Supporting Information

Highly efficient and stable pure-red phosphorescent organic light-emitting diodes based on heptacyclic bipolar hosts featuring an Armor-like structure

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1. Experimental details

Materials characterization.

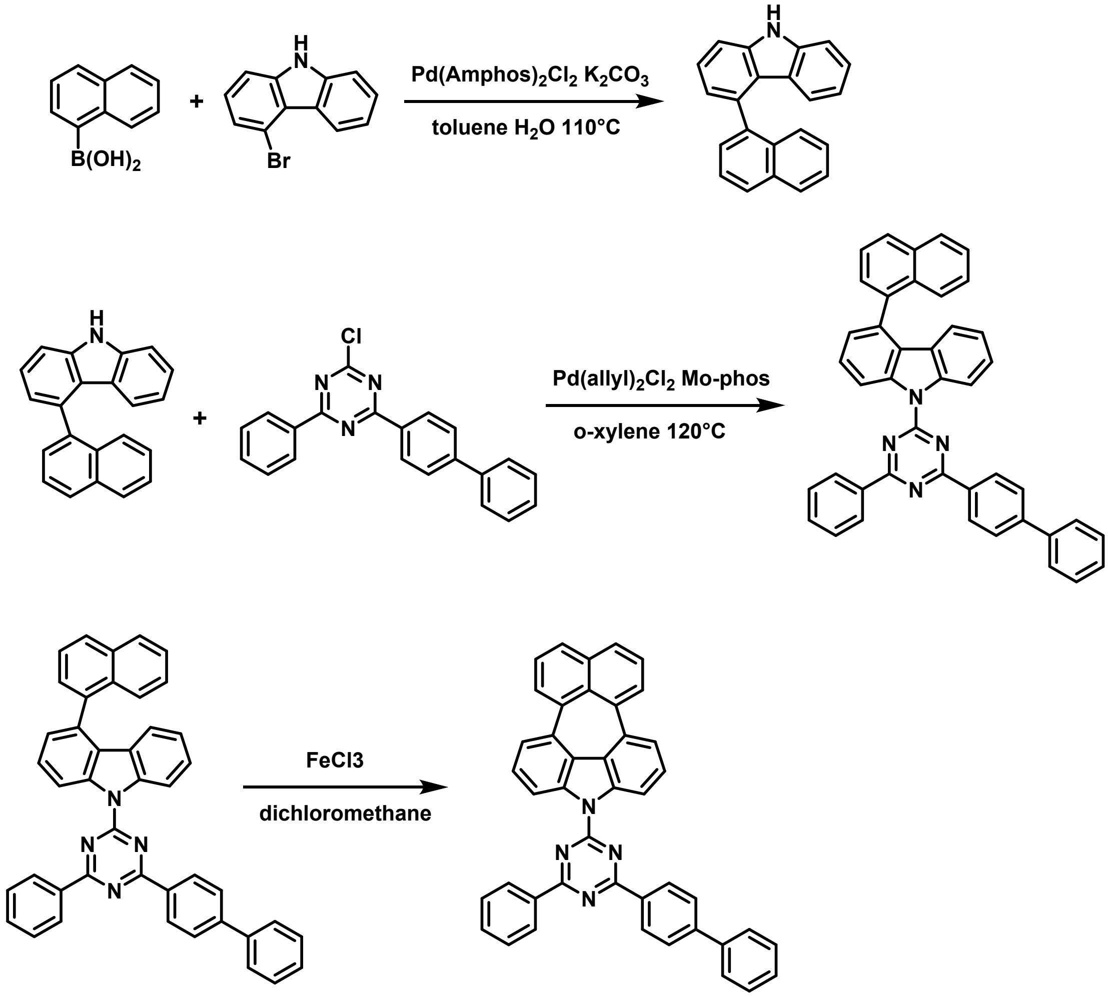
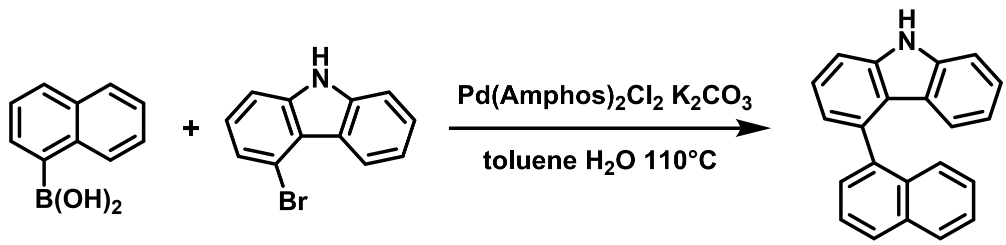
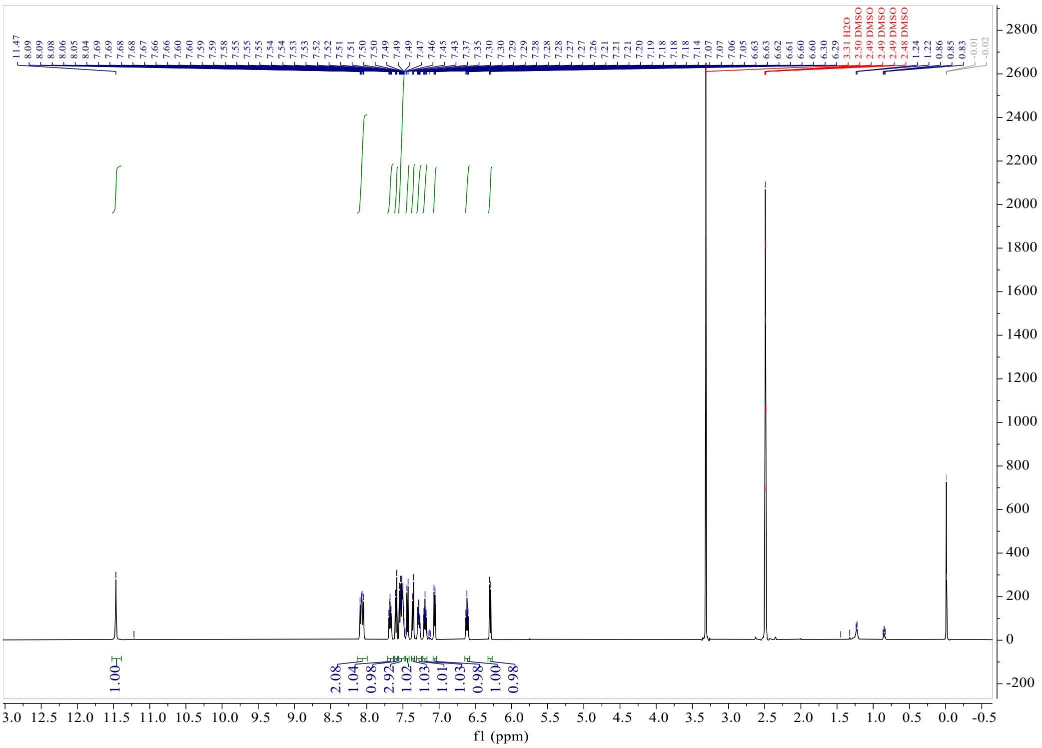


Fig. S1 The synthesis route and method for Hept-TRZ

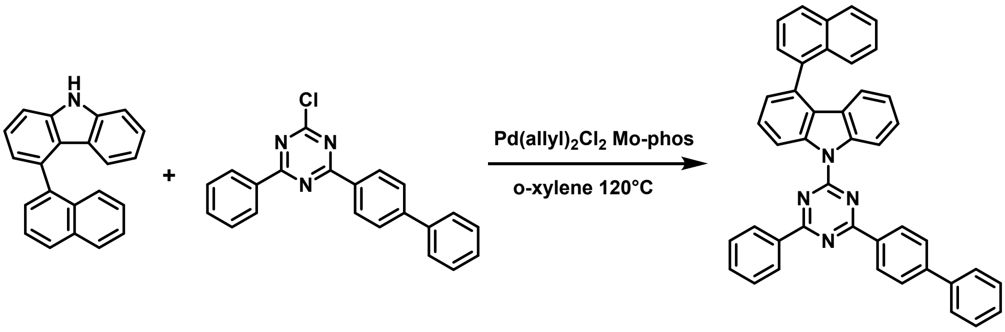
4-(naphthalen-1-yl)-9H-carbazole



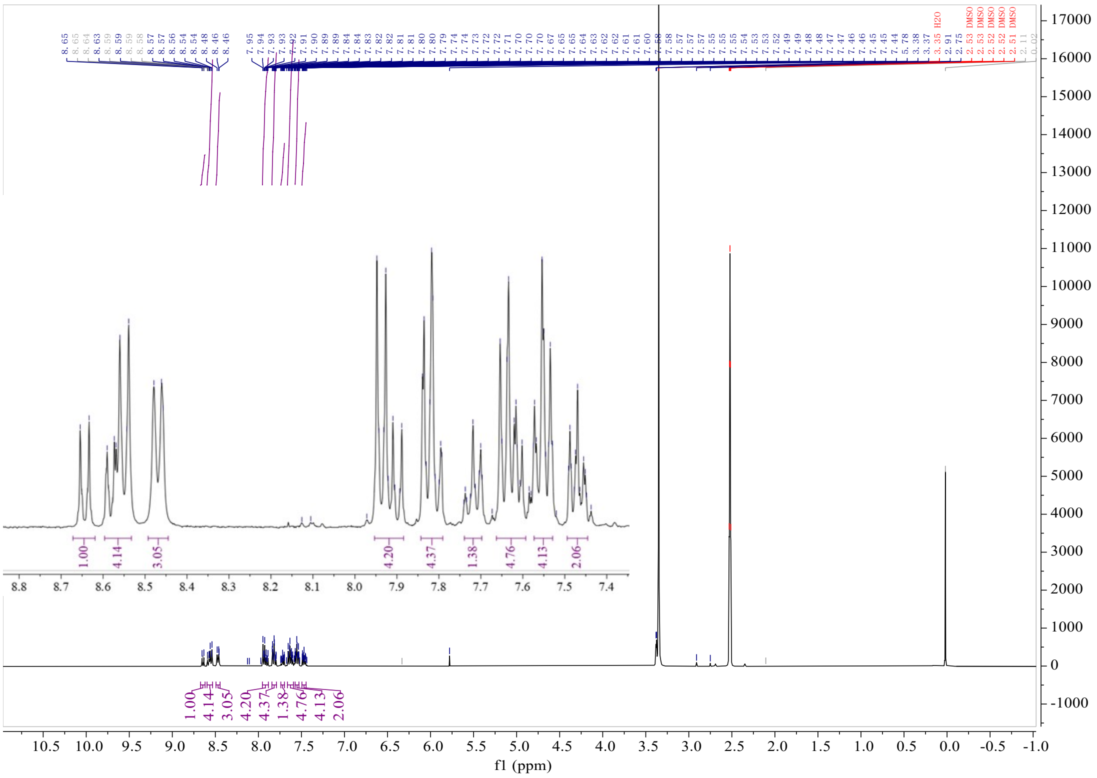
naphthalen-1-ylboronic acid (20 g, 0.12 mol) was dissolved in 500 ml of toluene in a flask under nitrogen, and 4-bromo-9H-carbazole (24.6 g, 0.10 mol), potassium carbonate (41.46 g, 0.3 mmol), water 150 ml and bis(di-tert-butyl(4-dimethylaminophenyl)phosphine)dichloropalladium(II) (0.35 g, 0.5 mmol) was added into the reaction mixture. The mixture was stirred at 110 °C for 24 h. After the reaction had finished, the mixture was washed three times with distilled water and extracted with dichloromethane. The organic layer was separated, dried over anhydrous magnesium sulfate, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography using eluent (n-hexane: dichloromethane = 4:1) to afford a white powder, yield 71%. 1H NMR (500 MHz, DMSO-d6) δ 11.47 (s, 1H), 8.13 – 7.99 (m, 2H), 7.68 (ddd, J = 9.5, 7.1, 2.6 Hz, 1H), 7.61 – 7.57 (m, 1H), 7.52 (dddt, J = 12.3, 8.0, 5.9, 2.0 Hz, 3H), 7.44 (d, J = 8.1 Hz, 1H), 7.36 (d, J = 8.5 Hz, 1H), 7.28 (ddt, J = 9.2, 6.9, 2.0 Hz, 1H), 7.23 – 7.17 (m, 1H), 7.06 (dd, J = 7.1, 2.1 Hz, 1H), 6.61 (td, J = 7.5, 2.2 Hz, 1H), 6.29 (d, J = 8.0 Hz, 1H).



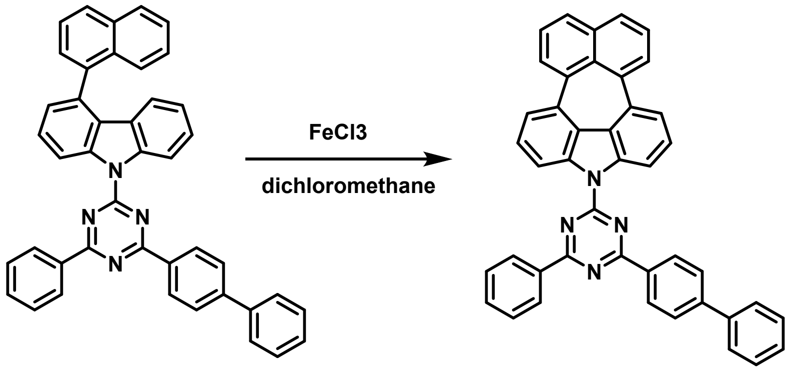
9-(4-([1,1'-biphenyl]-4-yl)-6-phenyl-1,3,5-triazin-2-yl)-4-(naphthalen-1-yl)-9H-carbazole



4-(naphthalen-1-yl)-9H-carbazole (14.7 g, 50 mmol) was dissolved in 300 ml of o-xylene in a flask under nitrogen, and 2-([1,1'-biphenyl]-4-yl)-4-chloro-6-phenyl-1,3,5-triazine (20.6 g, 60 mmol), bis(allyl)dichloropalladium (0.09 g, 0.25 mmol) and di-tert-butyl(2,2-diphenyl-1-methyl-1-cyclopropyl)phosphine (0.18 g, 0.5 mmol) was added into the reaction mixture. The mixture was stirred at 120 °C for 3 h. After the reaction had finished, the mixture was washed three times with distilled water and extracted with dichloromethane. The organic layer was separated, dried over anhydrous magnesium sulfate, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography using eluent (n-hexane: dichloromethane = 4:1) to afford a yellowish powder, yield 67%.1H NMR (400 MHz, DMSO-d6) δ 8.64 (d, J = 8.4 Hz, 1H), 8.57 (dd, J = 12.9, 7.6 Hz, 4H), 8.49 – 8.44 (m, 3H), 7.95 – 7.88 (m, 4H), 7.82 (tt, J = 8.5, 1.3 Hz, 4H), 7.74 – 7.70 (m, 1H), 7.66 – 7.59 (m, 5H), 7.55 (td, J = 8.2, 7.6, 1.9 Hz, 4H), 7.49 – 7.45 (m, 2H).



1-(4-([1,1'-biphenyl]-4-yl)-6-phenyl-1,3,5-triazin-2-yl)-1H-naphtho[1',8':5,6,7]cyclohepta[1,2,3,4-def]carbazole



9-(4-([1,1'-biphenyl]-4-yl)-6-phenyl-1,3,5-triazin-2-yl)-4-(naphthalen-1-yl)-9H-carbazole (3 g, 5 mmol) was dissolved in 80 ml of dichloromethane in a flask under nitrogen in 0°C. Dissolved ferric chloride (6.5 g, 40 mmol) in a solution of nitromethane: dichloromethane = 9:1. Slowly add the above-mentioned ferric chloride solution into the reaction system with vigorous stirring. The mixture was stirred for 2 h. After the reaction had finished, quench the reaction system with 200 mL of methanol and 200 mL of water. The mixture was washed three times with distilled water and extracted with dichloromethane. The organic layer was separated, dried over anhydrous magnesium sulfate, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography using eluent (n-hexane: dichloromethane = 6:1) to afford a yellow powder, yield 33%.

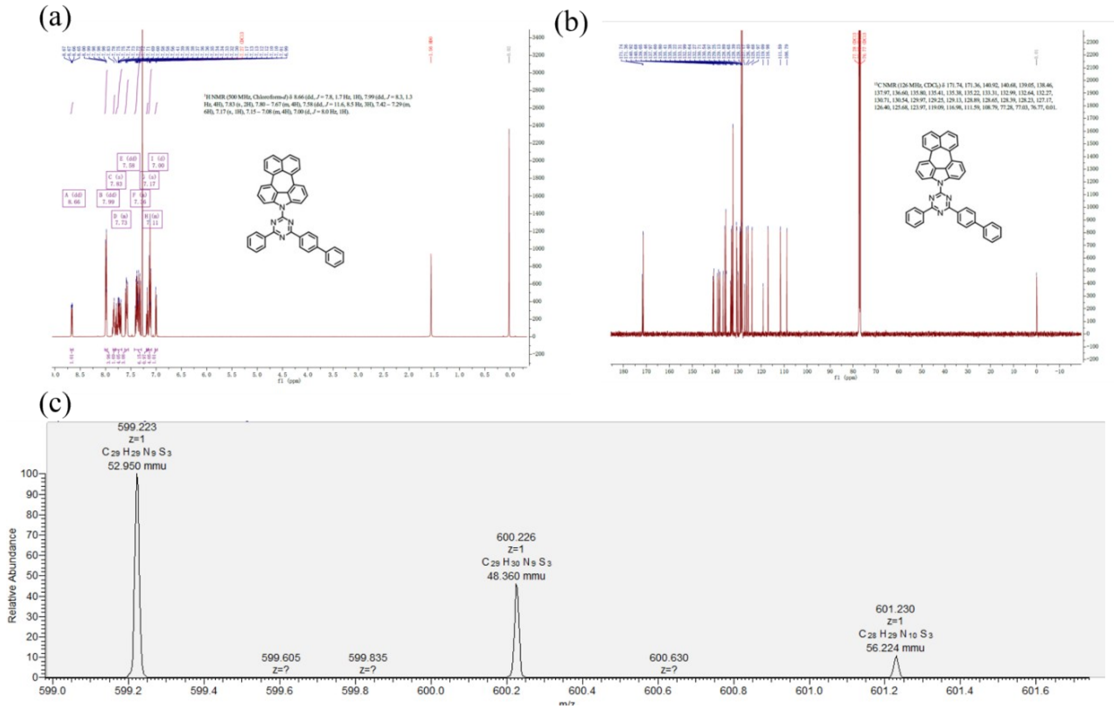


Fig S2 (a) Nuclear magnetic hydrogen spectroscopy, (b) nuclear magnetic carbon spectroscopy and (c) high-resolution mass spectra (HRMS).

The hydrogen nuclear magnetic resonance (^{1}H NMR) spectrum was recorded using chloroform-d ($CDCl_3$) as the solvent at a frequency of 500 MHz. The spectrum lists the chemical shifts of the hydrogen atoms in the compound, in parts per million (ppm), which can be used to infer the molecular structure[1]. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.66 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.99 (dd, *J* = 8.3, 1.3Hz, 4H), 7.83 (s, 2H), 7.80 – 7.67 (m, 4H), 7.58 (dd, *J* = 11.6, 8.5 Hz, 3H), 7.42 – 7.29 (m,6H), 7.17 (s, 1H), 7.15 – 7.08 (m, 4H), 7.00 (d, *J* = 8.0 Hz, 1H).

The carbon nuclear magnetic resonance (^{13}C NMR) spectrum presents the chemical environment of the carbon atoms in a compound, also using chloroform-d ($CDCl_3$) as the solvent, recorded at a frequency of 126 MHz. The spectrum displays a series of chemical shifts (δ), in ppm, providing detailed information about the chemical environments of the carbon atoms[2]. ^{13}C NMR (126 MHz, Chloroform-*d*) δ 171.74, 171.36, 140.92, 140.68, 139.05, 138.46,137.97, 136.60, 135.80, 135.41, 135.38, 135.22, 133.31, 132.99, 132.64, 132.27,130.71, 130.54, 129.97, 129.25, 129.13, 128.89, 128.65, 128.39, 128.23, 127.17,126.40, 125.68, 123.97, 119.09, 116.98, 111.59, 108.79, 77.28, 77.03, 76.77, 0.01.

The mass spectrum shows the results of the sample analyzed by the mass spectrometer.

The graph displays three main peaks, each representing ions with different mass-to-charge ratios (m/z).

PHOLED Characterization. To characterize the fabricated PHOLEDs, Keithley 2400 in conjunction with luminance colorimeter (BM-7A) within the F-Star Optical Measurement System were employed. Electroluminescence spectra and CIE coordinates were further determined using the PR-788 photometer. The forward viewing external quantum efficiency (ηext) was calculated based on the electroluminescent performance and electroluminescence spectra. This comprehensive process allowed for precise and reliable characterization of the PHOLEDs.

2. Cyclic voltammetry characterization

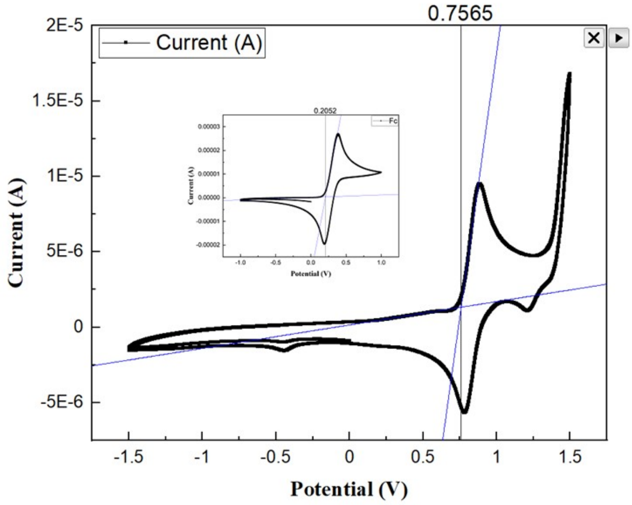


Fig.S3 Cyclic voltammetry (CV) measurements of Hept-TRZ. The inset is the CV of standard ferrocene.

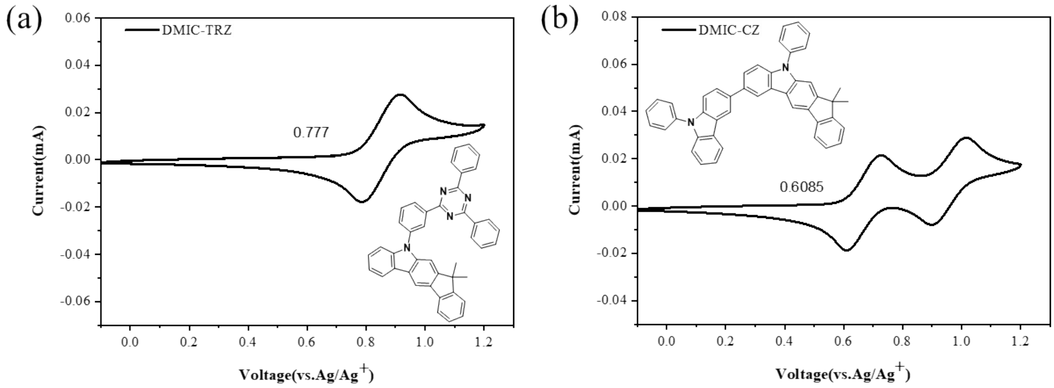
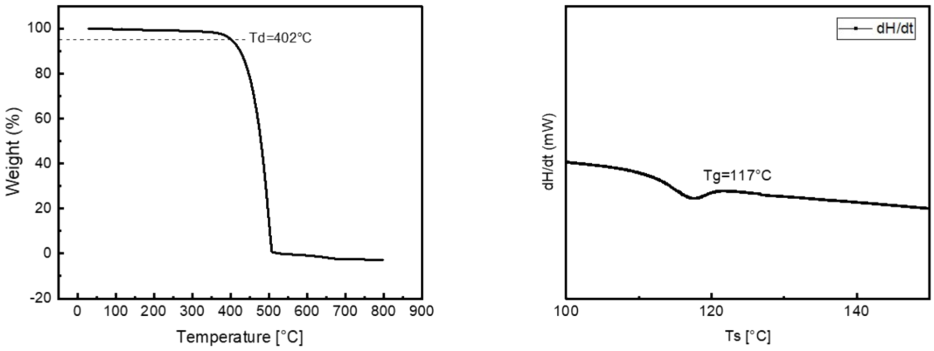


Fig.S4 Cyclic voltammetry (CV) measurements of DMIC-TRZ and DMIC-CZ.

3. Thermal stability characterization



(a) (b)

Fig. S5 (a) TGA and (b) DSC of Hept-TRZ. The Td value of Hept-TRZ is determined to be 402°C. Moreover, the glass transition temperature (Tg) value of heptacyclic is found to be 117°C.

4. Photophysical characterization

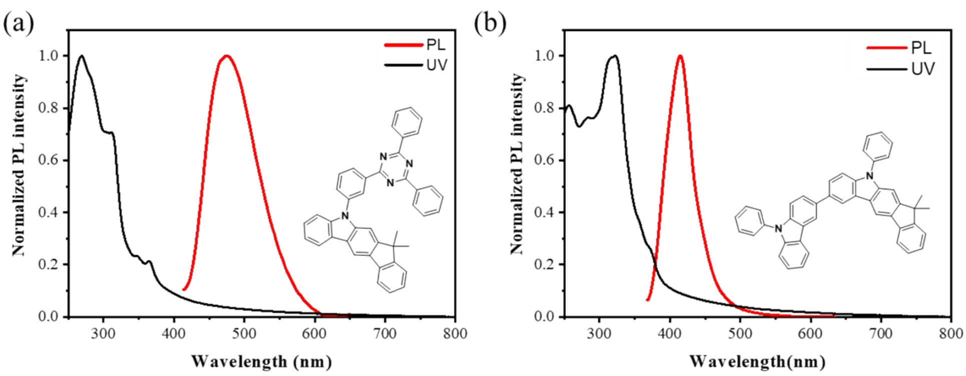


Fig.S6 Absorption spectrum and photoluminescence spectrum of two materials of co-host in thin film, (a) DMIC-TRZ and (b)DMIC-CZ.

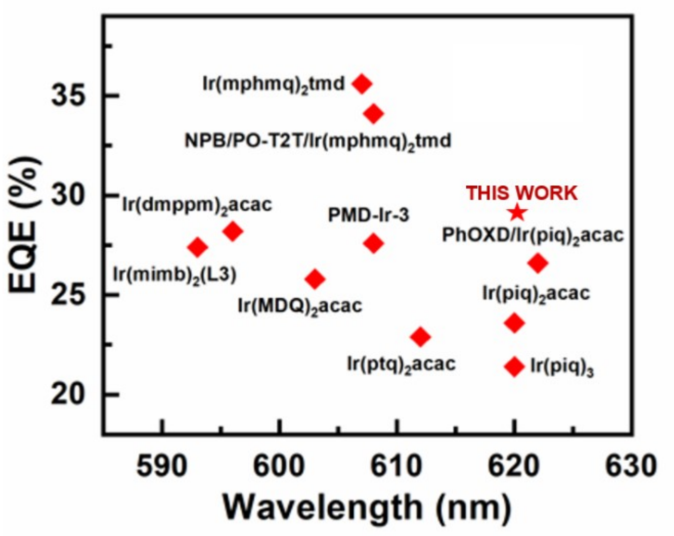


Fig. S7 Summary of existing phosphorescent OLED technologies

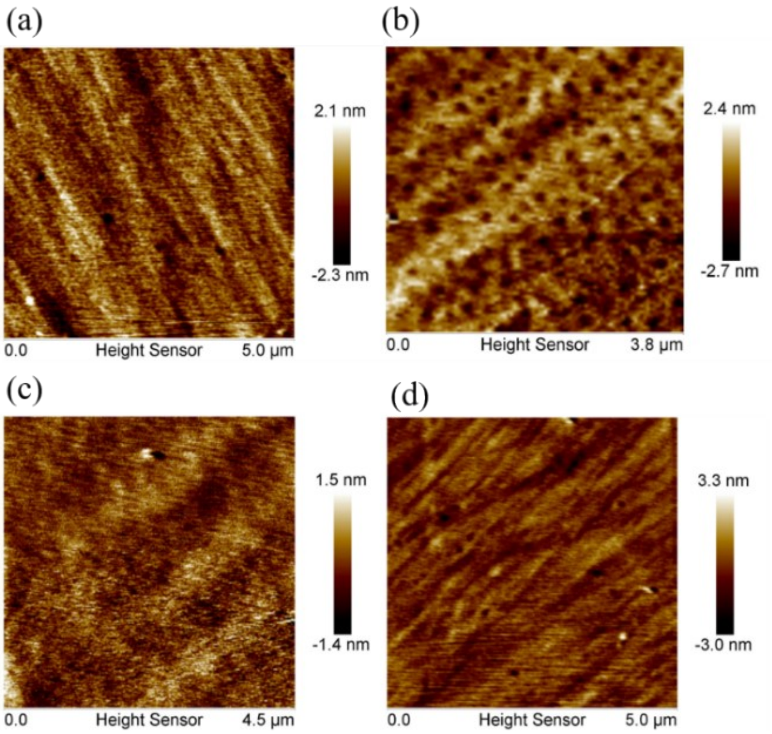


Fig. S8 Atomic force microscope images (5 um * 5 um) of a) fresh blend film of co-host. b) blend film of co-host after heating at 100 ℃ for 2 h. c) fresh blend film of Hept-TRZ. d) blend film of Hept-TRZ after heating at 100 ℃ for 2 h.

Table S1. Surface roughness of co-host and Hept-TRZ blend films before and after aging.

Film	R_q^a(nm)	R_q^b(nm)
CO-host	0.612	0.718
Hept-TRZ	0.399	0.592

[a]Surface roughness of fresh blend films. b Surface roughness of blend films heated at 100 ℃ for 2 h.

5. Theoretical simulations

Table S2 Frontier molecular orbital energy level

	HOMO/eV	LUMO/eV	HL-Gap/eV
DMIC-TRZ	-5.12	-1.97	3.15
DMIC-CZ	-4.91	-0.78	4.13
Hept-TRZ	-5.16	-1.97	3.19

*Calculated at B3LYP/6-31G(d) with D3BJ correction methods.

Table S3. Reorganization energy of hole and electron transport channels for studied host materials.

	DMIC-CZ	Hept-TRZ	DMIC-TRZ
λ_h (eV)	0.177	0.253	0.209
λ_e (eV)	0.165	0.390	0.350
$Ratio_{\lambda e/\lambda h}$	0.9	**1.5**	1.7
Priority	p-type	bipolar	n-type

Table S4. Bond dissociation energy (eV) of studied host materials.

	BDE_neu	BDE_+	BDE_-
DMIC-TRZ	3.83	4.14	2.70
DMIC-CZ	3.69	3.78	1.46
Hept-TRZ	3.90	4.48	2.80

Coordinates of optimized Hept-TRZ:

Ground state

C	6.62089300	-3.72430800	1.72703400
C	5.29573300	-3.26536700	1.65494800
C	4.87474600	-2.29120200	0.75279300
C	5.87624800	-1.60173100	-0.03434500
C	7.19385500	-2.19633100	-0.06130200
C	7.53979500	-3.24147700	0.83286200
C	5.70430400	-0.38250400	-0.79697700
C	6.68261000	-0.03893200	-1.72715300
C	7.90008900	-0.72736600	-1.85134600
C	8.17567200	-1.75010000	-0.98226900
C	3.40296100	-2.14405400	0.60598500
C	4.62551200	0.62054900	-0.59858800
C	2.55062700	-3.22337600	0.90607100
C	1.16305200	-3.07671900	0.94263700
C	0.53996600	-1.85393900	0.68924300
C	1.36584200	-0.79315100	0.32540900
C	2.76868800	-0.95297100	0.23132100
C	3.32600900	0.30144600	-0.18530300
C	2.27521200	1.24817200	-0.22999700
C	2.51169700	2.57502300	-0.58108100
C	3.83168500	2.92162900	-0.87295000
C	4.86049800	1.97847300	-0.88548500
H	6.88968400	-4.48821100	2.45058900

H	4.56242000	-3.70821800	2.31806800
H	8.55254600	-3.63384600	0.79992000
H	6.50748000	0.81425400	-2.37135500
H	8.62606600	-0.41176700	-2.59477500
H	9.14034000	-2.25015500	-0.98991300
H	2.97520500	-4.19962700	1.10755500
H	0.54853500	-3.93790200	1.18857900
H	-0.52965300	-1.73545100	0.75998200
H	1.71319700	3.29925100	-0.61373300
H	4.06247300	3.95613500	-1.11021700
H	5.86607900	2.30994400	-1.11542100
N	1.06209100	0.56943700	0.06269100
C	-0.20062600	1.13849300	0.08694800
N	-1.25250700	0.31428600	0.01098700
C	-2.45302300	0.91203600	0.03741000
N	-2.63839900	2.23821500	0.13535000
C	-1.51945300	2.97520200	0.20639600
N	-0.27679700	2.47165800	0.18439500
C	-1.65992100	4.44236100	0.32377400
C	-3.64691800	0.04948900	-0.05431500
C	-4.92913900	0.58920700	0.12300500
C	-6.05171200	-0.22419500	0.04324700
C	-5.93391800	-1.59958500	-0.22090900
C	-4.64520100	-2.13011900	-0.40359800
C	-3.51926200	-1.32188600	-0.32143200
C	-2.91944800	5.04335500	0.18517400
C	-3.05043000	6.42528400	0.28799500
C	-1.92857900	7.21936700	0.53645500
C	-0.67274600	6.62543300	0.68234700
C	-0.53664900	5.24442300	0.57550500
H	-5.02621700	1.65077000	0.31844500
H	-7.03861200	0.21292600	0.15986700
H	-4.52789900	-3.19359600	-0.58752700
H	-2.52994300	-1.73988800	-0.46754100
H	-3.77960500	4.41279500	-0.00720600
H	-4.02810200	6.88471000	0.17430900
H	-2.03285100	8.29770000	0.61834400
H	0.20041700	7.23977900	0.88218900
H	0.43037400	4.77067500	0.69887700
C	-7.13217600	-2.46403100	-0.30672900
C	-8.23449800	-2.25165100	0.53695900
C	-7.19515100	-3.51705700	-1.23367600
C	-9.36207700	-3.06564800	0.45701100
H	-8.19309400	-1.45973300	1.27881200

C	-8.32313500	-4.33036900	-1.31469900
H	-6.36400600	-3.67931000	-1.91340500
C	-9.41143300	-4.10843300	-0.46942700
H	-10.20046500	-2.89032700	1.12533200
H	-8.35546200	-5.13383900	-2.04522000
H	-10.29082100	-4.74290700	-0.53220400

Triplet state

C	6.54877700	-3.91662100	1.51274200
C	5.33890700	-3.32406300	1.67891700
C	4.85352700	-2.25830300	0.78222200
C	5.84399500	-1.57270200	-0.05862700
C	7.07877900	-2.30550300	-0.28678900
C	7.39328100	-3.47566900	0.46341300
C	5.71415200	-0.31558500	-0.70221500
C	6.68234500	0.06879400	-1.69057100
C	7.79220000	-0.68876800	-1.96988400
C	8.00895700	-1.86246100	-1.23801100
C	3.43340700	-2.10036000	0.72087300
C	4.65216400	0.68625100	-0.47110200
C	2.56283800	-3.14087200	1.16731600
C	1.18754300	-2.97758900	1.21783300
C	0.55746500	-1.77278900	0.87041600
C	1.38288300	-0.74424500	0.41694900
C	2.77905000	-0.91296200	0.28937600
C	3.33728300	0.34232500	-0.11093000
C	2.28625900	1.29341000	-0.15251600
C	2.52904500	2.62906400	-0.46198400
C	3.85546100	2.99028800	-0.70613500
C	4.88863600	2.05205100	-0.71587400
H	6.88151500	-4.70148900	2.18620400
H	4.70523900	-3.60444300	2.51265200
H	8.34427400	-3.96490800	0.27739500
H	6.49526800	0.96624500	-2.26625600
H	8.49022700	-0.38261700	-2.74324900
H	8.89677800	-2.46360900	-1.41371900
H	2.98467400	-4.09927000	1.44288300
H	0.57203200	-3.80734300	1.55421900
H	-0.50878700	-1.64257500	0.96374200
H	1.72855300	3.35092000	-0.49546200
H	4.08641800	4.03164300	-0.91057700
H	5.89787400	2.39191500	-0.91590100
N	1.07512500	0.61291000	0.12959900
C	-0.19298500	1.17197500	0.12397400

N	-1.23426200	0.33607500	0.03815200
C	-2.44138100	0.92047800	0.03224800
N	-2.64230600	2.24617800	0.10519400
C	-1.53298100	2.99584700	0.18908200
N	-0.28446300	2.50536500	0.20140100
C	-1.69175700	4.46297200	0.28175000
C	-3.62287700	0.04228100	-0.06719800
C	-4.91550700	0.57160500	0.05821400
C	-6.02606300	-0.25739600	-0.02856700
C	-5.88513400	-1.63860700	-0.24732800
C	-4.58581600	-2.15883800	-0.37726400
C	-3.47178600	-1.33497400	-0.28865100
C	-2.95269900	5.04834800	0.09676300
C	-3.10118400	6.43005500	0.17591700
C	-1.99586100	7.23965600	0.44728400
C	-0.73901100	6.66144900	0.63992600
C	-0.58532300	5.28068100	0.55639600
H	-5.03005300	1.63723500	0.21905600
H	-7.02079700	0.17090000	0.04691100
H	-4.45141100	-3.22595700	-0.52477300
H	-2.47366900	-1.74480500	-0.39259400
H	-3.80000200	4.40588100	-0.11248100
H	-4.07965600	6.87719900	0.02601100
H	-2.11384100	8.31780600	0.51078000
H	0.12108600	7.28790000	0.85800100
H	0.38234100	4.81947100	0.71655100
C	-7.07062600	-2.51976500	-0.34039600
C	-8.19910100	-2.29517200	0.46467900
C	-7.09493400	-3.60129700	-1.23580600
C	-9.31460300	-3.12495400	0.37790000
H	-8.18802600	-1.48053700	1.18262100
C	-8.21083600	-4.43040800	-1.32370900
H	-6.24273500	-3.77408000	-1.88622200
C	-9.32544200	-4.19605400	-0.51695000
H	-10.17380200	-2.93961200	1.01642000
H	-8.21303200	-5.25615000	-2.02968700
H	-10.19540600	-4.84285200	-0.58505600

Coordinates of optimized DMIC-TRZ:

Ground state

C	3.33356500	5.64526500	1.62158800
C	4.61264900	5.10701900	1.83846000
C	4.90667100	3.80249700	1.45180000
C	3.91455600	3.03622400	0.83295100

C	2.63469100	3.60317400	0.60146800
C	2.32739000	4.90348200	1.00512300
C	3.87001500	1.67239900	0.34665200
C	2.56106000	1.46133400	-0.16651800
N	1.82142100	2.64106800	-0.01244300
C	4.81459000	0.64101600	0.30592600
C	4.43083000	-0.57670900	-0.24718000
C	3.12533500	-0.76443800	-0.76934800
C	2.17699600	0.24513800	-0.74501700
C	5.17744000	-1.82814600	-0.41691600
C	4.33733800	-2.77529000	-1.03623200
C	2.95941900	-2.18090400	-1.31291700
C	6.48762600	-2.16328100	-0.07320100
C	6.95055000	-3.45095900	-0.35344700
C	6.11683500	-4.39046100	-0.96790000
C	4.80212700	-4.05381600	-1.31241800
C	2.64459200	-2.16970500	-2.82186300
C	1.85729800	-2.94048500	-0.54770700
C	0.46464200	2.80501100	-0.37401000
C	-0.46382800	1.82411400	-0.02619700
C	-1.80189700	1.94679700	-0.41369400
C	-2.22214100	3.08639700	-1.11242300
C	-1.29578700	4.07311900	-1.44172900
C	0.04766700	3.93233400	-1.09421000
C	-2.75028000	0.85631200	-0.09293500
N	-4.05080700	1.05152500	-0.34886200
C	-4.86108600	0.01941000	-0.05881100
N	-4.43980700	-1.14988000	0.44718000
C	-3.12051200	-1.25267700	0.66962700
N	-2.23895500	-0.27267700	0.41813400
C	-2.59898100	-2.52462200	1.21315800
C	-6.30807200	0.18306500	-0.31487600
C	-7.19770000	-0.86723700	-0.04424600
C	-8.55926000	-0.71127700	-0.28649900
C	-9.04661600	0.49286700	-0.79995300
C	-8.16551500	1.54239500	-1.07046900
C	-6.80316500	1.39027900	-0.83001400
C	-3.46704200	-3.59743200	1.46382700
C	-2.96976000	-4.79752300	1.96362300
C	-1.60346300	-4.93897200	2.21794000
C	-0.73467200	-3.87328400	1.97208000
C	-1.22796300	-2.67129000	1.47336100
H	3.11867500	6.66024800	1.94327100
H	5.37510400	5.71300100	2.31860400

H	5.89116300	3.38024900	1.63334000
H	1.33798200	5.32143900	0.85738300
H	5.81709700	0.79266000	0.69685400
H	1.18325900	0.09876000	-1.15359700
H	7.13981900	-1.43710600	0.40482300
H	7.96870400	-3.72521700	-0.09130000
H	6.49173200	-5.38791900	-1.17943200
H	4.15785800	-4.78790300	-1.79026300
H	1.68203100	-1.68131100	-3.01128300
H	3.41909400	-1.63177700	-3.37688700
H	2.58838400	-3.19230700	-3.21168600
H	1.79120400	-3.97943400	-0.88957400
H	2.06695400	-2.94595700	0.52656700
H	0.88019400	-2.47136100	-0.70454900
H	-0.15796500	0.95828400	0.54552100
H	-3.26346800	3.17517900	-1.39799000
H	-1.61471600	4.95081500	-1.99598800
H	0.77710300	4.67871300	-1.38946700
H	-6.80424000	-1.79489400	0.35436200
H	-9.24228900	-1.52891300	-0.07487000
H	-10.10985700	0.61311300	-0.98830200
H	-8.54194000	2.48015400	-1.46892800
H	-6.10707500	2.19550400	-1.03336700
H	-4.52399400	-3.47294900	1.25934300
H	-3.64738800	-5.62469900	2.15458500
H	-1.21699100	-5.87688800	2.60695100
H	0.32814700	-3.97915400	2.16790800
H	-0.56439600	-1.83742500	1.27877900

Triplet state

C	3.69035400	5.60652900	1.44823900
C	4.96394100	5.02893900	1.52467200
C	5.17023500	3.69932100	1.14543000
C	4.09182600	2.96382700	0.66274200
C	2.81899800	3.57328800	0.55520500
C	2.59216300	4.88181500	0.97923400
C	3.93969900	1.57843600	0.24329900
C	2.57359600	1.40111700	-0.10977500
N	1.89764800	2.61780000	0.07147400
C	4.83770200	0.52155400	0.13344500
C	4.35018100	-0.70333300	-0.33501600
C	2.99158900	-0.85557900	-0.71477400
C	2.08865000	0.18841600	-0.62174600
C	5.03105600	-1.97951400	-0.54088800

C	4.09754200	-2.91153300	-1.04225400
C	2.72061000	-2.27584800	-1.19903200
C	6.36026500	-2.34875200	-0.31931100
C	6.74804000	-3.65798100	-0.60283400
C	5.82192300	-4.58327700	-1.09945700
C	4.49050300	-4.21327800	-1.32143500
C	2.26105900	-2.28654900	-2.67140500
C	1.66887700	-2.97207800	-0.31106000
C	0.54192900	2.84005500	-0.16762500
C	-0.38277800	1.85488900	0.11738000
C	-1.74403100	2.01318200	-0.21391900
C	-2.14621800	3.27886300	-0.83391100
C	-1.21091200	4.25862100	-1.11235500
C	0.14227300	4.09308400	-0.79748300
C	-2.67512500	0.96752700	0.03770300
N	-3.98907600	1.16727800	-0.28036700
C	-4.79776500	0.13290500	-0.06793000
N	-4.41628300	-1.06507400	0.42820100
C	-3.09906100	-1.16684000	0.72826300
N	-2.20195800	-0.20705500	0.55821700
C	-2.62703100	-2.46302700	1.27648000
C	-6.23446800	0.30025100	-0.40027600
C	-7.13822300	-0.74963500	-0.18475800
C	-8.48662400	-0.59263400	-0.49718200
C	-8.94867700	0.61321200	-1.02795200
C	-8.05299100	1.66355000	-1.24443800
C	-6.70522700	1.50913500	-0.93286500
C	-3.49281300	-3.56341100	1.34182600
C	-3.04310900	-4.78429800	1.84077200
C	-1.72664800	-4.92046900	2.28508400
C	-0.86058300	-3.82513600	2.22965300
C	-1.30699000	-2.60539800	1.72908300
H	3.54524500	6.63163000	1.77443800
H	5.79644800	5.61440500	1.90236800
H	6.15183700	3.24428200	1.23837400
H	1.60050800	5.31656600	0.96258000
H	5.88335800	0.64806600	0.39846100
H	1.05687200	0.07142800	-0.92755400
H	7.08026900	-1.63283400	0.06770500
H	7.77689100	-3.96363500	-0.43649800
H	6.14068200	-5.59917500	-1.31424700
H	3.77847000	-4.93850600	-1.70625000
H	1.29991600	-1.77210000	-2.77749000
H	2.99361800	-1.78997100	-3.31509200

H	2.13357600	-3.31577100	-3.02369700
H	1.53059800	-4.01344100	-0.62075100
H	1.97751500	-2.96574600	0.73869000
H	0.69991200	-2.46899100	-0.38493700
H	-0.08863000	0.95364700	0.63687000
H	-3.19422800	3.41363400	-1.06990700
H	-1.52860500	5.17535800	-1.60168300
H	0.89555300	4.79183700	-1.13633000
H	-6.76338900	-1.67815500	0.22943800
H	-9.17908800	-1.41241700	-0.32576400
H	-10.00085900	0.73481200	-1.27132400
H	-8.40755700	2.60438800	-1.65688200
H	-5.99752300	2.31412800	-1.09389400
H	-4.51166800	-3.44089500	0.99357100
H	-3.72173800	-5.63195300	1.88345000
H	-1.37782300	-5.87267300	2.67576800
H	0.16333200	-3.92233100	2.58066600
H	-0.64822600	-1.74590900	1.68424400

Coordinates of optimized DMIC-CZ:

Ground state

C	8.54183000	-3.76572900	-1.48373500
C	7.72970300	-3.02636500	-2.34537500
C	7.01404500	-1.92899600	-1.86993900
C	7.09290200	-1.57922700	-0.51720000
C	7.89772400	-2.32519500	0.35127600
C	8.62681400	-3.40795800	-0.13709900
N	6.35792200	-0.47232000	-0.02798100
C	6.88158900	0.59667900	0.70868400
C	5.83092100	1.50076000	1.01328000
C	4.62201300	0.95192600	0.43313300
C	4.98516400	-0.26430700	-0.19890000
C	8.19943500	0.84849700	1.09391400
C	8.45078600	2.01501300	1.81346500
C	7.42010400	2.91324200	2.13792000
C	6.11062100	2.66372500	1.73715000
C	3.29079800	1.37042900	0.41711700
C	2.31849700	0.58982200	-0.21961900
C	2.71195800	-0.62343200	-0.82936400
C	4.03020700	-1.06665200	-0.82482100
C	0.90046600	1.01878700	-0.25003100
C	-0.13429200	0.08555800	-0.11219600
C	-1.46412000	0.50703900	-0.14667000
C	-1.76176800	1.88191800	-0.32347700

C	-0.74721100	2.83171400	-0.44525000
C	0.56921800	2.38343500	-0.41186900
C	-2.72973300	-0.18522600	-0.00984000
C	-3.75007300	0.80072800	-0.11229400
N	-3.15101700	2.05041800	-0.30207600
C	-3.07075200	-1.52955200	0.17115400
C	-4.42105000	-1.85877900	0.23901500
C	-5.42569600	-0.86418100	0.11767600
C	-5.11001200	0.47313900	-0.06241400
C	-5.07892500	-3.15715700	0.42071400
C	-6.47459300	-2.96276800	0.40818500
C	-6.81558100	-1.48812800	0.21300200
C	-4.54501600	-4.43550800	0.58755100
C	-5.41654600	-5.51614400	0.74116900
C	-6.80137000	-5.32298300	0.72833600
C	-7.33662300	-4.04001200	0.56098900
C	-7.61696900	-1.26646200	-1.08525400
C	-7.59561000	-0.92974600	1.41984100
C	-3.83619500	3.28130900	-0.44356300
C	-4.78906800	3.66619400	0.50651800
C	-5.46899700	4.87350800	0.35691600
C	-5.18924900	5.71129400	-0.72412400
C	-4.23025400	5.32987700	-1.66404800
C	-3.56096800	4.11431200	-1.53383800
H	9.10462100	-4.61514900	-1.85915200
H	7.66295600	-3.29438700	-3.39586000
H	6.40278500	-1.33188100	-2.53846400
H	7.93568400	-2.05790800	1.40207100
H	9.25131800	-3.98213600	0.54123400
H	9.00074200	0.16453600	0.83688000
H	9.46784100	2.23306200	2.12662100
H	7.65024700	3.81182100	2.70248500
H	5.31514100	3.36344700	1.97831200
H	3.00195000	2.28600500	0.92486000
H	1.96060500	-1.21833800	-1.33948500
H	4.30359800	-2.00313900	-1.29836500
H	0.10058200	-0.96192300	0.05250300
H	-0.97284300	3.88530500	-0.56794800
H	1.37171200	3.10364300	-0.53799100
H	-2.29930400	-2.29073900	0.25074700
H	-5.87734100	1.23313700	-0.16635100
H	-3.46949900	-4.59139300	0.59886500
H	-5.01418300	-6.51690800	0.87219900
H	-7.46612000	-6.17369300	0.84915100

H	-8.41424200	-3.89513600	0.55167500
H	-7.79965900	-0.19828200	-1.24885600
H	-7.07260600	-1.65843900	-1.94967900
H	-8.58745300	-1.77258900	-1.03072500
H	-8.56564200	-1.43014200	1.51772400
H	-7.03590000	-1.08022800	2.34799000
H	-7.77864800	0.14399700	1.29757100
H	-4.97984700	3.02253400	1.35880300
H	-6.20871200	5.16626100	1.09648100
H	-5.71486500	6.65522300	-0.83316200
H	-4.01109100	5.97325500	-2.51129000
H	-2.83488400	3.79710500	-2.27495600

Triplet state

C	8.55270700	-3.80402700	-1.39830600
C	7.74393200	-3.08319200	-2.27858900
C	7.02843100	-1.97455500	-1.82976000
C	7.10427400	-1.59497600	-0.48501100
C	7.90568000	-2.32205900	0.40228000
C	8.63461500	-3.41643500	-0.05975300
N	6.36924800	-0.47628800	-0.02246100
C	6.89357500	0.61049700	0.68763200
C	5.84323500	1.52165800	0.97094500
C	4.63401500	0.95868600	0.40499500
C	4.99717200	-0.27284700	-0.19742500
C	8.21165000	0.87090500	1.06590900
C	8.46360100	2.05443300	1.75691600
C	7.43328800	2.96050300	2.06004300
C	6.12347100	2.70176200	1.66626000
C	3.30320500	1.37652600	0.37883000
C	2.33037400	0.57948000	-0.23754300
C	2.72381900	-0.64901400	-0.81701900
C	4.04207500	-1.09076600	-0.80315400
C	0.91334500	1.00689300	-0.27794200
C	-0.12119500	0.06921000	-0.13542400
C	-1.44997700	0.48598600	-0.17718300
C	-1.74533900	1.85955300	-0.36772700
C	-0.73888600	2.81308000	-0.48714600
C	0.58155900	2.36972000	-0.44859900
C	-2.71636000	-0.21402800	-0.03012200
C	-3.72928500	0.77893900	-0.14365300
N	-3.14208200	2.01637400	-0.34629600
C	-3.04064800	-1.55063800	0.16333500
C	-4.46548500	-1.87990500	0.23898800

C	-5.46750500	-0.83868200	0.08497900
C	-5.13756400	0.46634800	-0.11014800
C	-5.10057800	-3.10337000	0.42837000
C	-6.53890700	-2.92312900	0.40409600
C	-6.86492400	-1.45129600	0.17394200
C	-4.56175400	-4.42189700	0.62631800
C	-5.43685800	-5.47643400	0.79049700
C	-6.83718700	-5.28609900	0.76613000
C	-7.38370300	-3.98584300	0.56857700
C	-7.64290300	-1.25027900	-1.14117700
C	-7.65462200	-0.85970300	1.35748100
C	-3.82387800	3.25390800	-0.43242700
C	-4.77510000	3.59844100	0.53640100
C	-5.45001100	4.81318100	0.43954100
C	-5.17065000	5.69529800	-0.60631000
C	-4.21503100	5.35134000	-1.56499100
C	-3.54705000	4.13142800	-1.48805900
H	9.11532800	-4.66237000	-1.75307500
H	7.67961000	-3.37467500	-3.32293600
H	6.41955800	-1.39185800	-2.51305600
H	7.94123200	-2.03118600	1.44689100
H	9.25651700	-3.97611300	0.63290200
H	9.01249000	0.18048700	0.82522700
H	9.48081700	2.27974200	2.06427700
H	7.66397700	3.87237700	2.60260100
H	5.32833200	3.40727700	1.89106400
H	3.01458900	2.30391600	0.86457600
H	1.97285500	-1.25710300	-1.31171400
H	4.31573700	-2.03828700	-1.25396600
H	0.11604800	-0.97517600	0.04275600
H	-0.96765500	3.86560200	-0.61192600
H	1.38151700	3.09151200	-0.57846500
H	-2.28464400	-2.32343300	0.23672700
H	-5.88364800	1.24111300	-0.24541300
H	-3.48750300	-4.57676000	0.64791900
H	-5.04522200	-6.47908800	0.94264100
H	-7.49959000	-6.13571000	0.89744300
H	-8.46256100	-3.85137400	0.54924700
H	-8.61797700	-1.74775600	-1.09054300
H	-7.81076000	-0.18395100	-1.33185500
H	-7.08844000	-1.66733200	-1.98720500
H	-8.63002400	-1.34991800	1.45252700
H	-7.10873400	-0.99742400	2.29576700
H	-7.82312400	0.21364600	1.21114200

H	-4.96435400	2.91994800	1.36127700
H	-6.18643100	5.07670000	1.19310600
H	-5.69395900	6.64422700	-0.67395400
H	-3.99819700	6.02849100	-2.38598200
H	-2.82769000	3.84227500	-2.24668000

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