atomic charge (ADCH) of [Ph$_8$Dz$_4$PzMg·DMSO]$_2$ (dimer with coordinated DMSO molecule)

Atom 1(C): 0.03398728	Atom 44(C): -0.25138842	Atom 87(H): 0.10410107
Atom 2(C): 0.01442596	Atom 45(C): -0.02476655	Atom 88(H): 0.14525776
Atom 3(C): 0.28713053	Atom 46(C): -0.22416020	Atom 89(H): 0.10974394
Atom 4(C): 0.00335813	Atom 47(C): 0.02517453	Atom 90(H): 0.11891238
Atom 5(C): 0.27772921	Atom 48(C): -0.17374800	Atom 91(H): 0.11645233
Atom 6(C): 0.04431991	Atom 49(C): -0.13950101	Atom 92(H): 0.28097173
Atom 7(C): 0.04663876	Atom 50(C): -0.52404298	Atom 93(H): 0.30057473
Atom 8(C): 0.20431000	Atom 51(C): 0.15723593	Atom 94(H): 0.20264936
Atom 9(C): -0.06685737	Atom 52(C): -0.05610596	Atom 95(H): 0.28600159
Atom 10(C): 0.19619456	Atom 53(C): -0.06112519	Atom 96(H): 0.20224018
Atom 11(C): -0.06004934	Atom 54(C): -0.06241166	Atom 97(H): 0.10474666
Atom 12(C): 0.05598729	Atom 55(C): -0.05443634	Atom 98(N): -0.20689652
Atom 13(C): 0.07266054	Atom 56(C): -0.34938121	Atom 99(N): -0.30513331
Atom 14(C): 0.14135916	Atom 57(C): -0.39879798	Atom 100(N): -0.19692560
Atom 15(C): -0.04081096	Atom 58(C): -0.17730118	Atom 101(N): -0.27351104
Atom 16(C): 0.19659257	Atom 59(C): -0.14511861	Atom 102(N): -0.23083012
Atom 17(C): -0.38268596	Atom 60(C): -0.52753836	Atom 103(N): -0.31066815
Atom 18(C): 0.02358555	Atom 61(C): 0.13079419	Atom 104(N): -0.31054476
Atom 19(C): 0.05481706	Atom 62(H): 0.12376437	Atom 105(N): -0.21728426
Atom 20(C): 0.20665976	Atom 63(H): 0.10836312	Atom 106(N): -0.22642458
Atom 21(C): -0.46434157	Atom 64(H): 0.11815043	Atom 107(N): -0.21877591
Atom 22(C): 0.26849680	Atom 65(H): 0.11484628	Atom 108(N): -0.22010526
Atom 23(C): -0.26949449	Atom 66(H): 0.30474801	Atom 109(N): -0.22795230
Atom 24(C): -0.36876717	Atom 67(H): 0.32857655	Atom 110(N): -0.21274374
Atom 25(C): -0.01781918	Atom 68(H): 0.28944860	Atom 111(N): -0.27124039
Atom 26(C): 0.14177671	Atom 69(H): 0.11703838	Atom 112(C): -0.45547251
Atom 27(C): -0.70518041	Atom 70(H): 0.11112435	Atom 113(C): -0.07013473
Atom 28(C): 0.16746911	Atom 71(H): 0.41417079	Atom 114(C): -0.06380393
Atom 29(C): -0.11891009	Atom 72(H): 0.25040892	Atom 115(C): -0.05666427
Atom 30(C): 0.18597723	Atom 73(H): 0.12239365	Atom 116(C): -0.34776176
Atom 31(C): -0.33493041	Atom 74(H): 0.29244264	Atom 117(C): -0.37371637
Atom 32(C): 0.23954063	Atom 75(H): 0.29498831	Atom 118(C): 0.15717310
Atom 33(C): 0.15386817	Atom 76(H): 0.22567981	Atom 119(C): -0.11841070
Atom 34(C): -0.12163967	Atom 77(H): 0.10511741	Atom 120(C): 0.15455119
Atom 35(C): 0.16379354	Atom 78(H): 0.05269547	Atom 121(C): -0.15720548
Atom 36(C): -0.64560935	Atom 79(H): 0.11016552	Atom 122(C): -0.00984622
Atom 37(C): -0.12860940	Atom 80(H): 0.05375129	Atom 123(C): -0.14423113
Atom 38(C): 0.24983419	Atom 81(H): 0.10244006	Atom 124(C): -0.12977212
Atom 39(C): -0.11727306	Atom 82(H): 0.05283187	Atom 125(C): -0.61383369
Atom 40(C): 0.27319611	Atom 83(H): 0.29366671	Atom 126(C): 0.25765248
Atom 41(C): -0.19860575	Atom 84(H): 0.20679472	Atom 127(H): 0.35697037
Atom 42(C): -0.22559982	Atom 85(H): 0.28476899	Atom 128(H): 0.10655462
Atom 43(C): -0.14824756	Atom 86(H): 0.20088122	Atom 129(H): 0.11855307

Atom 130(H): 0.11624936	Atom 188(C): -0.19727321	Atom 246(N): -0.21636619
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Atom 132(H): 0.29387954	Atom 190(C): -0.30142058	Atom 248(N): -0.20710629
Atom 133(H): 0.10407297	Atom 191(C): -0.04607478	Atom 249(N): -0.20944236
Atom 134(H): 0.05404834	Atom 192(C): 0.08484583	Atom 250(N): -0.23570018
Atom 135(H): 0.21595679	Atom 193(C): -0.50711349	Atom 251(N): -0.22227549
Atom 136(H): 0.30648619	Atom 194(C): -0.16959617	Atom 252(N): -0.27381366
Atom 137(H): 0.23782434	Atom 195(C): 0.20696110	Atom 253(C): -0.72958968
Atom 138(H): 0.10846981	Atom 196(C): -0.62133470	Atom 254(C): -0.51685103
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Atom 140(N): -0.23631815	Atom 198(C): -0.19743236	Atom 256(C): -0.68966197
Atom 141(Mg): 0.32847896	Atom 199(C): -0.20946325	Atom 257(C): -0.10762109
Atom 142(C): 0.03043250	Atom 200(C): -0.13321604	Atom 258(C): -0.18081718
Atom 143(C): 0.01225424	Atom 201(C): -0.65821578	Atom 259(C): 0.23931749
Atom 144(C): 0.29268543	Atom 202(C): 0.23078316	Atom 260(C): -0.11711503
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Atom 146(C): 0.27506389	Atom 204(H): 0.23779568	Atom 262(C): -0.10741299
Atom 147(C): 0.04859931	Atom 205(H): 0.10312309	Atom 263(C): -0.24284101
Atom 148(C): 0.05098942	Atom 206(H): 0.11584499	Atom 264(C): -0.19528208
Atom 149(C): 0.20793396	Atom 207(H): 0.26722738	Atom 265(C): -0.13946265
Atom 150(C): -0.36679369	Atom 208(H): 0.26263896	Atom 266(C): -0.74555325
Atom 151(C): 0.19448979	Atom 209(H): 0.35323995	Atom 267(C): 0.37924474
Atom 152(C): 0.08715426	Atom 210(H): 0.11569304	Atom 268(H): 0.48707399
Atom 153(C): 0.05544445	Atom 211(H): 0.11890234	Atom 269(H): 0.36364088
Atom 154(C): 0.06316486	Atom 212(H): 0.10887591	Atom 270(H): 0.12517946
Atom 155(C): 0.14641906	Atom 213(H): 0.15594174	Atom 271(H): 0.29582799
Atom 156(C): -0.05285989	Atom 214(H): -0.08928875	Atom 272(H): 0.30274329
Atom 157(C): 0.19565140	Atom 215(H): 0.17594954	Atom 273(H): 0.24692869
Atom 158(C): -0.33275937	Atom 216(H): 0.27411226	Atom 274(H): 0.10108751
Atom 159(C): 0.02454820	Atom 217(H): 0.19490200	Atom 275(H): 0.05399934
Atom 160(C): 0.04781072	Atom 218(H): 0.05338661	Atom 276(H): 0.25655485
Atom 161(C): 0.22279097	Atom 219(H): 0.10410138	Atom 277(H): 0.35114311
Atom 162(C): -0.25808067	Atom 220(H): 0.05185524	Atom 278(H): 0.29841619
Atom 163(C): 0.27138844	Atom 221(H): 0.10198377	Atom 279(H): 0.11221425
Atom 164(C): -0.47615316	Atom 222(H): 0.05290343	Atom 280(N): -0.22872684
Atom 165(C): -0.43910386	Atom 223(H): 0.10847815	Atom 281(N): -0.21899260
Atom 166(C): -0.02894873	Atom 224(H): 0.32856953	Atom 282(Mg): 0.32960492
Atom 167(C): -0.05375248	Atom 225(H): 0.26785157	Atom 283(S): 0.29987294
Atom 168(C): -0.06587397	Atom 226(H): 0.24869026	Atom 284(S): 0.30148433
Atom 169(C): 0.13062357	Atom 227(H): 0.11668324	Atom 285(C): -0.22546636
Atom 170(C): -0.11746393	Atom 228(H): 0.10711640	Atom 286(H): 0.08288785
Atom 171(C): 0.25854398	Atom 229(H): 0.33457006	Atom 287(H): 0.12386139
Atom 172(C): -0.18578643	Atom 230(H): 0.22623898	Atom 288(H): 0.13380141
Atom 173(C): 0.69217249	Atom 231(H): 0.09991663	Atom 289(C): -0.22729572
Atom 174(C): 0.26525854	Atom 232(H): 0.22617151	Atom 290(H): 0.13610003
Atom 175(C): -0.11764808	Atom 233(H): 0.31906638	Atom 291(H): 0.08380896
Atom 176(C): 0.23709221	Atom 234(H): 0.22384484	Atom 292(H): 0.12416598
Atom 177(C): -0.75213356	Atom 235(H): 0.22670042	Atom 293(C): -0.22571009
Atom 178(C): -0.05397133	Atom 236(H): 0.30313452	Atom 294(H): 0.13256471
Atom 179(C): 0.16024665	Atom 237(H): 0.29265835	Atom 295(H): 0.08437918
Atom 180(C): -0.12403901	Atom 238(H): 0.11871050	Atom 296(H): 0.12660822
Atom 181(C): 0.14982167	Atom 239(N): -0.20759517	Atom 297(C): -0.22793747
Atom 182(C): -0.13861347	Atom 240(N): -0.30685875	Atom 298(H): 0.13477503
Atom 183(C): -0.29071727	Atom 241(N): -0.20019877	Atom 299(H): 0.08527372
Atom 184(C): 0.02668769	Atom 242(N): -0.27633956	Atom 300(H): 0.12706759
Atom 185(C): -0.20854878	Atom 243(N): -0.24118963	Atom 301(O): -0.37095713
Atom 186(C): -0.16663738	Atom 244(N): -0.31141074	Atom 302(O): -0.36912006
Atom 187(C): -0.23430644	Atom 245(N): -0.30693720	

Table S20 Atomic dipole corrected Hirshfeld atomic charge (ADCH) of $[Ph_8Dz_4PzMg{\cdot}F^-]_2$ (dimer with coordinated F^- anion)

Atom 1(C): 0.01841595	Atom 5(C): 0.28383782	Atom 9(C): -0.07194000
Atom 2(C): 0.01054241	Atom 6(C): 0.00983706	Atom 10(C): 0.27897241
Atom 3(C): 0.28184704	Atom 7(C): 0.01745607	Atom 11(C): 0.35054289
Atom 4(C): -0.36076256	Atom 8(C): 0.27931926	Atom 12(C): 0.01126031

Atom 13(C): 0.01522474	Atom 79(H): 0.10105191	Atom 145(C): -0.50649949
Atom 14(C): 0.28880926	Atom 80(H): 0.05526169	Atom 146(C): 0.28169810
Atom 15(C): -1.23144338	Atom 81(H): 0.09647290	Atom 147(C): 0.01061441
Atom 16(C): 0.28972675	Atom 82(H): 0.05387241	Atom 148(C): 0.01755664
Atom 17(C): -0.26610863	Atom 83(H): 0.35062422	Atom 149(C): 0.28323594
Atom 18(C): 0.01194639	Atom 84(H): 0.28410854	Atom 150(C): -0.75582031
Atom 19(C): 0.01214046	Atom 85(H): 0.42449489	Atom 151(C): 0.28420807
Atom 20(C): 0.28187295	Atom 86(H): 0.31952837	Atom 152(C): 0.51669436
Atom 21(C): -0.51691522	Atom 87(H): 0.11827258	Atom 153(C): 0.01674854
Atom 22(C): 0.29015583	Atom 88(H): 0.40966347	Atom 154(C): 0.01013233
Atom 23(C): -0.31749538	Atom 89(H): 0.11037316	Atom 155(C): 0.28516212
Atom 24(C): -0.52347737	Atom 90(H): 0.13365031	Atom 156(C): -1.00854688
Atom 25(C): 0.02758489	Atom 91(H): 0.45046033	Atom 157(C): 0.28197998
Atom 26(C): 0.13195183	Atom 92(H): 0.39547133	Atom 158(C): -0.25950194
Atom 27(C): -0.69810230	Atom 93(H): 0.40480264	Atom 159(C): 0.01654045
Atom 28(C): 0.15215204	Atom 94(H): 0.23672953	Atom 160(C): 0.01125467
Atom 29(C): -0.12391843	Atom 95(H): 0.35638471	Atom 161(C): 0.28586727
Atom 30(C): 0.20008985	Atom 96(H): 0.34280731	Atom 162(C): -0.34773608
Atom 31(C): -0.24650025	Atom 97(H): 0.11954120	Atom 163(C): 0.28606416
Atom 32(C): 0.25781949	Atom 98(N): -0.26104977	Atom 164(C): -0.48243996
Atom 33(C): 0.15339990	Atom 99(N): -0.31195349	Atom 165(C): -0.47476460
Atom 34(C): -0.12944875	Atom 100(N): -0.26345075	Atom 166(C): -0.01406062
Atom 35(C): 0.19556576	Atom 101(N): -0.31308246	Atom 167(C): -0.06590230
Atom 36(C): -0.84666216	Atom 102(N): -0.26439691	Atom 168(C): -0.03891701
Atom 37(C): -0.22176357	Atom 103(N): -0.31448289	Atom 169(C): 0.15226507
Atom 38(C): 0.27726965	Atom 104(N): -0.31295822	Atom 170(C): -0.12336656
Atom 39(C): -0.12180773	Atom 105(N): -0.20877297	Atom 171(C): 0.22999812
Atom 40(C): 0.28745451	Atom 106(N): -0.20689575	Atom 172(C): -0.19563421
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Atom 42(C): -0.31027751	Atom 108(N): -0.22188441	Atom 174(C): 0.28612881
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Atom 44(C): -0.18751734	Atom 110(N): -0.20582357	Atom 176(C): 0.23494559
Atom 45(C): -0.05010413	Atom 111(N): -0.26161068	Atom 177(C): -0.69349452
Atom 46(C): -0.17609091	Atom 112(C): -0.79100045	Atom 178(C): -0.22668681
Atom 47(C): 0.01665843	Atom 113(C): -0.40726411	Atom 179(C): 0.19572928
Atom 48(C): -0.21770517	Atom 114(C): 0.26489060	Atom 180(C): -0.12368105
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Atom 50(C): -0.90249906	Atom 116(C): -0.21651829	Atom 182(C): -0.15387731
Atom 51(C): 0.46419807	Atom 117(C): -0.21948330	Atom 183(C): -0.30622940
Atom 52(C): -0.59748493	Atom 118(C): 0.25464531	Atom 184(C): -0.02783085
Atom 53(C): -0.03253978	Atom 119(C): -0.12112764	Atom 185(C): -0.03992236
Atom 54(C): 0.23950023	Atom 120(C): 0.18971374	Atom 186(C): -0.11311069
Atom 55(C): -0.93527609	Atom 121(C): -0.08475798	Atom 187(C): -0.10949302
Atom 56(C): -0.33612938	Atom 122(C): -0.33591166	Atom 188(C): -0.07986400
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Atom 59(C): -0.22691255	Atom 125(C): -0.63179168	Atom 191(C): -0.56152472
Atom 60(C): -0.79856528	Atom 126(C): 0.41966150	Atom 192(C): -0.27610563
Atom 61(C): 0.26224759	Atom 127(H): 0.45819465	Atom 193(C): -0.87906524
Atom 62(H): 0.31159586	Atom 128(H): 0.37226372	Atom 194(C): -0.51576491
Atom 63(H): 0.11210606	Atom 129(H): 0.14415186	Atom 195(C): 0.33165450
Atom 64(H): 0.14587333	Atom 130(H): 0.39267289	Atom 196(C): -0.80335855
Atom 65(H): 0.52383390	Atom 131(H): 0.38635657	Atom 197(C): -0.27387324
Atom 66(H): 0.48020302	Atom 132(H): 0.30460954	Atom 198(C): -0.18181332
Atom 67(H): 0.38003525	Atom 133(H): 0.09511049	Atom 199(C): -0.25368745
Atom 68(H): 0.31389392	Atom 134(H): 0.05447175	Atom 200(C): -0.26809291
Atom 69(H): 0.10388509	Atom 135(H): 0.26533238	Atom 201(C): -0.72153705
Atom 70(H): 0.12038246	Atom 136(H): 0.44195045	Atom 202(C): 0.29555890
Atom 71(H): 0.38717139	Atom 137(H): 0.14796393	Atom 203(H): 0.33606865
Atom 72(H): 0.21186088	Atom 138(H): 0.17226459	Atom 204(H): 0.38359076
Atom 73(H): 0.16318827	Atom 139(N): -0.19760536	Atom 205(H): 0.15351634
Atom 74(H): 0.36254375	Atom 140(N): -0.21135447	Atom 206(H): 0.43413708
Atom 75(H): 0.38112082	Atom 141(Mg): 0.36777738	Atom 207(H): 0.44070277
Atom 76(H): 0.26263937	Atom 142(C): 0.01547619	Atom 208(H): 0.30937719
Atom 77(H): 0.09613901	Atom 143(C): 0.00767002	Atom 209(H): 0.36138887
Atom 78(H): 0.05382883	Atom 144(C): 0.28501889	Atom 210(H): 0.09958669

Atom 211(H): 0.11021104	Atom 236(H): 0.34205229	Atom 261(C): 0.20662639
Atom 212(H): 0.11010629	Atom 237(H): 0.36064481	Atom 262(C): -0.11231648
Atom 213(H): 0.25312117	Atom 238(H): 0.10974219	Atom 263(C): -0.34255020
Atom 214(H): 0.13552697	Atom 239(N): -0.26132783	Atom 264(C): -0.26020126
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Atom 217(H): 0.24834581	Atom 242(N): -0.31314844	Atom 267(C): 0.44215679
Atom 218(H): 0.05438906	Atom 243(N): -0.26290430	Atom 268(H): 0.47454688
Atom 219(H): 0.09765737	Atom 244(N): -0.31462635	Atom 269(H): 0.33353623
Atom 220(H): 0.05349908	Atom 245(N): -0.31320579	Atom 270(H): 0.13296624
Atom 221(H): 0.09591708	Atom 246(N): -0.20780233	Atom 271(H): 0.45708812
Atom 222(H): 0.05468043	Atom 247(N): -0.18626861	Atom 272(H): 0.36780290
Atom 223(H): 0.09846450	Atom 248(N): -0.20020433	Atom 273(H): 0.30410915
Atom 224(H): 0.33627295	Atom 249(N): -0.21856676	Atom 274(H): 0.09448987
Atom 225(H): 0.34412410	Atom 250(N): -0.20730128	Atom 275(H): 0.05413930
Atom 226(H): 0.35150085	Atom 251(N): -0.21093806	Atom 276(H): 0.29490387
Atom 227(H): 0.09706503	Atom 252(N): -0.26322323	Atom 277(H): 0.44333215
Atom 228(H): 0.69681938	Atom 253(C): -0.74339246	Atom 278(H): 0.37945269
Atom 229(H): 0.43863267	Atom 254(C): -0.35721600	Atom 279(H): 0.15567580
Atom 230(H): 0.39116044	Atom 255(C): 0.27266151	Atom 280(N): -0.19416610
Atom 231(H): 0.09164184	Atom 256(C): -0.91714243	Atom 281(N): -0.20336222
Atom 232(H): 0.36249683	Atom 257(C): -0.28509751	Atom 282(Mg): 0.36802061
Atom 233(H): 0.36716074	Atom 258(C): -0.14414342	Atom 283(F): -0.54829594
Atom 234(H): 0.26949863	Atom 259(C): 0.24848695	Atom 284(F): -0.54823950
Atom 235(H): 0.27414378	Atom 260(C): -0.12201835	

UV-vis and fluorescence spectra

According to a previously described method all compounds obtained were exposed to F^- anions (as the tetrabutylammonium salt) to evaluate the possibility of 100% conversion of dimeric forms to monomeric ones monitoring the equilibrium shift by UV-vis spectroscopy.[12] Then, for two compounds, *t*Bu_8Dz_4PzMg in pyridine and $^{tBu}Ph_8Dz_4PzMg$ in DMSO, under conditions where they exist 100% in the monomeric forms without the addition of F^- anions, the effect of the TBAF addition on their fluorescence quantum yields was tested. It was shown that the coordination of F^- anions to the monomeric complexes slightly shifts the maxima in the absorption and fluorescence spectra but does not change the fluorescence quantum yield. Thus, we can conclude that it is possible to estimate the extent of dissociation using the ratio of fluorescence peak areas (G) of the complex before and after the addition of F^- anions. The ratio of fluorescence peak areas (Table S13) before and after the addition of F^- anions will correspond to the extent of dissociation (α) only if the dimeric form of the complex does not fluoresce. Thus, in pyridine, where the equilibrium is more shifted towards the dimeric forms of the complexes, we additionally recorded the fluorescence excitation spectra (Fig S15, dot blue line) for each case, in order to exclude the contribution of the probable dimeric form fluorescence to the observed fluorescence.

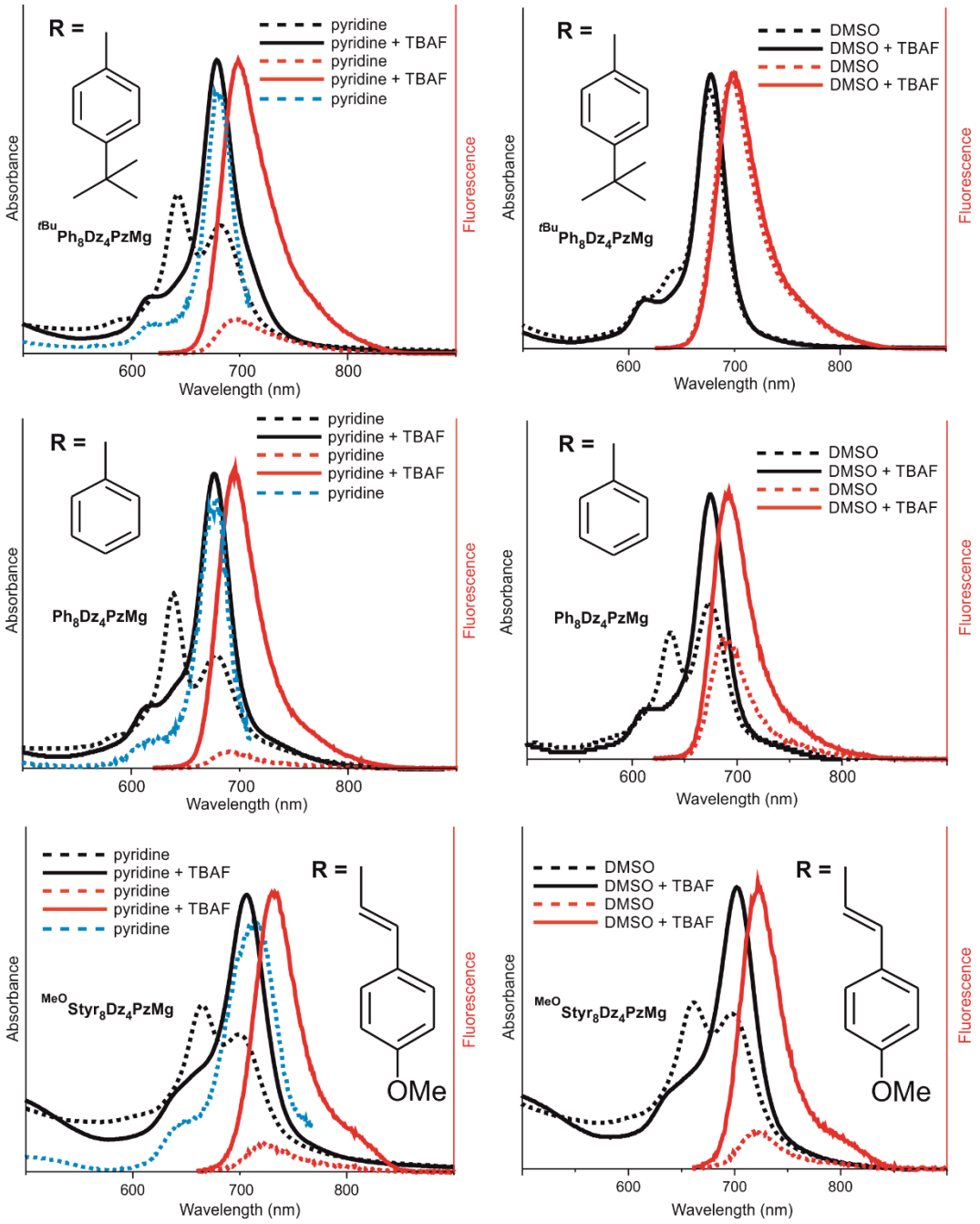

Fig. S19 UV-vis (black line), fluorescence (red line) and excitation (blue line) spectra of complexes under different conditions. λ_{ex} = 615 nm, λ_{em} = 730 nm for $^{tBu}Ph_8Dz_4PzMg$ and Ph_8Dz_4PzMg; λ_{ex} = 650 nm, λ_{em} = 790 nm for $^{MeO}Styr_8Dz_4PzMg$.

Table S21 Fluorescence data and determining the dissociation constant (K_d) of dimer in solution

Complex	Solvent	Temp., K	G(fluorescence), a.u.			$K_d \cdot 10^7$
			without TBAF (G)	with TBAF (G_F)	$G/G_F = \alpha$	
$^{tBu}Ph_8Dz_4PzMg$	DMSO	r.t.	22324	22826	0.98	1441
	pyridine		2745	21282	0.13	0.58
Ph_8Dz_4PzMg	DMSO	r.t.	9509	21184	0.45	11.05
	pyridine		1318	21448	0.06	0.11
$^{MeO}Styr_8Dz_4PzMg$	DMSO	r.t.	826	5836	0.14	0.68
	pyridine		1421	13177	0.11	0.41

$K_d = \frac{\alpha^2 \cdot c}{1-\alpha}$, C_M(complex) = 3 μM.

Spectroelectrochemistry

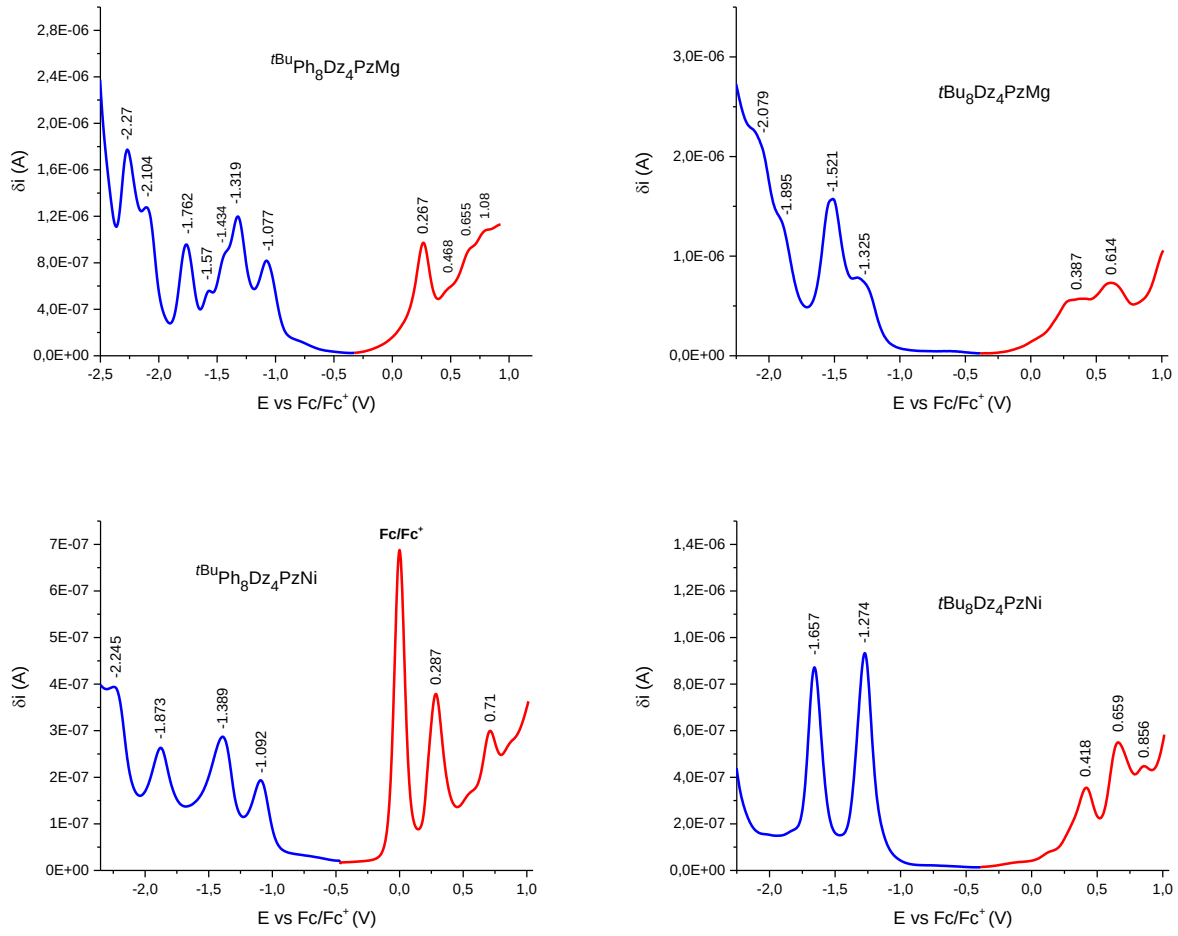

Fig. S20 CV of $^{tBu}Ph_8Dz_4PzMg$, tBu_8Dz_4PzMg, $^{tBu}Ph_8Dz_4PzNi$ and tBu_8Dz_4PzNi (2.1 mg in 10 mL DCM) in 0.1 M $TBAPF_6$ DCM solution. Measured vs Ag/Ag^+ (0.01 M AN) RE, converted to Fc/Fc^+ scale. WE: Pt 1mm diam.

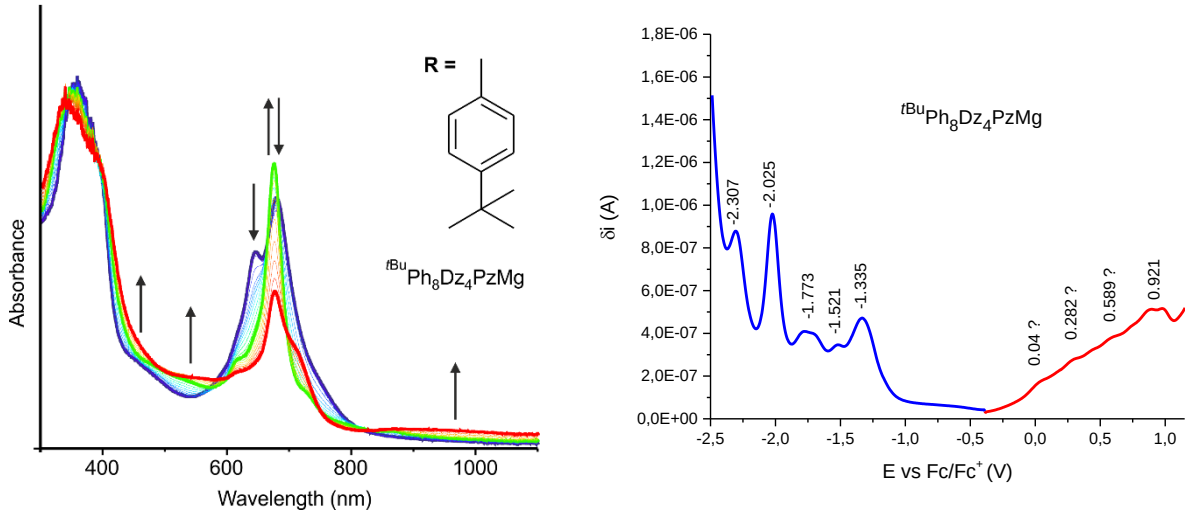

Fig. S21 Left: UV-Vis spectral changes for $^{t\text{Bu}}Ph_8Dz_4PzMg$ (20 μM) in DCM containing 0.1 M $[BuN_4][PF_6]$ during controlled potential oxidation (+0.7 V vs. Ag/Ag^+) and reduction (−0.2 V vs. Ag/Ag^+), respectively. Right: CV of $^{t\text{Bu}}Ph_8Dz_4PzMg$ (2.1 mg in 10 mL DCM) in 0.1 M $TBAPF_6$ DCM solution. Measured vs Ag/Ag^+ (0.01 M AN) RE, converted to Fc/Fc^+ scale. WE: Pt 1mm diam.

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