Electronic Supplementary Information *for*

Halogenated Tetraphenylethene with Enhanced Aggregation-Induced Emission: Anomalous Anti-Heavy-Atom Effect and Self-Reversible Mechanochromism

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1. Experimental Section

Synthesized of 1,1,2,2-Tetraphenylethene (TPE). 1,1,2,2-Tetraphenylethylene was synthesized and purified according to the previous procedure in the literature.[7] ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.10(m, J = 12 Hz, 12H), 7.03(m, J = 6 Hz, 8H). ^{13}C NMR (150 MHz, $CDCl_3$) δ(ppm) 143.91, 141.12, 131.52, 127.83, 126.60. MS (ESI) m/z: [M^+] 332.2 (calcd. for $C_{26}H_{20}$, 332.2).

Synthesized of 1,1,2,2-Tetra(4-fluorophenyl)ethene (TFPE). A certain amounts of Zn dust (1.84 g, 28 mmol) and $TiCl_4$ (1.58 mL, 14 mmol) were refluxed for 3 h in 100 mL of dry THF under N_2 atmosphere. A solution of 4,4'-Difluorobenzophenone (1.53 g, 7 mmol) in dry THF (30 mL) was added to the preceding suspension, and then the reaction was refluxed at 80 °C for 8 h. An aqueous solution containing 10% K_2CO_3 (50 mL) was added after the reaction mixture was cooled down to room temperature. The resulting product was extracted with ethyl acetate. The solvent was evaporated under vacuum and the crude product was purified by a silica gel column using pure petroleum ether as the eluent. TFPE was obtained in 90% yield (1.37 g). ^{1}H NMR(600 MHz, $CDCl_3$) δ (ppm) 6.94(d, J = 12 Hz, 8H), 6.81(d, J = 18 Hz, 8H). ^{13}C NMR (150 MHz, $CDCl_3$) δ(ppm) 162.56, 160.92, 139.30, 133.01, 115.23. HRMS (ESI) m/z [$M+Cl^-$] 439.0906 (calcd. for $C_{26}H_{16}F_4$, 404.1188).

Synthesis of 1,1,2,2-Tetra(4-chlorophenyl)ethene (TCPE). The synthesis of TCPE followed the synthesis procedure of TFPE with replacing 4,4'-difluorobenzophenone with 4,4'-dichlorobenzophenone. The crude product was finally purified by column chromatography to give a white solid (Yield 86%). Molecular formula: $C_{26}H_{16}Cl_4$. ^{1}H NMR(600 MHz, $CDCl_3$) δ (ppm) 7.10(d, J = 12 Hz, 8H), 6.90(d, J = 12 Hz, 8H). ^{13}C NMR (150 MHz, $CDCl_3$) δ(ppm) 141.12, 139.56, 132.99, 132.45, 128.33. HRMS (ESI) m/z [$M+Cl^-$] 502.9719 (calcd. for $C_{26}H_{16}Cl_4$, 468.0006).

Synthesis of 1,1,2,2-Tetra(4-Bromophenyl)ethene (TBPE). A similar procedure was applied to synthesis of TBPE using 4,4'-dibromobenzophenone as the initial reactant. A white powder in a yield of 80% was acquired after further purification using column chromatography. Molecular formula: $C_{26}H_{16}Br_4$. ^{1}H NMR(600 MHz, $CDCl_3$) δ (ppm) 7.23(d, J = 6 Hz, 8H), 6.82(d, J = 12 Hz, 8H). ^{13}C NMR (150 MHz, $CDCl_3$) δ(ppm) 141.67, 139.83, 132.96, 131.53, 121.53. HRMS (ESI) m/z: [M+Cl^-] 678.7687 (calcd. for $C_{26}H_{16}Br_4$, 643.7985).

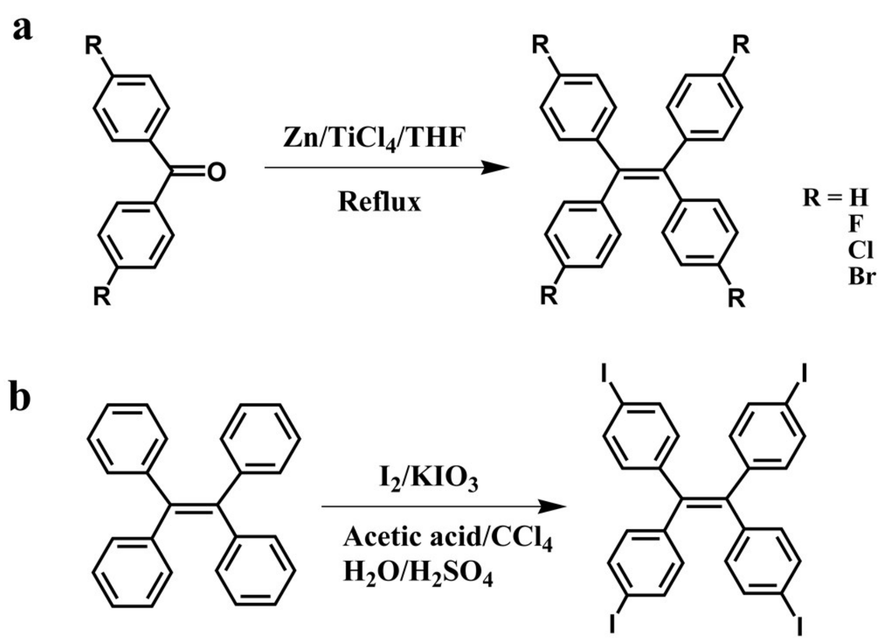
Synthesis of 1,1,2,2-Tetra(4-Iodophenyl)ethene (TIPE). A given amount of tetraphenylethylene (1.028 g, 3.1 mmol) was first dissolved in 20 ml THF, and then 1.718 g of iodate (9.8 mmol), 1.914 g of iodine (7.5 mmol), 4 mL of water and 80 mL of acetic acid were added. The resulting mixture was stirred at 80 ℃ for 12 h. Then the mixture was cooled to room temperature and iced water was added. The product was extracted with dichloromethane, and washed with sodium thiosulfate. The dichloromethane solution was dried with anhydrous magnesium sulfate, and further concentrated to solid under vacuum. The obtained crude product was recrystallized by ethyl acetate and petroleum ether. Yield: 0.68 g (66%). ^{1}H NMR(600 MHz, $CDCl_3$) δ (ppm) 7.44(d, J = 6 Hz, 8H), 6.69(d, J = 12 Hz, 8H). ^{13}C NMR (150 MHz, $CDCl_3$) δ(ppm) 142.26, 140.00, 137.68, 133.16, 93.24.

Characterization of Fluorescence Properties of All Samples. 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 fluorescence quantum yields of all samples were determined using an integrating sphere equipped in FLS980 spectrophotometer for at least three times.

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 ground state equilibrium geometries and the normal modes of vibration of the TPE derivatives were computed using density functional theory (DFT) with the hybrid B3LYP functional.[2] The basis set 6-31+G(d,p) level was used for C, H, F and Cl, and the basis set LanL2DZ was used for Br and I. NBO calculations were performed at the same level, and the visualization of HOMOs and LUMOs were conducted with Gview program. Excited state calculations were run at PBE0 functional with time-dependent density functional theory (TD-DFT).[3,4] The basis set 6-31+G(d,p) level was used for C, H, F and Cl, and the basis set LanL2DZ was used for Br and I.

3. Supplementary Schemes and Figures



Scheme S1. (a) Synthesis routes of TPE, TFPE, TCPE and TBPE, and (b) synthesis route of TIPE.

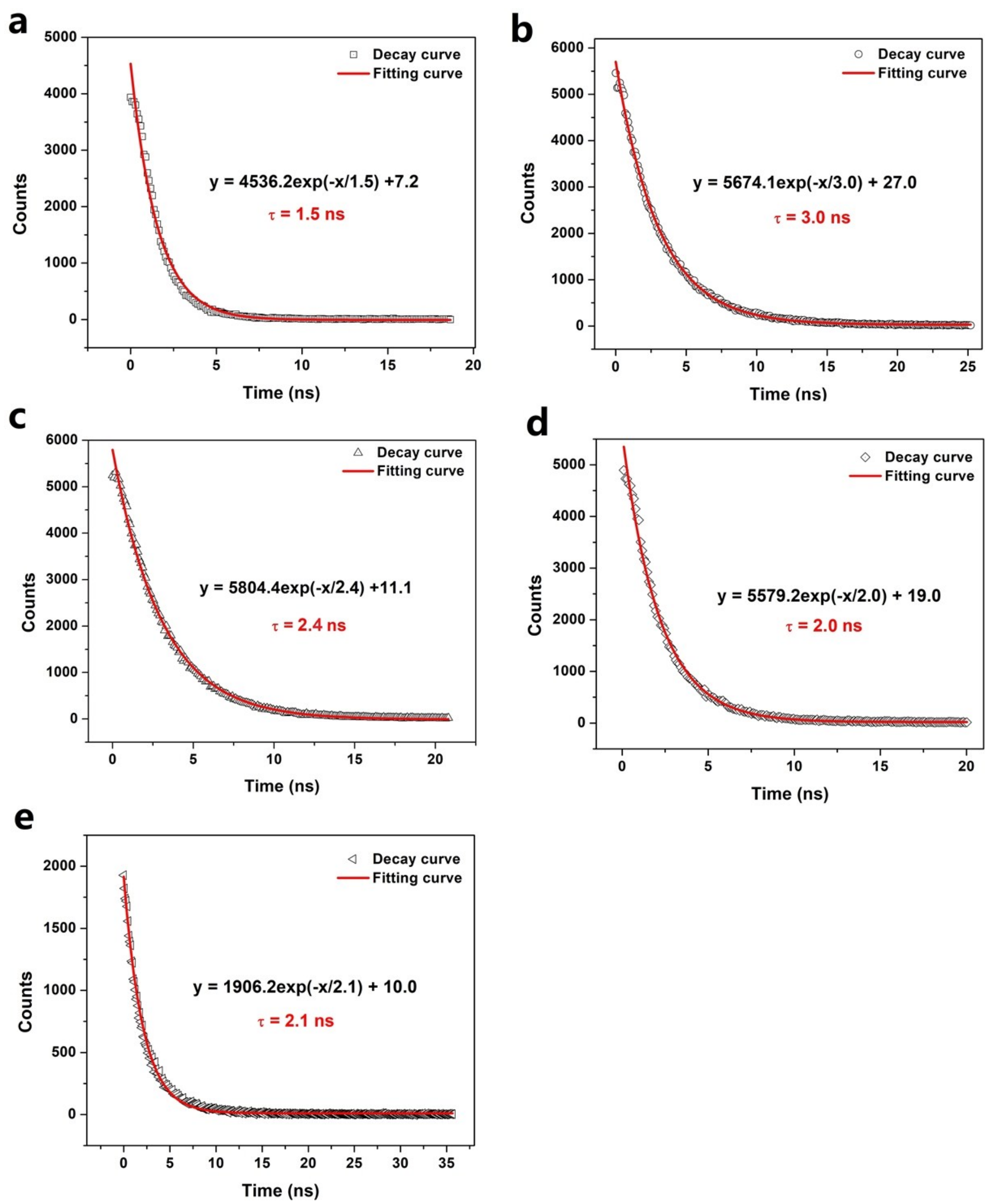


Figure S1. Time-resolved fluorescence decay curves of TPE (a), TFPE (b), TCPE (c), TBPE (d) and TIPE (e) in solid state.

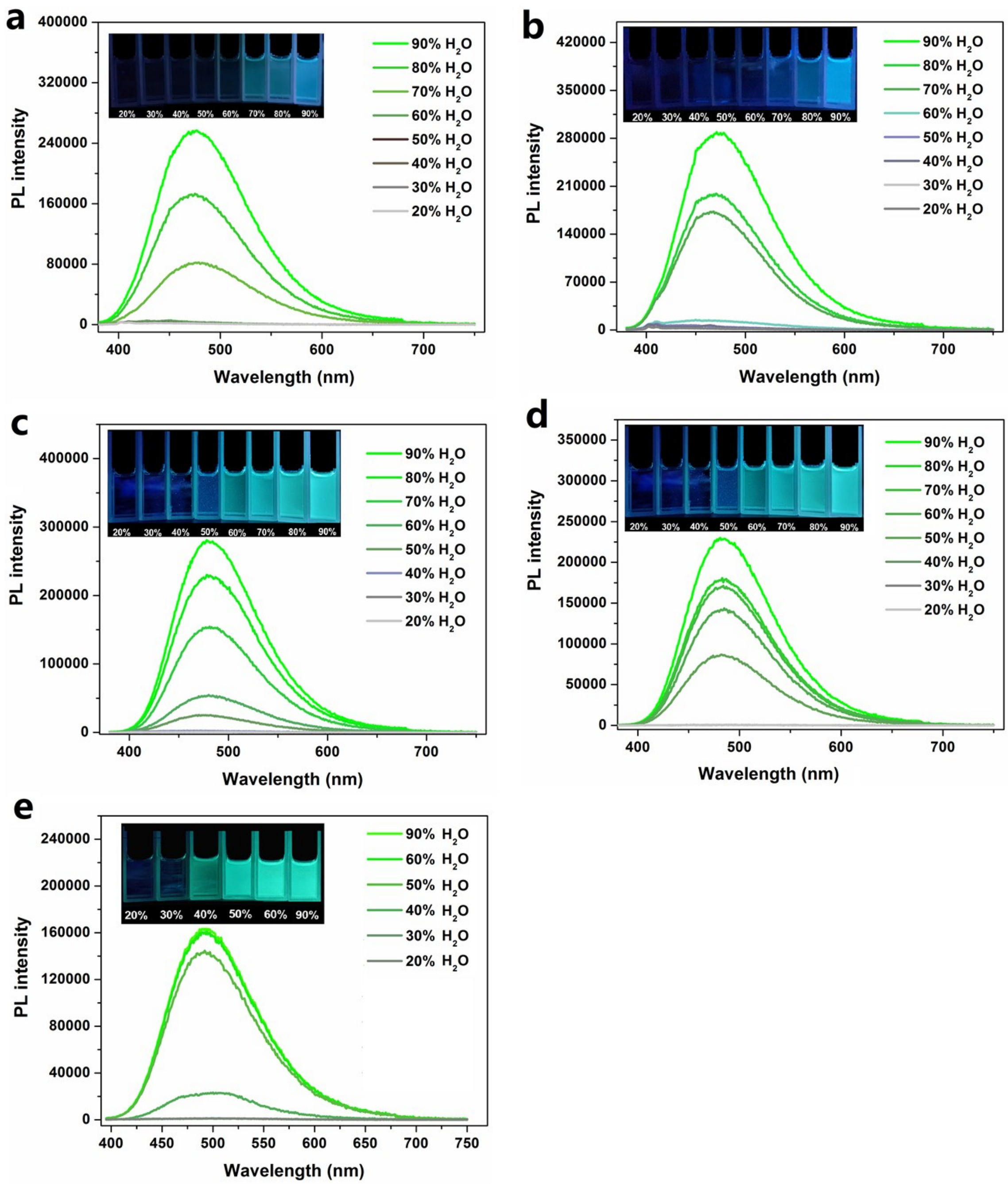


Figure S2. Aggregation-induced emission behaviors of TPE (a), TFPE (b), TCPE (c), TBPE (d) and TIPE (e) using water as the poor solvent.

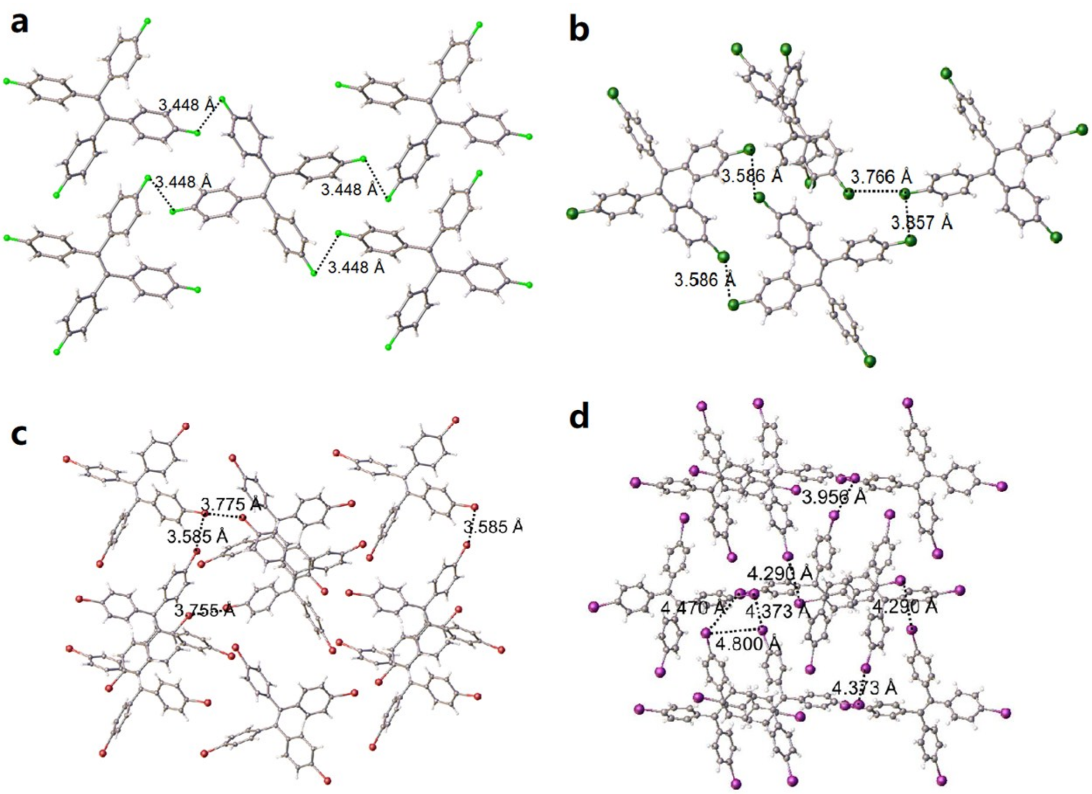


Figure S3. Crystal structures and molecular packing with labeled distances between halogen-halogen atoms of TFPE (a), TCPE (b), TBPE (c) and TIPE (d). Carbon, hydrogen, fluorine, chlorine, bromine and iodine atoms are represented in gray, white, green, olive, red and purple respectively.

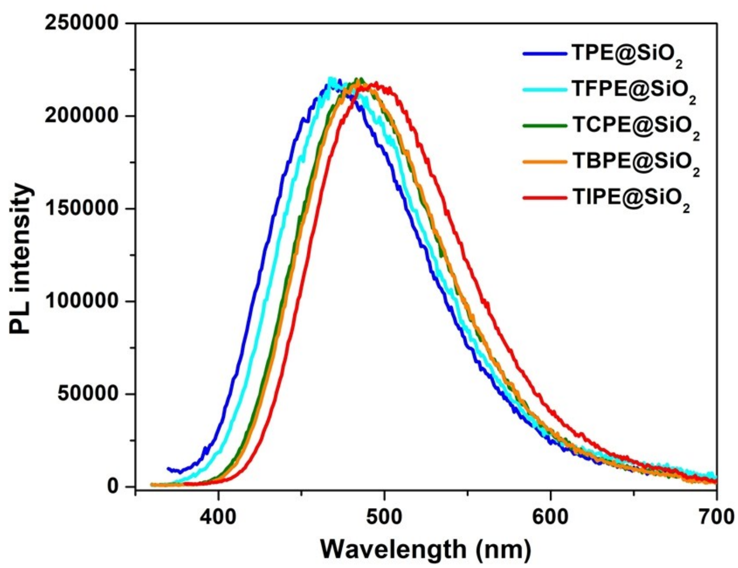


Figure S4. PL spectra of TPE, TFPE, TCPE, TBPE and TIPE dispersed in SiO_2.

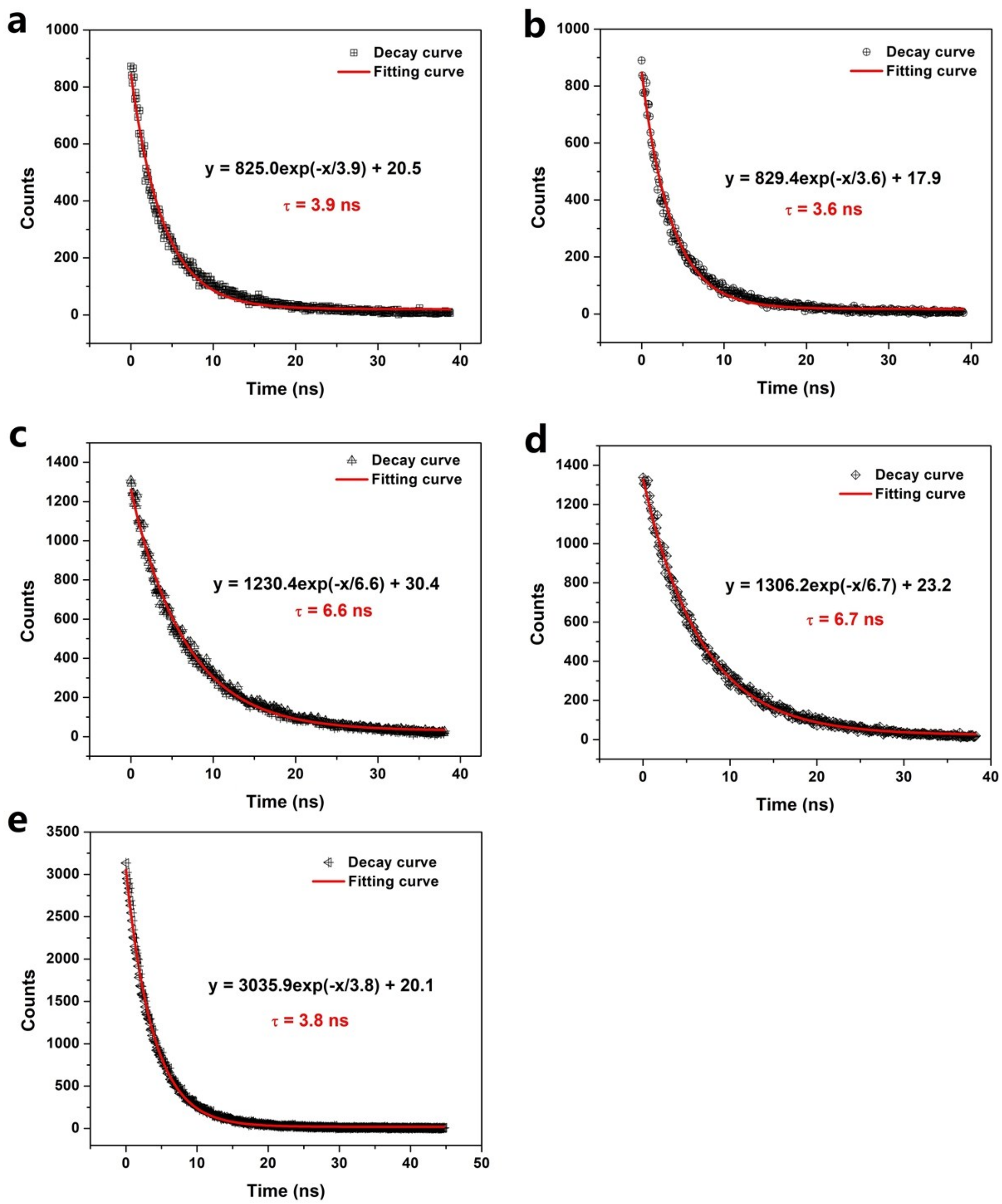


Figure S5. Time-resolved fluorescence decay curves of TPE (a), TFPE (b), TCPE (c), TBPE (d) and TIPE (e) dispersed in SiO_2.

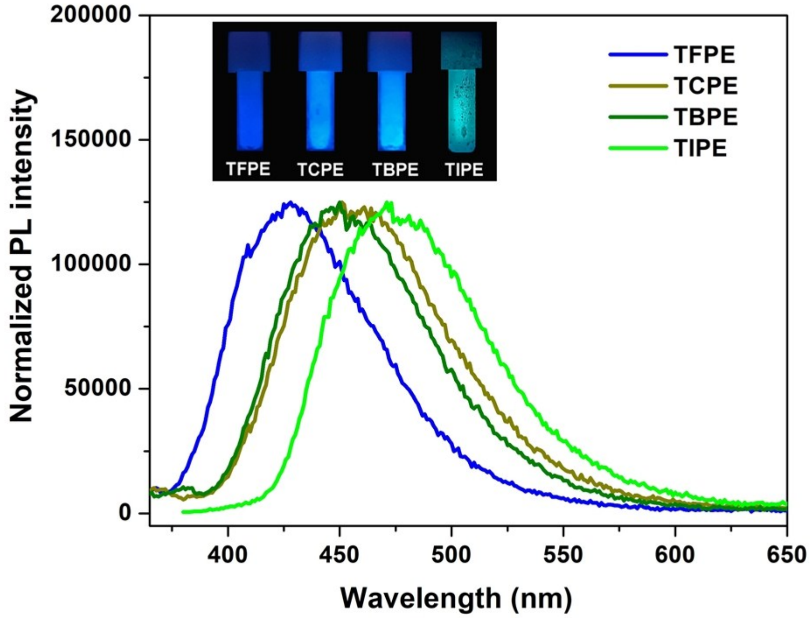


Figure S6. PL spectra and fluorescent images of TFPE, TCPE, TBPE and TIPE in THF at 77 K.

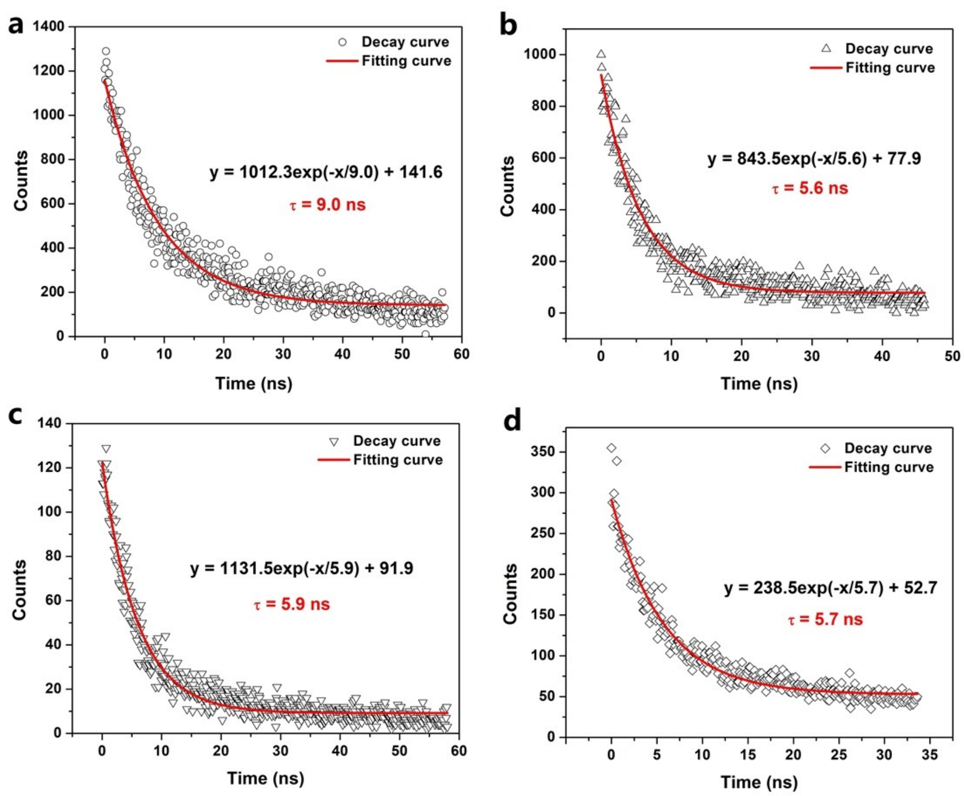


Figure S7. Time-resolved fluorescence decay curves of TFPE (a), TCPE (b), TBPE (c) and TIPE (d) in THF at 77 K.

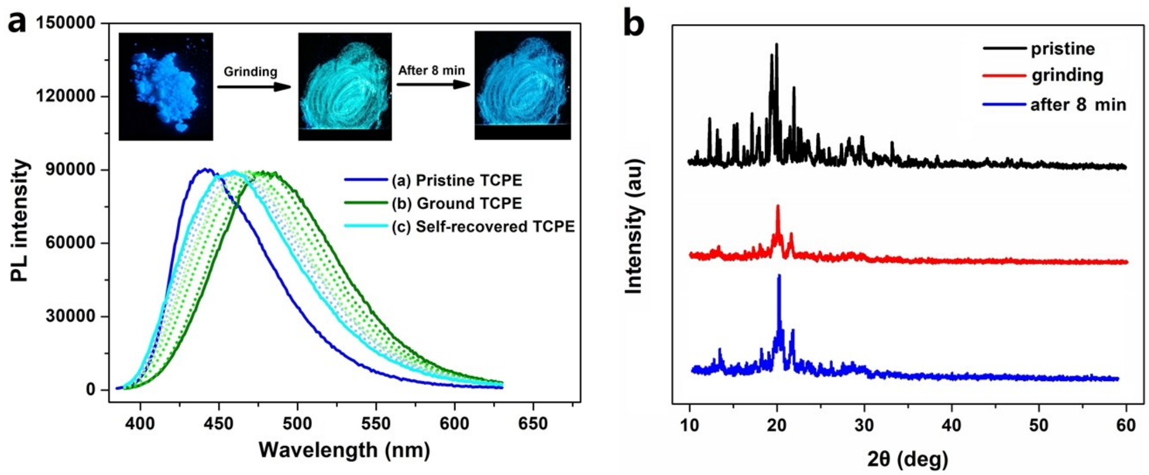


Figure S8. (a) PL spectra of pristine, ground and self-recovered TCPE solid within 8 min. Inset: photos of pristine crystals, ground crystals and self-recovered crystals of TCPE. (b) XRD patterns of pristine, grinding and self-recovered crystals of TCPE.

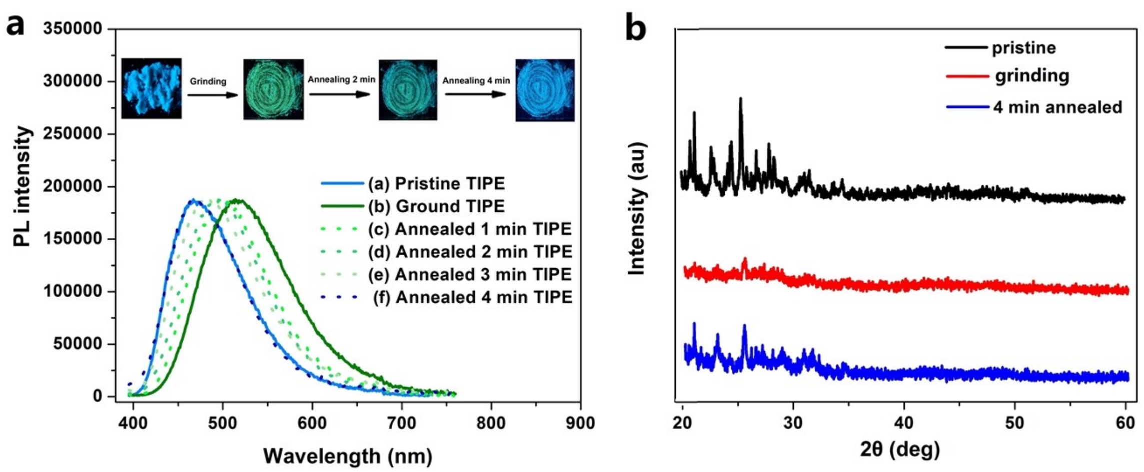


Figure S9. (a) PL spectra of pristine, ground and self-recovered TIPE solid within 8 min. Inset: photos of pristine crystals, ground crystals and annealed crystals of TIPE. (b) XRD patterns of pristine, grinding and self-recovered crystals of TIPE.

4. Supplementary Tables

Table S1. Contribution ratioes of different atoms to HOMOs and LUMOs of TPE, TFPE, TCPE, TBPE and TIPE

Compound	Center	Contribution to HOMO (%)	Contribution to LUMO (%)
TPE	C	98.86	95.77
	H	0.29	0.20
TFPE	C	94.59	94.40
	H	0.15	0.19
	F	4.76	2.11
TCPE	C	89.61	93.72
	H	0.14	0.18
	Cl	9.75	2.51
TBPE	C	82.74	84.98
	H	4.82	5.20
	Br	12.07	2.22
TIPE	C	82.16	94.26
	H	0.14	0.21
	I	17.30	2.30

Table S2. Excitation energies of first 20 states for TPE, TFPE, TCPE, TBPE and TIPE calculated with TDDFT at PBE0/6-31+G(d,p) level.

State No	TPE	TFPE	TCPE	TBPE	TIPE
1	2.3532 eV (T_1)	2.3352 eV (T_1)	2.2806 eV (T_1)	2.2852 eV (T_1)	2.2798 eV (T_1)
2	3.3232 eV (T_2)	3.3317 eV (T_2)	3.2235 eV (T_2)	3.2338 eV (T_2)	3.2157 eV (T_2)
3	3.3424 eV (T_3)	3.3529 eV (T_3)	3.2369 eV (T_3)	3.2471 eV (T_3)	3.2275 eV (T_3)
4	**3.4676 eV (T_4)**	**3.4831 eV (T_4)**	**3.3768 eV (T_4)**	**3.3840 eV (T_4)**	**3.3625 eV (T_4)**
5	**3.7072 eV (S_1)**	**3.6830 eV (S_1)**	**3.5553 eV (S_1)**	**3.5401 eV (S_1)**	**3.5043 eV (S_1)**
6	3.8032 eV (T_5)	3.8001 eV (T_5)	3.7564 eV (T_5)	3.7561 eV (T_5)	3.7414 eV (T_5)
7	4.0436 eV (T_6)	3.8263 eV (T_6)	3.8731 eV (T_6)	3.8912 eV (T_6)	3.8587 eV (T_6)
8	4.1787 eV (T_7)	3.9770 eV (T_7)	4.0343 eV (T_7)	4.0501 eV (T_7)	3.9471 eV (T_7)
9	4.2503 eV (T_8)	4.1109 eV (T_8)	4.1585 eV (T_8)	4.1679 eV (T_8)	3.9488 eV (T_8)
10	4.2655 eV (T_9)	4.1473 eV (S_2)	4.1814 eV (S_2)	4.1893 eV (S_2)	3.9498 eV (T_9)
11	4.3123 eV (T_{10})	4.1513 eV (T_9)	4.1862 eV (T_9)	4.1908 eV (T_9)	3.9619 eV (T_{10})
12	4.3450 eV (S_2)	4.3556 eV (S_3)	4.2885 eV (T_{10})	4.2681 eV (T_{10})	4.0386 eV (T_{11})
13	4.3906 eV (T_{11})	4.3622 eV (T_{10})	4.2999 eV (S_3)	4.2991 eV (S_3)	4.1494 eV (S_2)

14	4.4467 eV (S_3)	4.3971 eV (T_{11})	4.3415 eV (T_{11})	4.3328 eV (T_{11})	4.1494 eV (T_{12})
15	4.4721 eV (T_{12})	4.4909 eV (T_{12})	4.4154 eV (T_{12})	4.3932 eV (T_{12})	4.1741 eV (T_{13})
16	4.4745 eV (T_{13})	4.5388 eV (T_{13})	4.4167 eV (T_{13})	4.3963 eV (T_{13})	4.2216 eV (T_{14})
17	4.5107 eV (T_{14})	4.6051 eV (T_{14})	4.4313 eV (T_{14})	4.4178 eV (T_{14})	4.2607 eV (S_3)
18	4.5964 eV (T_{15})	4.6433 eV (S_4)	4.4887 eV (S_4)	4.4449 eV (S_4)	4.2966 eV (T_{15})
19	4.6342 eV (T_{16})	4.6824 eV (S_5)	4.5130 eV (T_{15})	4.4598 eV (T_{15})	4.3052 eV (S_4)
20	4.6483 eV (T_{17})	4.6957 eV (S_6)	4.5633 eV (T_{16})	4.5361 eV (T_{16})	4.3329 eV (T_{16})

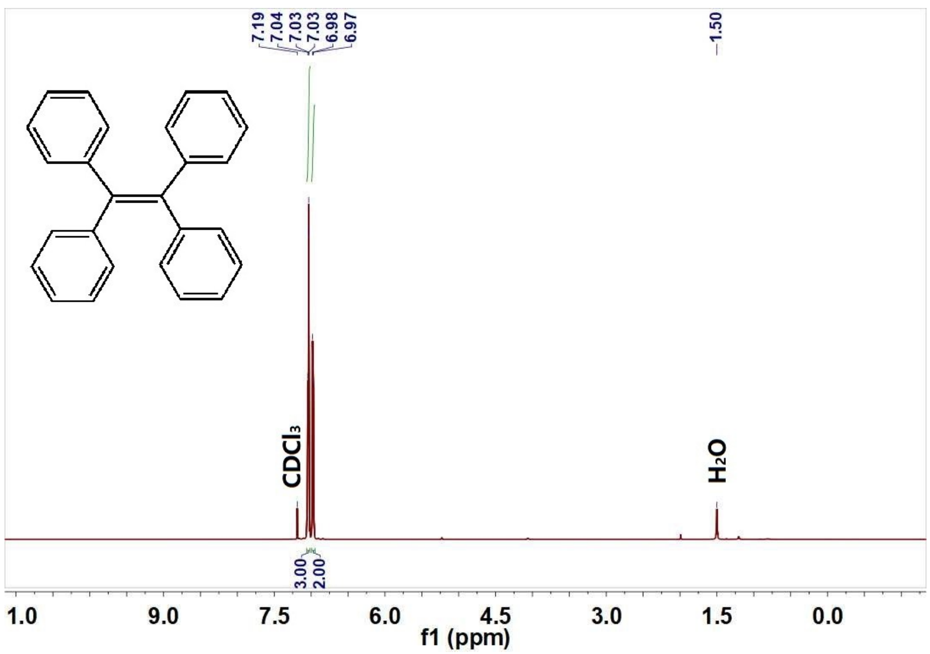
Table S3. Photophysical properties of TPE, TFPE, TCPE, TBPE and TIPE in different states

	λ_{ab} (nm)	λ_{em} (nm)	τ (ns)	Φ (%)	k_r (10^8 s^{-1})	k_{nr} (10^8 s^{-1})
			Crystal			
TPE	-	445	1.5	32.6	2.2	4.5
TFPE	-	438	3.0	58.6	2.0	1.3
TCPE	-	445	2.4	75.5	3.1	1.1
TBPE	-	452	2.0	64.4	3.2	1.8
TIPE	-	467	2.1	49.3	2.3	2.5
			Dispersed in SiO_2			
TPE	-	470	3.9	22.2	0.57	2.0
TFPE	-	470	3.6	5.2	**0.14**	**2.6**
TCPE	-	480	6.6	47.0	**0.71**	**0.81**
TBPE	-	485	6.7	54.3	**0.81**	**0.69**
TIPE	-	493	3.8	41.9	**1.10**	**1.53**
			In solution			
TPE	240 310	466	6.7	< 1	-	-
TFPE	231 304	460	6.5	< 1	-	-
TCPE	250 320	475	6.1	< 1	-	-
TBPE	253 323	510	5.3	< 1	-	-
TIPE	253 327	515	4.0	< 1	-	-

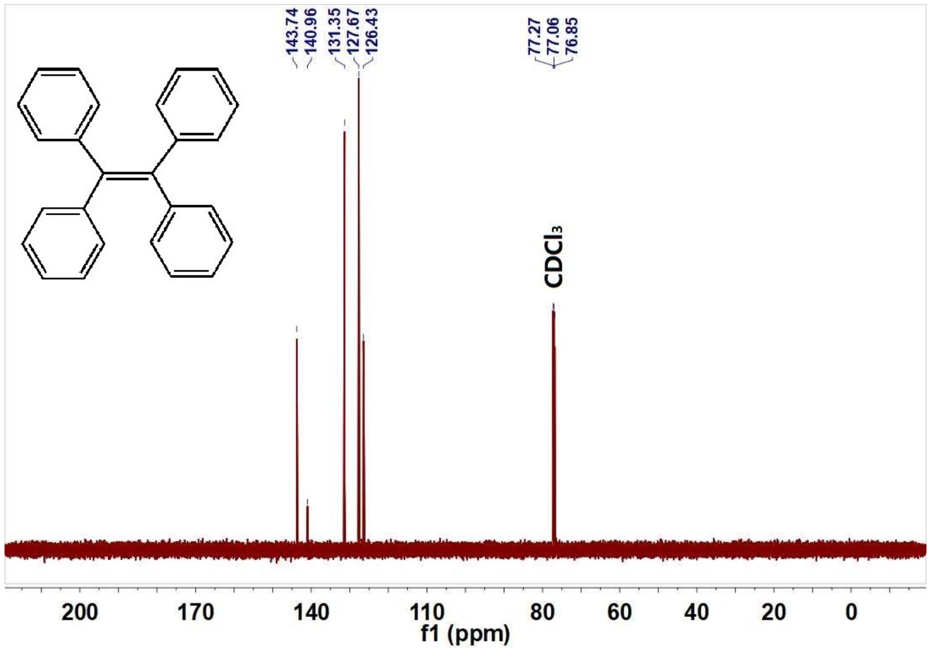
Table S4. Crystallographic data for TFPE, TCPE, TBPE and TIPE

source	TFPE	TCPE	TBPE	TIPE
CCDC No.	1948854	1948855	1948856	1958228
Chemical formula	$C_{26}H_{16}F_4$	$C_{26}H_{16}Cl_4$	$C_{26}H_{16}Br_4$ $2(C_4H_8O)$	$C_{26}H_{16}I_4$
Formula weight	404.39	470.19	792.24	836.02
Temperature (K)	289	298	293	273
wavelength (Å)	0.71073	1.54178	0.71073	0.71073
crystal system	orthorhombic	monoclinic	orthorhombic	orthorhombic
space group	Fdd2	P 21/n	P 21 21 21	P 21 21 21
a (Å)	18.5763	20.1695	9.3392	9.6191
b (Å)	40.241	9.8843	15.1764	17.2316
c (Å)	5.6042	23.3874	21.938	18.9386
α	90.00	90.00	90.00	90.00
β	90.00	92.701	90.00	90.00
γ	90.00	90.00	90.00	90.00
volume ($Å^3$)	4189.3	4657.4	3109.4	3139.1
Z	8	8	4	4
no. reflections collected	7647	60267	37711	33612
no. unique reflections	2344	8465	7120	8873
R_{int}	0.0224	0.0699	0.0964	0.0286
no. parameters	136	541	361	308
GOF on F^2	1.057	1.051	1.017	1.050
$R1$	0.0396	0.0708	0.0457	0.0427
$wR2$	0.1034	0.2078	0.0971	0.1383

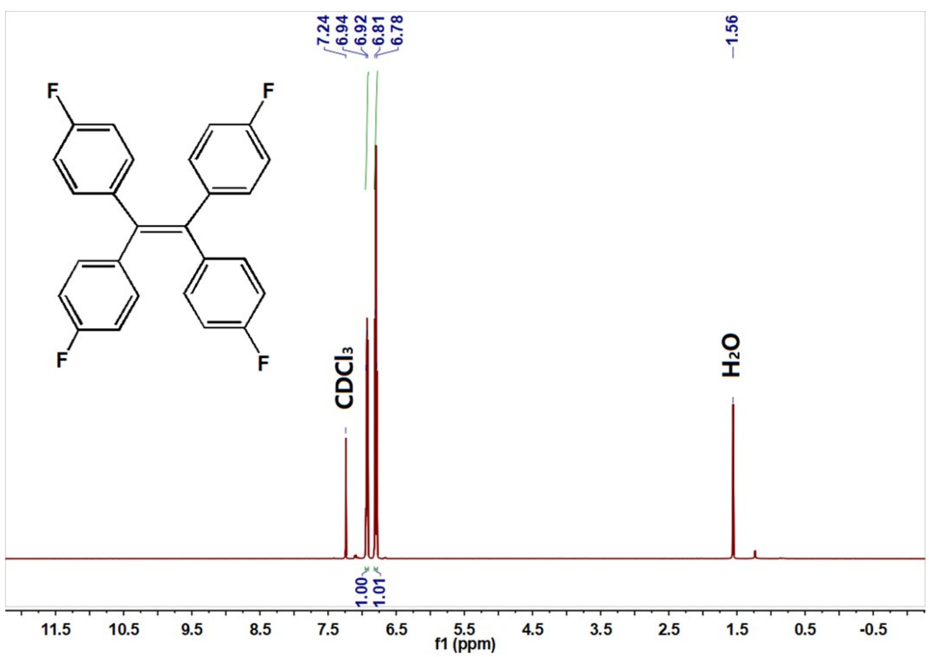
5. Spectra of Compounds



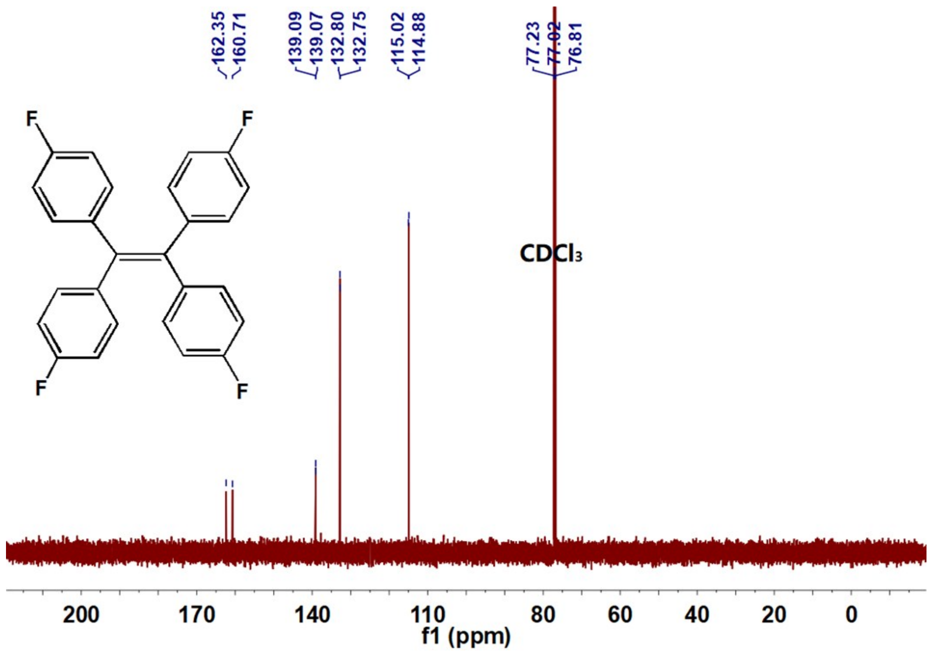
^{1}H NMR spectrum of 1,1,2,2-tetraphenylethene (TPE) in $CDCl_3$



^{13}C NMR spectrum of 1,1,2,2-tetraphenylethene (TPE) in $CDCl_3$



^{1}H NMR spectrum of 1,1,2,2-tetra(4-fluorophenyl)ethylene (TFPE) in $CDCl_3$



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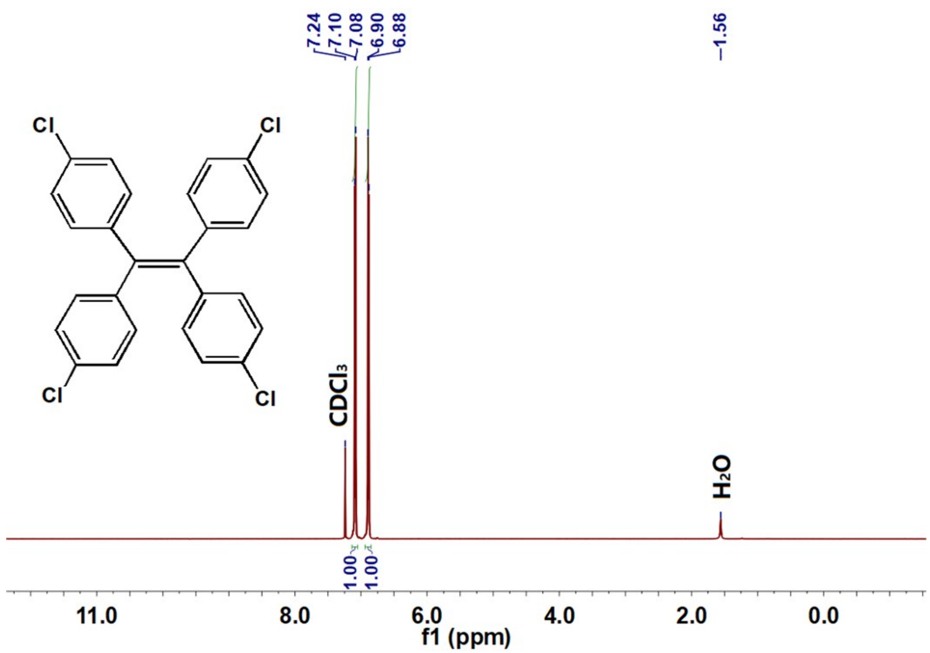

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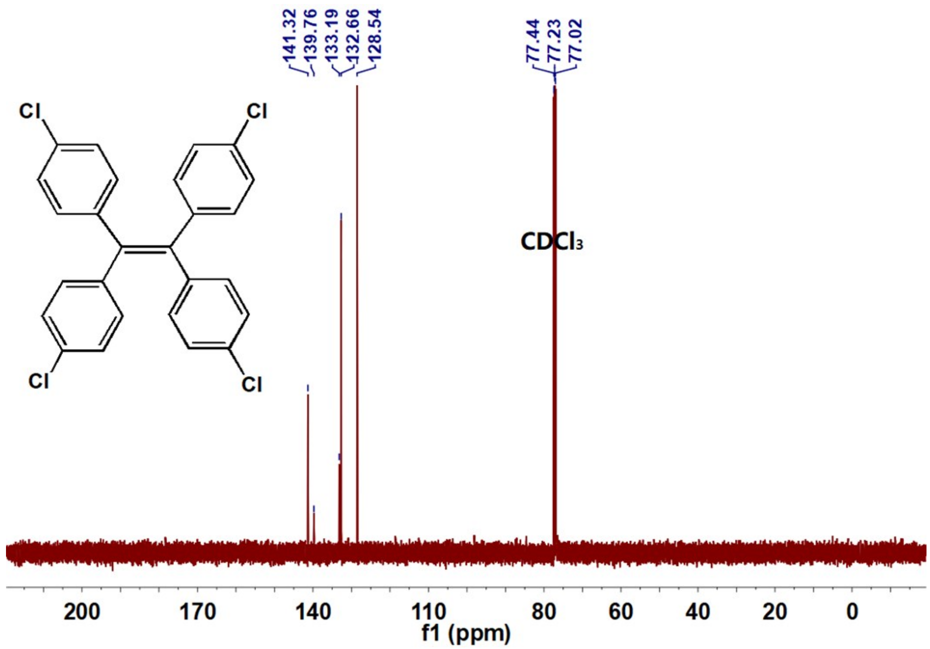

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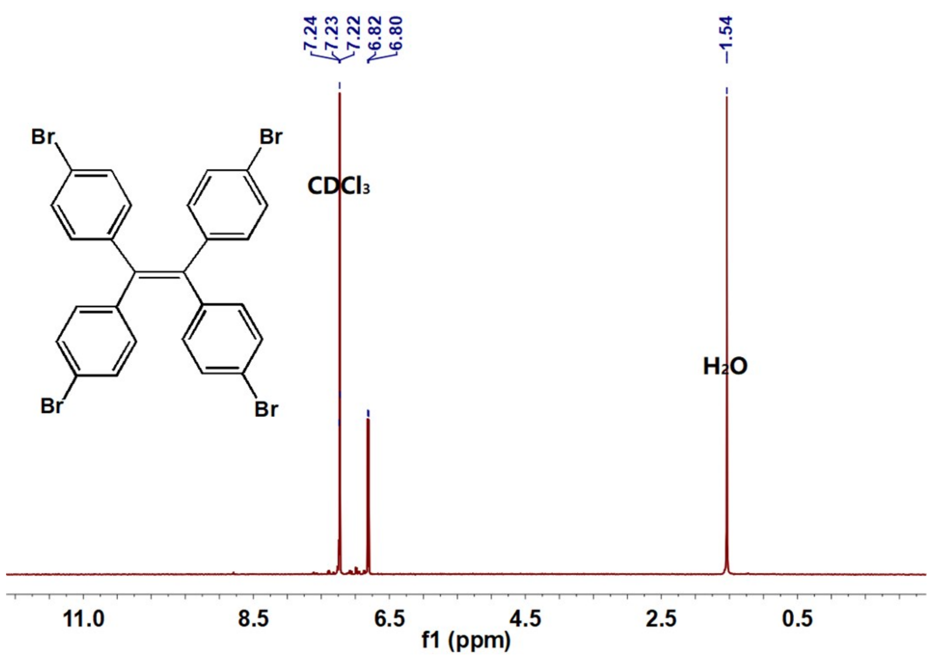

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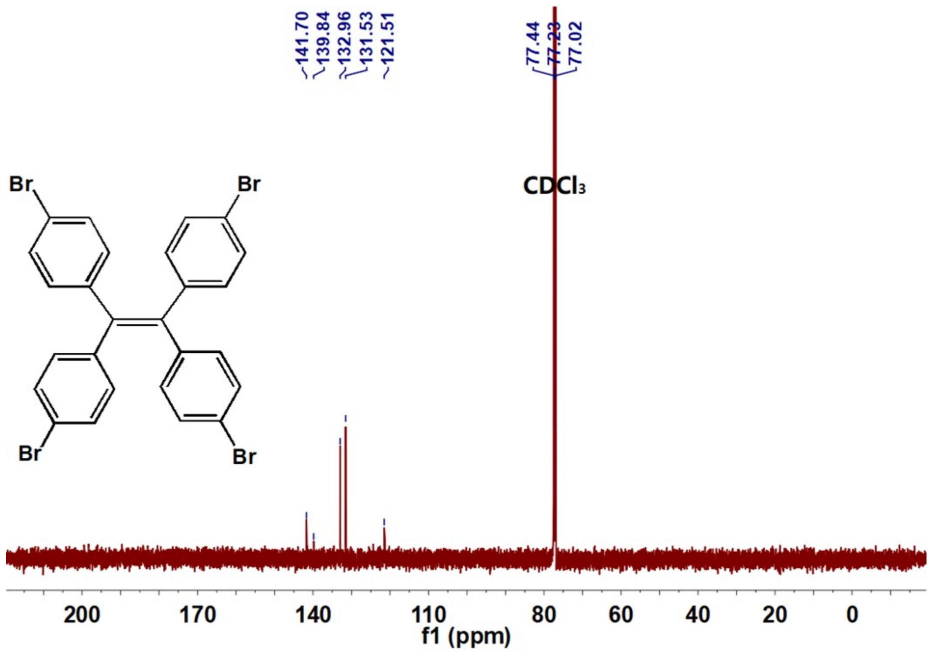

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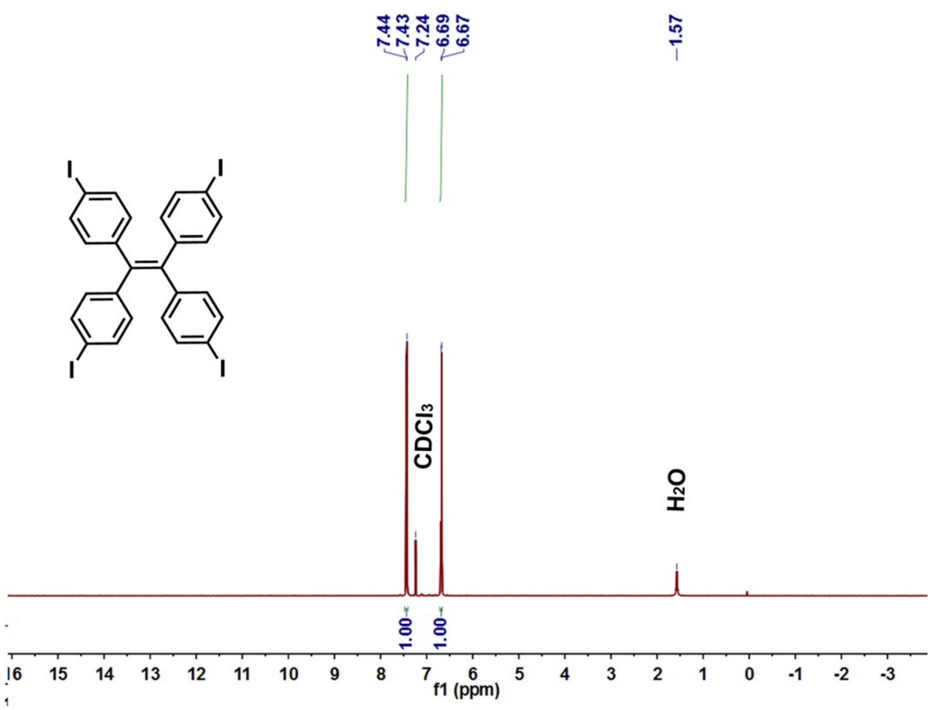

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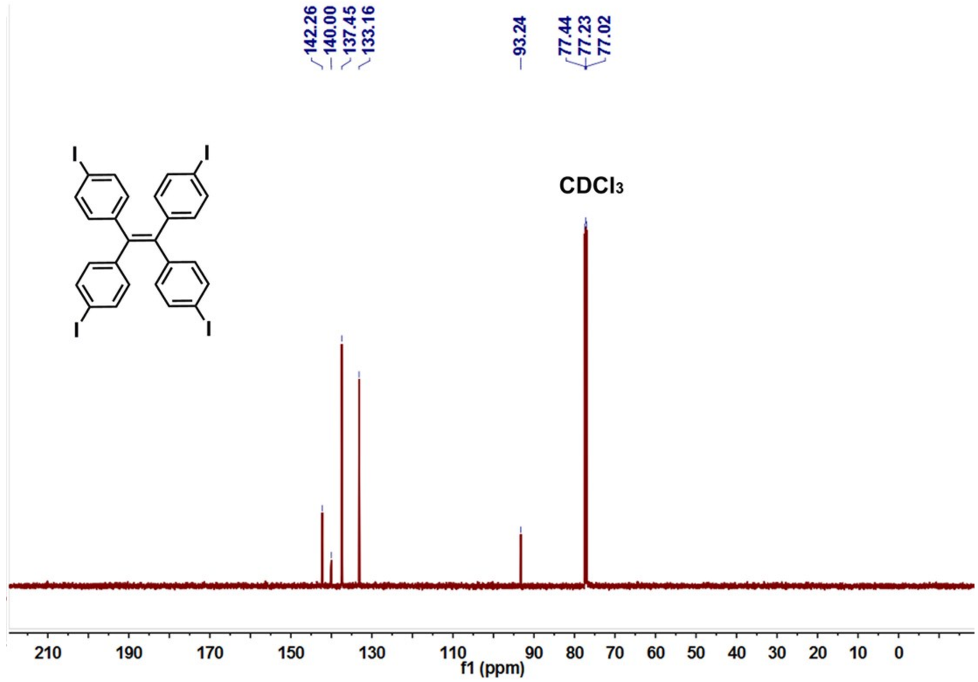

^{13}C NMR spectrum of 1,1,2,2-tetra(4-iodophenyl)ethylene (TIPE) in $CDCl_3$

6. Cartesian Coordinates

TPE

C	5.61546800	12.44776300	14.27613600
C	6.39406700	12.73758800	13.03157700
C	5.12501800	12.81464100	16.71282500
C	6.68423700	11.71092900	12.11463500
H	6.35301500	10.69841600	12.32678300
C	7.37670900	13.43820700	15.77011800
C	3.48049800	12.75589900	19.00689700
C	6.01533300	12.87387700	15.51172200
C	3.00716900	13.30964600	17.81413600
H	2.00368200	13.72309500	17.76531500
C	9.80502700	13.28717900	15.61559300
H	10.68751700	12.75099000	15.27793600
C	7.39571300	11.97432200	10.94333000
H	7.62014200	11.16300800	10.25641800
C	4.36513200	11.65500900	14.06030500
C	7.52873400	14.63054800	16.50099800
H	6.64544300	15.15054100	16.86034200

C	8.53761700	12.77061600	15.34202700
H	8.44268900	11.83918000	14.79325000
C	6.81004700	14.04339800	12.71856400
H	6.58084500	14.85263700	13.40451800
C	5.59562700	12.28116300	17.92642100
H	6.60823900	11.89167500	17.97945500
C	4.77948800	12.24119100	19.05778500
H	5.16030700	11.81285200	19.98080700
C	3.82045100	13.33732300	16.68009500
H	3.44473900	13.76953600	15.75816900
C	4.08581600	10.50754900	14.82300900
H	4.77994400	10.20468800	15.60047400
C	3.46105700	12.01166400	13.04320000
H	3.66897600	12.88201800	12.42751600
C	9.93979100	14.48551900	16.32218200
C	8.79484400	15.15520200	16.76434100
H	8.88714100	16.08431000	17.31993700
C	2.93309900	9.75520500	14.59180900
H	2.74087200	8.86989400	15.19148100
C	7.81213200	13.27660100	10.65082600
C	2.03187000	10.13550200	13.59346200
C	2.30155100	11.26811500	12.81932900
H	1.61118200	11.57068000	12.03684500
C	7.50983300	14.31092500	11.54088000
H	7.81761600	15.32887100	11.31868800
H	8.35969500	13.48385500	9.73590800
H	1.13330900	9.55171100	13.41563300
H	2.84714200	12.73209600	19.88902800
H	10.92595700	14.88922500	16.53284100

TFPE

C	5.61602100	12.44663400	14.27540300
C	6.39079200	12.74372500	13.03097000
C	5.12260800	12.82051400	16.70970100
C	6.67881300	11.72396700	12.10531900
H	6.34913700	10.70944400	12.30792400
C	7.37950900	13.43076900	15.77036400
C	3.48768300	12.77233600	18.97001600
C	6.01619900	12.87311700	15.51148400
C	2.99282900	13.32516200	17.79546400
H	1.98775100	13.73222100	17.76996200

C	9.81160000	13.26469100	15.60451900
H	10.70718700	12.74819100	15.27637200
C	7.38773100	11.98553500	10.93233600
H	7.62262300	11.20009800	10.22202100
C	4.36970400	11.64802400	14.06234800
C	7.53878600	14.61945900	16.50608600
H	6.66067300	15.14376600	16.87055200
C	8.53800300	12.76140600	15.33703900
H	8.44203300	11.83189200	14.78598800
C	6.80795800	14.05138100	12.72536700
H	6.58071600	14.85823400	13.41412200
C	5.58710200	12.29237600	17.92824100
H	6.59817100	11.90136800	17.99033800
C	4.77362300	12.25339000	19.06125200
H	5.12383100	11.83638800	19.99938900
C	3.81801800	13.34377500	16.67037300
H	3.44412600	13.77432500	15.74740500
C	4.09273800	10.50404300	14.83196300
H	4.78611400	10.20479200	15.61091300
C	3.46406700	11.99436800	13.04274500
H	3.66598500	12.86088000	12.42043200
C	9.91756200	14.45465500	16.31373500
C	8.80305100	15.14579200	16.77349300
H	8.92952700	16.06801000	17.33037700
C	2.94500200	9.74119400	14.61325300
H	2.73085700	8.85548800	15.20166900
C	7.78953000	13.29174800	10.68001200
C	2.06811700	10.13674400	13.61085400
C	2.30469900	11.25192300	12.81608100
H	1.59787200	11.52297800	12.03921300
C	7.50699000	14.33594900	11.55175800
H	7.82618500	15.34414600	11.31058400
F	8.47290700	13.55843100	9.53527300
F	0.94557400	9.40144000	13.39247400
F	2.69041700	12.74752300	20.07104800
F	11.15422900	14.95438000	16.57724500

TCPE

Cl	11.52666200	15.12356000	16.65102300
Cl	2.45068200	12.72619400	20.40996000
Cl	0.59462900	9.18965200	13.32397300

Cl	8.68947300	13.62896700	9.18797700
C	5.61637100	12.44591400	14.27563800
C	6.39214300	12.74073600	13.03213300
C	5.12396600	12.81779900	16.70998500
C	6.67670800	11.72168000	12.10569700
H	6.34451300	10.70729500	12.30556300
C	7.37812300	13.43236700	15.77024900
C	3.48048600	12.76346600	18.98631000
C	6.01642600	12.87242400	15.51191200
C	2.99591500	13.31463300	17.79984100
H	1.99204200	13.72299500	17.75820500
C	9.80950600	13.27674200	15.60300600
H	10.69616700	12.75084800	15.26606200
C	7.38715200	11.98211700	10.93415700
H	7.61164200	11.18404900	10.23482000
C	4.36913100	11.65019500	14.06216800
C	7.53603200	14.62010900	16.50643400
H	6.65839200	15.14384300	16.87324900
C	8.53846500	12.76842800	15.33608500
H	8.44788300	11.83847500	14.78459500
C	6.81527800	14.04547700	12.72585300
H	6.59229500	14.85532900	13.41267100
C	5.58948800	12.29145500	17.92807500
H	6.60125600	11.90218500	17.99201300
C	4.77600700	12.24993900	19.06016000
H	5.14356400	11.82908400	19.98974100
C	3.81834200	13.33658200	16.67356800
H	3.43969000	13.76741000	15.75251100
C	4.08666300	10.50826400	14.83135500
H	4.77657200	10.20508500	15.61204700
C	3.46543100	11.99652200	13.04182800
H	3.66774900	12.86173100	12.41760500
C	9.92992400	14.47097200	16.31415800
C	8.79902100	15.14910600	16.77092000
H	8.90549900	16.07314700	17.32868100
C	2.93715300	9.74980100	14.61067800
H	2.73468800	8.86811300	15.20893100
C	7.80294600	13.28712500	10.66655800
C	2.04879300	10.13536900	13.60640800
C	2.30495300	11.25678500	12.81625800
H	1.60979200	11.54351000	12.03469700

C	7.51526300	14.32567500	11.55253300
H	7.83168200	15.33819700	11.32701800

TBPE

Br	11.69642600	4.56867500	4.99187400
Br	2.33006700	7.04949300	8.87961800
Br	0.41425800	10.66248900	1.60203000
Br	8.78486300	6.09392600	-2.66010200
C	3.45864800	7.76310500	1.35089000
H	3.66446100	6.89866900	0.72634800
C	9.80390500	6.49073100	3.90922900
H	10.68794100	7.01700900	3.56647200
C	7.52900400	5.15255800	4.82250300
H	6.65150400	4.63077700	5.19307000
C	6.66758700	8.04343400	0.41567700
H	6.33281000	9.05777200	0.61269000
C	6.00989000	6.89756500	3.82408900
C	4.76894000	7.52350300	7.37249500
H	5.13960300	7.94639000	8.29974100
C	5.11729400	6.95305000	5.02223200
C	5.58303200	7.48141300	6.23923800
H	6.59459100	7.87186600	6.30302600
C	8.53151700	7.00031400	3.64424600
H	8.44119200	7.92929900	3.09063800
C	6.38568800	7.02547900	1.34399600
C	8.79293500	4.62167200	5.08563300
H	8.89553600	3.69893500	5.64595200
C	7.37973400	7.78185300	-0.75621600
H	7.60043900	8.58123900	-1.45505600
C	2.03845600	9.61625100	1.91649300
C	9.91847500	5.29950100	4.62208300
C	2.98864500	6.45505300	6.11234200
H	1.98576300	6.04506000	6.06691300
C	4.07337800	9.25381800	3.14179700
H	4.76179200	9.55991400	3.92299300
C	7.79589400	6.47754000	-1.01494000
C	2.92010600	10.00889000	2.92088200
H	2.71731200	10.88862100	3.52163000
C	6.81173400	5.72072500	1.04204000
H	6.59039600	4.91172600	1.73075000
C	3.81233300	6.43276700	4.98538300

H	3.43391600	6.00022600	4.06476000
C	2.29422100	8.49886200	1.12442300
H	1.60306100	8.20661700	0.34156000
C	7.51372600	5.43860300	-0.13109300
H	7.83153000	4.42526300	-0.35011100
C	4.35983300	8.11334900	2.37200100
C	3.47687900	7.00797600	7.29389200
C	7.37187500	6.33828200	4.08307200
C	5.60921200	7.32124100	2.58701800

TIPE

C	-1.50068300	2.56078200	-0.73366800
H	-0.78729900	2.79456600	-1.51879800
C	3.35213000	-2.00522600	1.28046400
H	4.06193000	-1.78264100	2.06975600
C	1.49590600	-2.58080000	-0.72163100
H	0.77461000	-2.82241900	-1.49702100
C	1.50857700	2.56336300	0.74502700
H	0.79574400	2.79773900	1.53048100
C	0.00324100	-0.68683000	0.00931000
C	-2.67239700	-3.32812000	0.63289400
H	-2.85766900	-4.13844600	1.32947500
C	-1.25110600	-1.48970100	-0.12216500
C	-1.51347800	-2.55879100	0.75212600
H	-0.80614200	-2.79160900	1.54306000
C	2.19696400	-1.23272700	1.14642700
H	2.02690100	-0.41520400	1.83973000
C	1.25632800	1.48738600	-0.12399800
C	2.65237300	-3.35467400	-0.60871000
H	2.82161800	-4.17784800	-1.29445300
C	2.66395400	3.33792200	0.62739800
H	2.84046100	4.15427500	1.31922900
C	-3.57323500	3.04861900	0.39535600
C	3.57781400	-3.05949800	0.39405300
C	-3.33407800	-2.00620800	-1.28874900
H	-4.02988700	-1.79256400	-2.09266000
C	-2.18087100	1.23431300	1.15729400
H	-2.00258900	0.42523900	1.85859500
C	3.57795500	3.05337000	-0.38872800
C	-3.33653500	2.00605800	1.29256400
H	-4.03810600	1.79190300	2.09139500

C	2.18977500	1.23272800	-1.14288700
H	2.01304500	0.42083400	-1.84125200
C	-2.17707600	-1.23746200	-1.14820100
H	-1.99170900	-0.43116000	-1.85080000
C	-2.65803600	3.33307800	-0.61982300
H	-2.83627400	4.14645100	-1.31471600
C	3.34367100	2.00656300	-1.28177500
H	4.04569700	1.79163000	-2.08017500
C	-1.24775400	1.48695400	0.13774400
C	-3.57927000	-3.04562200	-0.39026400
C	1.25375900	-1.49535500	0.13848500
C	0.00451600	0.68081400	0.00791000
I	5.34801100	-4.23907800	0.57908100
I	5.33967300	4.24327500	-0.58895700
I	-5.34516200	4.22517700	0.58217100
I	-5.34903200	-4.22326800	-0.59060800

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