Electronic Supplementary Information *for*

Dramatic Emission Enhancement of Aggregation-Induced Emission Luminogens by Dynamic Metal Coordination Bonds and Anti-Heavy-Atom Effect

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1. **Experimental Section.**
2. **Computational Methods.**
3. **Supplementary Schemes and Figure**

3.1. Scheme S1. Synthesis routes of DPDPE and Zn-DPDPE, Cd-DPDPE and Hg-DPDPE.

3.2. Figure S1. Time-resolved PL decay curve of DPDPE in solid at room temperature.

3.3. Figure S2. The change of UV-visible spectra of DPDPE (100 μM) in methanol in the presence of different amounts of Zn^{2+} (a), Cd^{2+} (b), and Hg^{2+} (c) respectively, and change of PL spectra of DPDPE (100 μM) in methanol in the presence of different amounts of Zn^{2+} (d), Cd^{2+} (e), and Hg^{2+} (f) respectively.

3.4. Figure S3. The asymmetric units of Zn-DPDPE, Cd-DPDPE and Hg-DPDPE.

3.5. Figure S4. Stacking patterns of Zn-DPDPE (a), Cd-DPDPE (b) and Hg-DPDPE (c) in crystal.

3.6. Figure S5. Time-resolved PL decay curves of Zn-DPDPE (a), Cd-DPDPE (b) and Hg-DPDPE (c) in solid at room temperature.

3.7. Figure S6. Natural transition orbitals of DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

3.8. Figure S7. Natural transition orbitals of Zn-DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

3.9. Figure S8. Natural transition orbitals of Cd-DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

3.10. Figure S9. Natural transition orbitals of Hg-DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

3.11. Figure S10. Controllable patterning demonstrations based on stimuli-responsive behaviours of DPDPE and its zinc complex. (a) A green pattern of mountain is written on a paper containing DPDPE with blue emission using zinc ion, and then is erased using EDTA. (b) The blue paper is firstly turned to green using zinc ion, then a yellow pattern of two leaves is drawn on the green paper using trifluoroacetic acid (TFA), and finally erased with triethenylamine (TEA). (c) The blue paper is firstly turned to green using zinc ion, and then a group of letters “ZJNU” is written on the green paper with quenched fluorescence using sodium sulfide.

3.12. Figure S11. (a) PL spectra of DPDPE on a paper in the presence of different compositions: DPDPE, DPDPE+Zn^{2+}, and DPDPE+Zn^{2+}+EDTA. (b) PL spectra of DPDPE on a paper in the presence of different compositions: DPDPE, DPDPE+Zn^{2+}, DPDPE+Zn^{2+}+TFA, and DPDPE+Zn^{2+}+TFA+TEA. (c) PL spectra of DPDPE on a

paper in the presence of different compositions: DPDPE, DPDPE+Zn^{2+}, and DPDPE+Zn^{2+}+Na_2S.

4. **Supplementary Tables**

4.1. Table S1. Crystallographic data for Zn-DPDPE, Cd-DPDPE, Hg-DPDPE.

4.2. Table S2. Photophysical properties of DPDPE, Zn-DPDPE, Cd-DPDPE and Hg-DPDPE in different states.

4.3. Table S3. Compositions of Natural Transition Orbitals of DPDPE, Zn-DPDPE, Cd-DPDPE and Hg-DPDPE for the $S_0 \rightarrow S_1$ transition.

4.4. Table S4. Contribution ratios of different groups to natural transition orbitals of DPDPE, Zn-DPDPE, Cd-DPDPE and Hg-DPDPE.

4.5. Table S5. Experimental and calculated absorption and emission maxima of DPDPE, Zn-DPDPE, Cd-DPDPE and Hg-DPDPE in different states.

5. **NMR and MS Spectra of Compounds**

5.1. Figure S9. ^1H NMR spectrum of DBDBE in $CDCl_3$.

5.2. Figure S10. ^{13}C NMR spectrum of DBDBE in $CDCl_3$.

5.3. Figure S11. ^1H NMR spectrum of DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.4. Figure S12. ^{13}C NMR spectrum of DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.5. Figure S13. ^1H NMR spectrum of Zn-DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.6. Figure S14. ^{13}C NMR spectrum of Zn-DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.7. Figure S15. ^1H NMR spectrum of Cd-DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.8. Figure S16. ^{13}C NMR spectrum of Cd-DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.9. Figure S17. ^1H NMR spectrum of Hg-DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.10.Figure S18. ^{13}C NMR spectrum of Hg-DBDPE in $CDCl_3/CD_3OD$ (3:2).

5.11.Figure S19.High-resolution mass spectrum of DPDBE.

5.12.Figure S20.High-resolution mass spectrum of DPDPE.

6. **Cartesian Coordinates**

7. **References**

1. Experimental Section

Synthesis of ((*Z*)-(1,2-diphenyl-)-(*Z*)-di(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl))ethene (DPDBE). To a degassed solution of diphenylacetylene (5.00 g, 28.0 mmol) and bis(pinacolato)diboron (14.25 g, 56.0 mmol) in DMF (150 ml) was added $Pt(PPh_3)_4$ (0.35 g, 1 mol%), and then the mixture was heated at 90°C for 24 h. After cooling to room temperature, the reaction mixture was extracted three times with ethyl acetate. The crude product of DPDBE was obtained after removal of the solvent under reduced pressure. DPDBE (10.00 g) was obtained by washing several times with ethanol as a white solid in a yield of 82%. Molecular formula: $C_{26}H_{34}B_2O_4$. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.07-7.05 (m, 6H), 6.95-6.94 (d, J=4 Hz, 4H), 1.32 (s, 24H). ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 141.27, 129.32, 127.44, 125.80, 84.08, 24.90. HRMS (EI) m/z: $[M+H]^+$ 433.2735 (calcd. 433.2643).

Synthesis of ((Z)-(1,2-diphenyl)-(Z)-1,2-dipyridin-4-yl)ethene (DPDPE). A mixture of **DPDBE** (2.00 g, 4.6 mmol), 4-bromopyridine (1.10 mL, 11.56 mmol), potassium carbonate (1.60 g, 11.56 mmol) and $Pd(PPh_3)_4$ (0.10 g, 0.10 mmol) in 150 mL of toluene/THF/water (8:6:1; v/v/v) was refluxed for 24 h under nitrogen. After cooling to room temperature, the reaction mixture was extracted three times with dichloromethane. The combined organic layers were washed with brine and then dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel using ethyl acetate/petroleum ether (2:3) as eluent. The final product DPDPE was obtained by recrystallization with ethanol as a white solid (1.10 g) in 72% yield. Molecular formula: $C_{24}H_{18}N_2$. ^{1}H NMR (400 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 8.34-8.33 (d, J=8 Hz, 4H), 7.18-7.16 (m, 6H), 7.06-7.05 (d, J=8 Hz, 4H), 7.01-6.99 (d, J=8 Hz, 4H). ^{13}C NMR (150 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 150.50, 149.74, 141.41, 140.60, 131.02, 128.12, 127.56, 125.69. HRMS (EI) m/z: $[M+H]^+$ 335.1541 (calcd. 335.1570), $[M+Na]^+$ 357.1361 (calcd. 357.1470).

Crystal growth of the complex of Zn^{2+} and DPDPE (Zn-DPDPE). To a solution of DPDPE (1.00 g, 3.00 mmol) in $CHCl_3$ (10 mL), a methanol solution of $Zn(OAc)_2 \cdot 2H_2O$ (1.37 g, 6.00 mmol) was added and the solution was stirred for 1 h at room temperature. After removal of the solvent under reduced pressure, the final product Zn-DPDPE was obtained as a white solid (0.95 g) in 62% yield.

The solid (20 mg) was dissolved in a mixed solution containing $CHCl_3$ (2 mL), methanol (1 mL) and petroleum ether (1 mL) to the saturated state, and then the resulting mixture was naturally evaporated at room temperature through several small pores. The cubic and colorless crystals were obtained, and then were selected for single-crystal X-ray diffraction analysis. ^{1}H NMR (400 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 8.48-8.46 (d, J=8 Hz, 8H), 7.20-7.19 (m, 20H), 7.00-6.99 (d, J=8 Hz, 8H), 2.05 (s, 12H). ^{13}C NMR (150 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 180.25, 153.34, 148.99, 141.00, 140.29, 130.82, 128.34, 128.09, 126.95, 21.83. CCDC No: 2170098.

Crystal growth of the complex of Cd^{2+} and DPDPE (Cd-DPDPE). To a solution of DPDPE (1.00 g, 3.00 mmol) in $CHCl_3$ (10 mL), a methanol solution of $Cd(OAc)_2{\cdot}2H_2O$ (1.60 g, 6.00 mmol) was added, and then the resulting solution was stirred for 1 h at room temperature. After removal of the solvent under reduced pressure, the final product Cd-DPDPE was obtained as a white solid (0.90 g) in 64% yield. The solid (20 mg) was dissolved in a mixed solution containing $CHCl_3$ (2 mL), methanol (1 mL) and petroleum ether (1 mL) to the saturated state, and then the resulting mixture was naturally evaporated at room temperature through several small pores. The cubic and colorless crystals were obtained, and then were selected for single-crystal X-ray diffraction analysis. ^{1}H NMR (400 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 8.38-8.37 (d, J=4 Hz, 8H), 7.19-7.17 (m, 12H), 7.12-7.10 (d, J=8 Hz, 8H), 6.99-6.97 (d, J=8 Hz, 8H), 2.04(s, 12H). ^{13}C NMR (150 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 180.62, 152.27, 149.05, 140.81, 140.66, 130.81, 128.23, 127.91, 126.50, 21.18. CCDC No: 2170097.

Crystal growth of the complex of Hg^{2+} and DPDPE (Hg-DPDPE). To a solution of DPDPE (1.00 g, 3.00 mmol) in $CHCl_3$ (10 mL), a methanol solution of $Hg(OAc)_2{\cdot}2H_2O$ (2.12 g, 6.00 mmol) was added, and then the solution was stirred for 1 h at room temperature. After removal of the solvent under reduced pressure, the final product Hg-DPDPE was obtained as a white solid (1.02 g) in 50% yields. The solid (20 mg) was dissolved in a mixed solution containing $CHCl_3$ (2 mL), methanol (1 mL) and petroleum ether (1 mL) to the saturated state, and then the resulting mixture was naturally evaporated at room temperature through several small pores. The cubic and colorless crystals were obtained, and then were selected for single-crystal X-ray diffraction analysis. ^{1}H NMR (400 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 8.50-8.49 (d, J = 4 Hz, 8H), 7.27-7.25 (m, 10H), 7.21-7.19 (d, J = 8 Hz,

10H), 6.99-6.97 (d, J=8 Hz, 8H), 2.08(s, 12H). ^{13}C NMR (150 MHz, $CDCl_3/CD_3OD$=3:2) δ (ppm) 180.62, 152.27, 149.05, 140.81, 140.66, 130.81, 128.23, 127.91, 126.50, 21.18. CCDC No: 2170096.

Characterization of UV-Visible and Fluorescence Properties of All Samples. UV−vis absorption spectra were recorded using an Agilent Cary 5000 UV-Vis-NIR spectrophotometer. Steady PL spectra of all samples were performed on an Edinburgh Instruments model FLS980 fluorescence spectrophotometer equipped with a xenon arc lamp using a front face sample holder. Time-resolved fluorescence measurements were conducted with EPL-series lasers. The absolute PL quantum yields of all samples were determined using an integrating sphere equipped in FLS980 spectrophotometer for at least three times.

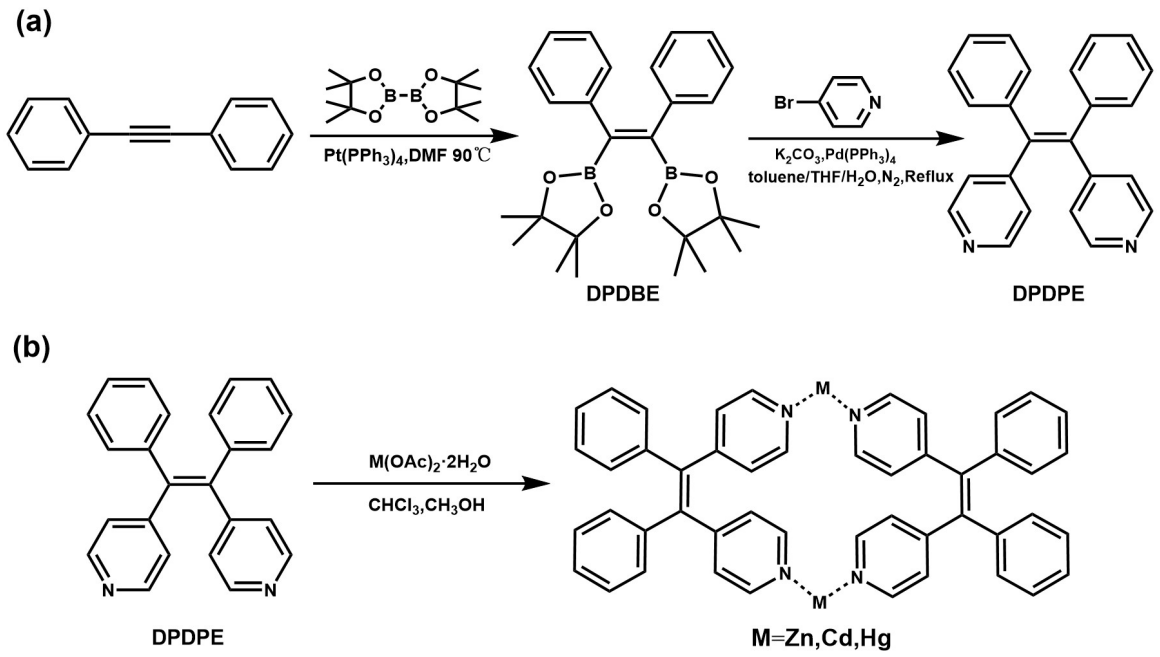
Controllable Patterning Application Based on Stimuli-Responsive Behaviours of Dynamic DPDPE-Metal Complexes. A paper was soaked with a solution of DPDPE at 100 μM, and then the paper was dried naturally. The paper retained white in daylight, but exhibited intense blue emission under UV light. After a pattern of mountain was drawn on the paper using a solution of zinc ion, the pattern with green color appeared while the background is with blue emission under UV light, and the mountain pattern can be easily erased with a solution of EDTA to return its initial state, during which a competitive coordination reaction occurs. After the paper soaked with DPDPE was further treated with a solution of zinc ion, the whole paper turned from blue to bright green color under the UV light. Then a pattern of two leaves was drawn on the paper using trifluoacetic acid, the yellow leaves appeared under the UV light, and then the pattern can be rapidly erased with triethylamine, during which a competition between a coordination reaction and an acid-base reaction takes place. The paper soaked with DPDPE can be treated using sodium sulfide to write a group of letters “ZJNU”, where the letters appeared with quenched fluorescence under the UV light, during which a competition between a coordination reaction and a precipitation reaction takes place and the formed precipitate ZnS can quench the fluorescence of DPDPE. The PL spectra during these controllable patterning demonstrations were recorded and displayed in Figure S11, which well supported the observed changes in emission colors. Therefore, controllable patterning can be achieved based on the distinct emission colors of DPDPE and its zinc complex on the paper by competitive reactions and dynamic

nature of these complexes.

2. Computational Details.

All the calculations were performed with density functional theory (DFT) and time-dependent density functional theory (TDDFT) implemented in Gaussian 09 program package.[1] The equilibrium geometries at S_0 and S_1 state and the normal modes of vibration of the single molecule of DPDPE, Zn-DPDPE, Cd-DPDPE and Hg-DPDPE were computed using density functional theory (DFT) with the hybrid M062X functional at 6-31+G(d,p) level.[2] Excitation energies, absorption maxima and emission maxima of all the four molecules were calculated using M062X functional with 6-31+G(d,p) level based on the optimized structure in acetonitrile with SCRF at S_0 and S_1 state.[3]

3. Supplementary Schemes and Figure



Scheme S1. Synthesis routes of DPDPE and Zn-DPDPE, Cd-DPDPE and Hg-DPDPE.

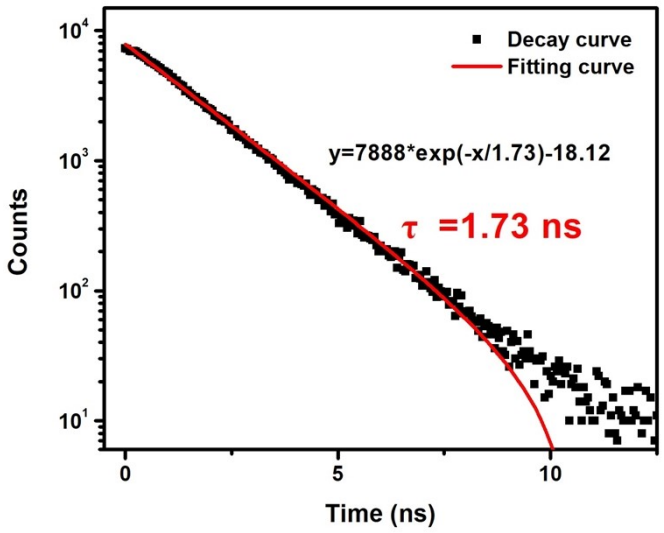


Figure S1. Time-resolved PL decay curve of DPDPE in solid at room temperature.

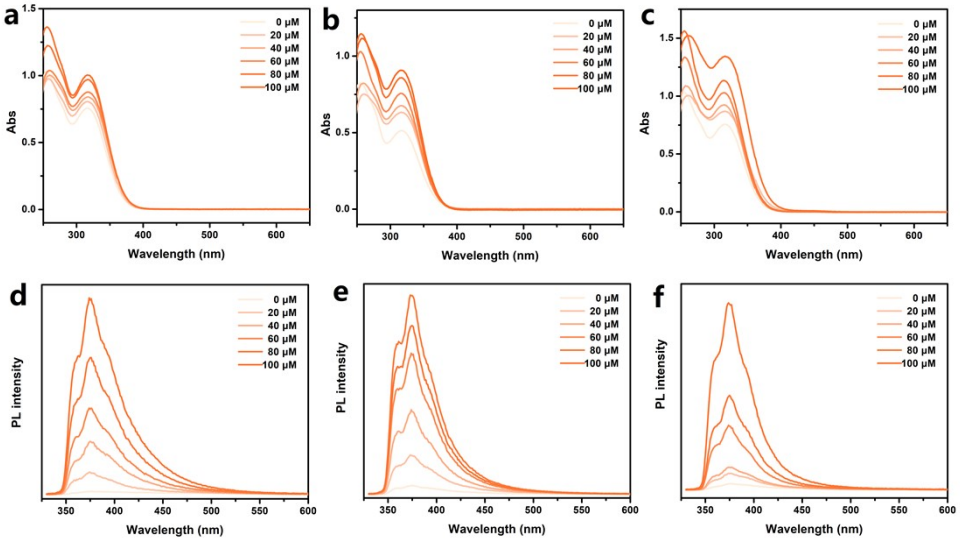


Figure S2. The change of UV-visible spectra of DPDPE (100 μM) in methanol in the presence of different amounts of Zn^{2+} (a), Cd^{2+} (b), and Hg^{2+} (c) respectively, and change of PL spectra of DPDPE (100 μM) in methanol in the presence of different amounts of Zn^{2+} (d), Cd^{2+} (e), and Hg^{2+} (f) respectively.

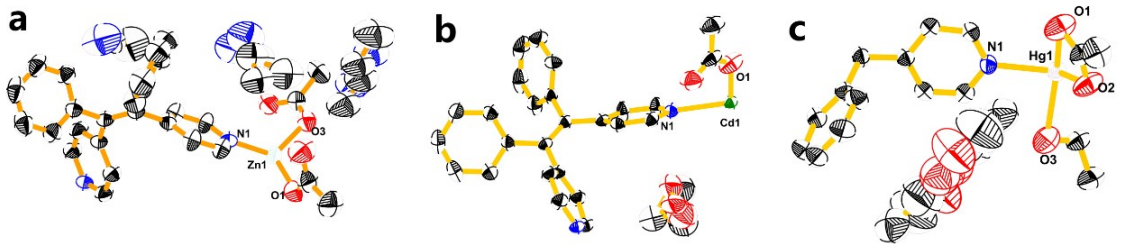


Figure S3.The asymmetric units of Zn-DPDPE (a), Cd-DPDPE (b) and Hg-DPDPE (c).

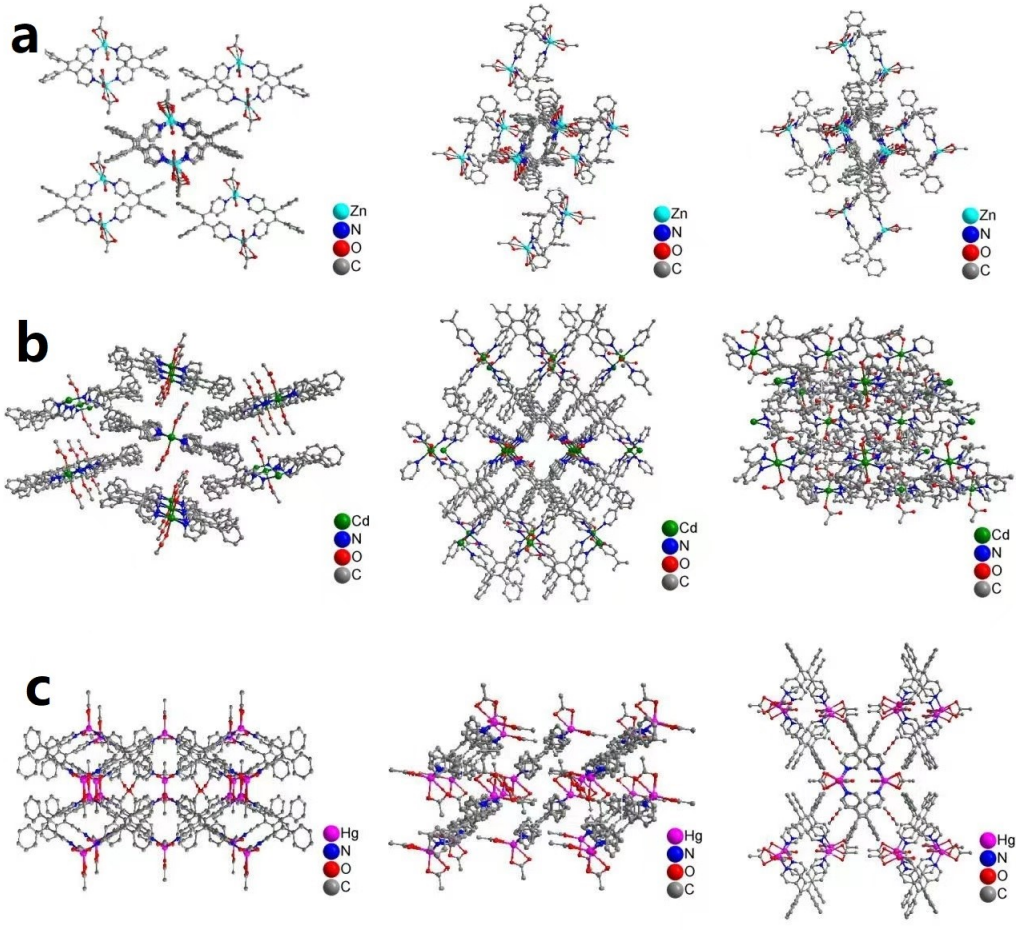


Figure S4. Stacking patterns of Zn-DPDPE (a), Cd-DPDPE (b) and Hg-DPDPE (c) in crystal.

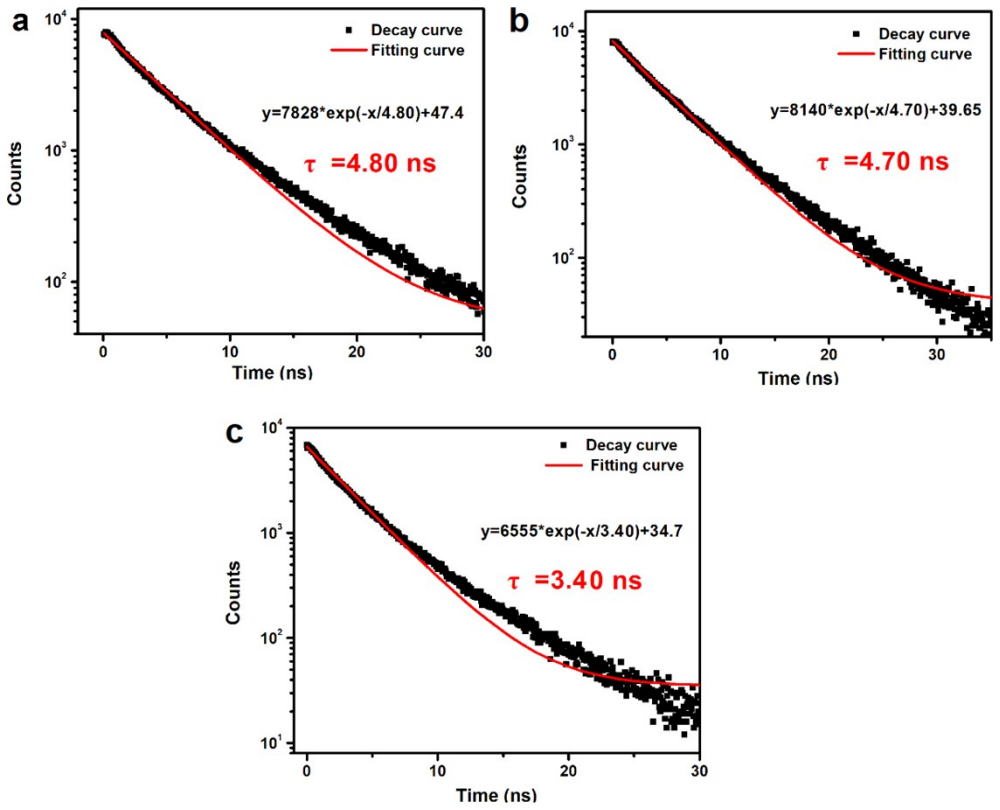


Figure S5. Time-resolved PL decay curves of Zn-DPDPE (a), Cd-DPDPE (b) and Hg-DPDPE (c) in solid at room temperature.

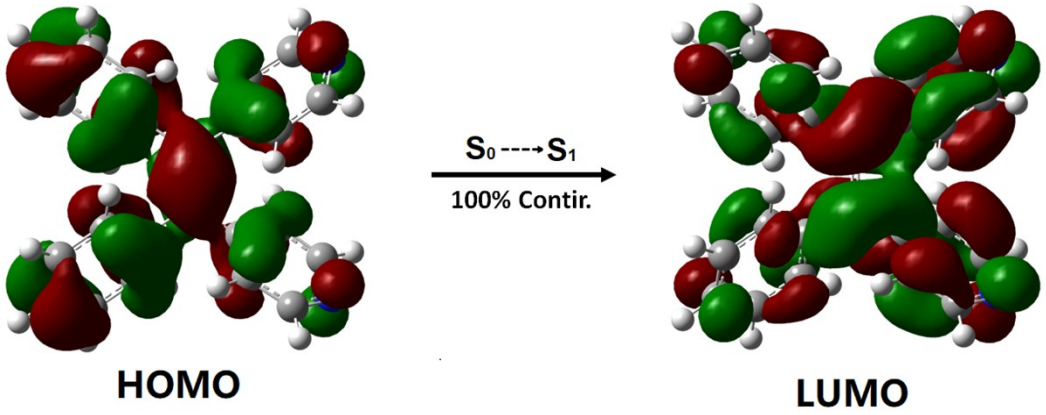


Figure S6. Natural transition orbitals of DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

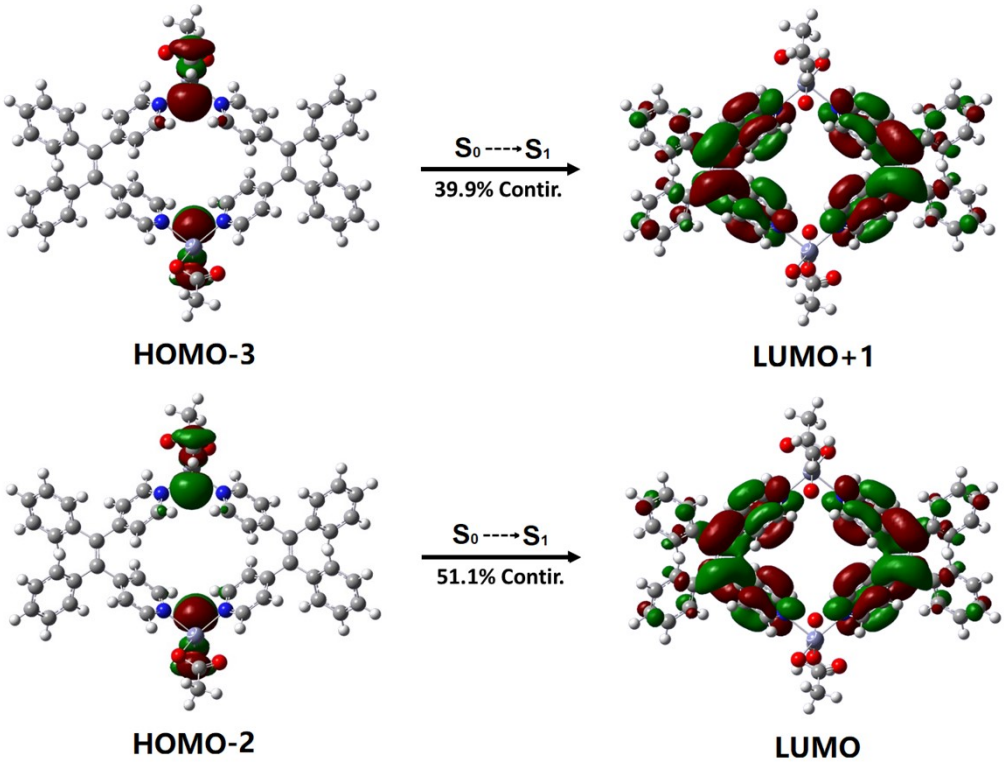


Figure S7. Natural transition orbitals of Zn-DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

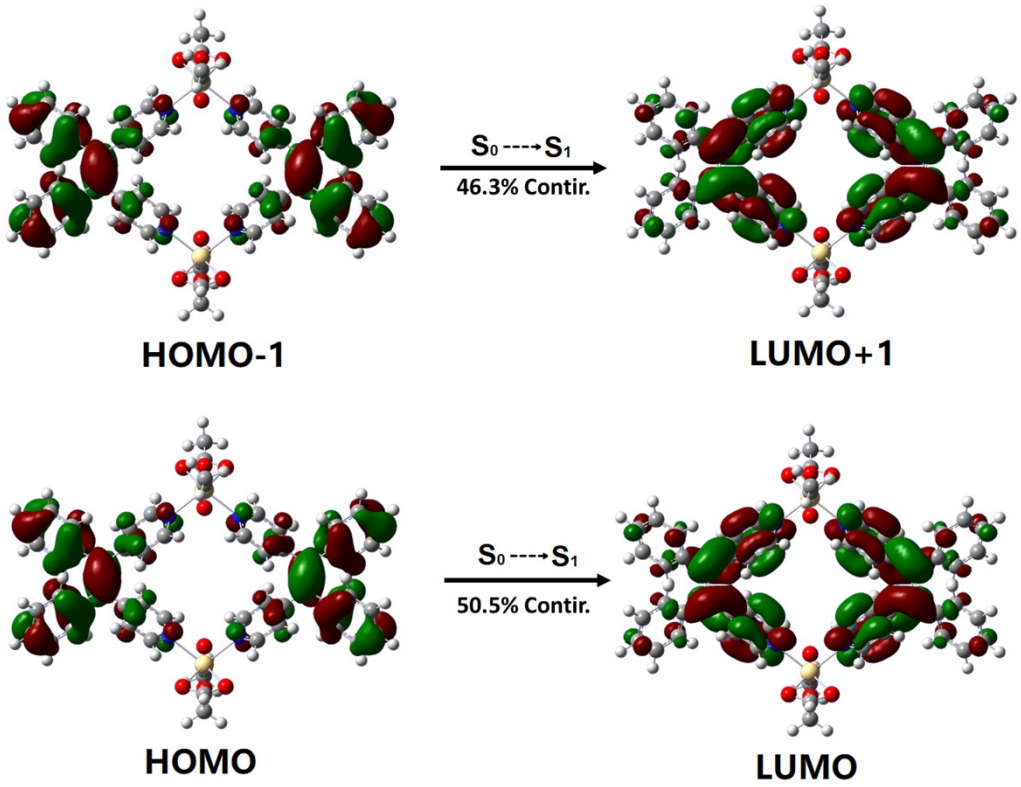


Figure S8. Natural Transition Orbitals of Cd-DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

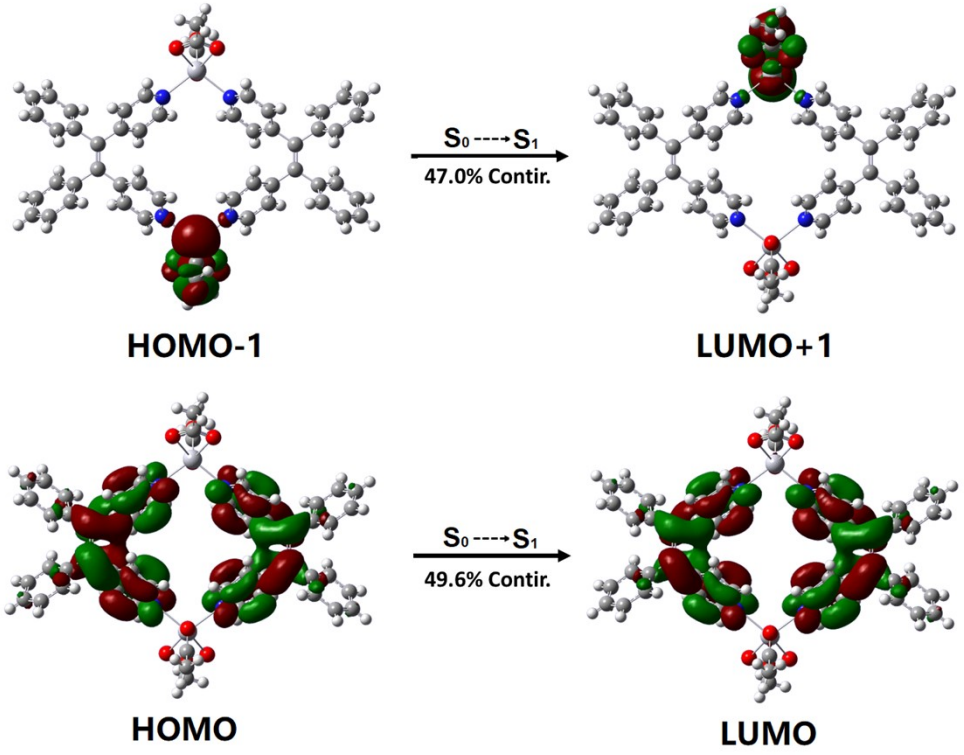


Figure S9. Natural Transition Orbitals of Hg-DPDPE for the transition from S_0 to S_1 with labeled contribution calculated with TDDFT.

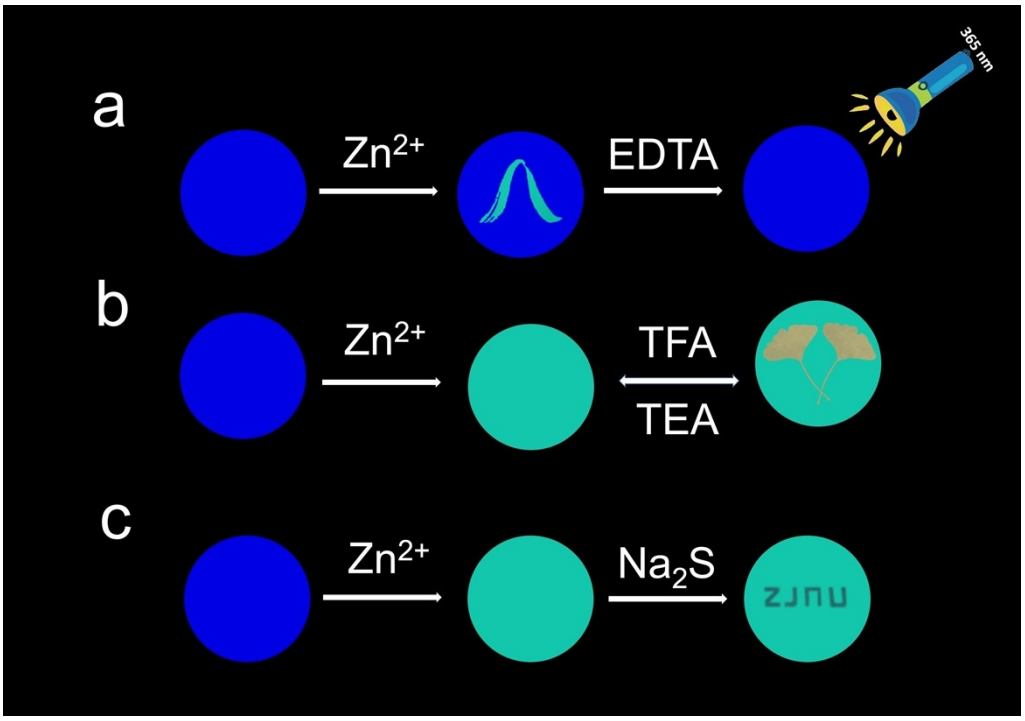


Figure S10. Controllable patterning demonstrations based on stimuli-responsive behaviours of DPDPE and its zinc complex. (a) A green pattern of mountain is written on a paper containing DPDPE with blue emission using zinc ion, and then is erased using EDTA. (b) The blue paper is firstly turned to green using zinc ion, then a yellow pattern of two leaves is drawn on the green paper using trifluoroacetic acid (TFA), and finally erased with triethenylamine (TEA). (c) The blue paper is firstly turned to green using zinc ion, and then a group of letters "ZJNU" is written on the green paper with quenched fluorescence using sodium sulfide.

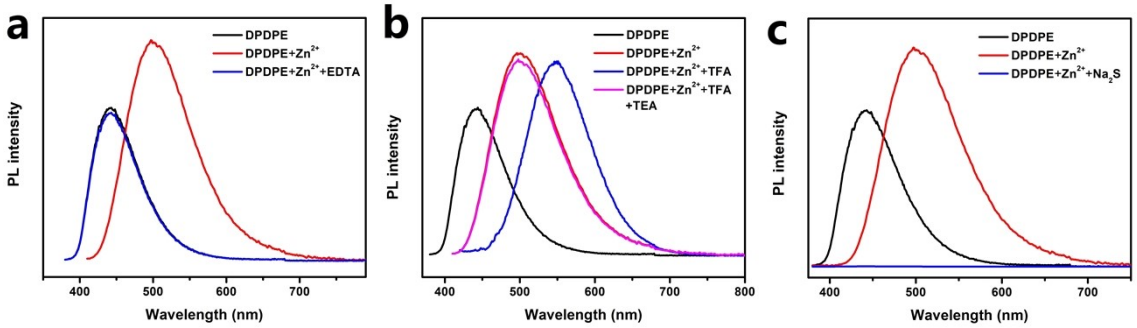


Figure S11. (a) PL spectra of DPDPE on a paper in the presence of different compositions: DPDPE, DPDPE+Zn^{2+}, and DPDPE+Zn^{2+}+EDTA. (b) PL spectra of DPDPE on a paper in the presence of different compositions: DPDPE, DPDPE+Zn^{2+}, DPDPE+Zn^{2+}+TFA, and DPDPE+Zn^{2+}+TFA+TEA. (c) PL spectra of DPDPE on a paper in the presence of different compositions: DPDPE, DPDPE+Zn^{2+}, and DPDPE+Zn^{2+}+Na_2S.

4. Supplementary Tables

Table S1. Crystallographic data for Zn-DPDPE, Cd-DPDPE and Hg-DPDPE.

source	Zn-DPDPE	Cd-DPDPE	Hg-DPDPE
CCDC	2170098	2170097	2170096
Formula	$C_{56}H_{48}N_4O_8Zn_2 \cdot 5(C_2H_3N)$	$C_{52}H_{42}CdN_4O_4 \cdot 2(H_2O) \cdot 2(CH_4O)$	$C_{56}H_{48}Hg_2N_4O_8 \cdot 2(C_4H_8O_2)$
$D_{calc.}$/ g cm^{-3}	1.249	1.345	1.628
μ/mm^{-1}	0.79	0.50	5.14
Formula Weight	1240.99	999.41	1482.37
Shape	block	block	block
Crystal System	triclinic	monoclinic	monoclinic
Space Group	P-1	$P2_1/n$	C2/m
a (Å)	8.1837 (18)	9.8170 (5)	17.1620 (12)
b (Å)	13.428 (3)	9.5192 (5)	21.5993 (15)
c (Å)	15.086 (4)	26.5971 (12)	8.1568 (5)
α	86.984 (8)	90	90
β	85.155 (8)	96.935 (2)	90.374 (2)
γ	89.371 (8)	90	90
wavelength (Å)	0.71073	0.71073	0.71073
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α
min/°	2.9	2.7	2.9
max/°	28.3	28.7	27.5
Measured Refl's.	48270	25598	11516
Ind't Refl's	8402	5647	3537
R_{int}	0.053	0.042	0.043
Parameters	457	344	224
GooF	1.034	1.042	1.077
wR_2 (all data)	0.1524	0.0860	0.0795
wR_2	0.1368	0.0778	0.0728
R_1 (all data)	0.0665	0.0455	0.0518
R_1	0.0482	0.0325	0.0361

Table S2. Photophysical properties of DPDPE, Zn-DPDPE, Cd-DPDPE and Hg-DPDPE in different states.

	λ_{ab} (nm)	λ_{em} (nm)	τ (ns)	Φ (%)	k_r (10^8 s^{-1})	k_{nr} (10^8 s^{-1})
solid powder						
DPDPE	—	443	1.73	12.6	0.73	5.05
Zn-DPDPE	—	500	4.80	70.2	1.46	0.62
Cd-DPDPE	—	494	4.70	65.2	1.39	0.74
Hg-DPDPE	—	472	3.40	68.4	2.0	0.93
In solution at 77 K						
DPDPE	—	449	4.33	—	—	—
Zn-DPDPE	—	502	6.38	—	—	—
Cd-DPDPE	—	497	6.41	—	—	—
Hg-DPDPE	—	487	6.01	—	—	—

Table S3. Compositions of Natural Transition Orbitals of DPDPE, Zn-DPDPE and Cd-DPDPE and Hg-DPDPE for the $S_0 \rightarrow S_1$ transition.

	NTOs	Contribution（%）
DPDPE	HOMO→LUMO	100
Zn-DPDPE	HOMO-3→LUMO+1	39.9
	HOMO-2→LUMO	51.1
Cd-DPDPE	HOMO-1→LUMO+1	46.3
	HOMO→LUMO	50.5
Hg-DPDPE	HOMO-1→LUMO+1	47.0
	HOMO→LUMO	49.6

Table S4. Contribution ratios of different groups to natural transition orbitals of DPDPE, Zn-DPDPE,

Cd-DPDPE and Hg-DPDPE.

Compound	Group	Contribution to HOMO(%)	Contribution to LUMO(%)
DPDPE		100	100
Compound	**Group**	**Contribution to HOMO-2(%)**	**Contribution to LUMO(%)**
Zn-DPDPE	DPDPE	1.85	99.58
	Zn	0.61	0.34
	CH_3COO^-	97.53	0.07
Compound	**Group**	**Contribution to HOMO (%)**	**Contribution to LUMO(%)**
Cd-DPDPE	DPDPE	99.94	99.95
	Cd	0.02	0.3
	CH_3COO^-	0.04	0.04
Compound	**Group**	**Contribution to HOMO (%)**	**Contribution to LUMO(%)**
Hg-DPDPE	DPDPE	0.83	99.53
	Hg	2.47	0.4
	CH_3COO^-	96.71	0.07

Table S5. Experimental and calculated absorption and emission maxima of DPDPE, Zn-DPDPE, Cd-DPDPE and Hg-DPDPE in different states.

	λ_{ab}^{exp} (nm)[a]	λ_{ab}^{cal} (nm)[b]	λ^{exp} (nm)[c]	λ^{cal} (nm)[d]
DPDPE	315	292.35	443	598.50
Zn-DPDPE	316	275.37	500	593.37
Cd-DPDPE	316	327.45	494	579.55
Hg-DPDPE	317	326.98	472	585.92

[a] Experimental absorption maximum in TCM/MeOH. [b] Calculated absorption maximum with TDDFT.
[c] Experimental emission maximum in solid. [d] Calculated emission maximum with TDDFT.

5. NMR and MS Spectra of Compounds

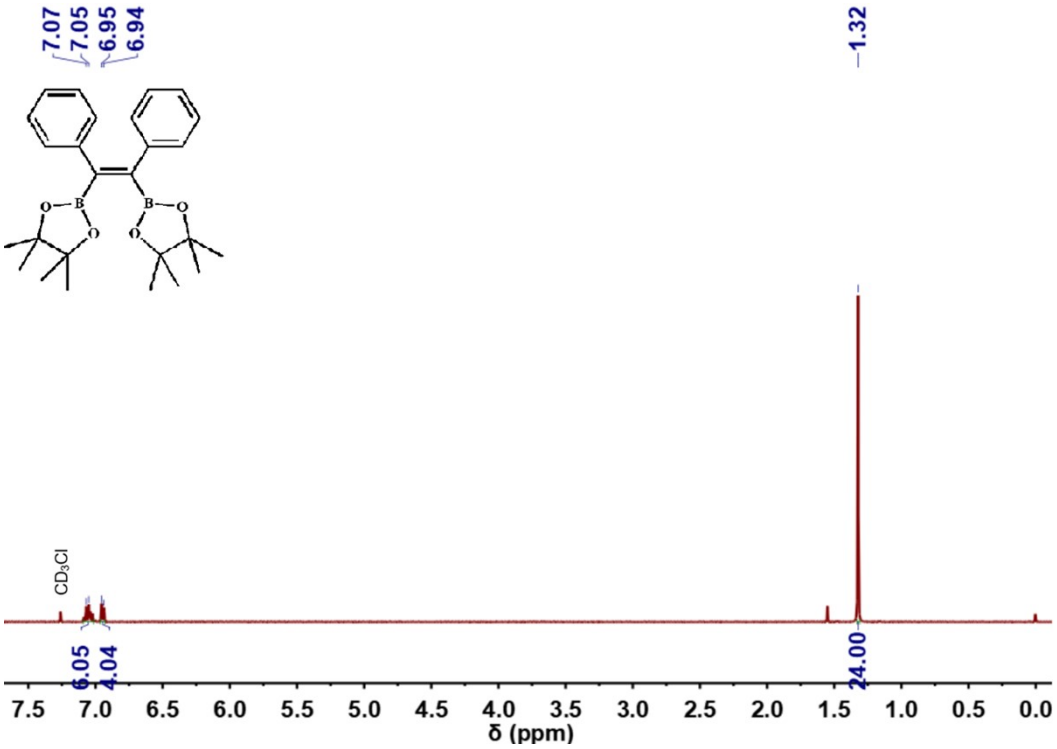


Figure S9. ^{1}H NMR spectrum of DPDBE in $CDCl_3$.

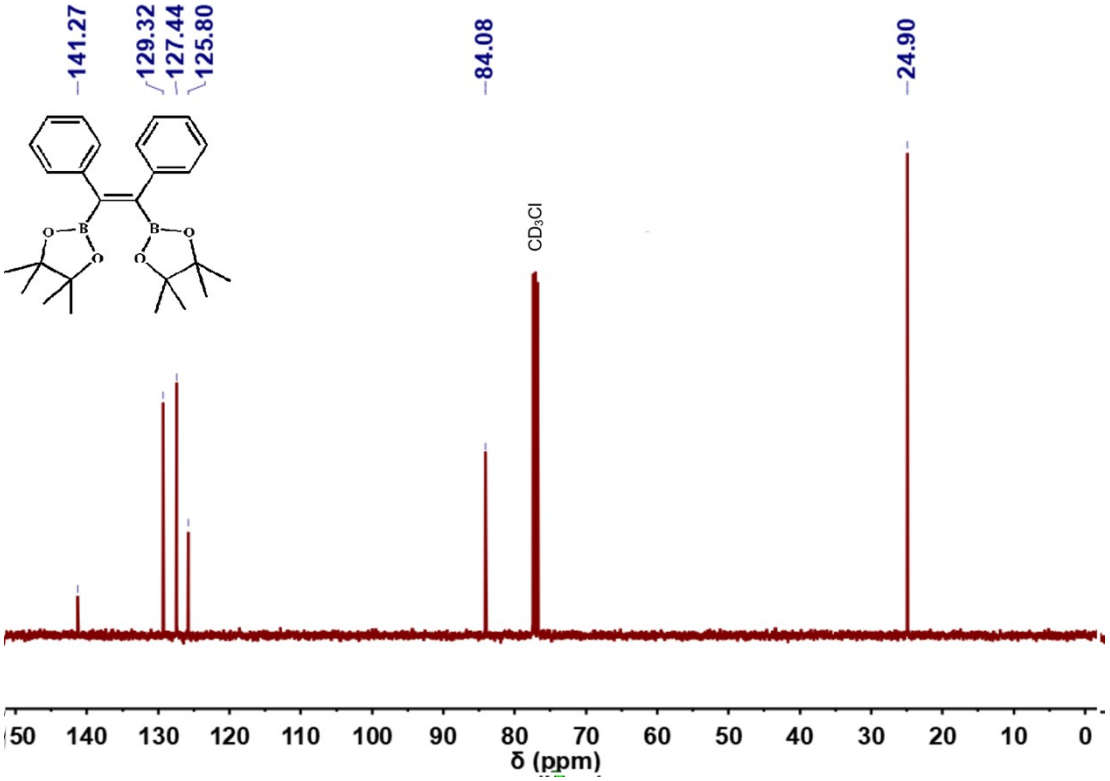


Figure S10. ^{13}C NMR spectrum of DBDBE in $CDCl_3$.

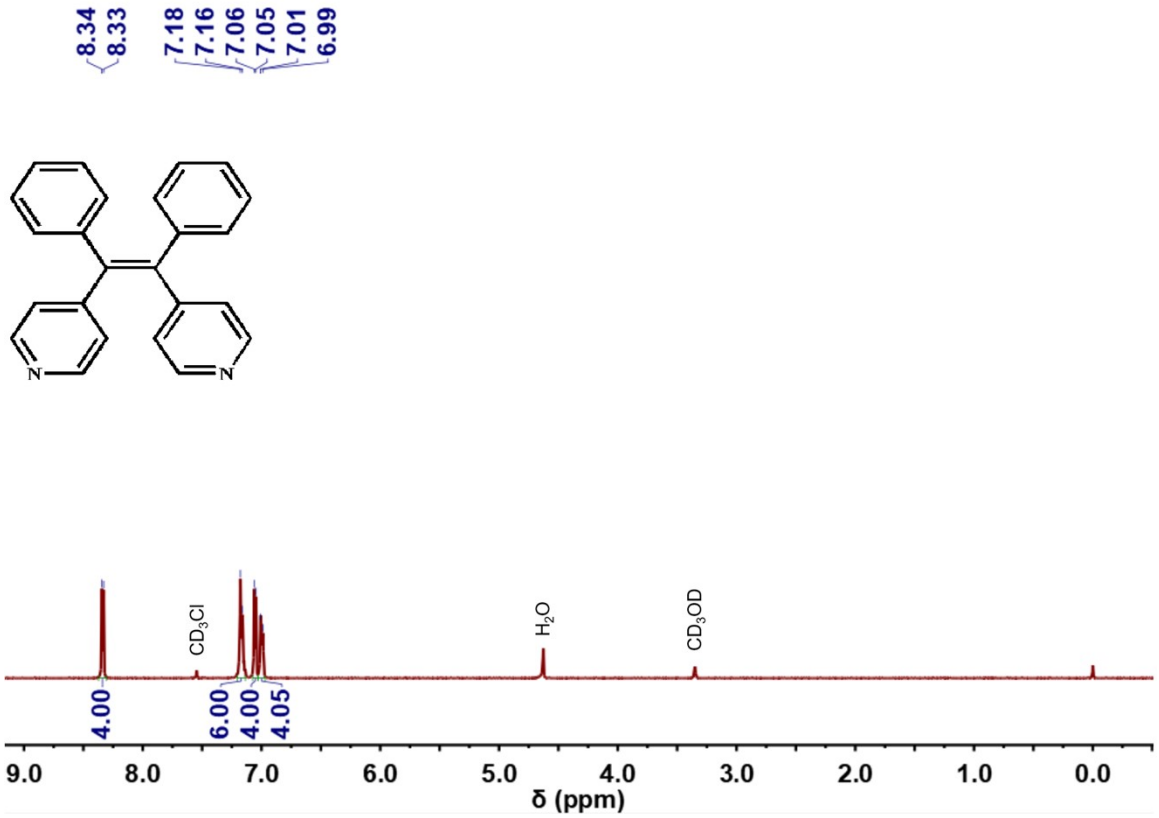


Figure S11. ^{1}H NMR spectrum of DPDPE in $CDCl_3/CD_3OD$ (3:2).

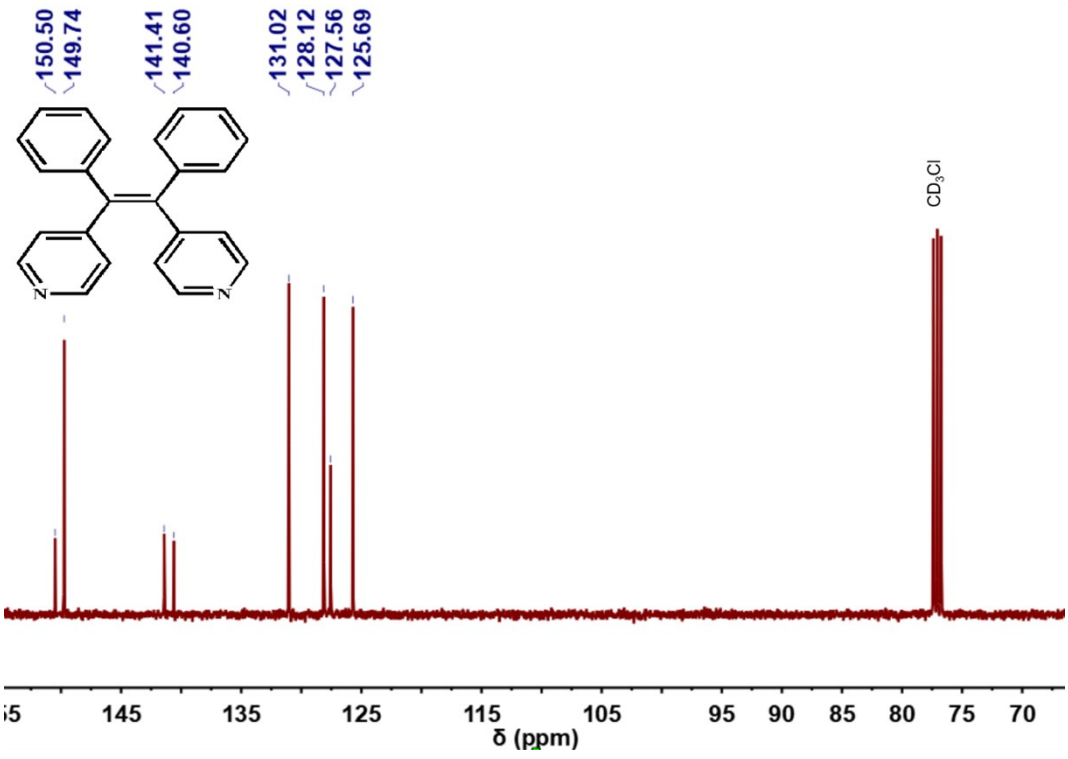


Figure S12. ^{13}C NMR spectrum of DPDPE in $CDCl_3/CD_3OD$ (3:2).

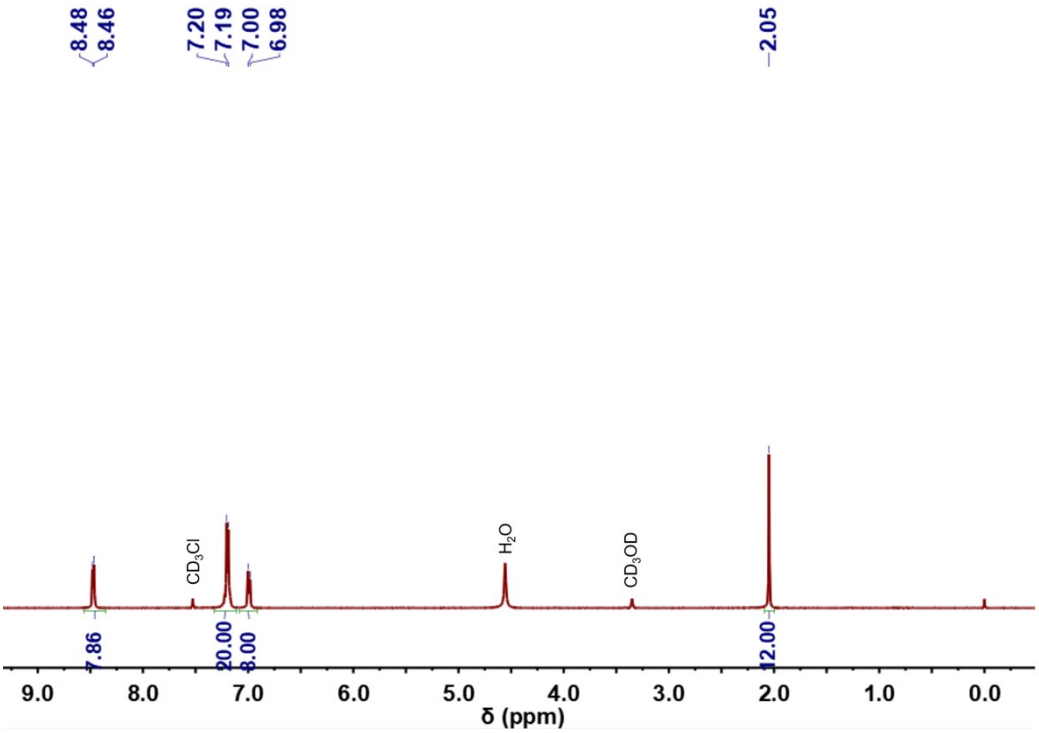


Figure S13. ^{1}H NMR spectrum of Zn-DPDPE in $CDCl_3/CD_3OD$(3:2).

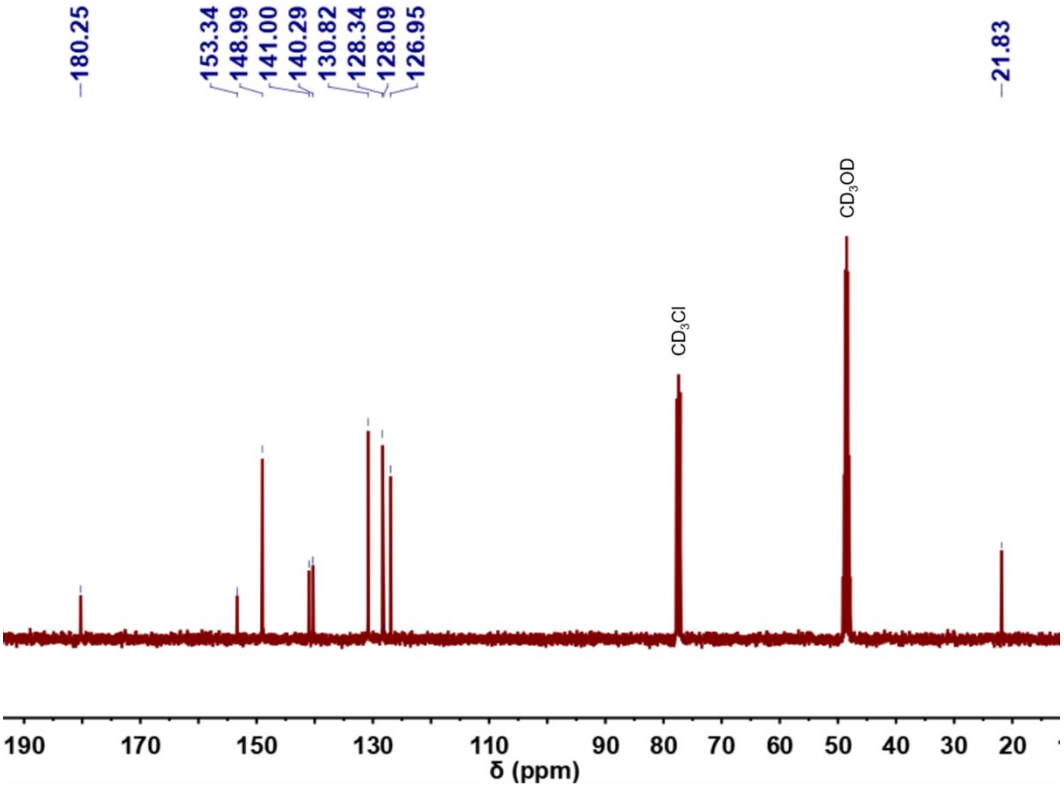


Figure S14. ^{13}C NMR spectrum of Zn-DPDPE in $CDCl_3/CD_3OD$ (3:2).

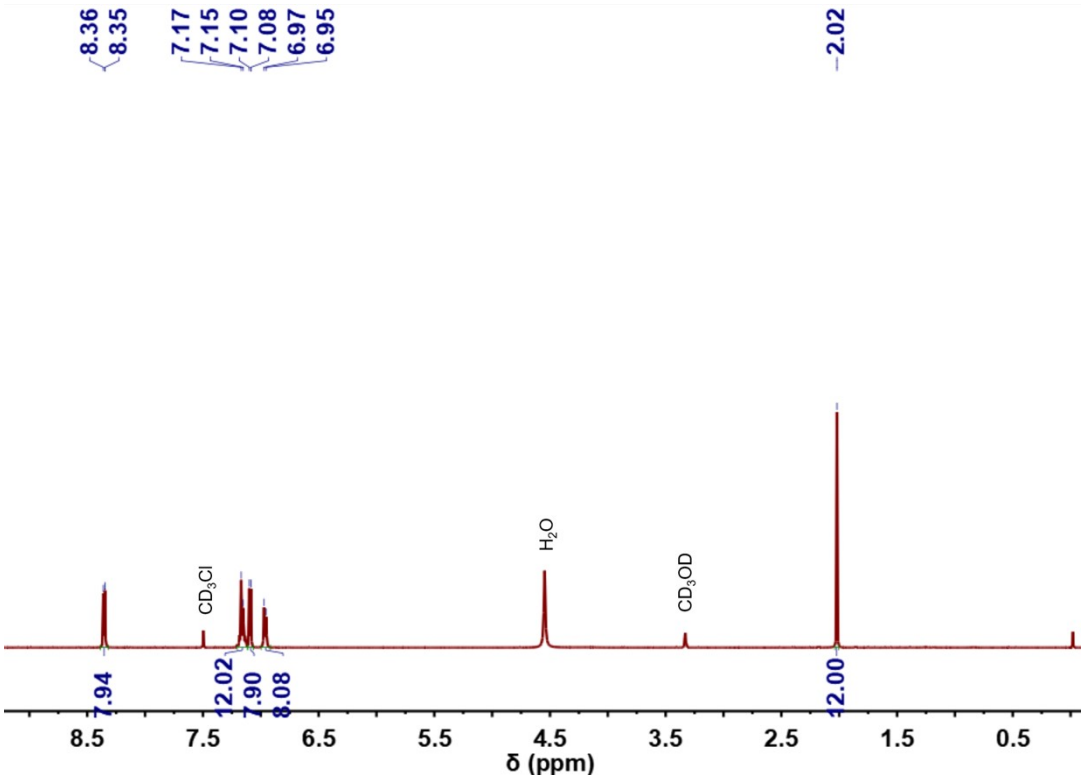


Figure S15. ^{1}H NMR spectrum of Cd-DPDPE in $CDCl_3/CD_3OD$ (3:2).

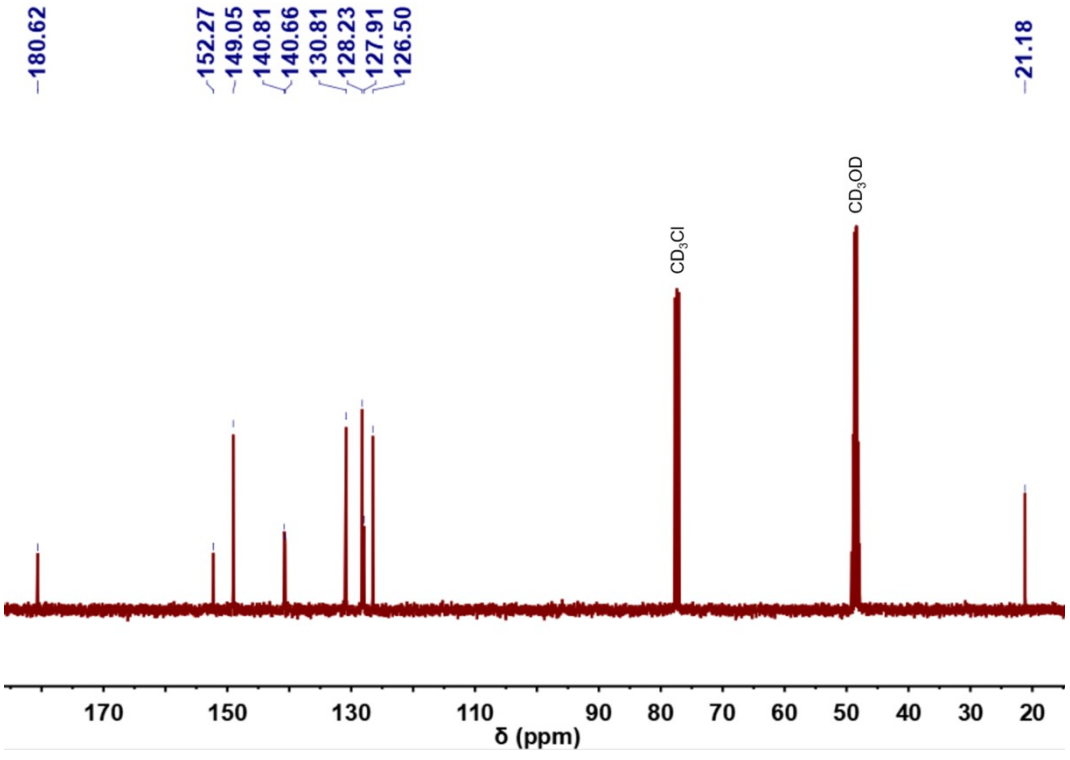


Figure S16. ^{13}C NMR spectrum of Cd-DPDPE in $CDCl_3/CD_3OD$ (3:2).

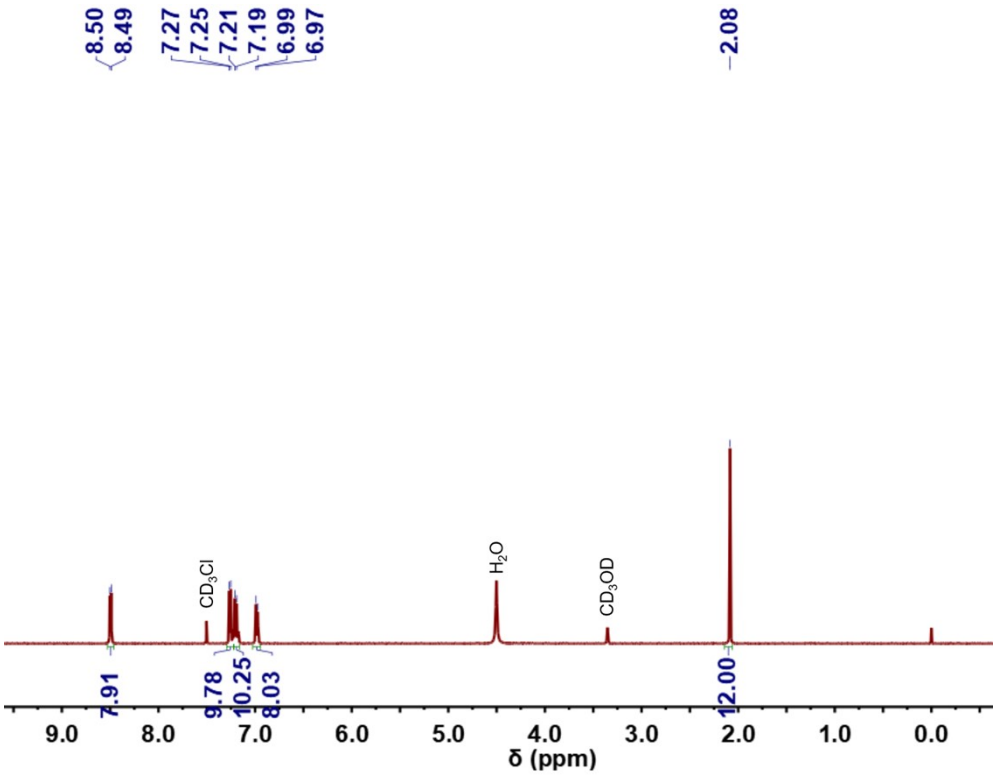


Figure S17. [1]H NMR spectrum of Hg-DPDPE in $CDCl_3/CD_3OD$ (3:2).

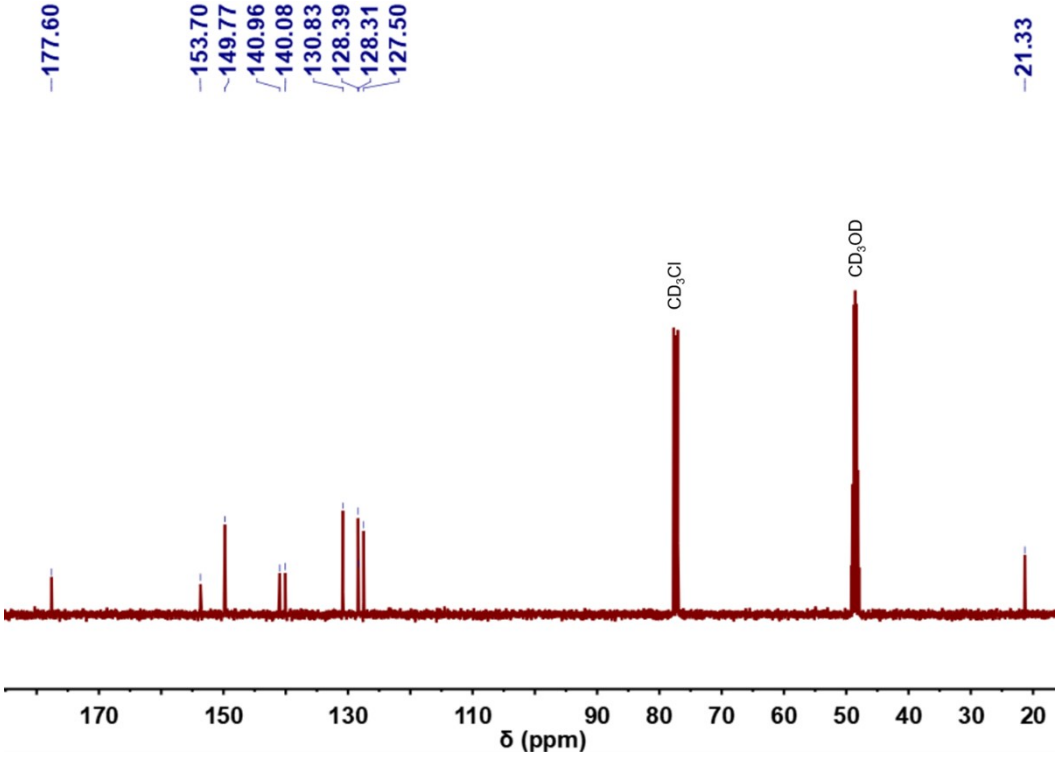


Figure S18. [13]C NMR spectrum of Cd-DPDPE in $CDCl_3/CD_3OD$ (3:2).

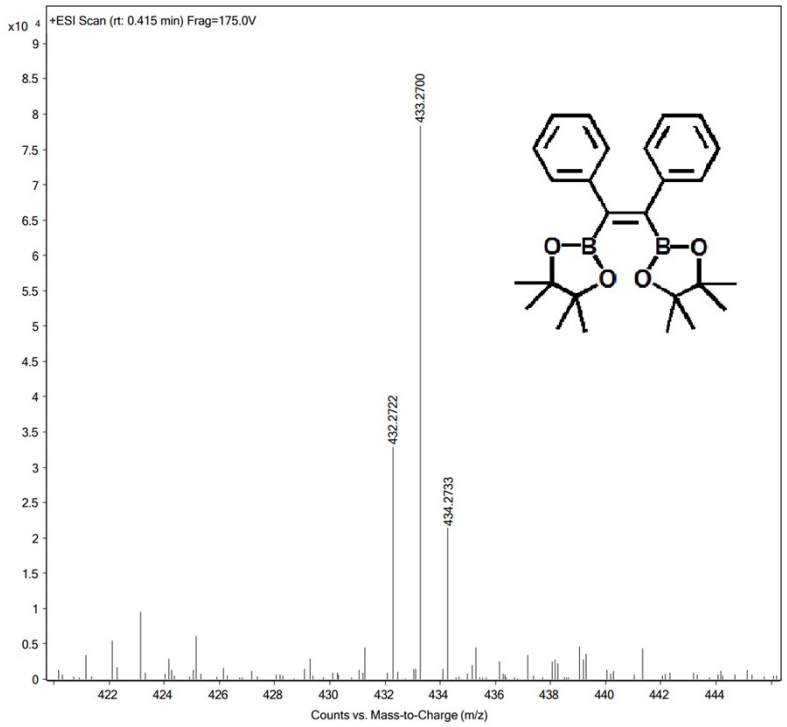


Figure S19. High-resolution mass spectrum of DPDBE.

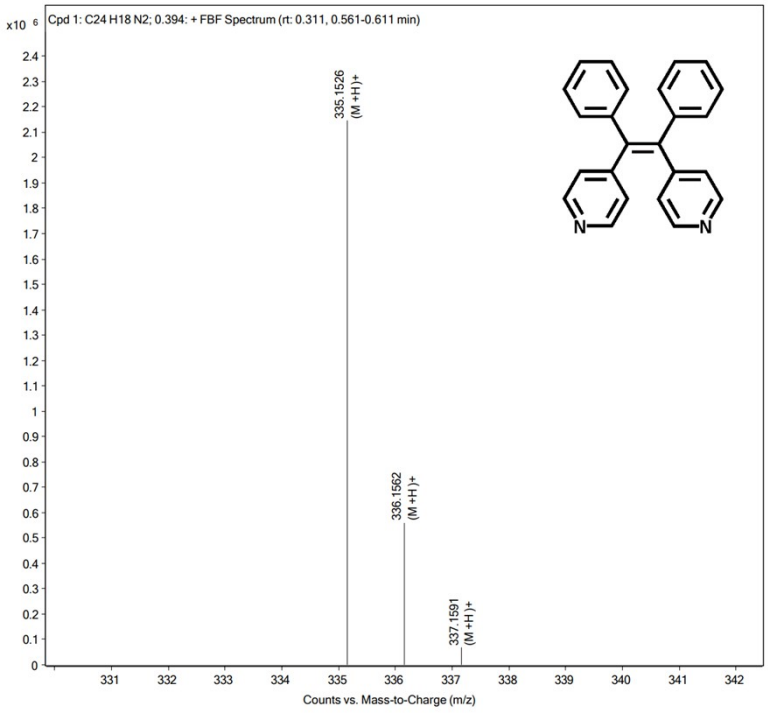


Figure S20. High-resolution mass spectrum of DPDPE.

6. Cartesian Coordinates

DPDPE

N	6.81620000	6.92990000	4.57080000
N	2.71550000	9.80550000	8.35330000
C	4.59770000	11.48980000	1.47180000
H	3.69390000	11.29660000	1.57880000
C	5.06560000	11.96590000	0.25700000
H	4.47260000	12.08810000	-0.44860000
C	6.38780000	12.25630000	0.08550000
H	6.69400000	12.57670000	-0.73260000
C	7.25420000	12.07260000	1.11610000
H	8.15610000	12.27030000	1.00470000
C	6.80230000	11.59620000	2.32640000
H	7.40370000	11.47140000	3.02440000
C	5.46770000	11.30250000	2.51630000
C	5.01680000	10.75590000	3.82720000
C	4.15710000	11.39020000	4.63430000
C	3.56400000	12.71850000	4.30420000
C	2.19960000	12.84210000	4.18630000
H	1.66270000	12.09440000	4.31790000
C	1.60520000	14.06020000	3.87500000
H	0.68150000	14.12160000	3.78930000
C	2.39270000	15.17050000	3.69500000
H	2.00470000	15.98970000	3.48790000
C	3.77450000	15.06180000	3.82480000
H	4.31070000	15.81250000	3.70730000
C	4.34940000	13.85110000	4.12550000
H	5.27370000	13.78870000	4.21050000
C	3.35310000	10.98320000	8.29120000
H	3.47690000	11.46580000	9.07640000
C	3.83020000	11.50580000	7.11240000
H	4.26020000	12.33060000	7.11270000
C	3.67540000	10.80920000	5.92280000
C	3.02600000	9.58470000	5.99730000
H	2.90630000	9.07350000	5.22960000
C	2.55900000	9.12740000	7.21030000
H	2.11470000	8.31060000	7.23570000
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H	7.52150000	7.81030000	6.17180000
C	6.38470000	9.18590000	5.25490000

H	6.50300000	9.85400000	5.89090000
C	5.61650000	9.42160000	4.13830000
C	5.44540000	8.37220000	3.25440000
H	4.92340000	8.48600000	2.49330000
C	6.04670000	7.16120000	3.49940000
H	5.91370000	6.46950000	2.89220000

Zn-DPDPE

Zn	7.63920000	5.07840000	4.84320000
O	7.70340000	4.77670000	2.08890000
O	6.77110000	3.70560000	3.73140000
O	9.57120000	6.20400000	6.40180000
O	9.56440000	4.89590000	4.67780000
N	2.75570000	7.28020000	10.43120000
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C	4.97420000	2.72030000	13.53010000
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C	4.50630000	2.24420000	14.74500000
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H	2.87790000	1.63340000	15.73460000
C	2.31770000	2.13750000	13.88580000
H	1.41580000	1.93980000	13.99730000
C	2.76960000	2.61390000	12.67560000
H	2.16820000	2.73860000	11.97760000
C	4.10420000	2.90760000	12.48570000
C	4.55510000	3.45420000	11.17480000
C	5.41480000	2.81990000	10.36770000
C	6.00790000	1.49160000	10.69780000
C	7.37230000	1.36800000	10.81570000
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H	7.45720000	5.89940000	7.76630000
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C	4.12650000	5.83780000	11.74760000
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C	3.52520000	7.04890000	11.50260000
H	3.65820000	7.74060000	12.10980000
C	10.17520000	5.57300000	5.55840000
C	11.67550000	5.55390000	5.56570000
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C	4.15710000	11.39020000	4.63430000
C	3.56400000	12.71850000	4.30420000
C	2.19960000	12.84210000	4.18630000
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H	6.50300000	9.85400000	5.89090000
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C	5.44540000	8.37220000	3.25440000
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C	2.87670000	11.53380000	13.37280000

H	3.11930000	12.30500000	12.85460000
H	2.13700000	11.75300000	13.94460000
H	3.62520000	11.26130000	13.90930000

Cd-DPDPE

Cd	-1.60570000	4.75960000	13.20130000
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O	-3.10060000	7.69720000	12.01260000
C	-1.86970000	7.76200000	12.07100000
C	-1.16510000	8.95380000	11.44340000
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H	-0.77510000	8.69100000	10.60680000
H	-0.47630000	9.26620000	12.03420000
O	-2.06870000	2.61780000	13.79560000
O	-0.11080000	1.82200000	14.38990000
C	-1.34170000	1.75720000	14.33150000
C	-2.04630000	0.56540000	14.95910000
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H	-2.43630000	0.82820000	15.79570000
H	-2.73510000	0.25300000	14.36830000
N	-0.03040000	5.28130000	14.93110000
N	0.12180000	4.19890000	11.60550000
Cd	8.21130000	4.75960000	13.20130000
N	6.63600000	4.23790000	11.47140000
O	8.67430000	6.90140000	12.60690000
O	6.71640000	7.69720000	12.01260000
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C	2.62680000	3.32510000	8.23440000
C	1.82160000	3.64200000	9.45500000
C	3.97120000	3.19940000	8.24680000
C	1.78730000	3.18510000	7.00880000
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H	2.93870000	4.23000000	5.72660000
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C	0.88650000	3.10330000	11.58940000
H	0.83620000	2.51720000	12.31000000
C	4.61260000	4.64060000	10.23700000
H	3.85410000	5.16570000	10.11660000
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H	5.08980000	0.30590000	4.96490000
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H	6.37220000	1.84830000	3.84840000
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C	4.85470000	6.72060000	15.85000000

H	4.32610000	7.48520000	15.81090000
C	4.47590000	5.74200000	20.60290000
H	3.66690000	5.28920000	20.67590000
C	1.88990000	6.75200000	19.37730000
C	1.08560000	4.57110000	15.16690000
H	1.25710000	3.83150000	14.62950000
C	5.57130000	4.74060000	16.94010000
H	5.55610000	4.15310000	17.66120000
C	-0.23110000	6.34650000	15.70980000
H	-0.98510000	6.86740000	15.55210000
C	5.71900000	6.41590000	14.81310000
H	5.76940000	7.00200000	14.09250000
C	1.99290000	4.87860000	16.16550000
H	2.75150000	4.35350000	16.28590000
C	2.07830000	8.00950000	19.91120000
H	2.64010000	8.61900000	19.49020000
C	6.38370000	4.48640000	15.84600000
H	6.88220000	3.70110000	15.83710000
C	5.31420000	5.81430000	21.70080000
H	5.06730000	5.40510000	22.49880000
C	1.02840000	5.87140000	20.01180000
H	0.86170000	5.03730000	19.63600000
C	6.51200000	6.48830000	21.61860000
H	7.07630000	6.53410000	22.35660000
C	6.03120000	7.00140000	19.33320000
H	6.29300000	7.39840000	18.53380000
C	1.41750000	8.35600000	21.09010000
H	1.51580000	9.21330000	21.43760000
C	0.62560000	7.44590000	21.74140000
H	0.23340000	7.67090000	22.55410000
C	6.86630000	7.09090000	20.44140000
H	7.66630000	7.56160000	20.38300000
C	0.41280000	6.22650000	21.20680000
H	-0.14610000	5.62120000	21.63820000
O	7.74830000	2.61780000	13.79560000
O	9.70620000	1.82200000	14.38990000
C	8.47530000	1.75720000	14.33150000
C	7.77070000	0.56540000	14.95910000
H	8.40650000	-0.13870000	15.10970000
H	7.38070000	0.82820000	15.79570000
H	7.08190000	0.25300000	14.36830000

Hg-DPDPE

Hg	11.93740000	10.79960000	5.06400000
N	10.87750000	8.97880000	6.01310000
O	12.15290000	10.79960000	2.82380000
O	10.05480000	10.79960000	3.22350000
C	9.02500000	5.50350000	7.70560000
C	8.89730000	7.73470000	6.48940000
H	7.97120000	7.66960000	6.42960000
C	9.62930000	6.74330000	7.13950000
C	9.63780000	4.25070000	7.15990000
O	14.05350000	11.89040000	5.59300000
C	9.55480000	8.81250000	5.93560000
H	9.05380000	9.45500000	5.48740000
C	10.99360000	10.79960000	2.43070000
C	11.57540000	8.05220000	6.63540000
H	12.49680000	8.15490000	6.70450000
C	14.64820000	10.79960000	5.71290000
C	10.98820000	6.92910000	7.18930000
H	11.52280000	6.29050000	7.60320000
C	10.23670000	3.30900000	7.95520000
H	10.24760000	3.41370000	8.87940000
C	16.11240000	10.79960000	5.93800000
H	16.54590000	11.25820000	5.21190000
H	16.42970000	9.89460000	5.97650000
H	16.31040000	11.24620000	6.76170000
C	10.22010000	2.90290000	5.24390000
H	10.19450000	2.76520000	4.32460000
C	9.62270000	4.06280000	5.78630000
H	9.22370000	4.69060000	5.22890000
C	10.81910000	1.99580000	6.02450000
H	11.22400000	1.24710000	5.65090000
C	10.83100000	2.18370000	7.35970000
H	11.24450000	1.55130000	7.90150000
C	10.73730000	10.79960000	0.93310000
H	10.47040000	11.67860000	0.65390000
H	10.03970000	10.17300000	0.72770000
H	11.54010000	10.54740000	0.47070000
N	6.17800000	8.97880000	10.30020000
C	8.03050000	5.50350000	8.60770000
C	8.15820000	7.73470000	9.82380000

H	9.08440000	7.66960000	9.88370000
C	7.42620000	6.74330000	9.17380000
C	7.41770000	4.25070000	9.15340000
C	7.50070000	8.81250000	10.37770000
H	8.00170000	9.45500000	10.82580000
C	5.48020000	8.05220000	9.67780000
H	4.55870000	8.15490000	9.60880000
C	6.06730000	6.92910000	9.12400000
H	5.53270000	6.29050000	8.71000000
C	6.81880000	3.30900000	8.35810000
H	6.80800000	3.41370000	7.43380000
C	6.83540000	2.90290000	11.06940000
H	6.86100000	2.76520000	11.98870000
C	7.43280000	4.06280000	10.52690000
H	7.83180000	4.69060000	11.08430000
C	6.23640000	1.99580000	10.28880000
H	5.83150000	1.24710000	10.66240000
C	6.22460000	2.18370000	8.95350000
H	5.81100000	1.55130000	8.41180000
H	10.47040000	9.92070000	0.65390000
H	10.03970000	11.42630000	0.72770000
H	11.54010000	11.05190000	0.47070000
O	14.05350000	9.70890000	5.59300000
H	16.54590000	10.34110000	5.21190000
H	16.42970000	11.70470000	5.97650000
H	16.31040000	10.35310000	6.76170000
Hg	5.11810000	10.79960000	11.24920000
O	4.90270000	10.79960000	13.48940000
O	7.00070000	10.79960000	13.08980000
O	3.00200000	11.89040000	10.72030000
C	6.06200000	10.79960000	13.88260000
C	2.40730000	10.79960000	10.60040000
C	0.94310000	10.79960000	10.37520000
H	0.50960000	11.25820000	11.10140000
H	0.62580000	9.89460000	10.33680000
H	0.74510000	11.24620000	9.55150000
C	6.31820000	10.79970000	15.38010000
H	6.58520000	11.67860000	15.65930000
H	7.01580000	10.17300000	15.58560000
H	5.51540000	10.54740000	15.84260000
H	6.58520000	9.92070000	15.65930000

H	7.01580000	11.42630000	15.58560000
H	5.51540000	11.05190000	15.84260000
O	3.00200000	9.70890000	10.72030000
H	0.50960000	10.34110000	11.10140000
H	0.62580000	11.70470000	10.33680000
H	0.74510000	10.35310000	9.55150000
N	6.17800000	12.62050000	10.30020000
C	8.03050000	16.09580000	8.60770000
C	8.15820000	13.86460000	9.82380000
H	9.08440000	13.92970000	9.88370000
C	7.42620000	14.85600000	9.17380000
C	7.41770000	17.34860000	9.15340000
C	7.50070000	12.78680000	10.37770000
H	8.00170000	12.14430000	10.82580000
C	5.48020000	13.54710000	9.67780000
H	4.55870000	13.44440000	9.60880000
C	6.06730000	14.67020000	9.12400000
H	5.53270000	15.30880000	8.71000000
C	6.81880000	18.29030000	8.35810000
H	6.80800000	18.18560000	7.43380000
C	6.83540000	18.69640000	11.06940000
H	6.86100000	18.83410000	11.98870000
C	7.43280000	17.53650000	10.52690000
H	7.83180000	16.90870000	11.08430000
C	6.23640000	19.60350000	10.28880000
H	5.83150000	20.35220000	10.66240000
C	6.22460000	19.41560000	8.95350000
H	5.81100000	20.04800000	8.41180000
N	10.87750000	12.62050000	6.01310000
C	9.02500000	16.09580000	7.70560000
C	8.89730000	13.86460000	6.48940000
H	7.97120000	13.92970000	6.42960000
C	9.62930000	14.85600000	7.13950000
C	9.63780000	17.34860000	7.15990000
C	9.55480000	12.78680000	5.93560000
H	9.05380000	12.14430000	5.48740000
C	11.57540000	13.54710000	6.63540000
H	12.49680000	13.44440000	6.70450000
C	10.98820000	14.67020000	7.18930000
H	11.52280000	15.30880000	7.60320000
C	10.23670000	18.29030000	7.95520000

H	10.24760000	18.18560000	8.87940000
C	10.22010000	18.69640000	5.24390000
H	10.19450000	18.83410000	4.32460000
C	9.62270000	17.53650000	5.78630000
H	9.22370000	16.90870000	5.22890000
C	10.81910000	19.60350000	6.02450000
H	11.22400000	20.35220000	5.65090000
C	10.83100000	19.41560000	7.35970000
H	11.24450000	20.04800000	7.90150000

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