Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

The catenation of a singlet diradical dication and modulation of diradical character by metal coordination

Ke Li[a‡], Zhongtao Feng[a‡], Huapeng Ruan[a], Quanchun Sun[a], Yue Zhao[a], and Xinping Wang[a*]

[a.] *State Key Laboratory of Coordination Chemistry, Jiangsu Key Laboratory of Advanced Organic Materials, School of Chemistry and Chemical Engineering, Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210023, China.*

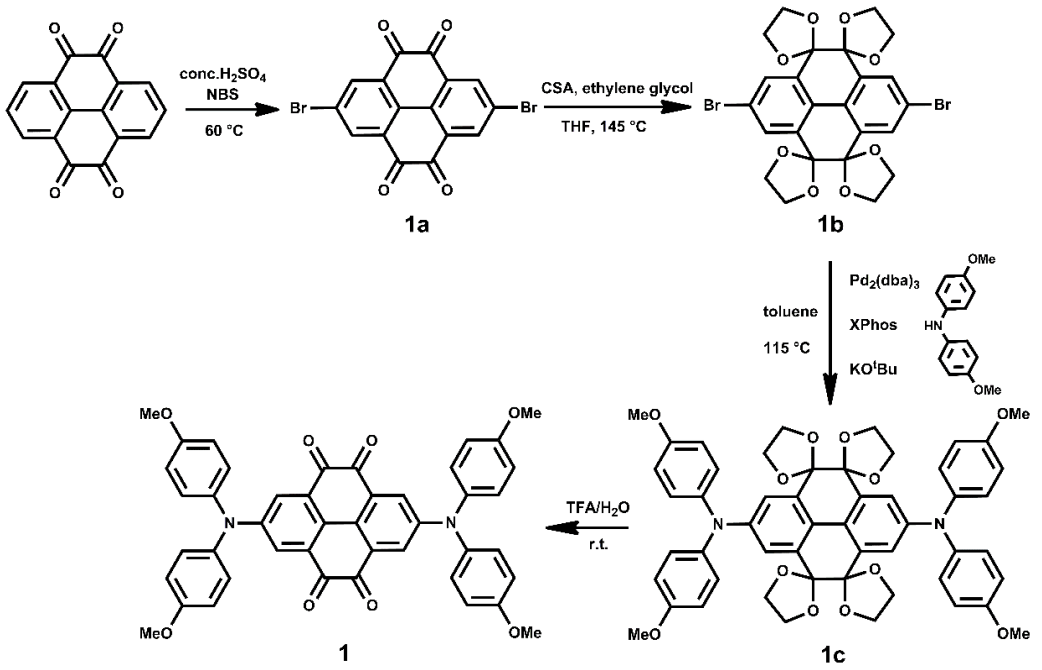
[‡] *These authors contributed equally to this work.*

E-mail: xpwang@nju.edu.cn

Contents

General Procedures

All experiments were carried out under a dry nitrogen atmosphere using standard Schlenk techniques and an Argon-filled glovebox. Solvents were dried by freshly distilling and degassed prior to use. 2,7-bis(bis(4-methoxyphenyl)amino)pyrene-4,5,9,10-tetraone (compound **1**) was prepared according to modified published procedures[1] and dried before use. Pyrenetetraone, $NOSbF_6$ and $AgSbF_6$ were purchased and used upon arrival. $Li[Al(OC(CF_3)_3)_4]$ and $Ag[Al(OC(CF_3)_3)_4]$ was synthesized according to literature methods[2]. The ^1H NMR and ^{13}C NMR spectra were obtained with a Bruker Ultra Shield 400 MHz spectrometer using $CDCl_3$ or CD_2Cl_2 as solvents and the data were listed in ppm referenced to internal standard TMS ($SiMe_4$). Elemental analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Science. Cyclic voltammetry was performed on a CHI660E electrochemical workstation with platinum as the working electrode and $Ag/AgNO_3$ (0.1 M in CH_3CN) as the reference electrode, and the measurements were carried out under an Argon atmosphere. For the single crystal X-ray structure analyses, the crystals were each mounted on an object slide in perfluorinated oil and measured in a cold N_2 flow. The data were collected on Bruker D_8 CMOS detectors at 120 or 130 K. The structures were solved by direct methods and all refined on F^2 with the Olex2. EPR spectra were obtained using Bruker EMX plus-6/1 X-band variable-temperature apparatus, and the spectra were simulated with the WinEPR SimFonia software packet. Magnetic measurements were performed using a Quantum Design SQUID VSM magnetometer with a field of 0.1 T. UV-Vis-NIR absorption spectrum were recorded on Lambda 750 spectrometer.



Scheme S1 Synthesis of **1a, 1b, 1c** and **1**.

Compound **1a**, **1b** were prepared according to published procedures[1a,1b], compound **1c**, **1** were prepared according to modified published procedures[1c].

Synthesis of 1c: 2,7-bis(bromo)-4,5,9,10-tetra(ethyleneglycol)ketal-pyrene (**1b**) (2.05 g, 3.438 mmol, 1.00 equiv), bis(4-methoxyphenyl)amine (1.66 g, 7.243 mmol, 2.10 equiv), $Pd_2(dba)_3$ (63.0 mg, 0.0688 mmol, 0.02 equiv), XPhos (65.6 mg, 0.1375 mmol, 0.04 equiv) and KO^tBu (1.16 g, 10.314 mmol, 3.00 equiv) were placed in a 125 mL sealed bottle in the glovebox, toluene (85 mL) was transferred to the bottle via syringe under stirring at room temperature. Afterwards, the reaction mixture was stirred at 115 °C for three days. The solvent was removed under reduced pressure, and the crude product was purified by chromatography (CH_2Cl_2:ethyl acetate = 100:1). Product **1c** was obtained as a pale yellow (or grey green) solid (2.5 g, 81.4%). ^{1}H NMR (CD_2Cl_2, 400 MHz): δ (ppm) 7.07 (s, 4H, Ar-*H*), 7.00 (d, 8H, *J*(H, H) = 9.0 Hz, Ar-*H*), 6.77 (d, 8H, *J*(H, H) = 9.0 Hz, Ar-*H*), 4.60-2.80 (b, 28H, C*H*$_2$, OC*H*$_3$). ^{13}C NMR (CD_2Cl_2, 100 MHz): δ (ppm) 156.49, 149.08, 140.51, 132.83, 126.95, 121.14, 117.89, 114.85, 92.69,

55.56, 31.34. Elemental analysis (%) calcd for $C_{52}H_{48}N_2O_{12}$: C: 69.94, H: 5.42, N: 3.14; found: C: 69.76, H: 5.89, N: 2.89.

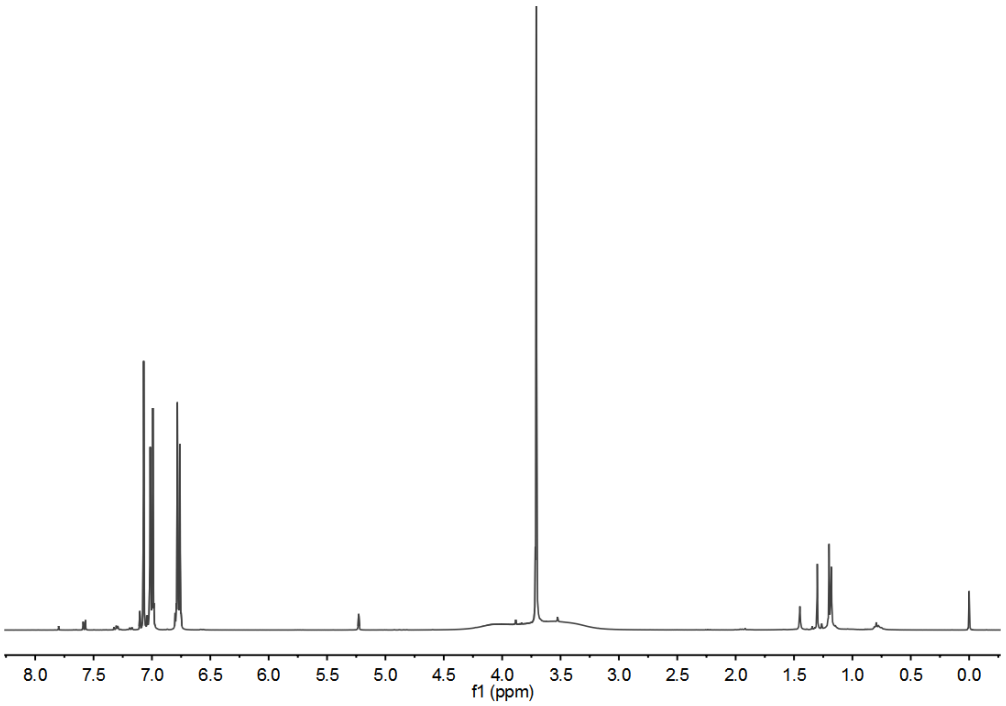


Fig. S1 ^{1}H NMR spectrum of **1c** in CD_2Cl_2 at room temperature.

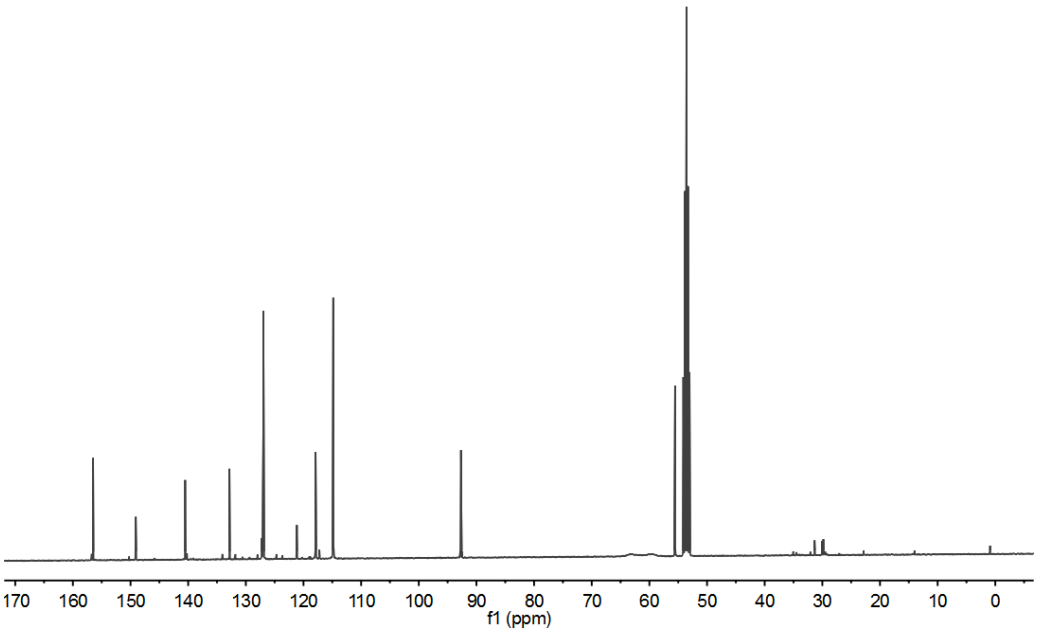


Fig. S2 ^{13}C NMR spectrum of 1c in CD_2Cl_2 at room temperature.

Synthesis of 1: Compound **1c** (1.57 g, 1.758 mmol) was suspended in 55 mL of H_2O in a 500 mL round bottom flask. Then 327 mL of TFA was added dropwise with a constant pressure dropping funnel and the reaction mixture was stirred at room temperature for three days. After that, pour the mixture into a large amount of distilled water, and the precipitated dark blue precipitate was filtered with a sand core funnel, the resulting crude product was washed with plenty of methanol and ethyl ether. The solvents were removed under reduced pressure. The product **1** was obtained as dark blue solid (1.08 g, 85.7%). ^{1}H NMR (CD_2Cl_2, 400 MHz): δ (ppm) 7.57 (s, 4H, Ar-*H*), 7.03 (d, 8H, *J*(H,H) = 8.9 Hz, Ar-*H*), 6.85 (d, 8H, *J*(H,H) = 8.9 Hz, Ar-*H*), 3.75 (s, 12H, OC*H*$_3$). ^{13}C NMR (CD_2Cl_2, 100 MHz): δ (ppm) 178.74, 138.39, 136.64, 130.95, 129.79, 127.85, 123.81, 115.40, 55.64, 29.84. Elemental analysis (%) calcd for $C_{44}H_{32}N_2O_8$: C: 73.73, H: 4.50, N: 3.91; found: C: 72.96, H: 4.00, N: 3.30.

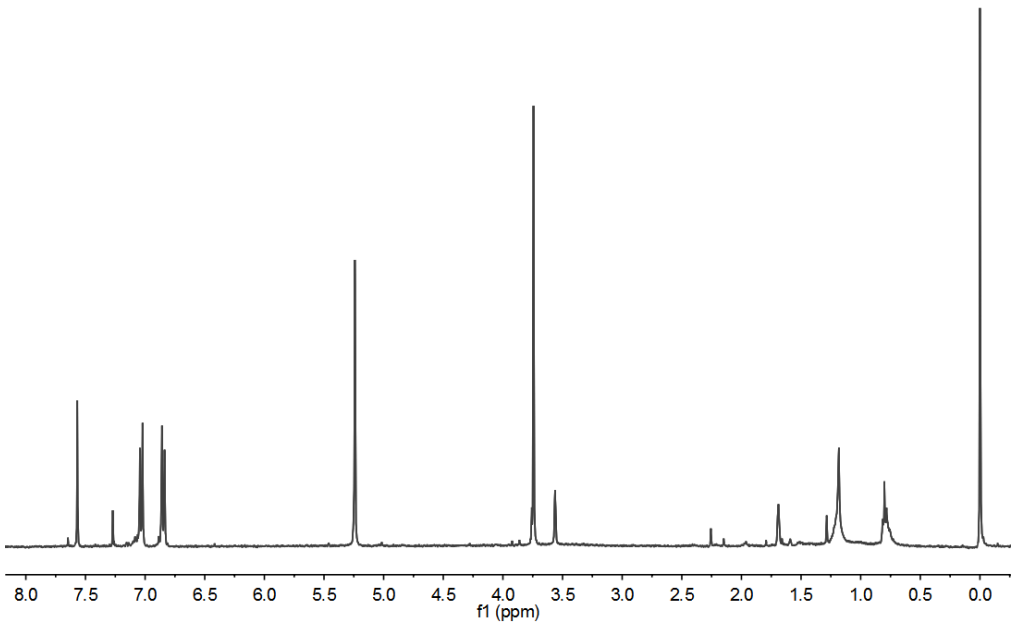


Fig. S3 ^{1}H NMR spectrum of **1** in CD_2Cl_2 at room temperature.

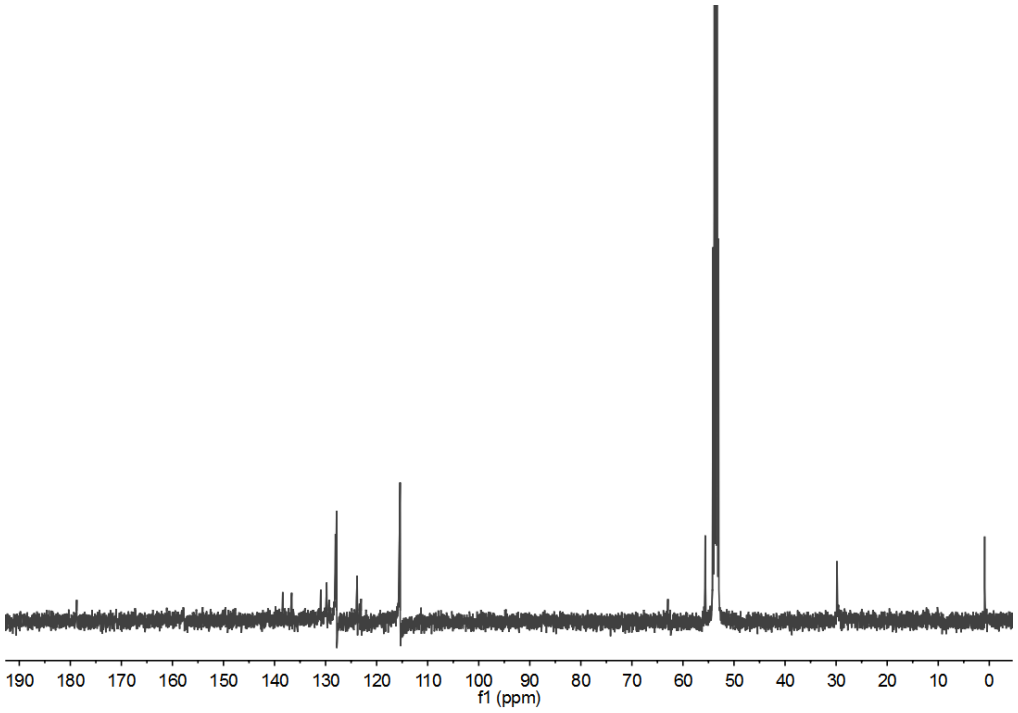


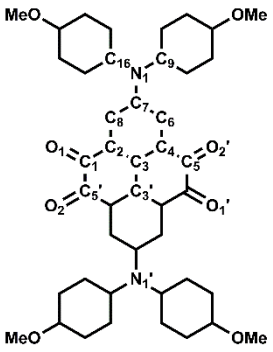
Fig. S4 ^{13}C NMR spectrum of 1 in CD_2Cl_2 at room temperature.

Synthesis of $1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$: Compound **1** (71.7 mg, 0.1 mmol), $NOSbF_6$ (53.2 mg, 0.2 mmol) and $Li[Al(OC(CF_3)_3)_4]$ (194.8 mg, 0.2 mmol) were placed in a 100ml Schlenk flask in the glovebox, CH_2Cl_2 (40 mL) was transferred to the flask via cannula under stirring at room temperature. The mixture turned dark purple quickly. After stirring for 24 h, filter to remove insoluble substance and the filtrate was concentrated to ca. 10 mL, then left at 5 °C refrigerator for a week affording **$1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$** as dark brown crystals. Washing them several times with toluene for purification. Yield: 160.8 mg, 60.6%. Elemental analysis (%) calcd for $C_{76}H_{32}Al_2F_{72}N_2O_{16}$: C: 34.43, H: 1.22, N: 1.06; found: C: 34.27, H: 1.28, N: 1.10.

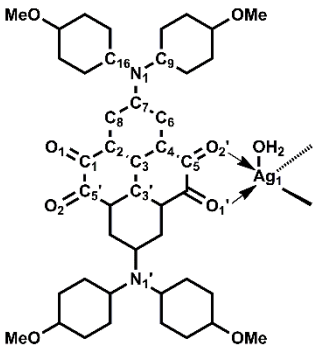
Synthesis of $(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$: Compound **1** (71.7 mg, 0.1 mmol), $AgSbF_6$ (140.9 mg, 0.41 mmol) were placed in a 100ml Schlenk flask in the glovebox, CH_2Cl_2 (35 mL) was transferred to the flask via cannula under stirring in the dark at room temperature. The mixture turned dark purple quickly. After stirring for 24 h, filter to remove insoluble substance and the filtrate was concentrated to ca. 15

mL, and left at room temperature for five days affording **$(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$** as dark brown crystals. Washing them several times with toluene for purification. Yield: 20.2 mg, 12.0%. Elemental analysis (%) calcd for ($C_{44}H_{34}AgF_{18}N_2O_9Sb_3$): C: 34.10, H: 2.21, N: 1.81; found: C: 34.47, H: 2.57, N: 1.68.

Table S1 Selected bond lengths (in Å) for **1**, **$1^{\bullet\bullet 2+}$** (in **$1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$**) and **$1Ag^{\bullet\bullet 3+}$** (in **$(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$**).



$1^{\bullet\bullet 2+}$



$1Ag^{\bullet\bullet 3+}$

	1		**$1^{\bullet\bullet 2+}$**	**$1Ag^{\bullet\bullet 3+}$**
	Calc.	X-ray	Calc.	X-ray
C1- O1	1.218	1.198(3)	1.204	1.205(11)
C1- C5´	1.552	1.538(4)	1.540	1.560(12)
C1-C2	1.485	1.484(4)	1.494	1.471(11)
C2-C3	1.413	1.402(4)	1.408	1.404(11)
C3-C3´	1.462	1.466(5)	1.473	1.459(16)
C3-C4	1.413	1.406(4)	1.407	1.417(11)
C4-C5	1.485	1.481(4)	1.494	1.458(11)
C5-O2	1.218	1.199(4)	1.204	1.201(10)
Ag1-O1´	-	-	-	2.397(6)
Ag1-O2´	-	-	-	2.460(6)
C4-C6	1.396	1.390(4)	1.390	1.376(11)
C6-C7	1.407	1.388(4)	1.399	1.397(12)
C7-C8	1.407	1.389(4)	1.399	1.386(11)

C7-N1	1.400	1.431(3)	1.416	1.424(10)
N1-C9	1.430	1.372(3)	1.399	1.376(11)
N1-C16	1.430	1.419(4)	1.402	1.437(11)

Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Center as supplementary publication CCDC- 2159584 for **$1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$**, and CCDC- 2159585 for **$(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$**.

Table S2 Crystal data and structure refinement for **$1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$** and **$(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$**.

	$1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$	**$1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-$**
Formula	$C_{39}H_{18}AlCl_2F_{36}NO_8$	$C_{46}H_{38}AgF_{18}N_2O_9Sb_3Cl_4$
Formula weight	1410.42	1719.70
Temperature/K	120	130
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a/Å	10.9911(15)	12.0834(14)
b/Å	14.4696(18)	14.7801(15)
c/Å	17.114(2)	16.8572(18)
α/°	95.559(4)	90.257(3)
β/°	101.930(4)	110.805(3)
γ/°	111.307(4)	99.213(3)
Volume/ Å^3	2436.3(6)	2771.8(5)
Z	2	2
ρ_{calc} g/cm^3	1.923	2.060
μ/mm^{-1}	0.343	2.103
F(000)	1388.0	1660.0
2θ range/°	4.12 to 55.054	3.938 to 55.04
collected data	21988	23416
Unique data	11097	12621
GOF on F^2	1.154	1.082
Final R indexes[I>=2σ (I)]	R_1 = 0.0600, ωR_2=0.1539	R_1 = 0.0779, ωR_2= 0.2002
Final R indexes[all data]	R_1=0.0765, ωR_2=0.1654	R_1= 0.1197, ωR_2= 0.2236
Completeness	0.991	0.991

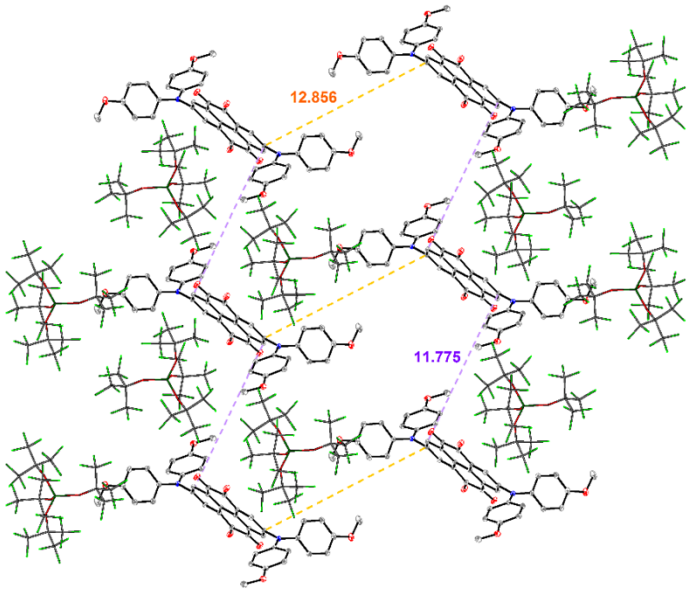


Fig. S5 Crystal packing diagram of $\mathbf{1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-}$ (Hydrogen atoms were omitted for the sake of clarity).

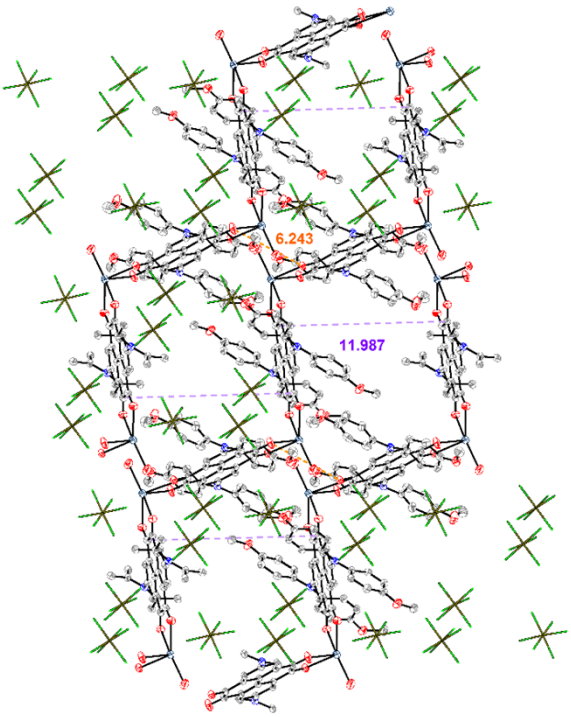


Fig. S6 Crystal packing diagram of $\mathbf{(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n}$ (Hydrogen atoms were omitted for the sake of clarity).

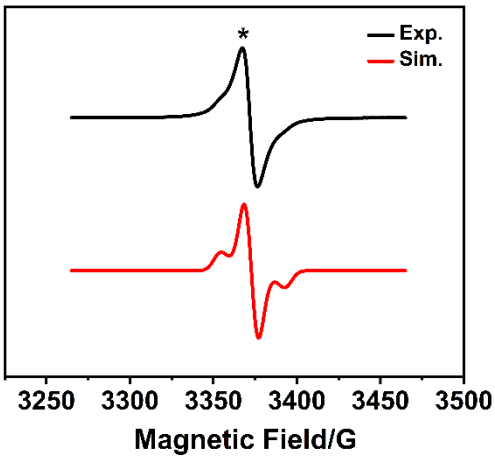


Fig. S7 Experimental (top, black) and simulated (bottom, red) powder EPR spectra of $(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$ at 298 K (υ = 9.4543 GHz). The central peak (with an asterisk) shows the signal due to the monoradical impurity.

SQUID measurements for the powder samples of $1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$ and $(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$ were carried out to determine their ground states (Fig. S8, S9). For $1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$, $\chi_M T$ is 0.69 $cm^3\ mol^{-1}$ K at 299 K and then slowly decreases upon cooling up to a minimum of 0.003 $cm^3\ mol^{-1}$ K at 1.8 K, indicating an antiferromagnetic interaction between two unpaired electrons. The experimental data were fitted to an equation corresponding to the Bleaney−Bowers model[3] for a diradical, giving the singlet−triplet energy gap $\Delta E_{OS\text{-}T} = 2J$ = -0.206 kcal/mol. SQUID curves indicate that both $(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$ and $1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$ are open-shell singlet ground state diradicals and the $\Delta E_{OS\text{-}T}$ of $(1Ag^{\bullet\bullet 3+}\cdot 3SbF_6^-)_n$ is smaller than that of $1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$.

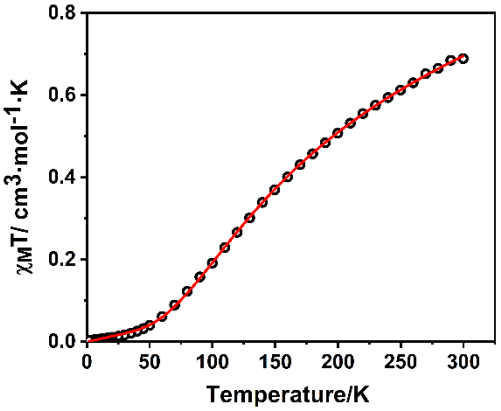


Fig. S8 Experimental $\chi_M T$ versus T data (black hollow circle) in the SQUID measurement for the powder sample of **$1^{\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$** and the fit (red solid line) using the Bleaney−Bowers equation with a coefficient of determination R^2 = 99.99%.

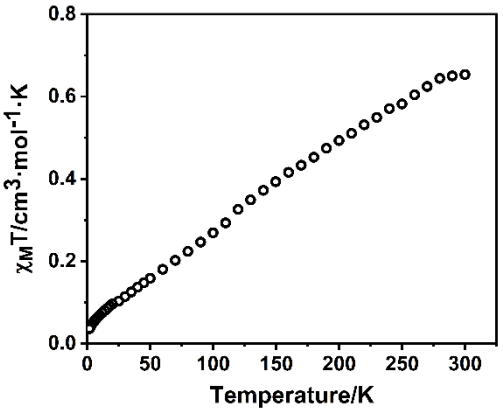


Fig. S9 Experimental $\chi_M T$ versus T data (black hollow circle) in the SQUID measurement for the powder sample of **$(1Ag^{\bullet 3+}\cdot 3SbF_6^-)_n$**.

Theoretical calculation details

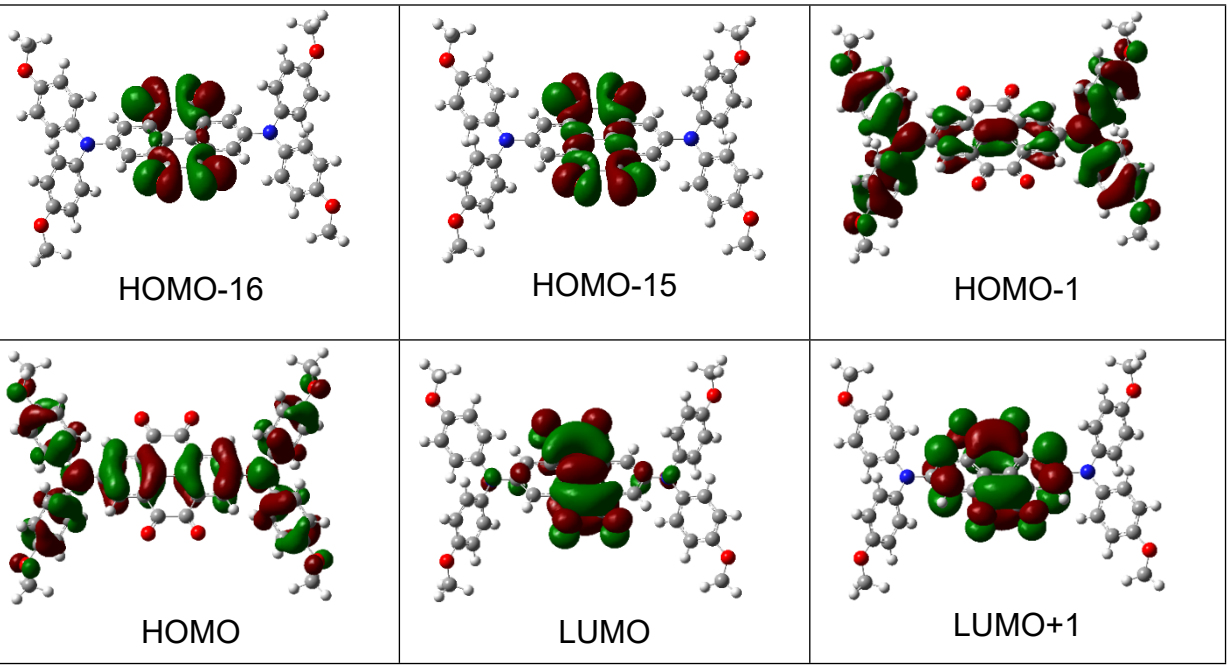
All the calculations were performed at the Gaussian 09 program. The geometry optimizations of the studied **$1^{\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$** were obtained at the (U)M062X/6-31G(d) level. Besides, the frequency calculations showed that there were no imaginary frequency. The UV-Vis-NIR absorption spectrum were calculated by using TD-DFT method at the UB3LYP/6-31G(d) level for **1** and at the UWB97XD/6-31G(d) level for **$1^{\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$**. CH_2Cl_2 was considered in the calculations by the polarizable continuum model (PCM)[4].

Table S3 Calculated absorption properties of UV-Vis-NIR absorption spectrum of **1** and **$1^{\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$**.

Molecules	Wavelength/nm	Transition	
	664	HOMO → LUMO	100%

1	324	HOMO-16 → LUMO+1 HOMO-15 → LUMO HOMO → LUMO +3	13% 31% 44%
	289	HOMO-1 → LUMO+7 HOMO → LUMO+6	11% 86%
$1^{\bullet\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$	833	HOMO-1 (α) → LUMO (α) HOMO-1 (β) → LUMO (β)	34% 34%
	551	HOMO (α) → LUMO+2 (α) HOMO (β) → LUMO+2 (β)	37% 37%
	457	HOMO-8 (α) → LUMO (α) HOMO-8 (β) → LUMO (β)	40% 40%
	354	HOMO-10 (α) → LUMO (α) HOMO-10 (β) → LUMO (β)	44% 44%
	299	HOMO-2 (α) → LUMO+1 (α) HOMO-2 (β) → LUMO+1 (β)	41% 41%
	255	HOMO-20 (α) → LUMO (α) HOMO-20 (β) → LUMO (β)	31% 31%

Table S4 Selected frontier molecular orbitals related to the electron transitions of UV-Vis-NIR absorption spectrum of neutral compound 1.



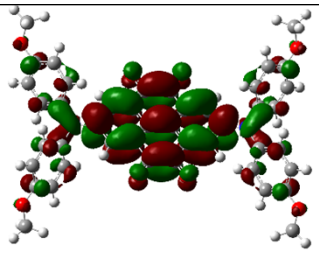
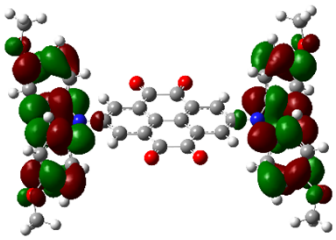
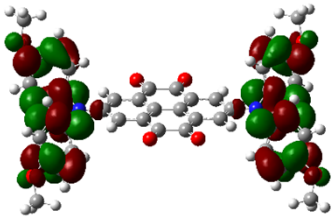
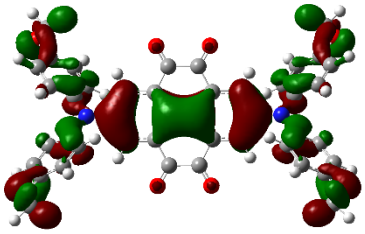
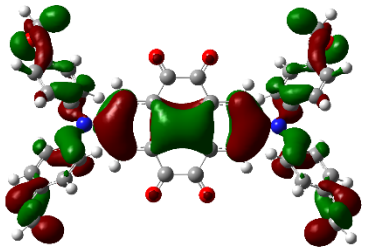
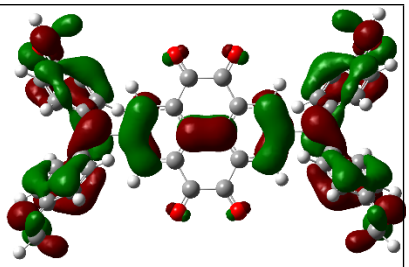
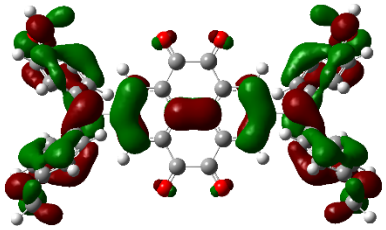
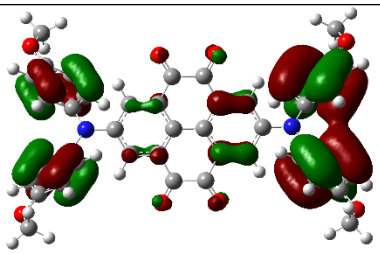
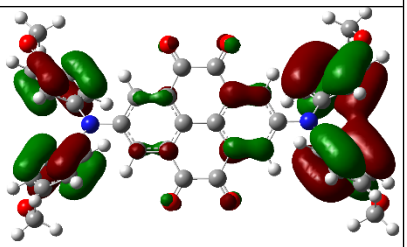
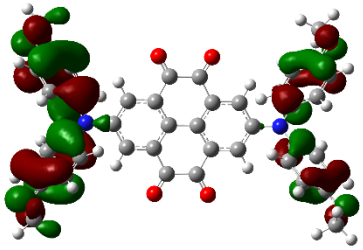
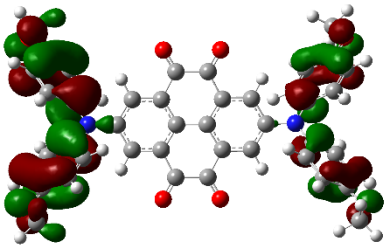
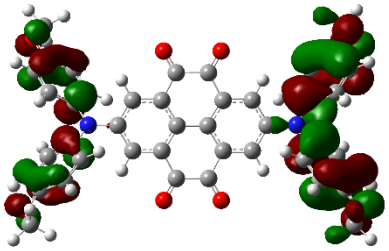
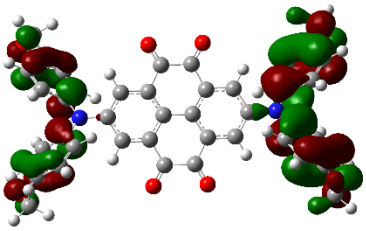
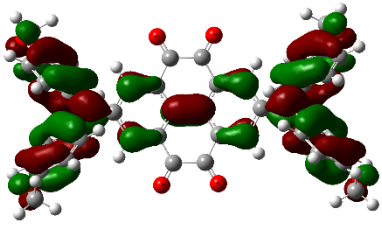
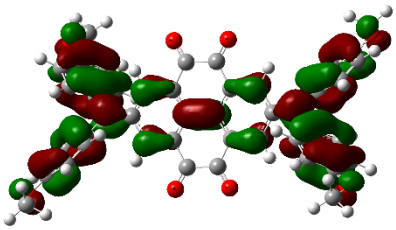
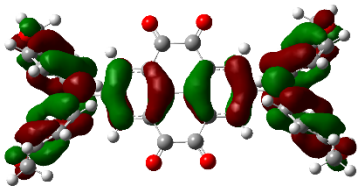
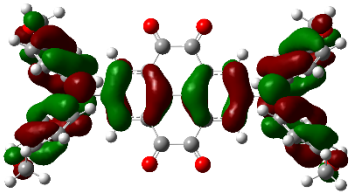
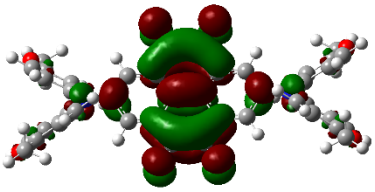
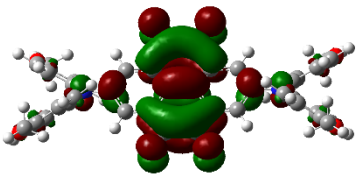
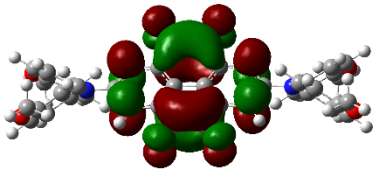
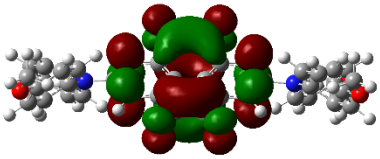
 LUMO+3	 LUMO+6	 LUMO+7

Table S5 Selected frontier molecular orbitals related to the electron transitions of UV-Vis-NIR absorption spectrum of $1^{\bullet 2+}\cdot 2[Al(OC(CF_3)_3)_4]^-$.

 HOMO-20 (α)	 HOMO-20 (β)	 HOMO-10 (α)
 HOMO-10 (β)	 HOMO-8 (α)	 HOMO-8 (β)
 HOMO-2 (α)	 HOMO-2 (β)	 HOMO-1 (α)

 HOMO-1 (β)	 HOMO (α)	 HOMO (β)
 LUMO (α)	 LUMO (β)	 LUMO+1 (α)
 LUMO+1 (β)	 LUMO+2 (α)	 LUMO+2 (β)

Optimized coordinates for the studied compounds

1

O	-1.36446000	3.25637900	-1.49593700
O	-1.36435100	-3.25610900	1.49661700
O	-7.98378500	-4.74119400	0.05926000
N	-4.99860000	-0.00000700	0.00022500
O	-7.98406600	4.74100700	-0.05930600
C	-1.47004000	1.09548900	-0.50094200
C	-0.73096300	0.00001000	0.00003700
C	-1.47000600	-1.09544500	0.50114300
C	-2.86555300	1.08942300	-0.50595100
H	-3.37059700	1.95606300	-0.91673300
C	-0.77596300	2.28712400	-1.05160200
C	-3.59836300	0.00003200	0.00017900

C	-0.77588500	-2.28703900	1.05184400
C	-6.75426900	-1.44269400	0.93556400
H	-6.96762000	-0.67755200	1.67559200
C	-2.86550900	-1.08934700	0.50630100
H	-3.37054400	-1.95593400	0.91720500
C	-6.75437300	1.44247300	-0.93528500
H	-6.96770400	0.67725300	-1.67523900
C	-5.73472200	-1.22617900	-0.00560400
C	-7.48941500	2.61881600	-0.92264900
H	-8.27887800	2.79358400	-1.64673100
C	-5.47467500	-2.21859600	-0.95519200
H	-4.69725700	-2.05984300	-1.69666700
C	-7.21203700	-3.61970400	-0.02146500
C	-5.73481500	1.22610700	0.00590200
C	-6.19484000	-3.41491300	-0.96118200
H	-5.96191300	-4.16629800	-1.70679200
C	-5.47482900	2.21864000	0.95538900
H	-4.69743700	2.06000300	1.69691600
C	-7.48926400	-2.61905900	0.92279200
H	-8.27871900	-2.79396400	1.64684800
C	-7.21223900	3.61958500	0.02148800
C	-6.19504600	3.41492200	0.96124300
H	-5.96217100	4.16638200	1.70679800
C	-7.73498000	-5.79536600	-0.85768500
H	-6.71256400	-6.18302800	-0.75851900
H	-7.90104000	-5.47587200	-1.89511300
H	-8.44592300	-6.58429900	-0.60608000
C	-7.73459600	5.79570000	0.85685800
H	-6.71203100	6.18283300	0.75718700
H	-7.90056100	5.47700800	1.89454500
H	-8.44526600	6.58475900	0.60488300

O	1.36446400	-3.25637600	1.49594200
O	1.36435400	3.25610800	-1.49662300
O	7.98377300	4.74120400	-0.05925600
N	4.99860300	0.00000700	-0.00022600
O	7.98406900	-4.74100600	0.05932800
C	1.47004400	-1.09550100	0.50091400
C	0.73096700	-0.00002000	-0.00006000
C	1.47001100	1.09544100	-0.50115600
C	2.86555700	-1.08943100	0.50593100
H	3.37060100	-1.95607300	0.91670900
C	0.77596700	-2.28714400	1.05155700
C	3.59836600	-0.00003500	-0.00018800
C	0.77588900	2.28703900	-1.05184700
C	6.75427100	1.44269800	-0.93556100
H	6.96762700	0.67755700	-1.67558700
C	2.86551300	1.08934500	-0.50630700
H	3.37054800	1.95593700	-0.91720100
C	6.75437600	-1.44246900	0.93529200
H	6.96770600	-0.67724600	1.67524300
C	5.73472100	1.22618000	0.00560500
C	7.48941800	-2.61881200	0.92266100
H	8.27887900	-2.79357700	1.64674500
C	5.47466700	2.21859800	0.95518900
H	4.69724500	2.05984400	1.69666100
C	7.21202800	3.61971100	0.02146800
C	5.73482000	-1.22610700	-0.00589800
C	6.19482700	3.41491800	0.96118100
H	5.96189500	4.16630300	1.70678900
C	5.47483300	-2.21864400	-0.95538000
H	4.69744100	-2.06001000	-1.69690800
C	7.48926200	2.61906600	-0.92278700

H	8.27871900	2.79397300	-1.64684000
C	7.21224300	-3.61958400	-0.02147200
C	6.19505000	-3.41492600	-0.96122900
H	5.96217500	-4.16638900	-1.70678000
C	7.73496000	5.79537700	0.85768500
H	6.71254200	6.18303500	0.75851400
H	7.90101700	5.47588600	1.89511500
H	8.44590000	6.58431200	0.60608100
C	7.73460100	-5.79570400	-0.85683100
H	6.71203600	-6.18283700	-0.75716000
H	7.90056700	-5.47701700	-1.89452000
H	8.44527100	-6.58476100	-0.60485100

$1^{\bullet\bullet 2+}$

O	-7.60231900	4.82331100	-0.30107500
O	-1.36919800	-3.04202900	-1.87929300
O	-1.36940100	2.78749800	2.25538900
O	-8.04555800	-4.59106100	-0.05953700
N	-4.96967000	-0.01460000	0.04217300
C	-0.73639700	-0.12059900	0.17753400
C	-2.85282700	-1.07205300	-0.56743100
H	-3.36820800	-1.82882600	-1.15274000
C	-1.46223000	0.86859800	0.86749100
C	-3.55608600	-0.07089600	0.11037000
C	-1.46374200	-1.09632200	-0.52935900
C	-2.85074800	0.89147400	0.84024000
H	-3.36704200	1.66716900	1.39915100
C	-6.84737600	1.43839500	0.59993800
H	-7.27528700	0.64704200	1.20706400
C	-5.60950700	1.22946600	-0.05112400
C	-0.77063900	-2.18283400	-1.28522900
C	-6.89315800	-1.27308800	-0.75881800

H	-7.17453400	-0.43308400	-1.38531200
C	-0.77027900	1.93592100	1.65103400
C	-7.48124900	2.65098800	0.49835400
H	-8.41882300	2.84411700	1.00761900
C	-5.72398700	-1.19333400	0.03412100
C	-7.63971300	-2.42323200	-0.76984300
H	-8.52512100	-2.51782400	-1.38871100
C	-5.67277000	3.49337700	-0.90947500
H	-5.22577900	4.27663600	-1.50918500
C	-5.03520000	2.27399600	-0.79978700
H	-4.10152400	2.10785000	-1.32762600
C	-6.90799500	3.69583300	-0.26109600
C	-5.33401800	-2.30327200	0.80857600
H	-4.45494200	-2.23750500	1.44197900
C	-7.25351000	-3.53296000	0.01630900
C	-6.08753800	-3.46002500	0.80618600
H	-5.78464600	-4.29504800	1.42571600
C	-7.09162400	5.93797900	-1.03004400
H	-7.82797800	6.72873600	-0.90585300
H	-6.99021400	5.68848300	-2.09057800
H	-6.12962400	6.25698500	-0.61790800
C	-7.73304000	-5.76192100	0.69466000
H	-8.52280800	-6.47435900	0.46697800
H	-7.73204300	-5.53773300	1.76535400
H	-6.76503000	-6.16786000	0.38648600
O	8.04568900	-4.59090000	-0.06059700
O	1.36927000	2.78747700	2.25545500
O	1.36917300	-3.04196000	-1.87935500
O	7.60240400	4.82326900	-0.30032500
N	4.96958900	-0.01461200	0.04231900
C	0.73631600	-0.12060100	0.17756300

C	2.85065400	0.89142700	0.84038000
H	3.36692900	1.66709000	1.39934900
C	1.46368100	-1.09632200	-0.52931500
C	3.55601400	-0.07092500	0.11050000
C	1.46213500	0.86857000	0.86757000
C	2.85276700	-1.07206500	-0.56734200
H	3.36814900	-1.82881400	-1.15267700
C	6.89295800	-1.27291400	-0.75921400
H	7.17414100	-0.43283400	-1.38568900
C	5.72396000	-1.19330700	0.03400300
C	0.77016500	1.93590900	1.65107000
C	6.84729200	1.43829000	0.60031400
H	7.27516700	0.64683000	1.20732900
C	0.77059700	-2.18282000	-1.28522900
C	7.63957200	-2.42301100	-0.77054300
H	8.52483700	-2.51748000	-1.38963500
C	5.60942600	1.22948800	-0.05078800
C	7.48121100	2.65087800	0.49890200
H	8.41878800	2.84390600	1.00820000
C	6.08783300	-3.46005700	0.80575300
H	5.78515600	-4.29515600	1.42528800
C	5.33424100	-2.30334900	0.80844000
H	4.45532200	-2.23770400	1.44207000
C	7.25361200	-3.53285100	0.01557400
C	5.03515800	2.27412300	-0.79931800
H	4.10146700	2.10806800	-1.32716400
C	6.90800700	3.69582900	-0.26043500
C	5.67276600	3.49350200	-0.90882900
H	5.22579700	4.27685000	-1.50843900
C	7.73344600	-5.76188100	0.69353600
H	8.52325400	-6.47420400	0.46562800

H	7.73262800	-5.53781000	1.76425400
H	6.76542300	-6.16789300	0.38549900
C	7.09162900	5.93813400	-1.02893800
H	7.82796600	6.72887800	-0.90456700
H	6.99017100	5.68894100	-2.08953900
H	6.12963600	6.25698000	-0.61665900

References:

1. (a) V. A. Kuehl, J. Yin, P. H. H. Duong, B. Mastorovich, B. Newell, K. D. Li-Oakey, B. A. Parkinson and J. O. Hoberg, *J. Am. Chem. Soc.*, 2018, **140**, 18200-18207; (b) P.-Y. Gu, Z. Wang, G. Liu, H. Yao, Z. Wang, Y. Li, J. Zhu, S. Li and Q. Zhang, *Chem. Mater.*, 2017, **29**, 4172-4175; (c) J. Merz, M. Dietz, Y. Vonhausen, F. Wober, A. Friedrich, D. Sieh, I. Krummenacher, H. Braunschweig, M. Moos, M. Holzapfel, C. Lambert and T. B. Marder, *Chem. Eur. J.*, 2020, **26**, 438-453.
2. I. Krossing, *Chem. Eur. J.*, 2001, **7**, 490-502.
3. B. Bleaney and K. D. Bowers, *Proc. R. Soc. London Ser. A*, 1997, **214**, 451-465.
4. (a) L. Frediani, Z. Rinkevicius and H. Agren, *J. Chem. Phys.*, 2005, **122**, 244104; (b) J. Tomasi, B. Mennucci and R. Cammi, *Chem Rev*, 2005, **105**, 2999-3093.