Electronic Supplementary Material

Simultaneously enhancing the planarity and electron-donating capability of donors for through-space charge transfer TADF towards deep-red emission

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General

All chemicals and materials, unless otherwise noted, were commercially available and used without further purification. All solvents for reactions and photophysical measurements were of HPLC grade. The chemical 3-(3,6-di-*tert*-butyl-9*H*-carbazol-1-yl)dibenzo[*a,c*]phenazine (CQX) and 3,3'-(3,6-di-tert-butyl-9H-carbazole-1,8-diyl)didibenzo[a,c]phenazine (C2QX) were prepared by following literature methods.[1]

^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ and CD_2Cl_2 solvent on a 500 MHz spectrometer (Bruker Daltonics, Germany) using tetramethylsilane (TMS) as the internal standard. High-resolution mass spectrometry was performed on AB SCIEX TripleTOF 6600 (Singapore). Thermogravimetric analysis (TGA) was performed on a TGA-Q50 Instrument (TA Instruments, America) with a heating rate of 10 ^{o}C/min from 60 to 800 ^{o}C under an argon atmosphere.

UV-vis absorption spectra were obtained on a Shimadzu UV-2600 spectrophotometer (Shimadzu, Japan) at room temperature. Room-temperature photoluminescence spectra were measured on a Hitachi F-7100 fluorescence spectrophotometer (Hitachi, Japan). Phosphorescence spectra were measured for doped films (5% in mCBP) at 77 K. The doped film samples were prepared by spin-coating chlorobenzene solutions. The transient PL characteristics were measured by a single photon counting spectrometer (Picoquant, FluoTime 300, Germany). The solid-state absolute photoluminescence quantum yields (PLQYs) were measured on a Hamamatsu UV-NIR absolute PL quantum yield spectrometer (C13534, Hamamatsu Photonics) equipped with a calibrated integrating sphere under argon atmosphere. Cyclic voltammetry (CV) measurements were carried out on a CHI600 electrochemical analyzer (Chenhua, China) at room temperature, with a conventional three-electrode system consisting of a glassy carbon working electrode, a platinum wire auxiliary electrode, and an Ag/AgCl standard electrode which was used as the reference electrode. Dichloromethane and tetrabutylammonium hexafluorophosphate (0.1 M) were used as the solvent and supporting electrolyte, respectively. The sweep speed was set as 100 mV s^{-1}.

Single Crystal Analysis

X-ray single-crystal diffraction data of all compounds were recorded on a Bruker D8 Venture diffractometer using Cu Kα radiation (λ = 1.54184 Å). The crystal was kept at 100.0 K during data collection. Using Olex2,[2] the structure was determined with the ShelXT[3] structure solution program using intrinsic phasing and refined with the ShelXL refinement package using least-squares minimization. Full crystallographic information in CIF format has been deposited at the Cambridge Crystallographic Data Center (CCDC) under deposition number 2223327 and 2223328.

Rate Constants Calculation

With the assumption $k' = k_{nr,T} + k_{r,T} \ll k_{RISC}$ ($k_{nr,T}$ and $k_{r,T}$ represent the rate constants of nonradiative decay and radiative decay from T_1 to S_0 states, respectively) and usual $k_p >> k_d$ (k_p and k_d represent the decay rate constants for prompt and delayed fluorescence, respectively), the rate constants of radiative decay ($k_{r,S}$) and nonradiative decay ($k_{nr,S}$) from S_1 to S_0 states, the rate constants of intersystem crossing (k_{ISC}) and reverse intersystem crossing (k_{RISC}) between the S_1 and T_1 states were calculated from the following six equations:[4]

$$k_p = \frac{1}{\tau_p}$$

$$k_d = \frac{1}{\tau_d}$$

$$k_{r,S} = \phi_p k_p + \phi_d k_d \approx \phi_p k_p$$

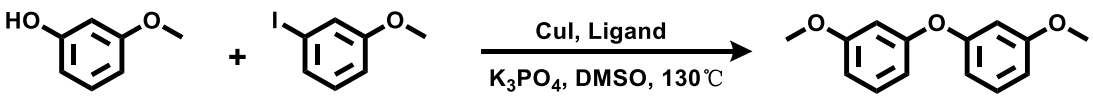
$$k_{nr,S} = \frac{1 - \phi_{PL}}{\phi_{PL}} k_{r,S}$$

$$k_{RISC} \approx \frac{k_p k_d \phi_{PL}}{k_{r,S}}$$

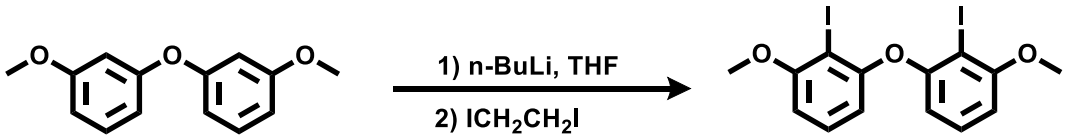
$$k_{ISC} \approx \frac{k_p k_d \phi_d}{k_{RISC} \phi_p}$$

Where τ_p and τ_d represent the experimentally determined prompt and delayed fluorescence decay time constants, respectively; ϕ_p and ϕ_p represent the prompt and delayed fluorescence components in the PLQY (ϕ_{PL}), respectively, and can be experimentally determined from typical PLQY and transient PL characteristics.

Synthesis and Characterization

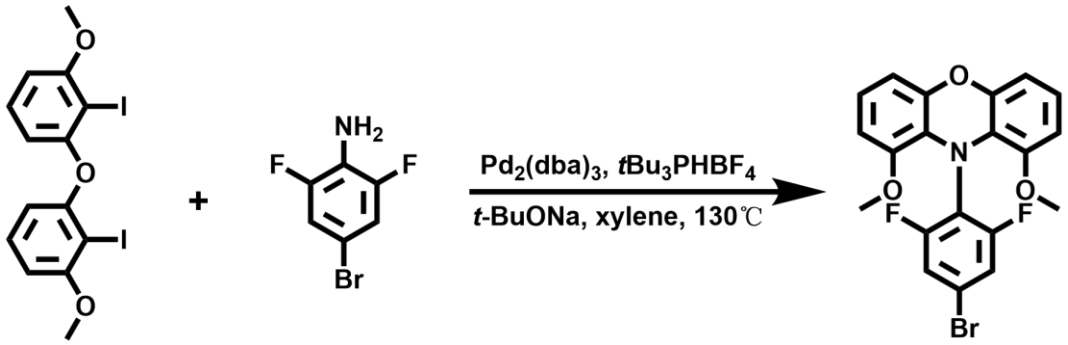


3,3'-oxybis(methoxybenzene): A mixture of CuI (813 mg, 4.27 mmol), pyridine-2-carboxylic acid (1.05 g, 8.54 mmol), 1-iodo-3-methoxybenzene (10.00 g, 42.7 mmol) and potassium phosphate (18.13 g, 85.4 mmol) was added to a 500 mL flame dried three-necked round bottom flask with a stirring bar. The flask was evacuated and filled with argon three times. DMSO (80 mL) and 3-methoxyphenol (51.3 mmol) were added under argon atmosphere. The reaction mixture was stirred at 130 °C for 48 h. The reaction mixture was cooled to room temperature and diluted with water (200 mL). The crude product was extracted with DCM (3 × 100 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, concentrated in vacuo and the residue was purified on silica-gel column chromatography using petroleum ether/EtOAc (v/v=100/1) as the eluent to give a colorless oil in 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 7.21 (t, *J* = 7.0, 6.5 Hz, 2H), 6.65 (ddd, *J* = 1.0, 1.0, 1.0, 0.5 Hz, 2H), 6.59 (m, 4H), 3.76 (s, 6H).

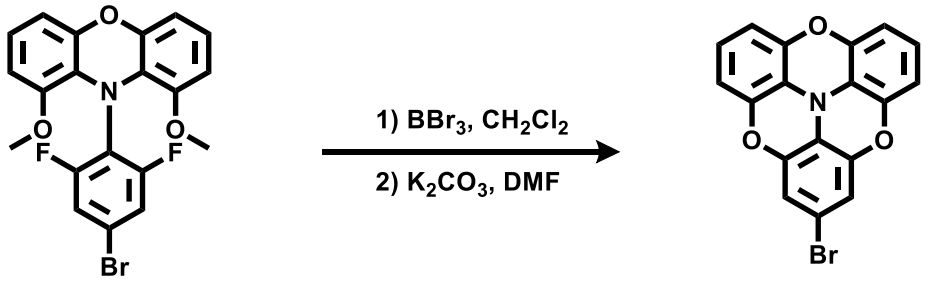


3,3'-oxybis(2-iodo-1-methoxybenzene): Under argon atmosphere, compound 3,3'-oxybis(methoxybenzene) (7.76 g, 33.7 mmol) was placed in a 250 mL dried two-necked round bottom flask with an ice/water bath. Tetrahydrofuran (40 mL) was added to the flask, then a 2.5 M hexane solution of n-butyllithium (30.6 mL, 76.5 mmol) was slowly added to the THF solution. After removing the ice/water bath, the mixture was stirred at room temperature for 2 h. Subsequently, the flask was placed into an ice/water bath again. A THF solution (40 mL) of 1,2-diiodo-ethane (21.00 g, 74.50 mmol) was slowly added to the mixture. The reaction was continued at room temperature for 4 h. Then the mixture was poured into 400 mL water and extracted with CH_2Cl_2. The organic layer was dried over sodium sulfate (Na_2SO_4), filtered, and concentrated under

reduced pressure. The resulting residue was washed with cold hexane to afford the desired compound as a white solid in 70% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 7.22 (t, *J* = 8.0, 8.5 Hz, 2H), 6.62 (d, *J* = 8.0 Hz, 2H), 6.42 (dd, *J* = 1.0, 0.5 Hz, 2H), 3.93 (s, 6H).



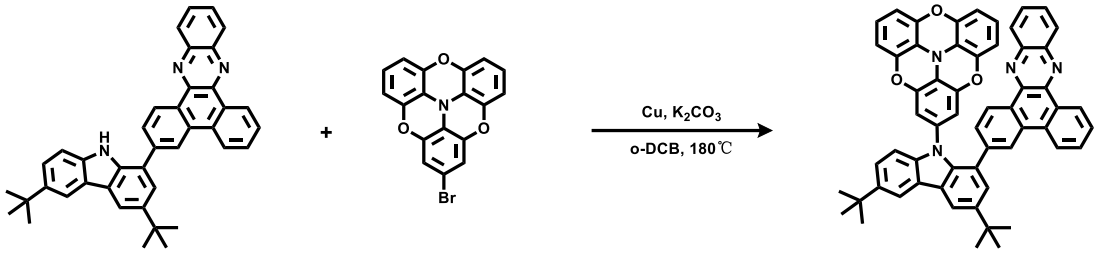
10-(4-bromo-2,6-difluorophenyl)-1,9-dimethoxy-10H-phenoxazine: Under argon atmosphere, a mixture of 3,3'-oxybis(2-iodo-1-methoxybenzene) (5.92 g, 12.28 mmol), 4-bromo-2,6-difluoroaniline (2.55 g, 12.28 mmol), $Pd_2(dba)_3$ (562 mg, 0.61 mmol), *t*Bu_3PHBF_4 (356 mg, 1.23 mmol) and *t*-BuONa (3.54 g, 36.84 mmol) in 15 mL dry xylene was stirred and refluxed for 24 h. After cooling to room temperature, the crude product was filtered through a celite pad and washed with DCM. The collecting filtrate was evaporated to remove the solvent and the residue was passed through a column chromatography on silica gel using DCM/petroleum ether (v/v=1/8) as the eluent to afford the product as a colorless powder (yield: 30%). ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 7.07 (d, *J* = 9.0 Hz 2H), 6.92 (t, *J* = 10.5, 10.5 Hz, 2H), 6.56 (dd, *J* = 1.0, 1.5 Hz, 2H), 6.44 (dd, *J* = 1.0, 1.0 Hz, 2H), 3.67 (s, 6H).



2-bromo-4,8,12-trioxa-3a2-azadibenzo[cd,mn]pyrene (TPXZ-Br): Under argon atmosphere, compound 10-(4-bromo-2,6-difluorophenyl)-1,9-dimethoxy-10H-phenoxazine (2.38 g, 5.49 mmol) was placed in a 250 mL two-necked flask. Dry CH_2Cl_2 (100 mL) was added to the flask. The mixture was cooled and stirred at -30 °C for 30 min. Then boron tribromide (BBr_3) (3.65 mL, 38.7 mmol)

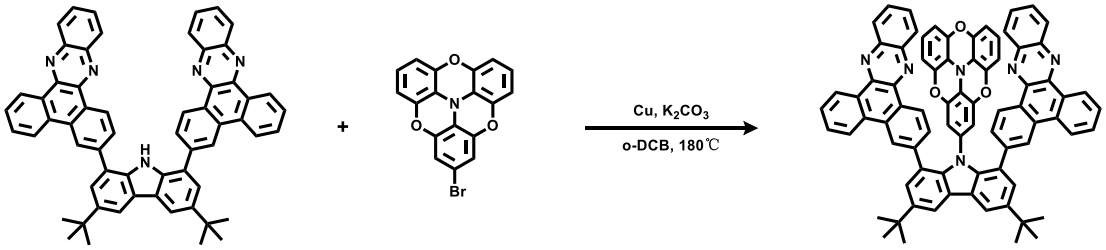
was added and the mixture was stirred for 24 h as the mixture was allowed to rise to room temperature. After the reaction ended, the mixture was poured into 200 mL of water and extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was used in the next reaction without further purification.

Under argon atmosphere, the product of the previous step (2.17 g, crude, 3.64 mmol) and K_2CO_3 (3.64 g, 26.40 mmol) were placed in a 250 mL two-necked flask. Dry DMF (100 mL) was added to the flask and the mixture was stirred at 100 °C for 12 h. After cooling to room temperature, the mixture was poured into 200 mL water and the resulting precipitate was collected by filtration. The precipitate was washed with water and EtOH to afford desired compound TPXZ-Br as a yellow solid (yield: 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 6.70 (t, *J* = 7.0, 7.0 Hz 2H), 6.61 (s, 2H), 6.45 (ddd, *J* = 1.0, 1.0, 0.5, 0.5 Hz, 4H).



TPXZ-QX: A mixture of 3-(3,6-di-tert-butyl-9H-carbazol-1-yl)dibenzo[a,c]phenazine (CQX, 558 mg, 1.00 mmol), TPXZ-Br (366 mg, 1.00 mmol), Cu powder (192 mg, 3.00 mmol), K_2CO_3 (415 mg, 3.00 mmol) in 10 mL dry o-dichlorobenzene was stirred and refluxed for 72 h under argon. After cooling to room temperature, the crude product was filtered through a celite pad and washed with DCM. The filtrate was concentrated to dryness. The collecting residue was purified by column chromatography on silica gel using DCM/petroleum ether (v/v=1/4) as the eluent to afford the product as a black powder. Yield: 71%. ^{1}H NMR (500 MHz, CD_2Cl_2) δ (ppm): 9.31 (d, *J* = 10.5 Hz, 1H), 9.05 (dd, *J* = 1.5, 1.0 Hz, 1H), 8.26 (m, 5H), 8.14 (m, 1H), 7.86 (pd, *J* = 2.0, 2.0, 2.0, 2.0, 2.0 Hz, 2H), 7.71 (dd, *J* = 1.5, 2.0 Hz, 1H), 7.66 (d, *J* = 2.5 Hz, 1H), 7.56 (m, 1H), 7.49 (dd, *J* = 2.5, 2.5 Hz, 1H), 7.38 (t, *J* = 9.0, 9.0 Hz, 1H), 7.23 (d, *J* = 11.0 Hz, 1H), 9.31 (d, *J* = 10.5 Hz, 1H), 5.99 (m, 8H), 1.56 (s, 9H), 1.48 (s, 9H). The ^{13}C NMR spectrum was not recorded due to its poor solubility. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{58}H_{42}N_4O_3$, 843.3330; found 843.3319. Anal. Calcd (%) for $C_{58}H_{42}N_4O_3$: C, 82.64;

H, 5.02; N, 6.65. Found: C, 82.47; H, 4.80; N, 6.54.



TPXZ-2QX: A mixture of 3,3'-(3,6-di-tert-butyl-9H-carbazole-1,8-diyl)didibenzo[a,c]phenazine (C2QX, 836 mg, 1.00 mmol), TPXZ-Br (366 mg, 1.00 mmol), Cu powder (192 mg, 3.00 mmol), K_2CO_3 (415 mg, 3.00 mmol) in 10 mL dry o-dichlorobenzene was stirred and refluxed for 72 h under argon. After cooling to room temperature, the crude product was filtered through a celite pad and washed with DCM. The filtrate was concentrated to dryness. The collecting residue was purified by column chromatography on silica gel using DCM/petroleum ether (v/v=1/4) as the eluent to afford the product as a black powder. Yield: 60%. ^{1}H NMR (500 MHz, Tetrahydrofuran-d8) δ (ppm): 9.00 (m, 4H), 8.14 (m, 10H), 7.43 (m, 12H), 5.36 (m, 8H), 1.56 (s, 18H). The ^{13}C NMR spectrum was not recorded due to its poor solubility. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{78}H_{52}N_6O_3$, 1121.4174; found 1121.4174. Anal. Calcd (%) for $C_{78}H_{52}N_6O_3$: C, 83.55; H, 4.67; N, 7.49. Found: C, 83.89; H, 4.68; N, 7.43.

Computational Details

The geometric optimization of ground-state (S_0) and the excited states (S_1 and T_1) were carried out with density functional theory (DFT) and time-dependent DFT (TD-DFT) methods in *Gaussian16* package.[5] The MN15[6] functional and 6-31G(d,p)[7,8] basis set were used for all atoms. Dispersion interaction was described using the D3BJ scheme with the specified parameter developed by Grimme and coworkers.[9-11] The solvent effects of toluene were considered using the polarizable continuum model (PCM).[12-14] Frequency analyses of all optimized geometries were performed at the same computational level to confirm that all geometries are present on the potential energy surfaces as true minima. The hole and electron density distribution analyses were performed to characterize the nature of the electronic states with the Multiwfn 3.8_dev package[15,16] and VMD 1.9.3 package[17]. The reduced density gradient (RDG)[18] was also analyzed by the Multiwfn 3.8_dev package. The RDG distribution is divided into three colors including blue, green and red, which represents strong electrostatic interactions like hydrogen-bonding interactions, van der Waals interactions like dispersion interaction, and repulsion interactions like steric effects between the atom of the ring, respectively. Besides, the peaks in the region of Sign(λ_2)ρ<0, =0 and >0 of the scatter graphs are in the blue, green, and red, respectively.

Intramolecular symmetry-adapted perturbation theory (I-SAPT)[19] was used to quantitatively describe the intramolecular interactions between the selected fragments. The version of I-SAPT exploited here is based on zero-order SAPT (SAPT0),[20] which considers Hartree-Fock wavefunctions and describes dispersion terms within second-order perturbation theory. A truncated aug-cc-pVDZ basis set (jun-cc-pVDZ) was used because of its reliable results for intramolecular and intermolecular noncovalent interactions demonstrated by earlier investigations.[21-24] All the I-SAPT computations were carried out with the Psi4 code.[25]

Figures

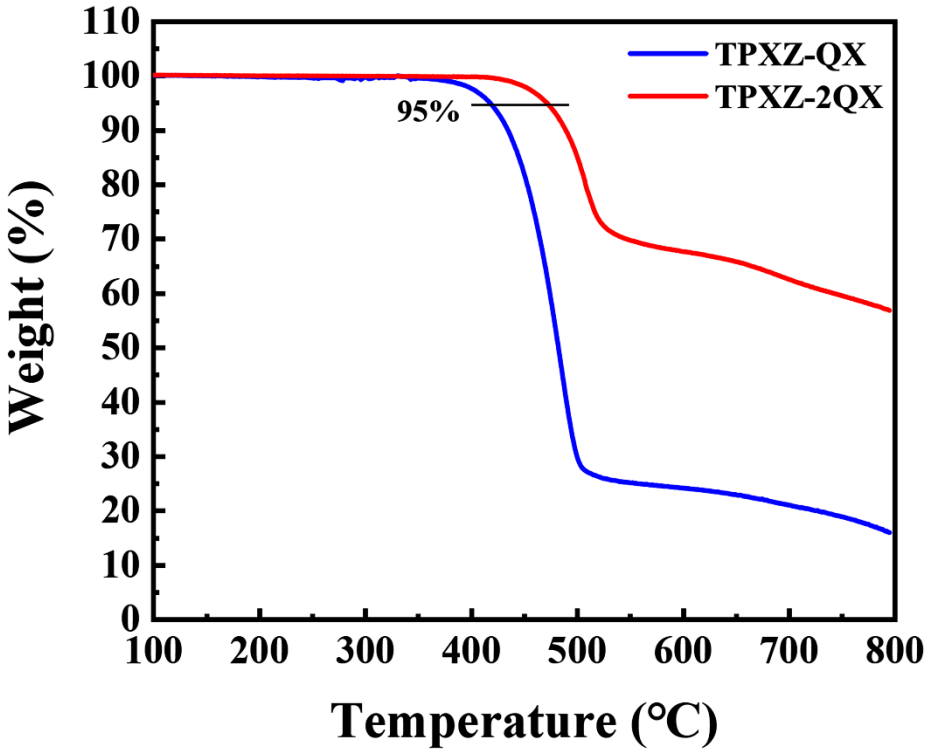


Fig. S1 Thermogravimetric (TGA) curves recorded for **TPXZ-QX** and **TPXZ-2QX**.

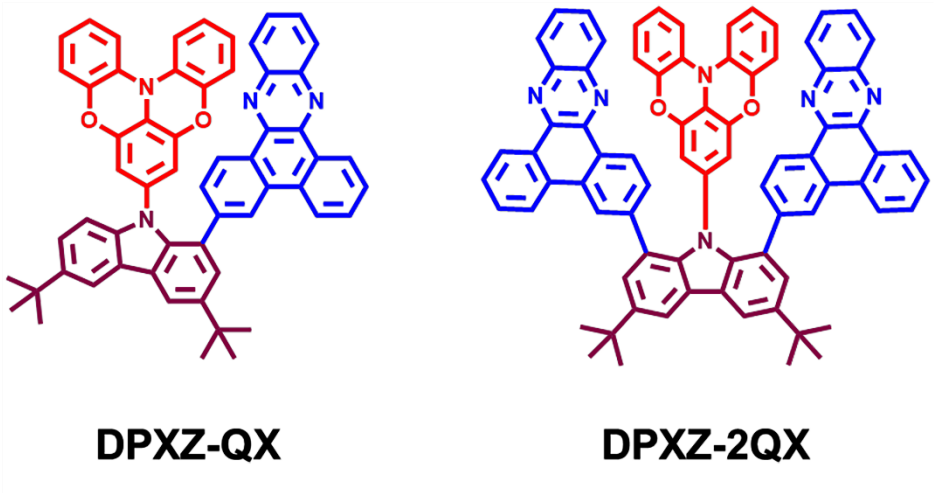


Fig. S2 Chemical structures of **DPXZ-QX** and **DPXZ-2QX** reported in reference.[1]

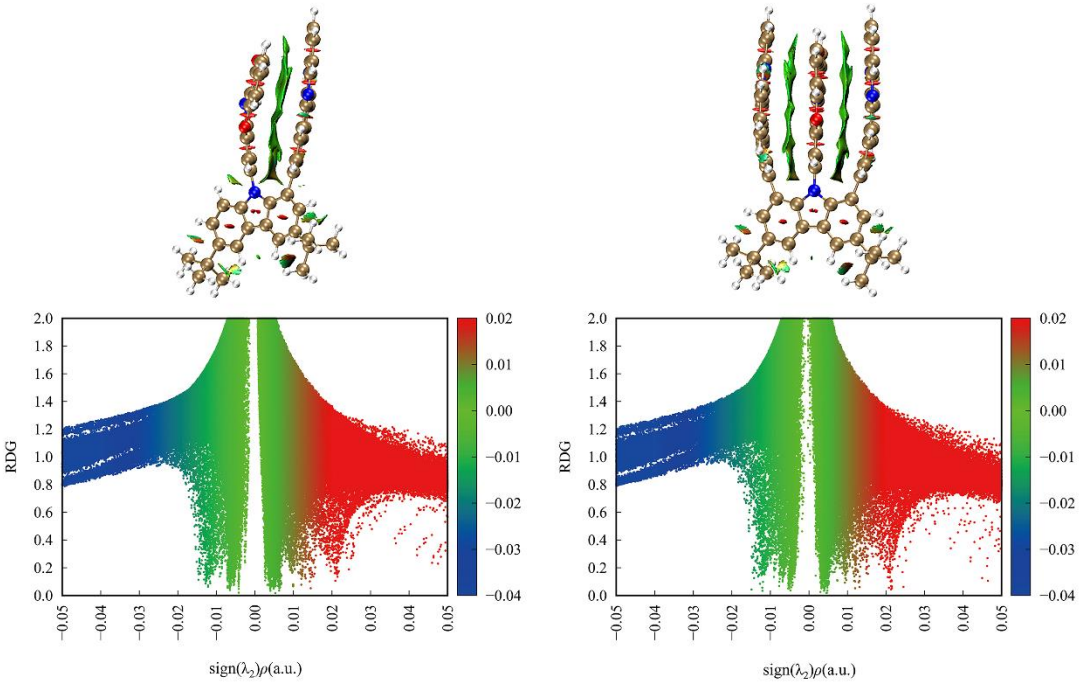


Fig. S3 Reduced density gradient (RDG) isosurfaces (isosurface value: 0.6) and scatter graphs of **TPXZ-QX** (left) and **TPXZ-2QX** (right) at their optimized ground state geometries.

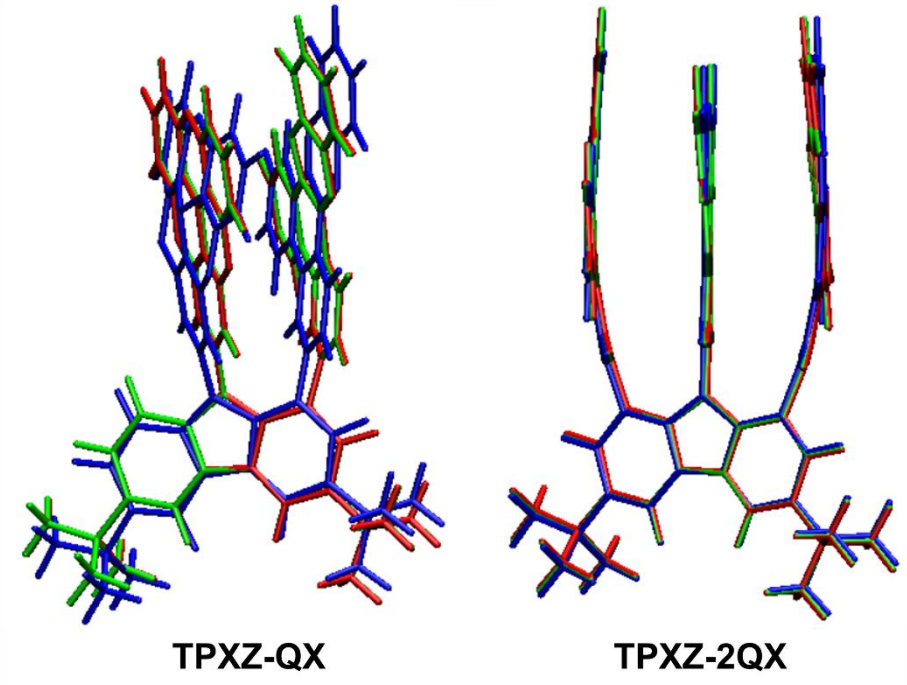


Fig. S4 Overlap graphs of the optimized S_0 (blue), S_1(red) and T_1 (green) states of the **TPXZ-QX** and **TPXZ-2QX**.

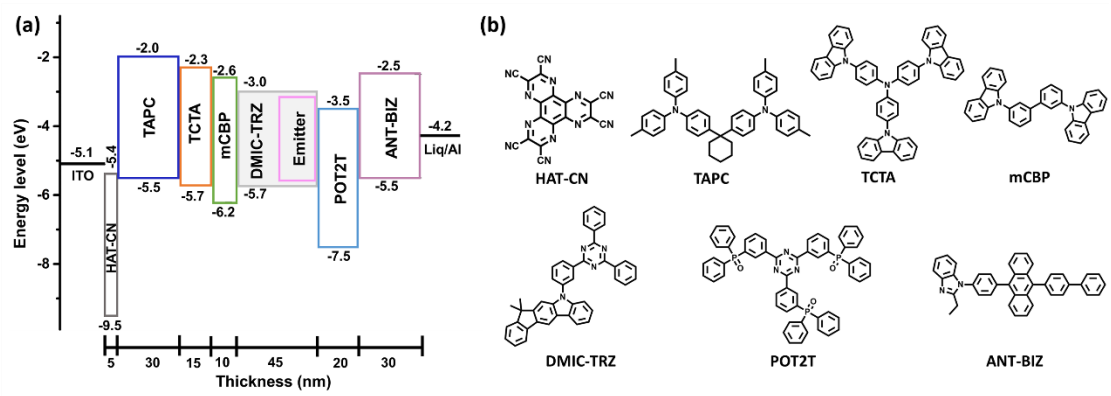


Fig. S5 (a) Device structure of the OLED doped with **TPXZ-QX** and **TPXZ-2QX**. (b) Chemical structures of the organic compounds used in the device fabrications.

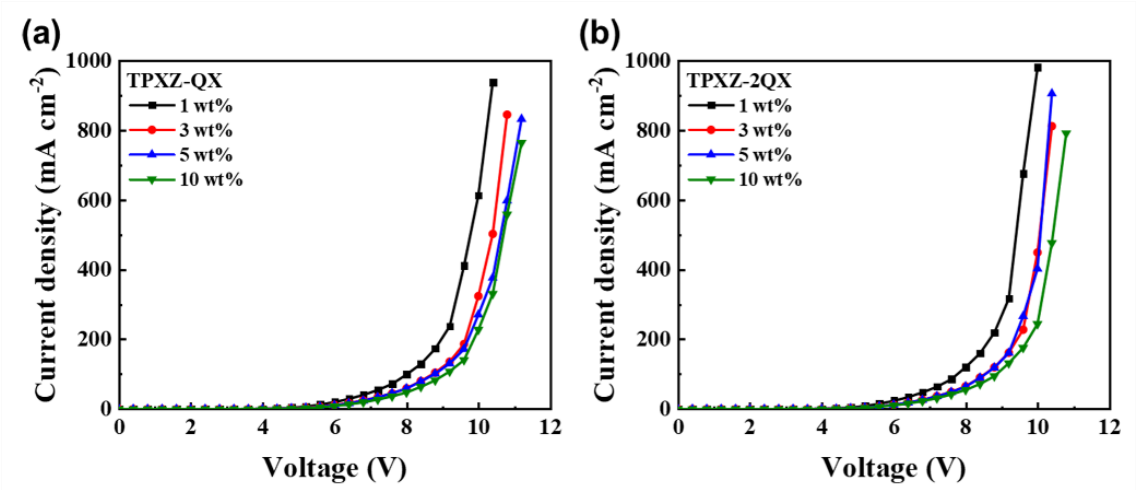


Fig. S6 (a) Current density-voltage curves of the devices doped with **TPXZ-QX** and **TPXZ-2QX**.

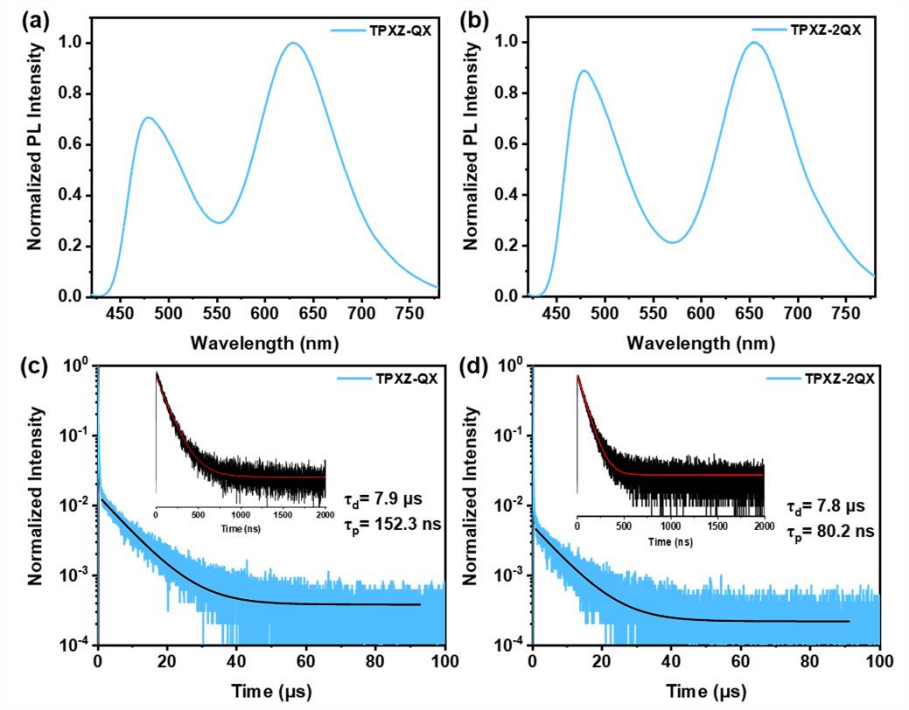


Fig. S7 (a and b) Photoluminescence spectra and (c and d) transient characteristics of **TPXZ-QX** and **TPXZ-2QX** in doped DMIC-TRZ film (3 wt%).

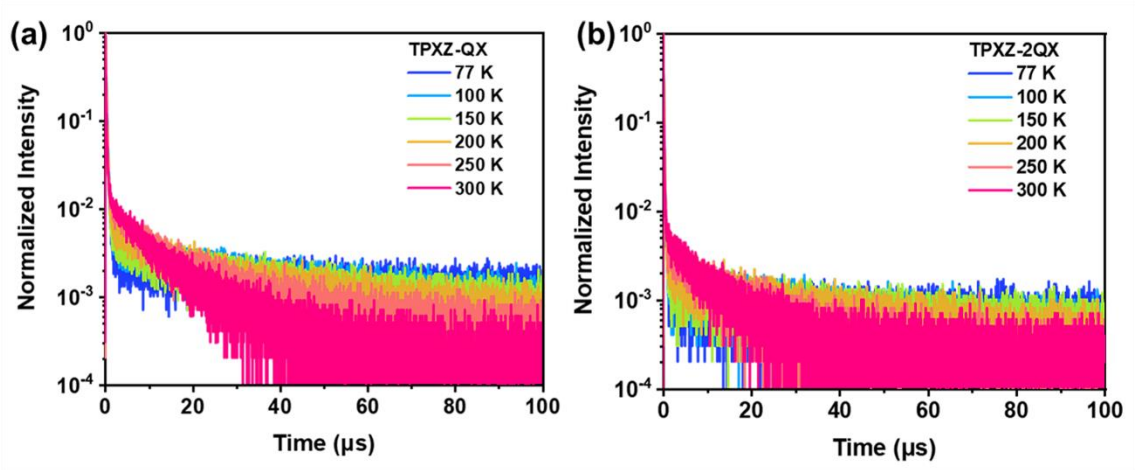


Fig. S8 The temperature-dependent transient PL characteristics of **TPXZ-QX** and **TPXZ-2QX** in 3 wt % DMIC-TRZ film.

Tables

Table S1. Crystallographic Data for **TPXZ-QX** and **TPXZ-2QX**.

Compound	**TPXZ-QX**	**TPXZ-2QX**
CCDC NO.	2223327	2223328
Formula	$C_{58}H_{42}N_4O_3\cdot(CH_2Cl_2)$	$C_{78}H_{52}N_6O_3\cdot(CHCl_3)$
Formula weight	927.88	1240.62
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/n$
a/Å	11.9390(13)	13.0796(4)
b/Å	12.0965(11)	32.0909(10)
c/Å	17.2673(16)	13.9618(4)
α/°	103.388(8)	90
β/°	108.096(9)	97.426(2)
γ/°	95.332(8)	90
Volume/Å^3	2269.0(4)	5811.1(3)
Z	2	4
ρ_{calc}g/cm^3	1.358	1.418
μ/mm^{-1}	0.197	1.914
F(000)	968.0	2576.0
Crystal size/mm^3	0.35 × 0.26 × 0.18	0.12 × 0.08 × 0.05
2Θ range (deg)	3.676-58.842	6.954-125.156
GOF on F^2	1.032	1.263
R_1/wR_2 [I>=2σ (I)]	0.0727/ 0.1914	0.0947/ 0.2807

Table S2. Summary of the Excited State Kinetic Parameters of **TPXZ-QX** and **TPXZ-2QX** in Doped mCBP Films.

Compound	Φ_{PL} (%)	τ_p (ns)	τ_d (μs)	Φ_p/Φ_d	$k_{r,S}$ ($\times10^6$ s^{-1})	$k_{nr,S}$ ($\times10^6$ s^{-1})	k_{ISC} ($\times10^6$ s^{-1})	k_{RISC} ($\times10^5$ s^{-1})
TPXZ-QX	41	94.4	6.9	0.34/0.07	3.60	5.18	1.81	1.75
TPXZ-2QX	32	42.2	7.2	0.29/0.03	6.87	14.6	2.22	1.53

Table S3. Electronic Interaction Energies (kcal/mol) between Selected Fragments in **DPXZ-2QX**, **TPXZ-QX** and **TPXZ-2QX** at their S_0, S_1 and T_1 minima by the I-SAPT Approach[a]

Compound	Frag 1	Frag 2	Minimum	Elst	Exch	Ind	Disp	Total
DPXZ-2QX	DPXZ	2QX	S_0	-22.3	80.2	-7.4	-76.3	-25.8
TPXZ-QX	TPXZ	QX	S_0	-13.0	45.6	-4.0	-43.5	-15.0
			S_1	-17.3	55.3	-5.1	-50.2	-17.3
			T_1	-19.3	60.0	-5.4	-52.5	-17.2
TPXZ-2QX	TPXZ	2QX	S_0	-27.9	97.2	-8.7	-93.8	-33.1
			S_1	-31.5	105.4	-9.2	-98.6	-33.9
			T_1	-34.4	112.2	-9.8	-101.6	-33.7

[a]The total interaction energies between the two fragments are decomposed into four terms: electrostatics (Elst), exchange-repulsion (Exch), induction/polarization (Ind), and dispersion (Disp)

Table S4. Calculated Vertical Emission Energies ($E_\perp$, eV), Wavelength (λ, nm), Oscillator Strengths (ƒ) and Electronic Configurations at the S_1 and T_1 Minima and Available Experiment Data of Two Complexes in Toluene.

Structure	State	$E_\perp$ (eV)	λ (nm)	ƒ	Configuration	Character	Exp. (eV)
				TPXZ-QX			
S_1-MIN	S_1	1.81	686	0.0113	LUMO→HOMO (98.9%)	^{1}CT	1.83
T_1-MIN	T_1	1.71	724	-	LUMO→HOMO (96.0%)	^{3}CT	-

TPXZ-2QX							
S_1-MIN	S_1	1.70	729	0.0103	LUMO→HOMO (99.2%)	^{1}CT	1.80
T_1-MIN	T_1	1.61	768		LUMO→HOMO (96.3%)	^{3}CT	

Table S5. Related Energies (eV) of the S_1, T_1 and T_2 States and Their Electronic Characteristics at the S_0, S_1 and T_1 Minima of Two Complexes in Toluene Solution.

Structure	S_0	S_1		T_1		T_2	
	Energy	Energy	Character	Energy	Character	Energy	Character
TPXZ-QX							
S_0-MIN	0.00	2.58	^{1}CT	2.46	^{3}LE	2.57	^{3}CT
S_1-MIN	0.27	2.08	^{1}CT	2.01	^{3}CT	2.44	^{3}LE
T_1-MIN	0.29	2.09	^{1}CT	2.00	^{3}CT	2.44	^{3}LE
TPXZ-2QX							
S_0-MIN	0.00	2.13	^{1}CT	2.05	^{3}CT	2.09	^{3}CT’
S_1-MIN	0.22	1.92	^{1}CT	1.85	^{3}CT	2.18	^{3}CT’
T_1-MIN	0.23	1.93	^{1}CT	1.84	^{3}CT	2.19	^{3}CT’

Table S6. Device Data of the Doped Red TSCT-TADF OLEDs (λ_{max} ≥ 580 nm) Based on Selected Representative Emitters in the Literature and Comparison with This Work.

Emitter	EQE_{max} [%]	$EQE_{1000cd\ m\text{-}2}$ [%]	$\lambda_{EL,max}$ [nm]	Ref.
TPXZ-2QX (1 wt%)	11.4	7.7	665	This work
TPXZ-QX (1 wt%)	13.8	11.7	632	This work
SAF36DCPP	16.12	10.32	604	[26]
SAF27DCPP	11.8	6.14	604	[26]
DPXZ-2QX (6 wt%)	23.2	14.4	609	[1]
DPXZ-2QX (12 wt%)	21.1	18.9	616	[1]
RD-2TF	10.3	7.8	626	[27]
P5-05	1.0	0.3	616	[28]

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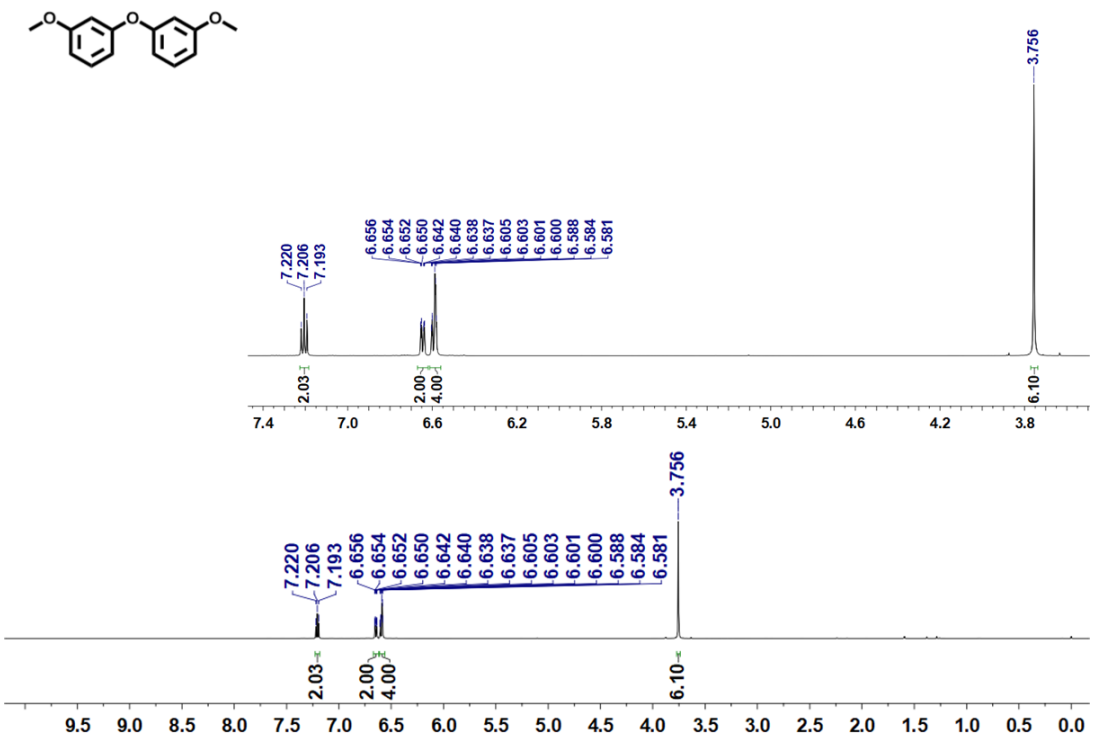
NMR Spectra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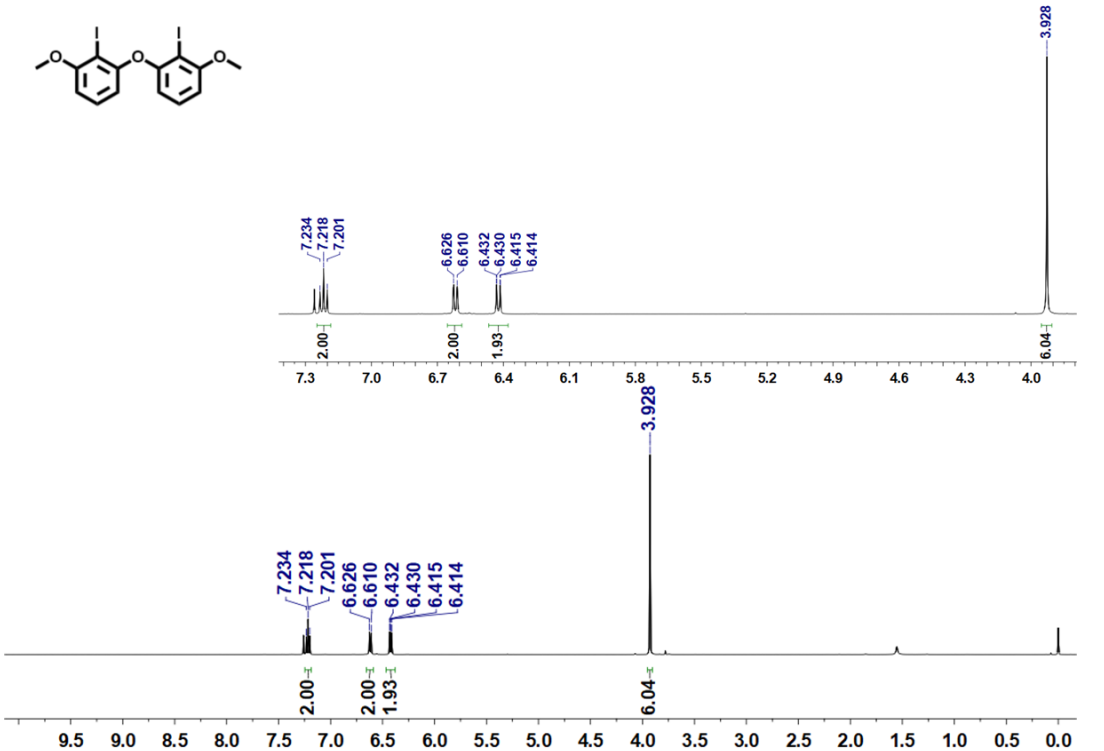
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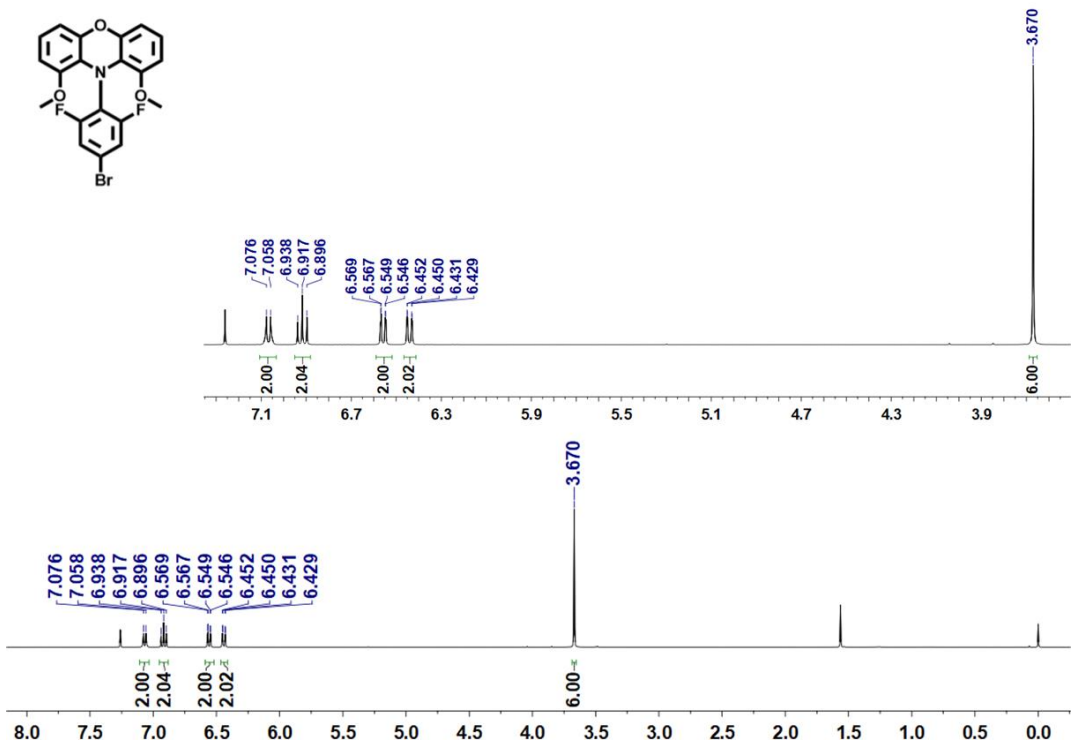
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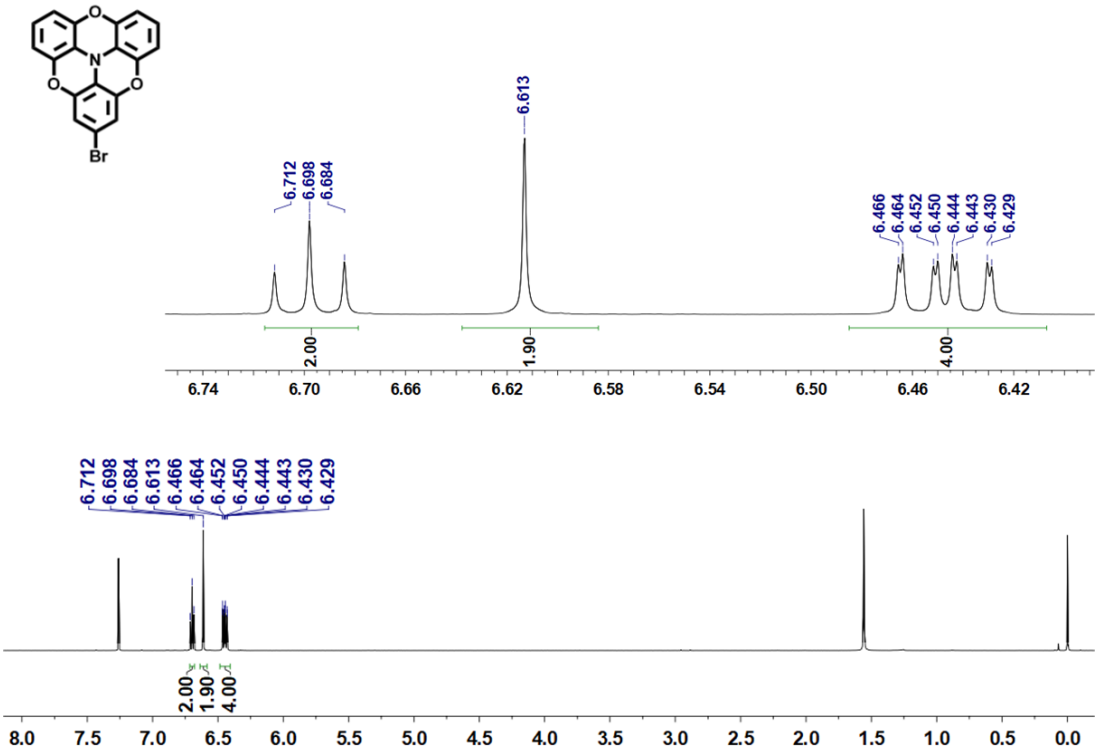
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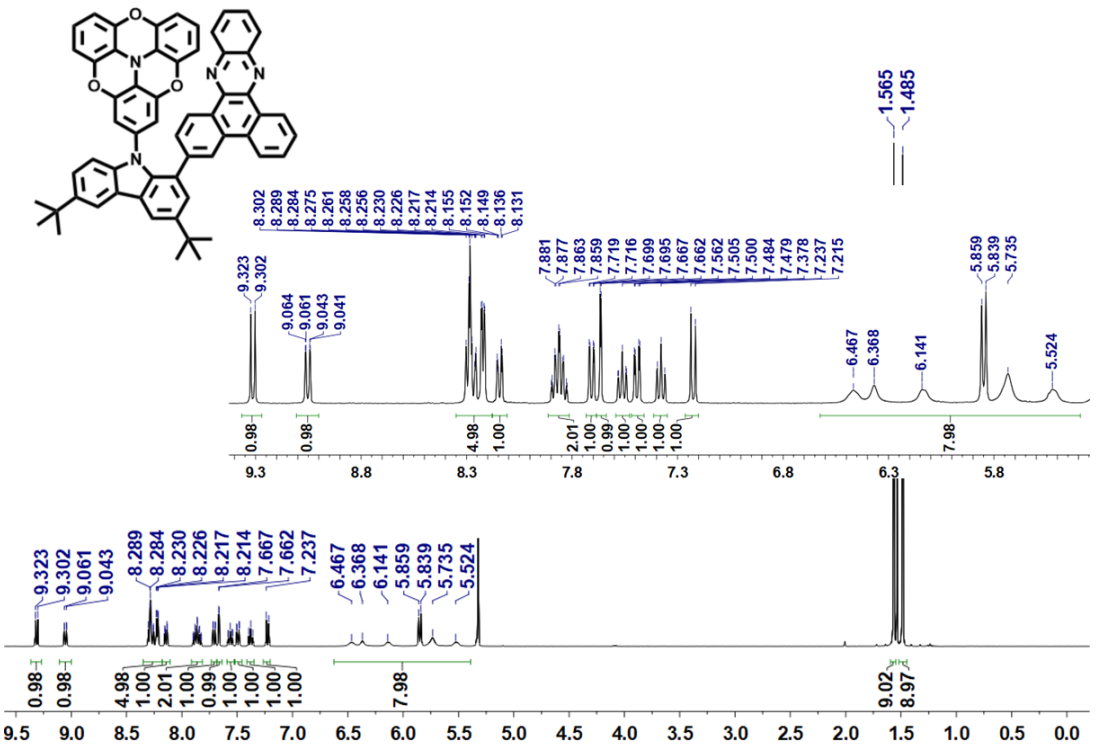

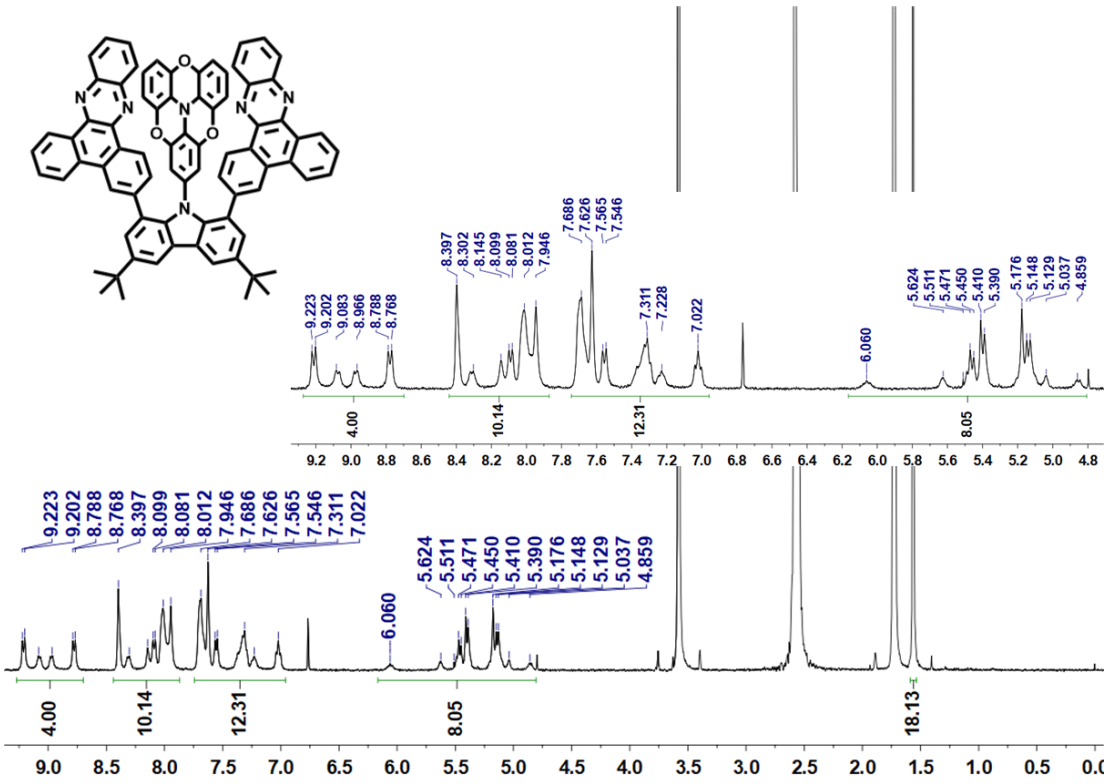

Cartesian Coordinates of Optimized Structures

In xyz format (unit: Angstrom)

TPXZ-QX

S0-MIN -2677.16522266 Hartree

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S1-MIN -2677.08894383 Hartree

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H	5.394868000	1.446542000	-4.321156000
C	-7.429990000	-3.499185000	-1.082891000
C	7.634588000	1.632315000	-0.804013000
H	8.676004000	1.378834000	-0.986364000
C	5.490578000	-0.123586000	-2.868984000
H	6.552992000	-0.304900000	-2.978190000
C	7.061951000	2.752860000	-1.429652000
H	7.661234000	3.368891000	-2.095774000
C	-5.433734000	5.413568000	-0.513691000
H	-4.384019000	5.689116000	-0.366158000
H	-6.037587000	6.324290000	-0.419364000
H	-5.545028000	5.029910000	-1.533934000
C	-8.169017000	-2.884002000	-2.283231000
H	-9.108052000	-3.421841000	-2.462135000
H	-7.557526000	-2.945948000	-3.190165000
H	-8.412770000	-1.830417000	-2.109212000
C	-7.191187000	-4.983050000	-1.378980000
H	-8.154415000	-5.479510000	-1.541191000
H	-6.690824000	-5.486117000	-0.543514000
H	-6.585829000	-5.122699000	-2.282030000
C	-8.324140000	-3.397249000	0.164265000
H	-8.569449000	-2.355951000	0.399328000
H	-7.826238000	-3.834011000	1.036941000
H	-9.264886000	-3.935995000	-0.002590000
O	5.396870000	-1.801589000	-1.180094000
H	-2.716264000	-3.175875000	-0.737278000

T1-MIN -2677.09187671 Hartree

O	1.231822000	-2.827814000	1.010321000
O	1.417204000	0.627496000	-2.326145000
N	-2.736833000	-0.375221000	-0.113597000
N	4.792085000	0.382344000	1.143738000
N	3.587528000	2.579864000	-0.237617000
N	2.695807000	-1.313138000	-0.806308000
C	-5.000847000	-0.659604000	-0.328472000
C	0.697619000	1.285995000	1.699440000
C	-3.751060000	-1.310250000	-0.371704000
C	1.350964000	0.297568000	2.548813000

C	-0.703550000	1.411764000	1.637085000
H	-1.333019000	0.755155000	2.233636000
C	2.906758000	1.826594000	0.647921000
C	-3.657776000	3.196352000	0.573450000
H	-3.223669000	4.158985000	0.840192000
C	2.733061000	0.029955000	2.350106000
C	3.507092000	0.760119000	1.362126000
C	-5.588405000	1.840339000	0.106557000
H	-6.659050000	1.701266000	-0.014272000
C	-5.053671000	3.094893000	0.390571000
C	-1.364746000	-0.639882000	-0.330645000
C	-0.655442000	0.100242000	-1.290621000
H	-1.149003000	0.864542000	-1.880146000
C	-1.325877000	2.255181000	0.726688000
C	-3.345586000	0.878448000	0.106992000
C	-4.739169000	0.736600000	-0.035249000
C	-2.781354000	2.117069000	0.472939000
C	1.478653000	2.065774000	0.806879000
C	0.657710000	-0.440569000	3.531613000
H	-0.392748000	-0.233664000	3.717211000
C	0.704262000	-0.109734000	-1.426636000
C	2.571506000	-3.049324000	0.850888000
C	-0.743163000	-1.639968000	0.430684000
H	-1.295272000	-2.189578000	1.185633000
C	0.613657000	-1.865845000	0.265833000
C	-6.170315000	-1.382003000	-0.565890000
H	-7.130518000	-0.869835000	-0.527638000
C	-0.534467000	3.113757000	-0.065922000
H	-1.021333000	3.793753000	-0.762230000
C	1.343859000	-1.087963000	-0.645227000
C	0.842013000	3.016437000	-0.021001000
H	1.475074000	3.615502000	-0.667929000
C	2.752222000	0.384099000	-2.504120000
C	5.512496000	1.168017000	0.289379000
C	-3.659083000	-2.665570000	-0.679526000
C	-5.915062000	4.352432000	0.533547000
C	4.912742000	2.276759000	-0.395720000
C	3.410277000	-0.587575000	-1.733029000
C	3.463375000	1.091097000	-3.458205000

H	2.956586000	1.852022000	-4.040245000
C	3.365997000	-0.961584000	3.137605000
H	4.420657000	-1.146364000	2.952526000
C	3.198665000	-4.033089000	1.601976000
H	2.615611000	-4.605138000	2.314542000
C	1.292319000	-1.410494000	4.288229000
H	0.734952000	-1.957895000	5.043621000
C	-6.110768000	-2.748815000	-0.856839000
C	3.320154000	-2.291339000	-0.057965000
C	6.871867000	0.869845000	0.043098000
H	7.295970000	0.017920000	0.569393000
C	-4.844166000	-3.362203000	-0.912087000
H	-4.771595000	-4.419637000	-1.145951000
C	-5.756465000	4.930951000	1.949712000
H	-6.077001000	4.204507000	2.704526000
H	-6.370264000	5.833703000	2.056261000
H	-4.717155000	5.204197000	2.160691000
C	4.695828000	-2.508185000	-0.225726000
C	5.707389000	3.042332000	-1.272035000
H	5.229229000	3.879598000	-1.774565000
C	4.570358000	-4.230444000	1.437732000
H	5.066086000	-4.991428000	2.031473000
C	2.661230000	-1.673026000	4.087853000
H	3.163106000	-2.431966000	4.683254000
C	-7.400448000	4.063428000	0.297385000
H	-7.578033000	3.666618000	-0.708896000
H	-7.972201000	4.992592000	0.398840000
H	-7.792645000	3.346608000	1.028036000
C	5.328035000	-3.481737000	0.530966000
H	6.392345000	-3.642740000	0.404099000
C	4.776354000	-0.855473000	-1.914748000
C	4.823087000	0.812529000	-3.630773000
H	5.384934000	1.377682000	-4.366776000
C	-7.411018000	-3.519665000	-1.109468000
C	7.630428000	1.636719000	-0.833872000
H	8.676517000	1.393821000	-1.002964000
C	5.487518000	-0.156912000	-2.876065000
H	6.548261000	-0.345284000	-2.990511000
C	7.045686000	2.729446000	-1.493164000

H	7.639045000	3.335720000	-2.173155000
C	-5.460338000	5.402644000	-0.493975000
H	-4.411532000	5.682185000	-0.347436000
H	-6.067767000	6.310616000	-0.396078000
H	-5.571721000	5.021417000	-1.515113000
C	-8.149073000	-2.902826000	-2.309573000
H	-9.084284000	-3.445171000	-2.494899000
H	-7.533686000	-2.956603000	-3.214399000
H	-8.399549000	-1.851543000	-2.131211000
C	-7.162609000	-5.000622000	-1.412185000
H	-8.122344000	-5.501686000	-1.580904000
H	-6.662767000	-5.505165000	-0.577297000
H	-6.552763000	-5.132144000	-2.313432000
C	-8.310667000	-3.429359000	0.134615000
H	-8.563016000	-2.390720000	0.373969000
H	-7.813567000	-3.867581000	1.007023000
H	-9.247591000	-3.972777000	-0.038600000
O	5.403074000	-1.799440000	-1.151975000
H	-2.699531000	-3.170313000	-0.742847000

TPXZ-2QX

S0-MIN -3553.87127801 Hartree

O	0.875965000	-1.214918000	2.086036000
O	0.874850000	1.206616000	-2.088783000
N	-3.296520000	-0.012017000	-0.004359000
N	3.925083000	2.921167000	1.321372000
N	2.397282000	-4.208379000	0.645064000
N	2.378415000	4.208026000	-0.644595000
N	3.941779000	-2.915863000	-1.318911000
N	2.267751000	-0.003374000	-0.001200000
C	-5.463053000	-0.740603000	-0.031890000
C	-0.270248000	2.816203000	1.511488000
C	-4.111162000	-1.151327000	-0.076391000
C	0.538373000	2.287794000	2.623508000
C	-1.651439000	2.578646000	1.429285000
H	-2.146821000	1.975578000	2.184457000
C	1.811047000	3.593833000	0.382953000
C	-4.867887000	3.390239000	0.140306000

H	-4.622220000	4.449324000	0.208596000
C	1.947637000	2.333622000	2.551791000
C	2.603483000	2.955498000	1.398587000
C	-6.509139000	1.639980000	0.027087000
H	-7.535173000	1.284183000	-0.010191000
C	-6.222867000	3.001949000	0.065374000
C	-1.872056000	-0.008144000	-0.002993000
C	-1.190282000	0.568775000	-1.077999000
H	-1.730132000	1.013501000	-1.907976000
C	-2.404515000	2.987460000	0.332412000
C	-0.253775000	-2.826768000	-1.514661000
C	0.366452000	-3.519350000	-0.450607000
C	-4.119087000	1.121590000	0.067729000
C	1.828974000	-3.596786000	-0.383519000
C	2.620472000	-2.955511000	-1.398114000
C	1.963770000	-2.336134000	-2.552186000
C	-5.465929000	0.706683000	0.023395000
C	-3.800276000	2.494709000	0.173813000
C	0.348693000	3.510604000	0.447840000
C	-0.047433000	1.697889000	3.759253000
H	-1.127776000	1.665453000	3.858119000
C	0.196543000	0.595587000	-1.056491000
C	-1.636012000	-2.594418000	-1.434163000
H	-2.132765000	-1.993051000	-2.189780000
C	0.554412000	-2.295213000	-2.625531000
C	2.257468000	-1.172974000	2.098875000
C	3.748895000	-4.194269000	0.723404000
C	-1.189840000	-0.582677000	1.073083000
H	-1.729478000	-1.029841000	1.901885000
C	-0.032056000	-1.707258000	-3.761951000
H	-1.112398000	-1.678651000	-3.862053000
C	0.197041000	-0.605211000	1.053371000
C	-6.494262000	-1.680352000	-0.035214000
H	-7.527525000	-1.338345000	0.001372000
C	-2.389324000	-3.006430000	-0.338512000
C	-1.793798000	3.777330000	-0.657344000
H	-2.383459000	4.120989000	-1.504015000
C	0.884068000	-0.003975000	-0.001259000
C	-0.431864000	4.026142000	-0.600416000

H	0.073671000	4.568583000	-1.393024000
C	2.256570000	1.171201000	-2.098533000
C	-1.776642000	-3.795164000	0.651154000
H	-2.366118000	-4.141965000	1.496690000
C	-0.413723000	-4.038596000	0.596157000
H	0.092693000	-4.579624000	1.389174000
C	4.514137000	3.534361000	0.268084000
C	-3.787082000	-2.519426000	-0.180726000
C	-7.307003000	4.082759000	0.050474000
C	3.730174000	4.199481000	-0.720794000
C	2.963051000	0.575786000	-1.055023000
C	2.944289000	1.737322000	-3.163802000
H	2.380331000	2.199178000	-3.967468000
C	2.729983000	1.786515000	3.582905000
H	3.810296000	1.816733000	3.475732000
C	2.945495000	-1.734658000	3.166291000
H	2.381932000	-2.198000000	3.969378000
C	0.732832000	1.165792000	4.774813000
H	0.253000000	0.718057000	5.640727000
C	-6.202085000	-3.045777000	-0.071574000
C	4.402084000	-4.841688000	1.807472000
H	3.781657000	-5.342995000	2.544777000
C	5.947025000	-3.501430000	-0.138335000
H	6.512344000	-2.969737000	-0.898265000
C	2.963460000	-0.575982000	1.055942000
C	5.929771000	3.515258000	0.144244000
H	6.495988000	2.985456000	0.904823000
C	2.745420000	-1.786214000	-3.582338000
H	3.825712000	-1.812785000	-3.473914000
C	4.531703000	-3.526391000	-0.264488000
C	0.747548000	-1.172323000	-4.776537000
H	0.267177000	-0.726197000	-5.642989000
C	-4.850372000	-3.427637000	-0.145870000
H	-4.589781000	-4.480759000	-0.211588000
C	-7.222567000	4.918934000	1.338552000
H	-7.373744000	4.288321000	2.221597000
H	-7.996230000	5.696497000	1.332661000
H	-6.250003000	5.413117000	1.436262000
C	4.356130000	-0.530745000	1.065278000

C	4.382482000	4.850122000	-1.803477000
H	3.761231000	5.349196000	-2.541598000
C	4.341247000	-1.673182000	3.181109000
H	4.885426000	-2.115111000	4.009942000
C	6.550080000	-4.135015000	0.920072000
H	7.632163000	-4.121594000	1.017005000
C	5.771718000	-4.814203000	1.898089000
H	6.271913000	-5.310302000	2.725167000
C	2.130650000	1.205476000	4.687498000
H	2.742148000	0.775750000	5.475852000
C	-8.714133000	3.484927000	-0.040376000
H	-8.841586000	2.893102000	-0.954169000
H	-9.452872000	4.294027000	-0.057117000
H	-8.936180000	2.845205000	0.821581000
C	5.053307000	-1.075056000	2.138437000
H	6.137849000	-1.049096000	2.127971000
C	4.355935000	0.537220000	-1.061311000
C	4.340321000	1.681943000	-3.175896000
H	4.884226000	2.127183000	-4.003134000
C	2.145394000	-1.207115000	-4.687579000
H	2.756324000	-0.775203000	-5.475182000
C	-7.345983000	-4.064866000	-0.046987000
C	6.531923000	4.151888000	-0.912821000
H	7.614206000	4.142986000	-1.008002000
C	5.052887000	1.085967000	-2.132356000
H	6.137511000	1.064893000	-2.119641000
C	5.752356000	4.828364000	-1.891791000
H	6.251876000	5.326929000	-2.717791000
C	-7.097036000	5.004187000	-1.162841000
H	-6.118959000	5.496291000	-1.130722000
H	-7.866632000	5.785589000	-1.178825000
H	-7.161845000	4.436650000	-2.097757000
C	-8.265427000	-3.836358000	-1.258343000
H	-9.091691000	-4.557719000	-1.244945000
H	-7.712349000	-3.962328000	-2.195605000
H	-8.697340000	-2.829713000	-1.251413000
C	-6.841561000	-5.510417000	-0.095492000
H	-7.697386000	-6.194115000	-0.065674000
H	-6.196619000	-5.741536000	0.760104000

H	-6.282312000	-5.712741000	-1.016115000
C	-8.162002000	-3.884759000	1.244156000
H	-8.587370000	-2.877701000	1.313333000
H	-7.534634000	-4.049595000	2.127093000
H	-8.990147000	-4.603648000	1.269532000
O	5.057320000	0.004156000	0.002376000

S1-MIN -3553.80080348 Hartree

O	-0.910540000	1.041638000	2.125598000
O	-0.846532000	-1.297881000	-2.074652000
N	3.279904000	0.033373000	0.004379000
N	-3.721522000	-2.807081000	1.342170000
N	-2.628895000	4.054408000	0.678673000
N	-2.180617000	-4.187653000	-0.639622000
N	-4.134222000	2.797201000	-1.336628000
N	-2.272428000	-0.118846000	-0.002999000
C	5.394025000	0.907084000	-0.052134000
C	0.495658000	-2.869921000	1.573720000
C	4.018296000	1.229727000	-0.056150000
C	-0.289632000	-2.362181000	2.690993000
C	1.878104000	-2.627453000	1.460924000
H	2.385788000	-2.036264000	2.219966000
C	-1.613141000	-3.578763000	0.425000000
C	5.089479000	-3.255802000	0.066324000
H	4.918746000	-4.329307000	0.133030000
C	-1.706040000	-2.371222000	2.591947000
C	-2.376969000	-2.932362000	1.427817000
C	6.603068000	-1.394175000	-0.065805000
H	7.600341000	-0.966258000	-0.118443000
C	6.412004000	-2.772588000	-0.040908000
C	1.862528000	-0.051827000	0.020609000
C	1.199059000	-0.652268000	-1.055484000
H	1.751494000	-1.077580000	-1.885730000
C	2.600607000	-2.995067000	0.335224000
C	0.065639000	2.746413000	-1.471979000
C	-0.578579000	3.419111000	-0.408787000
C	4.186881000	-1.047899000	0.029901000
C	-2.041372000	3.481297000	-0.361901000
C	-2.812282000	2.860081000	-1.402461000

C	-2.133765000	2.265886000	-2.557326000
C	5.496088000	-0.537303000	-0.032207000
C	3.963925000	-2.437617000	0.135680000
C	-0.160369000	-3.517019000	0.494114000
C	0.300700000	-1.818372000	3.852388000
H	1.382028000	-1.826426000	3.959040000
C	-0.184926000	-0.711656000	-1.038954000
C	1.453884000	2.555109000	-1.384150000
H	1.978748000	1.986636000	-2.146145000
C	-0.722629000	2.210168000	-2.596133000
C	-2.277600000	1.011478000	2.119165000
C	-3.979527000	4.017446000	0.744085000
C	1.165151000	0.501584000	1.103945000
H	1.695390000	0.952375000	1.935722000
C	-0.116664000	1.615793000	-3.719665000
H	0.964941000	1.563997000	-3.791306000
C	-0.217385000	0.477390000	1.094842000
C	6.363266000	1.909178000	-0.059562000
H	7.415887000	1.630727000	-0.054435000
C	2.187890000	2.985729000	-0.282197000
C	1.964476000	-3.759622000	-0.667079000
H	2.536499000	-4.079468000	-1.535878000
C	-0.894639000	-0.133966000	0.026375000
C	0.609397000	-4.012515000	-0.583500000
H	0.079163000	-4.537369000	-1.372001000
C	-2.212666000	-1.254149000	-2.118429000
C	1.545870000	3.743114000	0.713624000
H	2.121496000	4.104258000	1.562354000
C	0.178165000	3.948154000	0.650860000
H	-0.348073000	4.473830000	1.441197000
C	-4.317482000	-3.442993000	0.286981000
C	3.609847000	2.574812000	-0.137000000
C	7.567832000	-3.774707000	-0.097668000
C	-3.544985000	-4.146956000	-0.696124000
C	-2.942469000	-0.674247000	-1.067478000
C	-2.886218000	-1.777295000	-3.207551000
H	-2.318785000	-2.237109000	-4.008376000
C	-2.477148000	-1.841140000	3.652183000
H	-3.557778000	-1.854768000	3.537170000

C	-2.983055000	1.546360000	3.185553000
H	-2.436473000	1.981459000	4.014257000
C	-0.469611000	-1.300228000	4.878305000
H	0.011104000	-0.897047000	5.765687000
C	5.986619000	3.254689000	-0.063183000
C	-4.650377000	4.610460000	1.848708000
H	-4.044787000	5.102753000	2.604021000
C	-6.158255000	3.297455000	-0.148095000
H	-6.710181000	2.782844000	-0.929145000
C	-2.975008000	0.437007000	1.048683000
C	-5.721680000	-3.394924000	0.145476000
H	-6.278086000	-2.848070000	0.903509000
C	-2.897039000	1.746814000	-3.617322000
H	-3.978906000	1.798228000	-3.541615000
C	-4.743320000	3.365270000	-0.270378000
C	-0.878017000	1.103600000	-4.759707000
H	-0.382150000	0.654085000	-5.615268000
C	4.613654000	3.550143000	-0.105573000
H	4.284617000	4.584921000	-0.151610000
C	7.575446000	-4.628783000	1.181347000
H	7.706068000	-3.999147000	2.068339000
H	8.400897000	-5.350178000	1.145061000
H	6.642667000	-5.190644000	1.297702000
C	-4.376759000	0.394127000	1.033257000
C	-4.222568000	-4.784614000	-1.758565000
H	-3.615112000	-5.317472000	-2.486294000
C	-4.378288000	1.475225000	3.172258000
H	-4.933442000	1.887347000	4.008633000
C	-6.777572000	3.871334000	0.934164000
H	-7.858468000	3.823430000	1.030446000
C	-6.017986000	4.536518000	1.938006000
H	-6.532834000	4.986795000	2.781878000
C	-1.873849000	-1.311922000	4.775867000
H	-2.482285000	-0.907644000	5.581378000
C	8.927144000	-3.079372000	-0.217665000
H	8.987990000	-2.469049000	-1.126207000
H	9.719219000	-3.834914000	-0.265662000
H	9.128480000	-2.436526000	0.647081000
C	-5.085669000	0.906690000	2.109155000

H	-6.168854000	0.874986000	2.092525000
C	-4.345265000	-0.617409000	-1.102950000
C	-4.281603000	-1.692801000	-3.242122000
H	-4.812013000	-2.111476000	-4.090839000
C	-2.277060000	1.171536000	-4.713401000
H	-2.872323000	0.767570000	-5.527223000
C	7.064227000	4.343131000	-0.044850000
C	-6.360158000	-4.019503000	-0.918867000
H	-7.442920000	-3.973567000	-1.006646000
C	-5.019442000	-1.114398000	-2.206665000
H	-6.102560000	-1.091865000	-2.219163000
C	-5.604984000	-4.719331000	-1.875201000
H	-6.103727000	-5.217615000	-2.703096000
C	7.388422000	-4.694475000	-1.317111000
H	6.447743000	-5.253075000	-1.265638000
H	8.209246000	-5.420496000	-1.363258000
H	7.389012000	-4.113407000	-2.246004000
C	7.964319000	4.195733000	-1.283017000
H	8.743756000	4.967320000	-1.274553000
H	7.380744000	4.304742000	-2.203762000
H	8.458517000	3.218490000	-1.307271000
C	6.468661000	5.754351000	-0.050689000
H	7.280237000	6.489983000	-0.024352000
H	5.830513000	5.926553000	0.823724000
H	5.877220000	5.940137000	-0.954573000
C	7.922516000	4.189123000	1.222011000
H	8.412649000	3.210261000	1.259111000
H	7.309231000	4.296310000	2.123475000
H	8.703816000	4.958602000	1.242151000
O	-5.043279000	-0.105428000	-0.046666000

T1-MIN -3553.80371077 Hartree

O	-0.908360000	1.026901000	2.128494000
O	-0.843437000	-1.289356000	-2.085251000
N	3.284930000	0.029540000	0.001941000
N	-3.747917000	-2.773161000	1.341942000
N	-2.606418000	4.055688000	0.678576000
N	-2.213680000	-4.143403000	-0.646895000
N	-4.111411000	2.796182000	-1.335749000

N	-2.269624000	-0.145020000	0.004222000
C	5.405401000	0.887628000	-0.052649000
C	0.470470000	-2.847169000	1.567054000
C	4.031753000	1.219764000	-0.059688000
C	-0.312674000	-2.332790000	2.683527000
C	1.854669000	-2.616199000	1.457681000
H	2.366667000	-2.032044000	2.218995000
C	-1.642127000	-3.546946000	0.417708000
C	5.065105000	-3.272999000	0.075691000
H	4.885013000	-4.344877000	0.143769000
C	-1.730179000	-2.342335000	2.587316000
C	-2.401873000	-2.899945000	1.425991000
C	6.596077000	-1.424902000	-0.057646000
H	7.597447000	-1.006591000	-0.109961000
C	6.392376000	-2.801400000	-0.028855000
C	1.866603000	-0.052451000	0.018943000
C	1.201354000	-0.640332000	-1.066205000
H	1.754605000	-1.055556000	-1.901163000
C	2.576682000	-2.987555000	0.332001000
C	0.088239000	2.746631000	-1.471746000
C	-0.555752000	3.416092000	-0.406456000
C	4.183417000	-1.057003000	0.032114000
C	-2.018512000	3.478878000	-0.359850000
C	-2.789280000	2.856943000	-1.400160000
C	-2.110904000	2.263935000	-2.555678000
C	5.496937000	-0.557501000	-0.028795000
C	3.947166000	-2.444297000	0.138637000
C	-0.187888000	-3.492554000	0.487654000
C	0.279088000	-1.786986000	3.842409000
H	1.360557000	-1.792783000	3.947184000
C	-0.180141000	-0.705461000	-1.048145000
C	1.476429000	2.555376000	-1.384927000
H	2.000645000	1.987948000	-2.148182000
C	-0.699786000	2.212718000	-2.596929000
C	-2.274894000	1.001662000	2.117760000
C	-3.957246000	4.021942000	0.741672000
C	1.169015000	0.492594000	1.105231000
H	1.698096000	0.940761000	1.939276000
C	-0.093638000	1.624293000	-3.723466000

H	0.988033000	1.576953000	-3.797166000
C	-0.214217000	0.464047000	1.097324000
C	6.380865000	1.883943000	-0.059023000
H	7.431790000	1.599146000	-0.051579000
C	2.210993000	2.982935000	-0.282324000
C	1.936821000	-3.745166000	-0.672308000
H	2.507014000	-4.066589000	-1.541565000
C	-0.891392000	-0.146283000	0.027727000
C	0.579392000	-3.989253000	-0.589867000
H	0.046664000	-4.508023000	-1.380829000
C	-2.209843000	-1.252803000	-2.125130000
C	1.569373000	3.737394000	0.715939000
H	2.145167000	4.095961000	1.565663000
C	0.201501000	3.942285000	0.654336000
H	-0.324518000	4.465733000	1.446326000
C	-4.349006000	-3.414678000	0.295402000
C	3.631755000	2.567387000	-0.139029000
C	7.539188000	-3.814202000	-0.080016000
C	-3.580859000	-4.111773000	-0.695590000
C	-2.940776000	-0.683808000	-1.069193000
C	-2.883059000	-1.771817000	-3.216934000
H	-2.314634000	-2.222939000	-4.022052000
C	-2.500154000	-1.809571000	3.648368000
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C	-2.981226000	1.552682000	3.176871000
H	-2.434219000	1.993729000	4.002160000
C	-0.489881000	-1.266522000	4.868755000
H	-0.007362000	-0.860809000	5.753944000
C	6.012595000	3.231747000	-0.063895000
C	-4.628933000	4.621429000	1.842313000
H	-4.023545000	5.114616000	2.597220000
C	-6.136325000	3.305771000	-0.152842000
H	-6.687921000	2.789898000	-0.933312000
C	-2.972725000	0.420700000	1.050550000
C	-5.755643000	-3.375717000	0.166546000
H	-6.308969000	-2.833591000	0.929944000
C	-2.874283000	1.745236000	-3.615839000
H	-3.956208000	1.792569000	-3.538008000
C	-4.720856000	3.368344000	-0.271944000

C	-0.855007000	1.112672000	-4.763720000
H	-0.359112000	0.667777000	-5.621700000
C	4.641384000	3.536301000	-0.107110000
H	4.319080000	4.573218000	-0.152691000
C	7.535243000	-4.665569000	1.200821000
H	7.669113000	-4.035254000	2.086848000
H	8.354089000	-5.394641000	1.168483000
H	6.596992000	-5.218590000	1.315668000
C	-4.374909000	0.387236000	1.030433000
C	-4.260639000	-4.748277000	-1.754292000
H	-3.655958000	-5.272465000	-2.490447000
C	-4.375856000	1.489965000	3.159362000
H	-4.931636000	1.914616000	3.989102000
C	-6.756505000	3.886508000	0.925260000
H	-7.837836000	3.843018000	1.018851000
C	-5.997036000	4.552868000	1.928367000
H	-6.512358000	5.008519000	2.769084000
C	-1.894345000	-1.279082000	4.769744000
H	-2.500885000	-0.872838000	5.575633000
C	8.905182000	-3.131633000	-0.197403000
H	8.974491000	-2.524169000	-1.107248000
H	9.690447000	-3.894517000	-0.241040000
H	9.109637000	-2.488489000	0.666383000
C	-5.083467000	0.915123000	2.099057000
H	-6.166812000	0.892118000	2.078343000
C	-4.343038000	-0.623988000	-1.105425000
C	-4.278520000	-1.693687000	-3.248445000
H	-4.809064000	-2.109426000	-4.098564000
C	-2.254240000	1.175125000	-4.714514000
H	-2.849579000	0.771123000	-5.528280000
C	7.097180000	4.313301000	-0.045044000
C	-6.398597000	-4.007044000	-0.891146000
H	-7.482478000	-3.971051000	-0.968191000
C	-5.016624000	-1.120144000	-2.209506000
H	-6.099819000	-1.098147000	-2.221672000
C	-5.646832000	-4.697162000	-1.855940000
H	-6.148715000	-5.197812000	-2.680340000
C	7.355202000	-4.735005000	-1.298022000
H	6.409510000	-5.285240000	-1.248122000

H	8.169733000	-5.468319000	-1.340285000
H	7.363551000	-4.155936000	-2.228122000
C	7.997610000	4.159499000	-1.282202000
H	8.782039000	4.926028000	-1.273399000
H	7.415655000	4.271759000	-2.203585000
H	8.485446000	3.179033000	-1.305459000
C	6.510737000	5.728342000	-0.052382000
H	7.327023000	6.458764000	-0.026090000
H	5.873114000	5.905351000	0.821454000
H	5.921060000	5.917180000	-0.956787000
C	7.953279000	4.154773000	1.222746000
H	8.437125000	3.172829000	1.261018000
H	7.339781000	4.266466000	2.123523000
H	8.739457000	4.919282000	1.243159000
O	-5.042457000	-0.110221000	-0.050291000