Supporting Information

Rational Design and Syntheses of Aniline-Based Diradical Dications: Isolable Congeners of Quinodimethane Diradicals

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Table of Contents

Experimental Section

General Considerations. All experiments were carried out under an atmosphere of dry nitrogen or argon by using standard Schlenk techniques and a glovebox. Solvents were dried by standard methods and freshly distilled prior to use. The NMR spectra were recorded on a Bruker DRX 400 MHz NMR spectrometer referenced to residual solvent signals as internal standards (^{1}H NMR: CD_2Cl_2, 5.32 ppm and $^{13}C\{^1H\}$ NMR: CD_2Cl_2, 53.84 ppm). Cyclic voltammetry was performed on a CHI660E electrochemical workstation with platinum as the working and counter electrodes, Ag/Ag^+ as the reference electrode and 0.1 M $^nBu_4N[BAr^F_4]$ (Ar^F=3,5-$(CF_3)_2C_6H_3$) as the supporting electrolyte, and the measurement was carried out under a nitrogen atmosphere. UV/Vis spectra were recorded on the Lambda 750 spectrometer. Element analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. EPR spectra were obtained using a Bruker plus-6/1 X-band variable-temperature apparatus. Magnetic measurements were performed using a Quantum Design SQUID VMS magnetometer with a field of 0.1T. The X-ray single crystal diffraction data were collected on Bruker D8 CMOS detectors at 123 K. 4,4''-Diamino-*p*-terphenyl (Compound **1**) was purchased from Alfa-Aesar and used as received. Compounds $Li[Al(OR_{Cl})_4]$ (OR_{Cl} = $OC(CCl_3)(CF_3)_2$),[1] $Li[Al(OR_H)_4]$ (OR_H = $OC(CH_3)(CF_3)_2$),[2] $Li[Al(OR_F)_4]$ (OR_F = $OC(CF_3)_3$),[2] 4-(diphenylmethylene)amino-3,5-dimethylphenyl-boronic acid,[3] 4-(diphenylmethylene)amino-3,5-diisopropylphenyl-boronic acid[3] and compound **3**[4] were prepared according to the reported procedures.

Syntheses of neutral 4,4''-*p*/*m*-terphenyldiamines. Degassed DME (110 mL) and water (27.5 mL) were added into a Schlenk flask charged with the 4-(diphenylmethylene)amino-3,5-dialkylphenyl-boronic acid (22 mmol), $Pd(PPh_3)_4$ (0.35g, 0.30 mmol), Na_2CO_3 (6.36 g, 60 mmol), and *p*/*m*-dibromobenzene (2.36 g, 10 mmol). After addition, the flask was sealed and heated to 100 °C overnight. The reaction mixture was allowed to cool down to room temperature to deposit yellow flocculent precipitate, which was extracted with ethyl acetate (80 ml × 2), dried with anhydrous Na_2SO_4 and purified by column chromatography on silica gel with a mixture of hexane and toluene (1:1) as eluent. The off-white intermediate diimine obtained was dissolved in THF (50 mL), followed by addition of HCl (2 M, 25 mL). After the reaction mixture was stirred at 60 °C for 3 hours, the solvent was removed by rotary evaporator. The white solid was thoroughly washed with diethyl ether to remove the generated benzophenone. To a suspension of the remains in diethyl ether (50 mL) was added an aqueous KOH solution (1.0 N, 75 mL) and the mixture was stirred for 3 hours at room temperature. The phases were separated and the aqueous phase was extracted with diethyl ether (3 × 50 ml). The combined organic phase was washed with water and dried over anhydrous $MgSO_4$. The solvent was removed with rotary evaporator to give white crude product, which was further chromatographed on silica gel using a mixture of hexane and ethyl acetate (15:1) as eluent to yield the corresponding terphenyldiamine as a white powder.

Neutral 2: yield: 64%; ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.57 (s, 4H, Ar-*H*), 7.25 (s, 4H, Ar-*H*), 3.70 (br, 4H, NH_2), 2.25 (s, 12H, CH_3) ppm; ^{13}C NMR (100 MHz, CD_2Cl_2): δ 143.0, 139.4, 130.4, 126.9, 126.7, 122.3, 18.0 ppm; Elemental analysis for $C_{22}H_{24}N_2$ (%): Calcd: C 83.50, H 7.64, N 8.85; Found: C 82.91, H 7.73, N 8.49. m.p. 238–240 °C.

Neutral 4: Yield: 73%; ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 (s, 1H, Ar-*H*), 7.43 (m, 3H, Ar-*H*), 7.28 (s, 4H, Ar-*H*), 3.71 (br, 4H, NH_2), 2.26 (s, 12H, CH_3) ppm; ^{13}C NMR (100 MHz, CD_2Cl_2): δ 143.1, 142.2, 131.0, 129.3, 127.2, 124.7, 124.4, 122.3, 17.9 ppm; Elemental analysis for $C_{22}H_{24}N_2$ (%): Calcd: C 83.50, H 7.64, N 8.85; Found: C 82.70, H 7.96, N 8.14. m.p. 144–146 °C.

Neutral 5: Yield: 78%; ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.71 (s, 1H, Ar-*H*), 7.45 (m, 3H, Ar-*H*), 7.32 (s, 4H, Ar-*H*), 3.90 (br, 4H, N*H*$_2$), 3.00 (septet, *J* = 6.8 Hz, 4H, C*H*), 1.33 (d, *J* = 6.8 Hz, 24H, C*H*$_3$) ppm; ^{13}C NMR (100 MHz, CD_2Cl_2): δ 143.2, 140.6, 133.2, 131.8, 129.2, 125.5, 124.9, 122.2, 28.5, 22.7 ppm; Elemental analysis for $C_{30}H_{40}N_2$ (%): Calcd: C 84.06, H 9.41, N 6.54; Found: C 84.16, H 9.58, N 6.34. m.p. 179–181 °C.

Syntheses of Dication Salts. Under anaerobic and anhydrous conditions, a CH_2Cl_2 (≈ 15 ml) solution of $AgSbF_6$ was dropwise added into the mixture of 4,4''-*p*/*m*-terphenyldiamine and lithium polyfluorinated alkoxy aluminate in CH_2Cl_2 (≈ 30 ml). The resultant solution was stirred overnight at room temperature and then filtered to remove the gray precipitate (Ag metal and $LiSbF_6$). The filtrate was then concentrated and stored at around –30 °C for 1 day to afford blue crystals.

1^{2+}·2[Al(OR$_{Cl}$)$_4$]$^-$: 1 (0.057 g, 0.22 mmol), $AgSbF_6$ (0.155 g, 0.45 mmol) and Li[Al(OR$_{Cl}$)$_4$] (0.527 g, 0.45 mmol). Yield: 0.434 g, 82%; m.p. 231–233 °C; UV/Vis (CH_2Cl_2): λ_{max} = 536 nm; Elemental analysis for $C_{50}H_{16}N_2O_8F_{48}Al_2Cl_{24}$ (%): Calcd: C 23.19, H 0.62, N 1.08; Found: C 24.03, H 1.00, N 1.40.

2^{2+}·2[Al(OR$_H$)$_4$]$^-$·CH$_2$Cl$_2$: 2 (0.063 g, 0.20 mmol), $AgSbF_6$ (0.144 g, 0.42 mmol) and Li[Al(OR$_H$)$_4$]. Yield: 0.263 g, 69%; m.p. 237–240 °C; UV/Vis (CH_2Cl_2): λ_{max} = 542 nm; Elemental analysis for $C_{55}H_{50}N_2O_8F_{48}Al_2Cl_2$ (%): Calcd: C 34.70, H 2.65, N 1.47; Found: C 34.96, H 2.75, N 1.55.

3^{2+}·2[Al(OR$_H$)$_4$]$^-$: 3 (0.081 g, 0.19 mmol), $AgSbF_6$ (0.138 g, 0.40 mmol), and Li[Al(OR$_H$)$_4$] (0.303 g, 0.40 mmol). Yield: 0.278 g, 76%; m.p. 225–227 °C; UV/Vis (CH_2Cl_2): λ_{max} = 540 nm; Elemental analysis for $C_{62}H_{64}N_2O_8F_{48}Al_2$ (%): Calcd: C 38.56, H 3.34, N 1.45; Found: C 38.33, H 3.38, N 1.47.

4^{2+}/5^{2+}·2[Al(OR$_F$)$_4$]$^-$: 4/5 (0.063 g, 0.20 mmol for **4**; 0.086 g, 0.20 mmol for **5**), $AgSbF_6$ (0.144 g, 0.42 mmol) and Li[Al(OR$_F$)$_4$] (0.409 g, 0.42 mmol). Unfortunately, no crystals precipitated from the mother liquor even after standing for a long time and several times of further concentration. Finally the solution was allowed to warm up to room temperature and dilut to specific concentrations under nitrogen for subsequent UV/Vis and EPR measurements.

(**Note**: The *the elemental analysis and HRMS characterizations of* ***4***$^{2+}$ *and* ***5***$^{2+}$ *failed due to their highly reactive nature and consequent unclear destabilization processes.*)

NMR Spectra

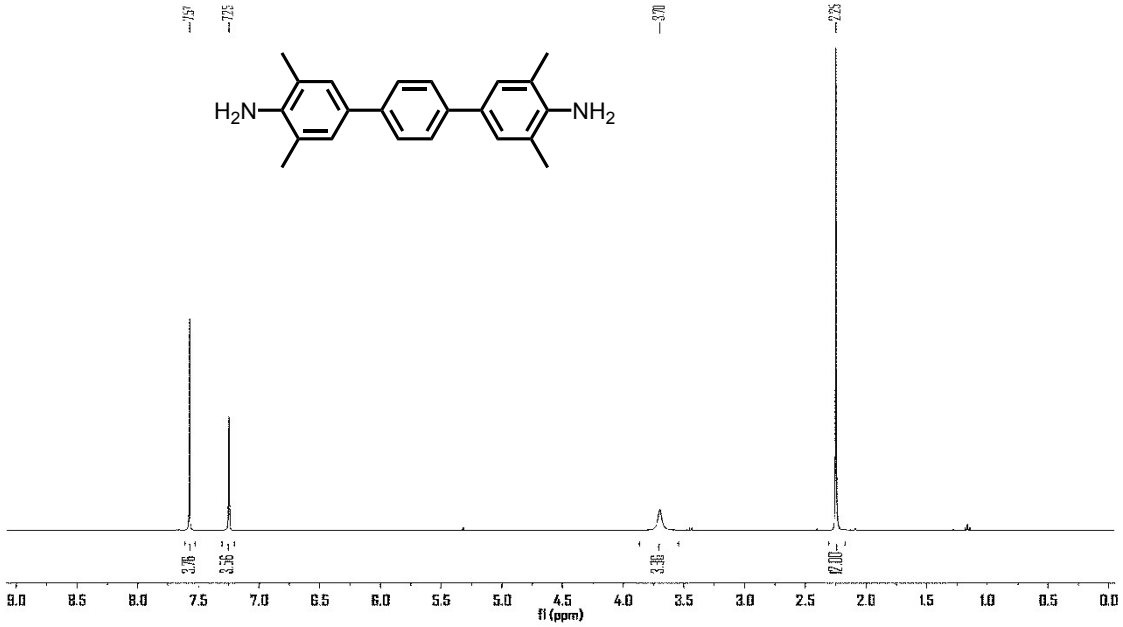


Figure S1. ^{1}H NMR spectrum of compound **2** in CD_2Cl_2.

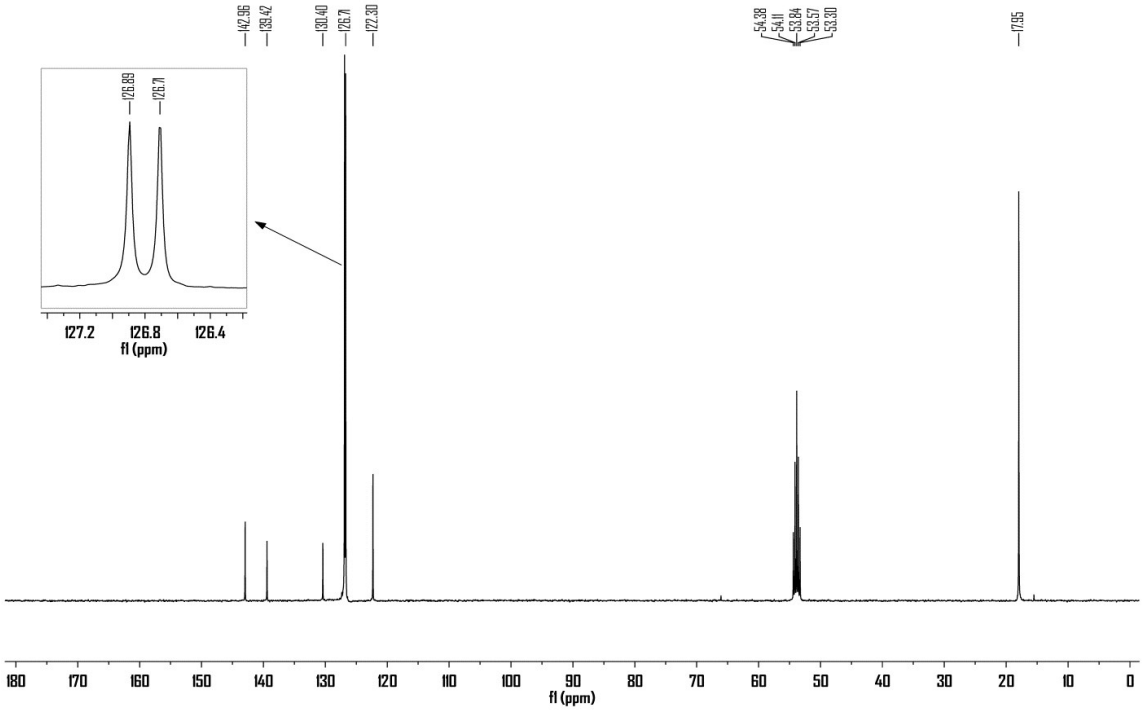


Figure S2. ^{13}C NMR spectrum of compound **2** in CD_2Cl_2.

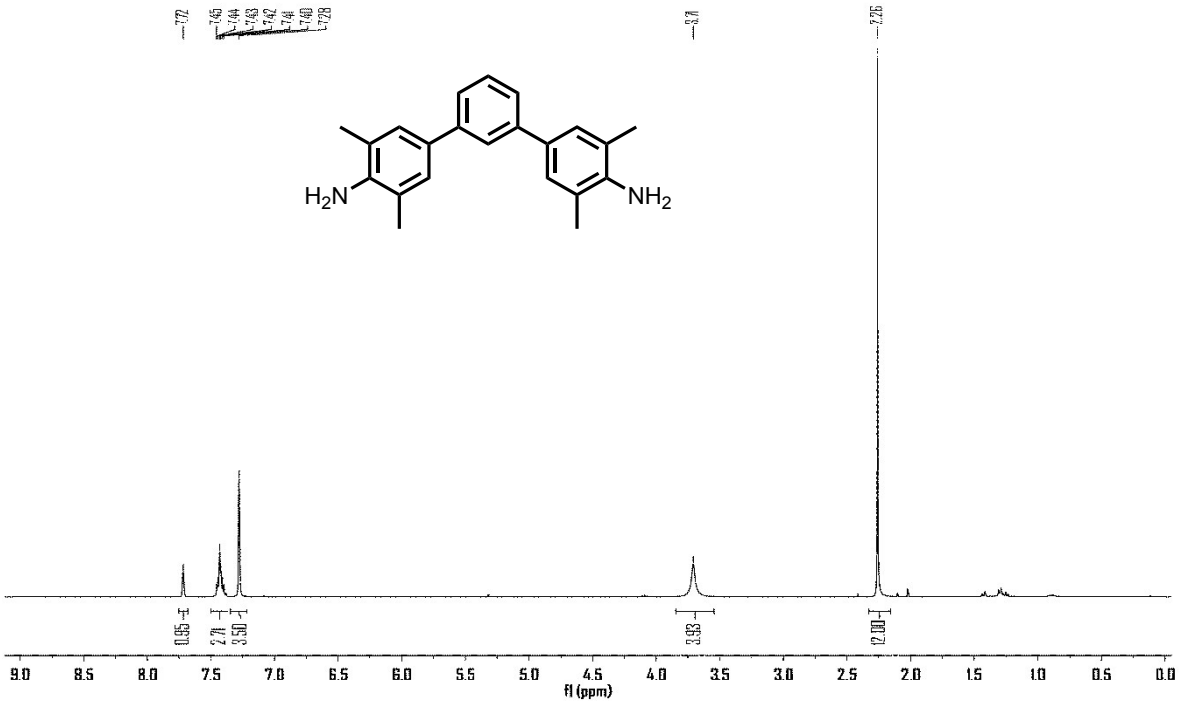


Figure S3. ^{1}H NMR spectrum of compound **4** in CD_2Cl_2.

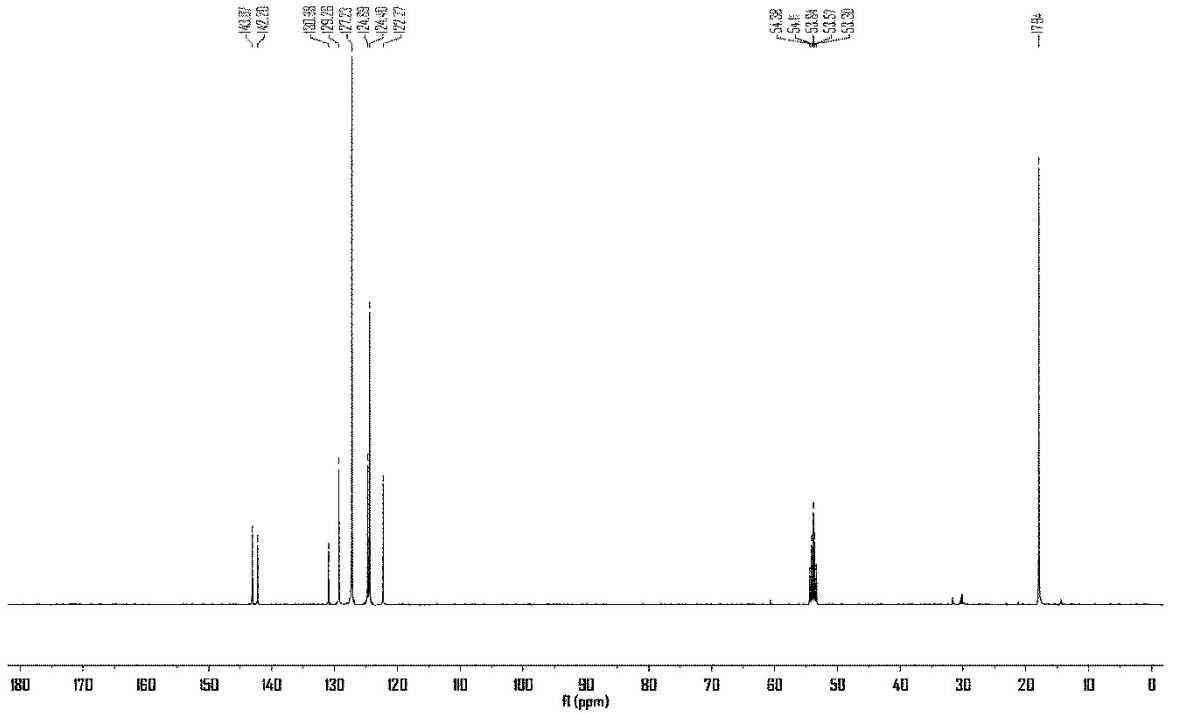


Figure S4. ^{13}C NMR spectrum of compound **4** in CD_2Cl_2.

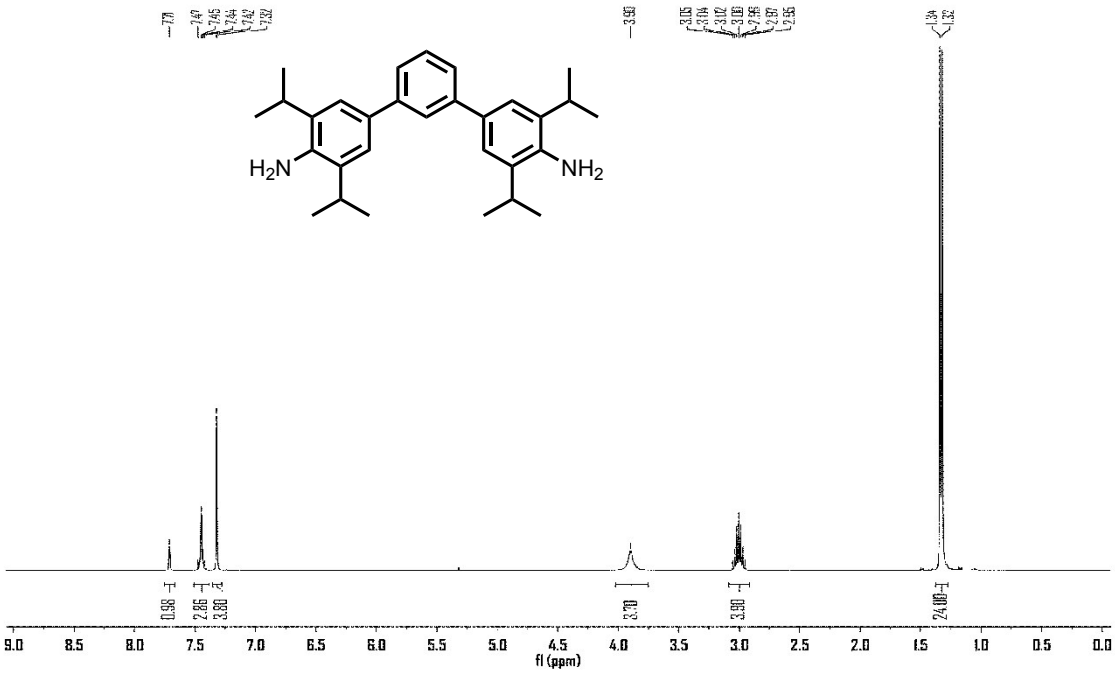


Figure S5. ^{1}H NMR spectrum of compound **5** in CD_2Cl_2.

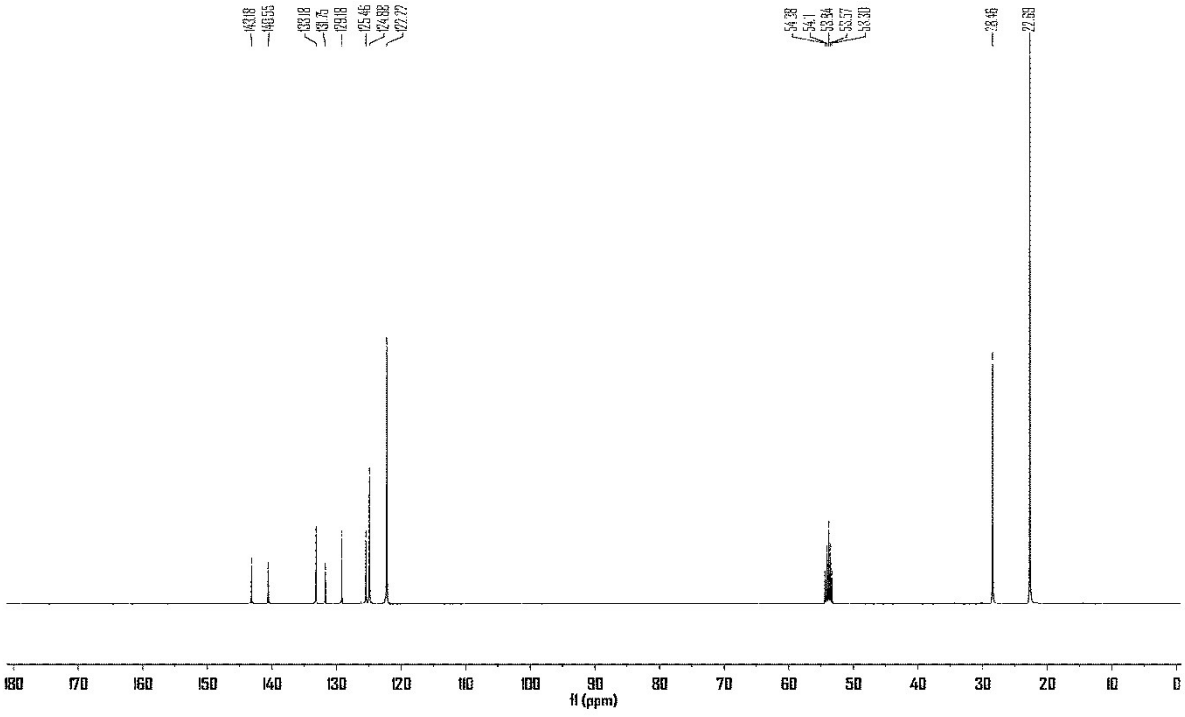


Figure S6. ^{13}C NMR spectrum of compound **5** in CD_2Cl_2.

X-ray Structural Determinations

Table S1. Crystal data and structure refinement.

	$\mathbf{1}^{2+}\bullet 2[Al(OR_{Cl})_4]^-$	$\mathbf{2}^{2+}\bullet 2[Al(OR_{H})_4]^-\bullet CH_2Cl_2$	$\mathbf{3}^{2+}\bullet 2[Al(OR_{H})_4]^-$
CCDC	1975308	1975310	1975311
Formula	$C_{50}H_{16}Al_2Cl_{24}F_{48}N_2O_8$	$C_{55}H_{50}Al_2Cl_2F_{48}N_2O_8$	$C_{31}H_{32}AlF_{24}NO_4$
*M*r [g mol^{-1}]	2589.41	1903.83	965.55
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*P* 2(1)/n	*P* 2(1)/n	*P* 2(1)/c
Z	4	2	4
Temp. (K)	123(2)	123(2)	123(2)
μ (mm^{-1})	0.985	0.293	0.206
a (Å)	18.3924(18)	17.1492(7)	13.8150(7)
b (Å)	11.3080(16)	10.1598(5)	14.6000(7)
c (Å)	39.3507(14)	20.7661(8)	19.3430(10)
β (°)	94.605(3)	98.0722(11)	97.0995(15)
V [Å^3]	8157.8(14)	3582.3(3)	3871.6(3)
*R*1 (I>2σ(I))	0.0466	0.0540	0.0402
*wR*2 (all data)	0.1048	0.1518	0.1052
GOF	1.047	1.043	1.021
Largest diff. Peak/hole, e•Å^{-3}	0.374/-0.520	0.531/-0.485	0.738/-0.634

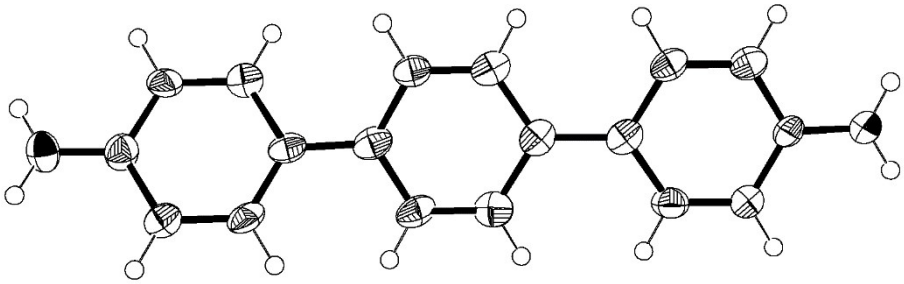


Figure S7. Ortep drawing of $\mathbf{1}^{2+}$ with ellipsoids given at the 50% probability level.

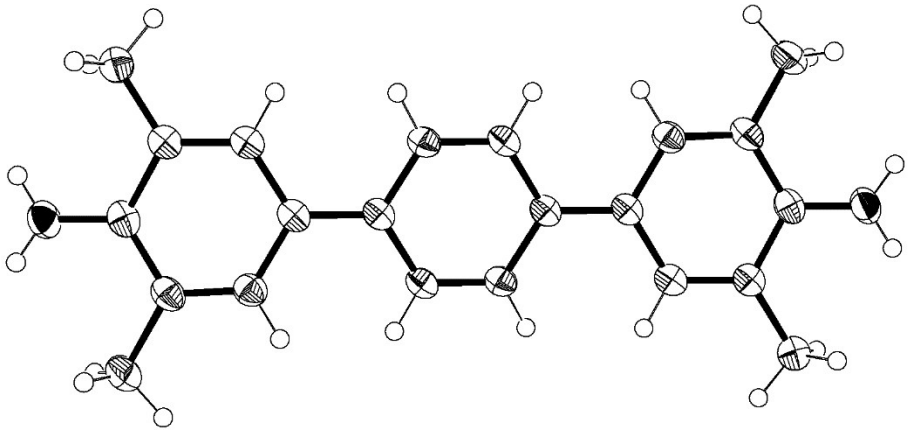


Figure S8. Ortep drawing of $\mathbf{2}^{2+}$ with ellipsoids given at the 50% probability level.

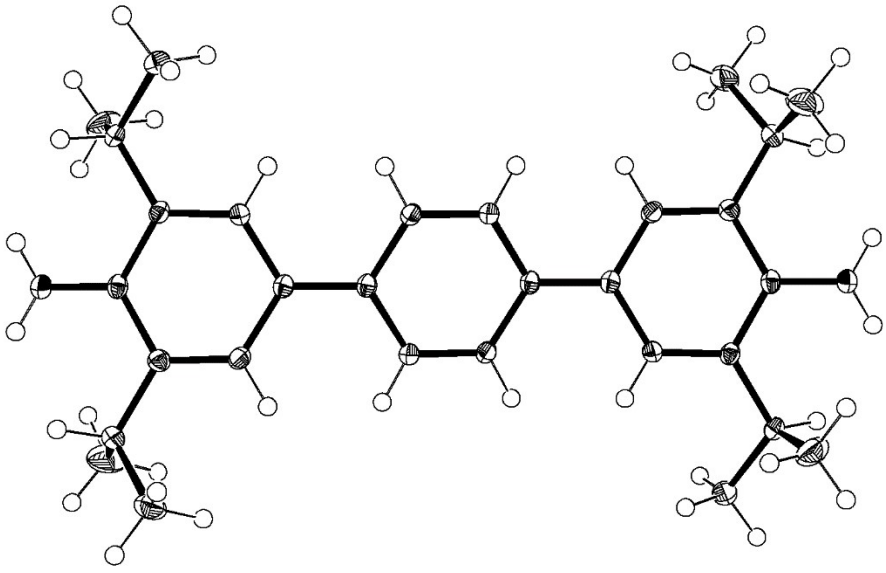
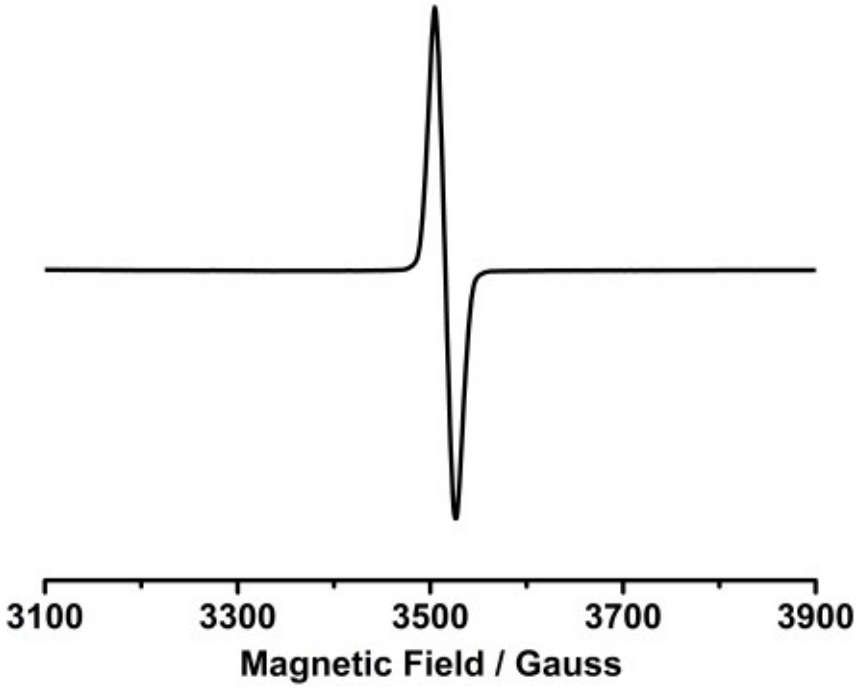


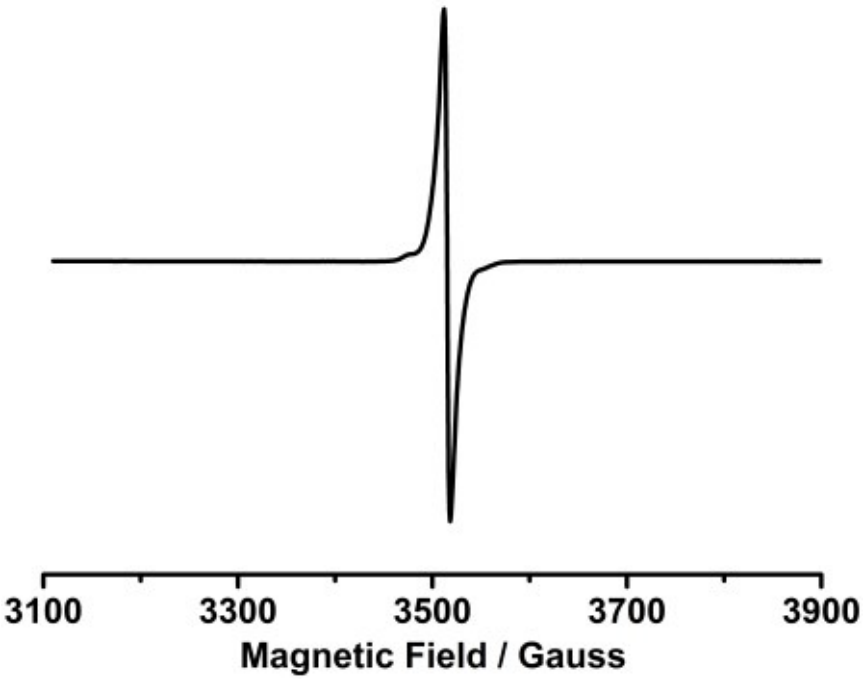
Figure S9. Ortep drawing of $\mathbf{3}^{2+}$ with ellipsoids given at the 50% probability level.

EPR Spectra

(a)



(b)



(c)

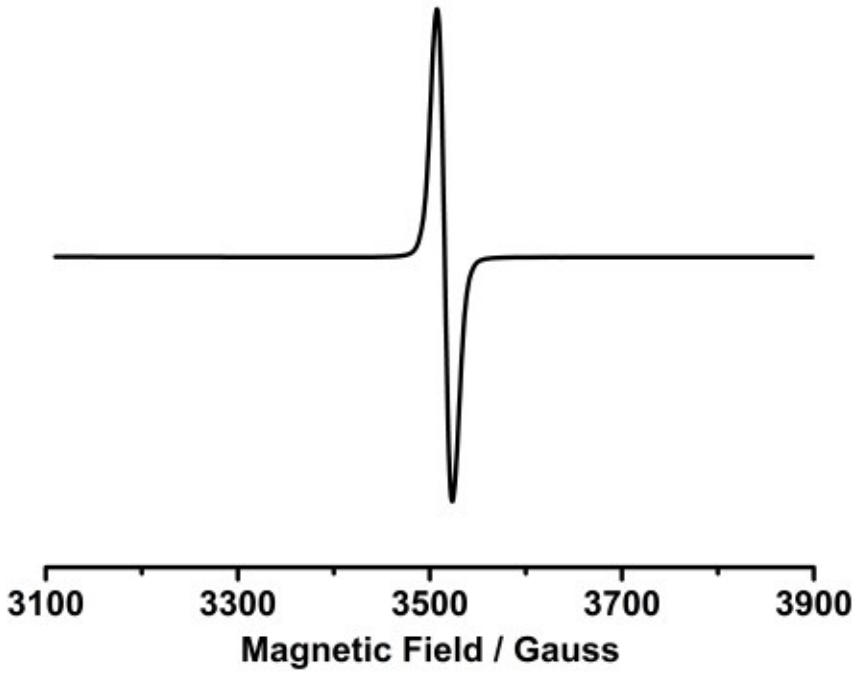


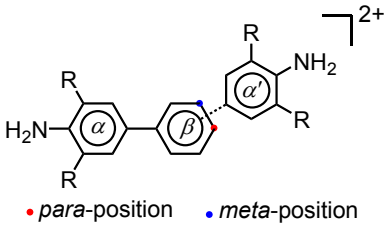
Figure S10. Powder EPR spectra of $\mathbf{1}^{2+}$ (a), $\mathbf{2}^{2+}$ (b), and $\mathbf{3}^{2+}$ (c) at 298K.

(The centered single-peak signal is reasonably attributed to corresponding monoradical impurity in each case)

Calculation Details

All the geometry optimizations were carried out at the (U)WB97XD/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. The UV-vis absorption spectra were calculated using time-dependent DFT (TD-DFT) method and polarized continuum model (PCM) was adopted to consider solvent effects. All calculations were performed with the Gaussian 09 program suite.[5] The ACID[6] plots were generated with Gaussian09 using the CSGT method[7] and AICD 2.0.0. ACID is a method to visualize conjugation and ring currents in molecules. Clockwise ring currents correspond to aromatic systems and counter-clockwise ring currents to antiaromatic systems. Systems with no evident ring current are considered non-aromatic.

Table S2. The NICS values for the phenyl rings in $\mathbf{1}^{2+}$–$\mathbf{5}^{2+}$.



Dication		$\mathbf{1}^{2+}$	$\mathbf{2}^{2+}$	$\mathbf{3}^{2+}$	$\mathbf{4}^{2+}$	$\mathbf{5}^{2+}$
ring α	NICS(0)	0.11	0.91	1.00	1.31	0.77
	$NICS(1)_{zz}$	−5.36	−2.54	−2.76	−1.85	−1.55
ring β	NICS(0)	−2.41	−3.52	−3.77	−4.73	−4.81
	$NICS(1)_{zz}$	−13.67	−15.91	−16.32	−16.17	−15.15
ring α′	NICS(0)	0.11	0.91	1.00	1.31	0.20
	$NICS(1)_{zz}$	−5.36	−2.76	−2.76	−1.85	−2.42

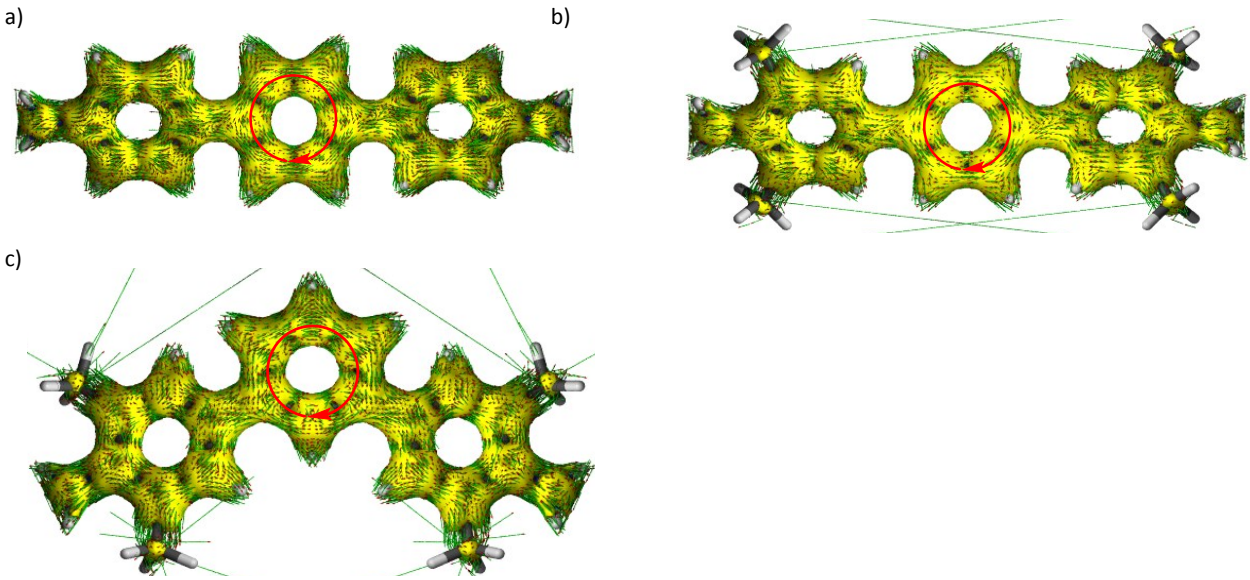


Figure S11. ACID plots of the the open-shell singlet states of $\mathbf{1}^{2+}$ (a), $\mathbf{2}^{2+}$ (b) and triplet states of $\mathbf{4}^{2+}$ (c) calculated at the level of CSGT-UWB97XD/6-31G(d) The magnetic field is perpendicular to the central phenyl plane and points out through the paper during ACID calculations. The circles labeled by red arrows indicate the clockwise ring current flow.

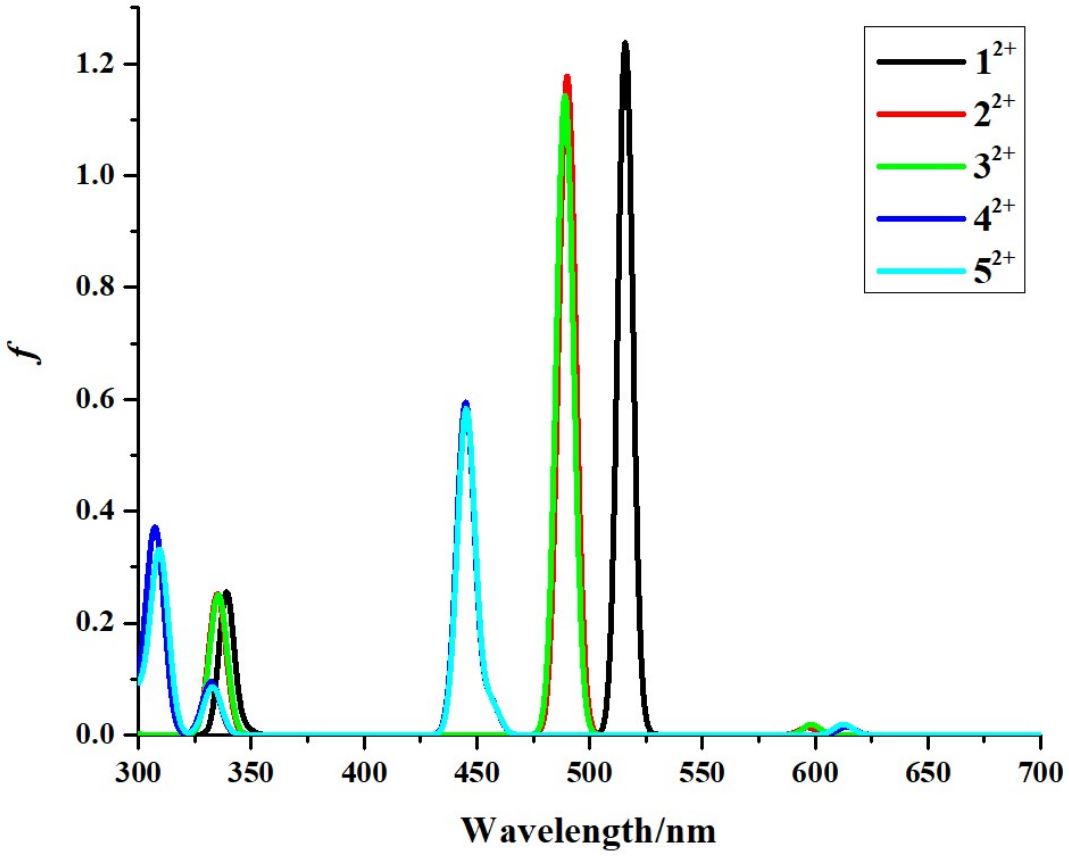


Figure S12. The calculated UV/Vis absorption spectra of $\mathbf{1}^{2+}$-$\mathbf{5}^{2+}$ in CH_2Cl_2.

Table S3. TD-DFT calculated absorption wavelengths (*λ*), oscillator strengths (*f*), and assignments for the electronic transition configurations .

1^{2+}

	λ (nm)	*f*	Assignment
S4	515.8	1.238	HOMO(α) → LUMO(α) (29%), HOMO(β) → LUMO(β) (29%) HOMO-2(α) → LUMO(α) (16%), HOMO-2(β) → LUMO(β) (16%)
S7	339.0	0.2548	HOMO(α) → LUMO+1(α) (18%), HOMO(β) → LUMO+1(β) (18%) HOMO-5(α) → LUMO(α) (11%), HOMO-5(β) → LUMO(β) (11%)

2^{2+}

	λ (nm)	*f*	Assignment
S4	490.0	1.178	HOMO(α) → LUMO(α) (27%), HOMO(β) → LUMO(β) (27%)
S6	335.0	0.2412	HOMO(α) → LUMO+1(α) (20%), HOMO(β) → LUMO+1(β) (20%)

3^{2+}

	λ (nm)	*f*	Assignment
S4	489.0	1.143	HOMO(α) → LUMO(α) (27%), HOMO(β) → LUMO(β) (27%)
S6	335.4	0.2426	HOMO(α) → LUMO+1(α) (20%), HOMO(β) → LUMO+1(β) (20%)

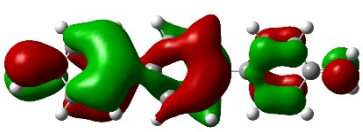
4^{2+}

	λ (nm)	*f*	Assignment
S1	614.1	0.0024	HOMO-3(β) → LUMO(β)(51%), HOMO-2(β) → LUMO+1(β) (45%)
S2	614.0	0.0123	HOMO-2(β) → LUMO(β)(51%), HOMO-3(β) → LUMO+1(β) (45%)
S3	455.9	0.0601	HOMO(β) → LUMO+1(β)(46%), HOMO-1(β) → LUMO(β) (21%)
S4	445.0	0.5932	HOMO(β) → LUMO(β) (56%), HOMO-1(β) → LUMO+1(β) (23%)
S6	332.2	0.0947	HOMO(α) → LUMO(α) (12%), HOMO-4(β) → LUMO(β) (12%)

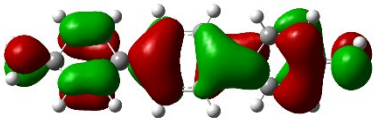
5^{2+}

	λ (nm)	*f*	Assignment
S1	613.7	0.01	HOMO-2(β) → LUMO(β)(48%), HOMO-2(β) → LUMO+1(β) (46%)
S3	456.1	0.0576	HOMO(β) → LUMO+1(β)(46%), HOMO-1(β) → LUMO(β) (20%)
S4	445.2	0.5932	HOMO(β) → LUMO(β) (56%), HOMO-1(β) → LUMO+1(β) (23%)
S8	309.5	0.0947	HOMO(α) → LUMO+1(α)(28%), HOMO-1(α) → LUMO(α) (26%)

1^{2+}-OS



HOMO-5(α)



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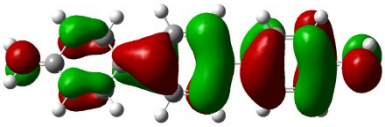
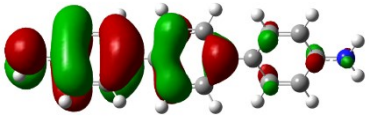
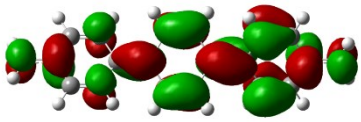


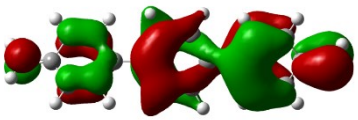
HOMO(α)



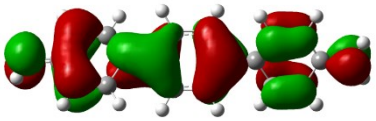
LUMO(α)



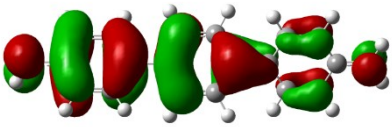
LUMO+1(α)



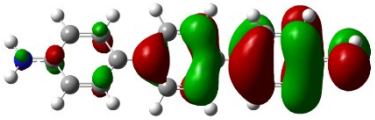
HOMO-5(β)



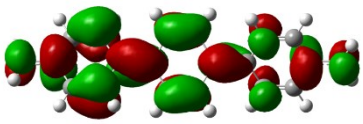
HOMO-2(β)



HOMO(β)



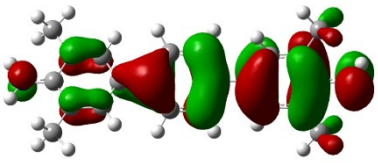
LUMO(β)



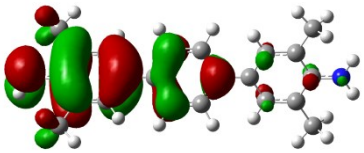
LUMO+1(β)

Figure S13. Selected frontier molecular orbitals for **1**$^{2+}$-OS.

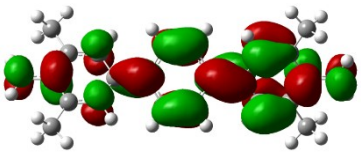
2^{2+}-OS



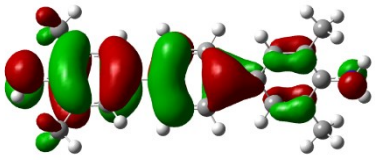
HOMO(α)



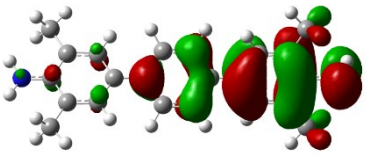
LUMO(α)



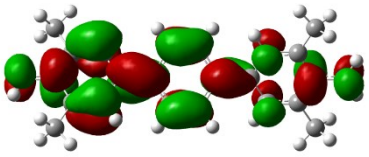
LUMO+1(α)



HOMO(β)



LUMO(β)



LUMO+1(β)

Figure S14. Selected frontier molecular orbitals for **2**$^{2+}$-OS.

3^{2+}-OS

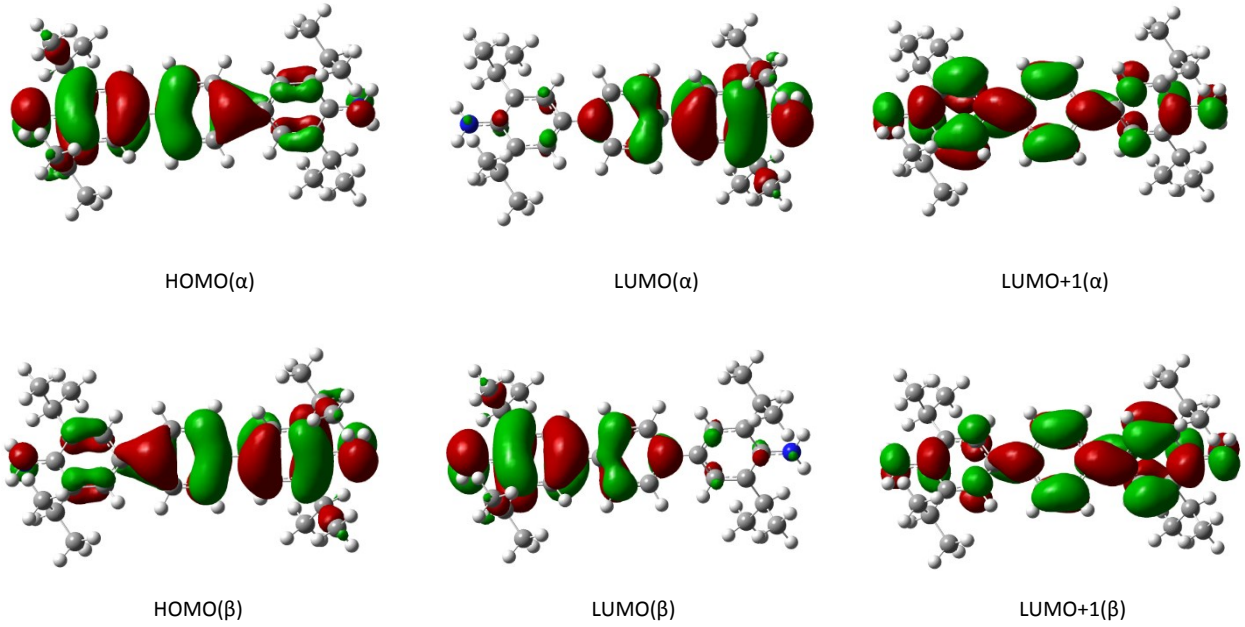


Figure S15. Selected frontier molecular orbitals for **3**$^{2+}$-OS.

4^{2+}-T

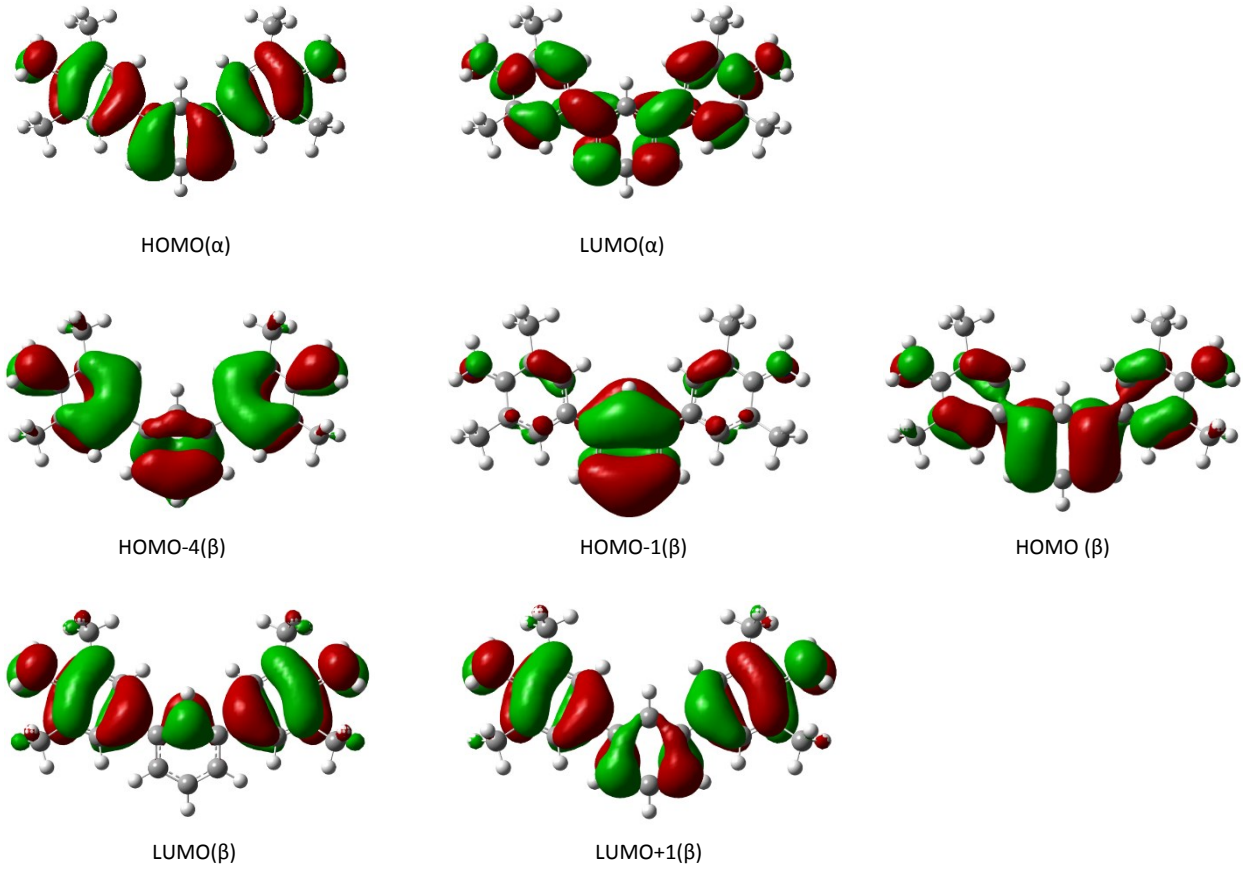
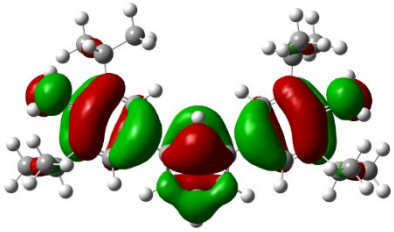
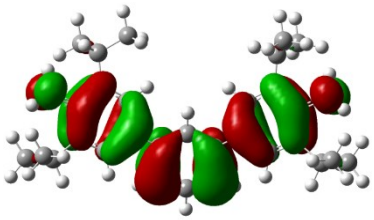


Figure S16. Selected frontier molecular orbitals for **4**$^{2+}$-T.

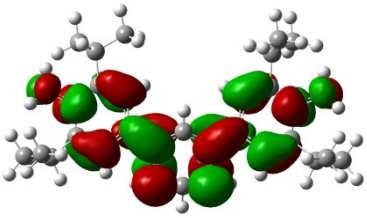
5^{2+}-T



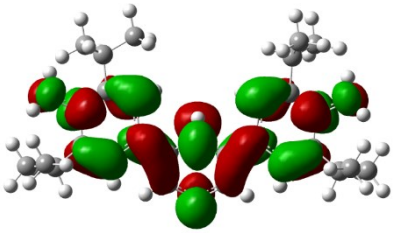
HOMO-1(α)



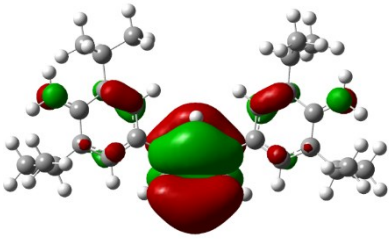
HOMO(α)



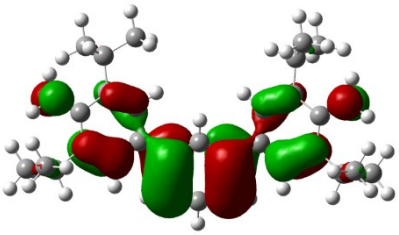
LUMO(α)



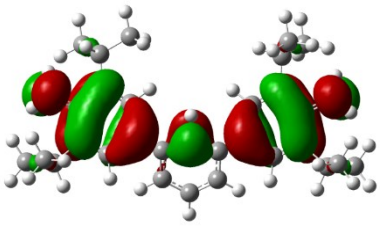
LUMO+1(α)



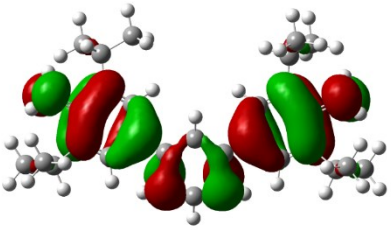
HOMO-1(β)



HOMO(β)



LUMO(β)



LUMO+1(β)

Figure S17. Selected frontier molecular orbitals for **5**$^{2+}$-T.

Table S4. The number of imaginary frequencies (**#** Imag. Freq.), absolute energy values (E_{abs}) and zero-point energy values (E_{zero}) of optimized structures of dications $\mathbf{1}^{2+}$-$\mathbf{5}^{2+}$ with different spin states calculated at the (U)WB97XD/6-31G(d) level.

	# Imag. Freq.	E_{abs}/Hartree	E_{zero}/Hartree
$\mathbf{1}^{2+}$-CS	0	-804.214828	-803.911942
$\mathbf{1}^{2+}$-OS	0	-804.226899	-803.925322
$\mathbf{1}^{2+}$-T	0	-804.221972	-803.920828
$\mathbf{2}^{2+}$-CS	0	-961.462758	-961.047397
$\mathbf{2}^{2+}$-OS	0	-961.478415	-961.064027
$\mathbf{2}^{2+}$-T	0	-961.474654	-961.060815
$\mathbf{3}^{2+}$-CS	0	-1275.892399	-1275.245615
$\mathbf{3}^{2+}$-OS	0	-1275.909052	-1275.263965
$\mathbf{3}^{2+}$-T	0	-1275.905579	-1275.260673
$\mathbf{4}^{2+}$-CS	0	-961.423501	-961.009051
$\mathbf{4}^{2+}$-OS	0	-961.471223	-961.057372
$\mathbf{4}^{2+}$-T	0	-961.472286	-961.058377
$\mathbf{5}^{2+}$-CS	0	-1275.844733	-1275.200690
$\mathbf{5}^{2+}$-OS	0	-1275.894912	-1275.251084
$\mathbf{5}^{2+}$-T	0	-1275.895879	-1275.251947

Coordinates for Calculated Geometries:

1^{2+}-CS

C	5.699917	0.000002	-0.000005	C	0.675456	-1.224516	0.025098
C	4.970432	1.235893	0.010920	H	1.175124	-2.183394	0.053768
H	5.515562	2.174209	0.021549	C	-2.849433	-0.000025	0.000006
C	3.616057	1.227398	0.009204	C	-3.616023	1.227338	0.013433
H	3.113258	2.185330	0.021879	H	-3.113177	2.185189	0.030049
C	2.849424	0.000014	0.000004	C	-4.970400	1.235847	0.015380
C	3.616046	-1.227376	-0.009203	H	-5.515515	2.174124	0.029687
H	3.113234	-2.185302	-0.021875	C	-5.699903	0.000014	-0.000005
C	4.970420	-1.235883	-0.010926	C	-4.970434	-1.235840	-0.015386
H	5.515542	-2.174204	-0.021558	H	-5.515575	-2.174101	-0.029697
C	1.451224	0.000009	0.000008	C	-3.616057	-1.227368	-0.013430
C	0.675425	1.224515	-0.025088	H	-3.113243	-2.185235	-0.030047
H	1.175065	2.183406	-0.053764	N	7.020086	-0.000004	-0.000009
C	-0.675481	1.224502	-0.024898	H	7.553567	-0.860984	-0.007476
H	-1.175177	2.183364	-0.053780	H	7.553575	0.860971	0.007455
C	-1.451235	-0.000026	0.000008	N	-7.020075	0.000032	-0.000009
C	-0.675451	-1.224537	0.024908	H	-7.553546	0.860985	0.010545
H	-1.175116	-2.183413	0.053788	H	-7.553570	-0.860905	-0.010567

1^{2+}-OS

C	5.697752	0.000023	0.000043	C	0.689089	1.210482	0.009995
C	4.972693	-1.099627	-0.564652	H	1.206051	2.163514	-0.006976
H	5.517137	-1.926332	-1.010196	C	-2.872409	0.000027	-0.000021
C	3.609588	-1.092448	-0.550452	C	-3.609533	-1.092400	0.550438
H	3.082692	-1.920116	-1.011096	H	-3.082585	-1.920061	1.011038
C	2.872409	-0.000047	-0.000005	C	-4.972637	-1.099624	0.564687
C	3.609514	1.092397	0.550446	H	-5.517039	-1.926351	1.010243
H	3.082548	1.920055	1.011032	C	-5.697753	0.000002	0.000018
C	4.972617	1.099642	0.564701	C	-4.972673	1.099638	-0.564679
H	5.517004	1.926381	1.010252	H	-5.517103	1.926350	-1.010229
C	1.418681	-0.000044	-0.000043	C	-3.609569	1.092437	-0.550473
C	0.689036	-1.210543	-0.010048	H	-3.082656	1.920097	-1.011114
H	1.205945	-2.163600	0.006984	N	7.024259	0.000057	0.000065
C	-0.689089	-1.210512	0.010000	H	7.558270	0.766890	0.393121
H	-1.206049	-2.163545	-0.006971	H	7.558323	-0.766750	-0.392971
C	-1.418681	0.000015	-0.000046	N	-7.024259	-0.000009	0.000039
C	-0.689035	1.210513	-0.010058	H	-7.558284	-0.766832	0.393097
H	-1.205945	2.163570	0.006964	H	-7.558309	0.766804	-0.393004

1^{2+}-T

C	5.695817	0.000041	-0.000009	C	0.692877	-1.207376	-0.007791
C	4.972649	1.000959	0.727010	H	1.217167	-2.157474	0.008218
H	5.517529	1.752284	1.290235	C	-2.880149	-0.000029	-0.000007
C	3.606344	0.991637	0.715115	C	-3.606356	0.991723	-0.715009
H	3.069101	1.737123	1.291235	H	-3.069129	1.737273	-1.291060
C	2.880152	-0.000042	0.000000	C	-4.972661	1.001038	-0.726891
C	3.606398	-0.991664	-0.715141	H	-5.517548	1.752422	-1.290030
H	3.069201	-1.737156	-1.291295	C	-5.695819	0.000037	0.000023
C	4.972704	-1.000911	-0.727037	C	-4.972693	-1.000993	0.726929
H	5.517626	-1.752191	-1.290280	H	-5.517603	-1.752344	1.290089
C	1.408053	-0.000050	-0.000020	C	-3.606388	-0.991737	0.715024
C	0.692886	1.207278	0.007774	H	-3.069185	-1.737294	1.291088
H	1.217187	2.157372	-0.008207	N	7.024258	0.000078	-0.000010
C	-0.692875	1.207283	-0.007698	H	7.558565	-0.697523	-0.506304
H	-1.217166	2.157381	0.008378	H	7.558527	0.697708	0.506285
C	-1.408054	-0.000041	-0.000004	N	-7.024260	0.000069	0.000038
C	-0.692884	-1.207371	0.007688	H	-7.558536	0.697751	-0.506177
H	-1.217181	-2.157466	-0.008375	H	-7.558559	-0.697585	0.506268

2^{2+}-CS

C	5.682254	0.000070	0.000015	C	3.612931	1.224739	0.049038
C	4.971037	-1.257582	-0.052892	H	3.098959	2.176204	0.094905
C	3.613075	-1.224844	-0.049022	C	4.970888	1.257638	0.052917
H	3.099232	-2.176373	-0.094899	C	1.452395	-0.000124	-0.000002
C	2.852176	-0.000094	0.000006	C	0.675795	-1.222666	-0.002032

H	1.174754	-2.182269	0.000674
C	-0.675836	-1.222643	0.002086
H	-1.174834	-2.182227	-0.000553
C	-1.452395	-0.000077	-0.000007
C	-0.675794	1.222462	-0.002095
H	-1.174763	2.182063	0.000547
C	0.675836	1.222439	0.002029
H	1.174845	2.182021	-0.000668
C	-2.852176	-0.000042	-0.000009
C	-3.613043	-1.224810	0.049024
H	-3.099168	-2.176323	0.094889
C	-4.971003	-1.257584	0.052895
C	-5.682254	0.000049	-0.000010
C	-4.970921	1.257636	-0.052917
C	-3.612963	1.224773	-0.049045
H	-3.099023	2.176253	-0.094912
N	7.005150	0.000147	0.000020
H	7.538339	0.858992	0.035785
H	7.538440	-0.858635	-0.035742

N	-7.005150	0.000092	-0.000010
H	-7.538418	-0.858704	0.035755
H	-7.538362	0.858923	-0.035774
C	-5.741948	2.546958	-0.111442
H	-6.376469	2.597324	-1.004717
H	-6.378310	2.676766	0.772496
H	-5.065574	3.402655	-0.148889
C	-5.742115	-2.546856	0.111419
H	-6.376637	-2.597183	1.004695
H	-6.378487	-2.676620	-0.772518
H	-5.065796	-3.402597	0.148862
C	5.741880	2.546981	0.111447
H	6.376395	2.597363	1.004724
H	6.378242	2.676806	-0.772489
H	5.065482	3.402660	0.148891
C	5.742183	-2.546833	-0.111419
H	6.376709	-2.597139	-1.004693
H	6.378557	-2.676584	0.772519
H	5.065887	-3.402592	-0.148867

2^{2+}-OS

C	5.680900	0.000003	0.000019
C	4.971406	1.088755	0.632760
C	3.603285	1.060740	0.604884
H	3.062273	1.857336	1.104280
C	2.876204	-0.000014	-0.000004
C	3.603309	-1.060756	-0.604888
H	3.062318	-1.857351	-1.104308
C	4.971430	-1.088755	-0.632739
C	1.416327	-0.000010	-0.000020
C	0.690214	1.208537	0.009524
H	1.210609	2.160074	-0.006938
C	-0.690191	1.208550	-0.009572
H	-1.210566	2.160097	0.006899
C	-1.416327	0.000014	-0.000023
C	-0.690214	-1.208532	0.009544
H	-1.210609	-2.160070	-0.006901
C	0.690191	-1.208545	-0.009549
H	1.210566	-2.160092	0.006940
C	-2.876203	0.000018	-0.000010
C	-3.603309	1.060747	-0.604915
H	-3.062320	1.857334	-1.104349
C	-4.971430	1.088743	-0.632770
C	-5.680901	-0.000006	0.000006
C	-4.971405	-1.088745	0.632768

C	-3.603285	-1.060727	0.604895
H	-3.062272	-1.857314	1.104305
N	7.009883	0.000012	0.000030
H	7.543764	-0.744171	-0.430962
H	7.543748	0.744202	0.431029
N	-7.009883	-0.000017	0.000012
H	-7.543765	0.744156	-0.430994
H	-7.543747	-0.744200	0.431026
C	-5.732880	-2.196009	1.302688
H	-6.364072	-1.817415	2.116015
H	-6.372215	-2.733164	0.591151
H	-5.049730	-2.927096	1.737925
C	-5.732932	2.195989	-1.302690
H	-6.364127	1.817378	-2.116007
H	-6.372268	2.733139	-0.591149
H	-5.049800	2.927084	-1.737940
C	5.732931	-2.196015	-1.302637
H	6.364129	-1.817420	-2.115958
H	6.372263	-2.733154	-0.591085
H	5.049798	-2.927116	-1.737876
C	5.732881	2.196029	1.302663
H	6.364072	1.817448	2.115997
H	6.372218	2.733172	0.591118
H	5.049732	2.927124	1.737887

2^{2+}-T

C	5.680755	-0.000000	0.000005
C	4.971979	1.005668	0.759058
C	3.601217	0.977080	0.731332
H	3.052827	1.707126	1.317850
C	2.882523	-0.000018	-0.000014
C	3.601240	-0.977100	-0.731361
H	3.052871	-1.707141	-1.317904
C	4.972003	-1.005674	-0.759063
C	1.408456	-0.000008	-0.000035
C	0.693025	1.206301	0.007297
H	1.219270	2.155380	-0.007804
C	-0.692993	1.206319	-0.007301
H	-1.219209	2.155412	0.007870
C	-1.408457	0.000027	-0.000030
C	-0.693025	-1.206282	0.007264
H	-1.219270	-2.155361	-0.007860
C	0.692993	-1.206300	-0.007340
H	1.219210	-2.155393	0.007799
C	-2.882522	0.000033	0.000002
C	-3.601250	0.977140	-0.731301
H	-3.052892	1.707207	-1.317820
C	-4.972014	1.005703	-0.758997
C	-5.680756	-0.000007	0.000032
C	-4.971968	-1.005707	0.759032

C	-3.601206	-0.977106	0.731302
H	-3.052809	-1.707180	1.317779
N	7.011063	0.000010	0.000012
H	7.545003	-0.687139	-0.517452
H	7.544987	0.687170	0.517480
N	-7.011063	-0.000029	0.000045
H	-7.545012	0.687140	-0.517385
H	-7.544979	-0.687217	0.517484
C	-5.731769	-2.028628	1.552407
H	-6.364677	-1.559203	2.315614
H	-6.369378	-2.646417	0.907862
H	-5.047314	-2.702181	2.070437
C	-5.731862	2.028587	-1.552375
H	-6.364787	1.559129	-2.315547
H	-6.369460	2.646383	-0.907826
H	-5.047437	2.702138	-2.070448
C	5.731840	-2.028530	-1.552486
H	6.364743	-1.559046	-2.315659
H	6.369459	-2.646340	-0.907970
H	5.047408	-2.702073	-2.070560
C	5.731792	2.028541	1.552484
H	6.364696	1.559071	2.315665
H	6.369405	2.646358	0.907970
H	5.047344	2.702075	2.070549

3^{2+}-CS

C	-5.678949	0.000657	-0.181250	C	-5.743662	2.573644	-0.119158
C	-4.968021	-1.264423	-0.164916	H	-6.578293	2.491839	-0.830762
C	-3.610556	-1.223867	-0.144039	C	-5.743502	-2.572610	-0.138163
H	-3.086881	-2.169139	-0.150786	H	-6.575557	-2.483819	-0.851906
C	-2.852284	0.000888	-0.140759	C	4.927830	3.786245	-0.575594
C	-3.610718	1.225474	-0.148740	H	4.473755	3.626723	-1.558584
H	-3.087479	2.170901	-0.135019	H	4.142037	4.041079	0.144505
C	-4.968238	1.265832	-0.161893	H	5.584618	4.656773	-0.647518
C	-1.452552	0.001095	-0.135962	C	6.312749	2.817607	1.293187
C	-0.675916	-1.218603	-0.059924	H	6.916871	1.984165	1.666726
H	-1.175511	-2.175016	0.016249	H	6.939065	3.713887	1.295551
C	0.675908	-1.218600	-0.059930	H	5.495321	2.973768	2.004189
H	1.175509	-2.175011	0.016238	C	4.925883	-3.780785	-0.603138
C	1.452538	0.001100	-0.135974	H	4.142429	-4.042073	0.117213
C	0.675909	1.220970	-0.209453	H	4.468266	-3.612107	-1.582927
H	1.175476	2.177306	-0.286913	H	5.582197	-4.650754	-0.685383
C	-0.675928	1.220967	-0.209448	C	6.317719	-2.830276	1.269647
H	-1.175500	2.177301	-0.286903	H	6.944546	-3.726169	1.260857
C	2.852271	0.000893	-0.140782	H	6.922547	-2.000310	1.649747
C	3.610537	-1.223864	-0.144079	H	5.502902	-2.994056	1.981950
H	3.086858	-2.169134	-0.150837	C	-6.312733	2.817664	1.293170
C	4.968002	-1.264425	-0.164978	H	-6.939048	3.713945	1.295509
C	5.678936	0.000652	-0.181283	H	-6.916849	1.984236	1.666749
C	4.968229	1.265829	-0.161912	H	-5.495294	2.973852	2.004154
C	3.610710	1.225477	-0.148758	C	-4.927837	3.786233	-0.575664
H	3.087475	2.170906	-0.135020	H	-4.142036	4.041093	0.144417
N	-7.002154	0.000679	-0.226319	H	-4.473773	3.626674	-1.558653
H	-7.534556	0.859159	-0.250021	H	-5.584624	4.656760	-0.647613
H	-7.534697	-0.857682	-0.250853	C	-6.317513	-2.830400	1.269802
N	7.002143	0.000663	-0.226278	H	-6.922261	-2.000466	1.650095
H	7.534680	-0.857703	-0.250780	H	-6.944357	-3.726281	1.261028
H	7.534554	0.859139	-0.249931	H	-5.502579	-2.994268	1.981951
C	5.743658	2.573639	-0.119142	C	-4.925982	-3.780746	-0.603280
H	6.578279	2.491857	-0.830759	H	-4.468530	-3.611998	-1.583133
C	5.743479	-2.572613	-0.138244	H	-4.142407	-4.042084	0.116922
H	6.575425	-2.483885	-0.852121	H	-5.582308	-4.650710	-0.685478

3^{2+}-OS

C	-5.676057	-0.159696	-0.140979	C	5.794409	-2.063563	-1.436101
C	-4.938969	-1.227528	0.506943	H	6.636517	-1.606147	-1.975216
C	-3.572085	-1.152440	0.483333	C	-5.794416	2.063556	-1.436107
H	-3.000925	-1.925103	0.983178	H	-6.636541	1.606135	-1.975191
C	-2.876869	-0.076942	-0.126403	C	-5.675991	-2.343646	1.225281
C	-3.627840	0.955906	-0.743992	H	-6.531877	-2.640227	0.601761
H	-3.097578	1.754084	-1.248885	C	4.836842	3.611016	1.412735
C	-4.996606	0.949495	-0.782361	H	4.404814	3.957262	0.468818
C	-1.415813	-0.037452	-0.123859	H	4.031401	3.460330	2.139546
C	-0.658258	-1.225479	-0.114456	H	5.472792	4.409270	1.803545
H	-1.154420	-2.190014	-0.131260	C	6.202108	1.844818	2.587545
C	0.722248	-1.188945	-0.132755	H	6.830259	0.951511	2.506405
H	1.268556	-2.125975	-0.117278	H	6.792236	2.629631	3.068482
C	1.415809	0.037456	-0.123862	H	5.363442	1.599178	3.246408
C	0.658255	1.225483	-0.114466	C	5.003945	-2.851161	-2.484993
H	1.154417	2.190018	-0.131278	H	4.219682	-3.463091	-2.026479
C	-0.722252	1.188949	-0.132762	H	4.549968	-2.193854	-3.232641
H	-1.268560	2.125979	-0.117290	H	5.678722	-3.535911	-3.004778
C	2.876865	0.076946	-0.126410	C	6.352351	-3.019084	-0.359974
C	3.627835	-0.955906	-0.743993	H	6.986796	-3.776609	-0.828099
H	3.097572	-1.754088	-1.248879	H	6.944925	-2.508609	0.406555
C	4.996601	-0.949496	-0.782365	H	5.530327	-3.532523	0.148493
C	5.676053	0.159698	-0.140989	C	-6.352321	3.019113	-0.359993
C	4.938966	1.227537	0.506924	H	-6.986769	3.776632	-0.828124
C	3.572083	1.152448	0.483317	H	-6.944882	2.508668	0.406566
H	3.000924	1.925115	0.983159	H	-5.530279	3.532558	0.148439
N	-7.005595	-0.204388	-0.156344	C	-5.003965	2.851117	-2.485037
H	-7.558337	0.514935	-0.602966	H	-4.219683	3.463048	-2.026556
H	-7.518097	-0.964945	0.269516	H	-4.550015	2.193786	-3.232680
N	7.005592	0.204380	-0.156339	H	-5.678745	3.535864	-3.004823
H	7.558333	-0.514953	-0.602947	C	-6.202071	-1.844817	2.587588
H	7.518095	0.964934	0.269525	H	-6.830210	-0.951500	2.506476
C	5.675990	2.343656	1.225257	H	-6.792199	-2.629629	3.068528
H	6.531858	2.640256	0.601722	H	-5.363386	-1.599200	3.246435

C	-4.836855	-3.611018	1.412727	H	-4.031394	-3.460350	2.139520
H	-4.404855	-3.957261	0.468796	H	-5.472806	-4.409268	1.803544

3^{2+}-T

C	5.674774	0.181099	-0.130022	C	5.794082	-1.883622	-1.665815
C	4.938113	1.167894	0.636132	H	6.638682	-1.370382	-2.147789
C	3.568930	1.087544	0.612662	C	5.673778	2.202012	1.467920
H	2.990608	1.796478	1.193344	H	6.528861	2.565106	0.879480
C	2.882286	0.088566	-0.115086	C	-4.831648	-3.439728	1.791238
C	3.625620	-0.861965	-0.852274	H	-4.396406	-3.883073	0.890470
H	3.088758	-1.598996	-1.437788	H	-4.028107	-3.209849	2.498971
C	4.996885	-0.850182	-0.891782	H	-5.466503	-4.193564	2.263553
C	1.408326	0.042976	-0.111331	C	-6.202224	-1.559986	2.768386
C	0.655951	1.226277	-0.103722	H	-6.833650	-0.683101	2.590622
H	1.153852	2.190605	-0.118838	H	-6.789554	-2.290635	3.331116
C	-0.729501	1.183934	-0.117923	H	-5.364824	-1.241349	3.396829
H	-1.285437	2.116025	-0.104028	C	-5.003896	2.545950	-2.798362
C	-1.408323	-0.042980	-0.111340	H	-4.217797	3.204041	-2.413080
C	-0.655948	-1.226281	-0.103706	H	-4.551994	1.807275	-3.467038
H	-1.153849	-2.190609	-0.118808	H	-5.678569	3.168443	-3.391410
C	0.729504	-1.183938	-0.117898	C	-6.347993	2.955486	-0.702813
H	1.285440	-2.116029	-0.103982	H	-6.979330	3.658271	-1.253248
C	-2.882283	-0.088570	-0.115104	H	-6.942680	2.535591	0.115315
C	-3.625612	0.861947	-0.852314	H	-5.523991	3.519303	-0.254567
H	-3.088747	1.598969	-1.437837	C	6.347976	-2.955519	-0.702726
C	-4.996877	0.850163	-0.891832	H	6.979318	-3.658312	-1.253145
C	-5.674771	-0.181104	-0.130057	H	6.942649	-2.535629	0.115413
C	-4.938115	-1.167886	0.636118	H	5.523958	-3.519327	-0.254496
C	-3.568932	-1.087536	0.612656	C	5.003924	-2.545979	-2.798303
H	-2.990613	-1.796459	1.193356	H	4.217811	-3.204059	-2.413033
N	7.005510	0.229467	-0.142140	H	4.552045	-1.807303	-3.466992
H	7.558319	-0.434030	-0.668495	H	5.678603	-3.168483	-3.391334
H	7.517338	0.936681	0.368544	C	6.202190	1.560042	2.768411
N	-7.005508	-0.229466	-0.142174	H	6.833612	0.683146	2.590682
H	-7.558314	0.434025	-0.668540	H	6.789518	2.290701	3.331130
H	-7.517338	-0.936668	0.368524	H	5.364778	1.241429	3.396849
C	-5.673786	-2.201988	1.467921	C	4.831644	3.439767	1.791191
H	-6.528857	-2.565103	0.879477	H	4.396421	3.883092	0.890404
C	-5.794069	1.883591	-1.665886	H	4.028090	3.209911	2.498917
H	-6.638655	1.370340	-2.147874	H	5.466497	4.193611	2.263497

4^{2+}-CS

C	0.000000	-0.434594	-0.077975	H	-1.752299	1.534208	-0.612156
C	-1.220455	-1.094795	-0.253537	C	-4.970525	0.855992	0.225089
C	-1.193477	-2.475017	-0.634177	C	-6.107031	-1.345404	0.824888
C	0.000000	-3.145808	-0.843427	H	-5.874406	-2.404952	0.944664
C	1.193478	-2.475018	-0.634169	H	-6.511809	-0.992396	1.781362
C	1.220454	-1.094796	-0.253533	H	-6.898291	-1.271555	0.068407
H	0.000001	0.585561	0.286386	C	-3.933673	3.103762	-0.387606
H	-2.123942	-3.002519	-0.814316	H	-4.265692	3.630315	0.515930
H	0.000001	-4.181383	-1.163589	H	-2.973786	3.534051	-0.678314
H	2.123943	-3.002522	-0.814300	H	-4.644981	3.323873	-1.193298
C	2.497601	-0.441779	-0.112420	C	6.107023	-1.345400	0.824922
C	3.672606	-1.172044	0.236165	H	6.511795	-0.992380	1.781394
C	2.620546	0.965869	-0.295513	H	5.874396	-2.404946	0.944710
C	4.884866	-0.570301	0.421982	H	6.898288	-1.271561	0.068445
H	3.607742	-2.239161	0.420082	C	3.933682	3.103753	-0.387652
C	3.807449	1.626308	-0.150379	H	4.265694	3.630320	0.515878
H	1.752305	1.534199	-0.612190	H	4.644997	3.323849	-1.193341
C	4.970525	0.855990	0.225085	H	2.973798	3.534038	-0.678375
C	-2.497601	-0.441777	-0.112421	N	6.139529	1.469082	0.378435
C	-3.672610	-1.172045	0.236147	H	6.977409	0.962307	0.630890
C	-2.620543	0.965874	-0.295493	H	6.241927	2.465824	0.243576
C	-4.884871	-0.570302	0.421966	N	-6.139529	1.469084	0.378440
H	-3.607751	-2.239164	0.420050	H	-6.241924	2.465828	0.243595
C	-3.807445	1.626314	-0.150356	H	-6.977411	0.962307	0.630883

4^{2+}-OS

C	0.000000	-0.429935	-0.203633	C	0.000001	-3.054065	-1.147379
C	1.218209	-1.085707	-0.421244	C	-1.202297	-2.406885	-0.897958
C	1.202298	-2.406885	-0.897957	C	-1.218208	-1.085707	-0.421245

H	-0.000001	0.573870	0.211609	H	3.124430	3.502413	-0.896295
H	2.134428	-2.920415	-1.111212	H	4.320445	3.637880	0.390685
H	0.000001	-4.064402	-1.541077	H	4.823714	3.226437	-1.264551
H	-2.134427	-2.920414	-1.111214	C	5.971623	-1.360034	1.156404
C	-2.501371	-0.415750	-0.155746	H	6.308592	-0.955216	2.118623
C	-2.669172	0.967730	-0.412059	H	5.687750	-2.399994	1.325029
C	-3.599532	-1.154295	0.352207	H	6.824445	-1.364895	0.466209
C	-3.861368	1.610744	-0.200678	C	-4.046731	3.068823	-0.506432
H	-1.841792	1.530579	-0.832246	H	-4.320448	3.637881	0.390670
C	-4.817693	-0.577245	0.600495	H	-3.124438	3.502408	-0.896315
H	-3.465622	-2.205713	0.584876	H	-4.823723	3.226428	-1.264562
C	-4.964293	0.831880	0.315711	C	-5.971619	-1.360033	1.156414
C	2.501371	-0.415750	-0.155745	H	-6.308581	-0.955217	2.118636
C	2.669170	0.967732	-0.412052	H	-6.824446	-1.364891	0.466225
C	3.599534	-1.154295	0.352203	H	-5.687747	-2.399995	1.325034
C	3.861366	1.610746	-0.200671	N	-6.136636	1.422179	0.531693
H	1.841788	1.530582	-0.832235	H	-6.283591	2.405768	0.342910
C	4.817695	-0.577244	0.600492	H	-6.933919	0.909569	0.887622
H	3.465626	-2.205714	0.584869	N	6.136637	1.422180	0.531691
C	4.964293	0.831882	0.315711	H	6.933922	0.909569	0.887615
C	4.046725	3.068827	-0.506419	H	6.283591	2.405769	0.342908

4^{2+}-T

C	0.000000	-0.438511	-0.203495	H	3.492127	-2.210554	0.560343
C	1.220621	-1.098854	-0.403636	C	4.959519	0.841554	0.299555
C	1.202900	-2.433285	-0.848157	C	4.012843	3.078479	-0.487999
C	0.000000	-3.085453	-1.080556	H	3.081947	3.508523	-0.860999
C	-1.202900	-2.433285	-0.848157	H	4.294576	3.641385	0.410493
C	-1.220621	-1.098854	-0.403636	H	4.778016	3.249107	-1.255240
H	0.000000	0.574017	0.189101	C	5.995624	-1.349288	1.106555
H	2.133686	-2.952677	-1.051451	H	6.341562	-0.950089	2.067913
H	0.000000	-4.104805	-1.450337	H	5.722730	-2.393082	1.269524
H	-2.133686	-2.952677	-1.051452	H	6.839471	-1.340864	0.405459
C	-2.498795	-0.422457	-0.149847	C	-4.012843	3.078479	-0.488000
C	-2.653255	0.966296	-0.392686	H	-4.294576	3.641385	0.410493
C	-3.612399	-1.156226	0.334276	H	-3.081947	3.508523	-0.860999
C	-3.843005	1.616105	-0.193246	H	-4.778015	3.249106	-1.255241
H	-1.817157	1.528287	-0.796132	C	-5.995624	-1.349288	1.106556
C	-4.828078	-0.571302	0.572409	H	-6.341563	-0.950088	2.067913
H	-3.492127	-2.210554	0.560344	H	-6.839471	-1.340865	0.405459
C	-4.959519	0.841554	0.299555	H	-5.722729	-2.393081	1.269526
C	2.498795	-0.422457	-0.149847	N	-6.129530	1.439329	0.505568
C	2.653255	0.966296	-0.392686	H	-6.265768	2.425918	0.324981
C	3.612399	-1.156226	0.334276	H	-6.935676	0.929899	0.845549
C	3.843005	1.616105	-0.193246	N	6.129530	1.439329	0.505568
H	1.817157	1.528287	-0.796132	H	6.935677	0.929899	0.845549
C	4.828078	-0.571302	0.572409	H	6.265768	2.425919	0.324983

5^{2+}-CS

C	-0.076812	-0.754917	0.002011	C	3.761547	1.081974	0.814683
C	1.130649	-1.454094	-0.078237	H	1.695791	0.870351	1.171420
C	1.078176	-2.880080	-0.182993	C	4.926504	0.459572	0.213890
C	-0.126085	-3.562801	-0.136848	N	-6.182920	1.311834	-0.085899
C	-1.305707	-2.845817	-0.021453	H	-6.258520	2.241773	-0.472471
C	-1.308082	-1.415728	0.015114	H	-7.030811	0.905403	0.279838
H	-0.058208	0.326870	0.055463	N	6.106897	1.061040	0.304401
H	1.996366	-3.453343	-0.245064	H	6.216464	1.943680	0.780307
H	-0.145247	-4.645230	-0.190276	H	6.940168	0.650809	-0.089847
H	-2.243796	-3.389482	-0.014054	C	-6.184398	-1.390526	1.093909
C	-2.576220	-0.727329	-0.027449	C	-7.291233	-1.700546	0.068736
C	-2.669879	0.587264	-0.560485	C	-6.722798	-0.709240	2.365151
C	-3.768388	-1.325909	0.469931	H	-5.803593	-2.365037	1.419365
C	-3.843474	1.284972	-0.607570	H	-6.882468	-2.187531	-0.821217
H	-1.783857	1.037354	-0.991398	H	-8.018883	-2.379466	0.521744
C	-4.976669	-0.684314	0.491330	H	-7.851442	-0.820025	-0.264298
H	-3.721498	-2.313904	0.915808	H	-5.921097	-0.531141	3.087515
C	-5.029812	0.650477	-0.063168	H	-7.219220	0.249412	2.179699
C	2.421982	-0.819328	0.031245	H	-7.463713	-1.361018	2.836178
C	3.595329	-1.408068	-0.519965	C	-3.941697	2.653370	-1.258715
C	2.564883	0.431376	0.692386	C	-4.568357	2.536705	-2.663960
C	4.825519	-0.812575	-0.471084	C	-2.603288	3.393135	-1.338088
H	3.516648	-2.343882	-1.063088	H	-4.592397	3.279726	-0.631389

H	-5.537727	2.027906	-2.661720	H	4.343782	1.460739	3.490112
H	-4.710613	3.531801	-3.094463	H	5.727980	2.230736	2.710193
H	-3.902870	1.972517	-3.324876	H	4.491466	3.224206	3.463353
H	-2.110173	3.446361	-0.362197	C	6.010721	-1.500984	-1.136745
H	-1.922674	2.923879	-2.057078	C	7.095293	-1.959844	-0.143845
H	-2.775639	4.415508	-1.683969	C	6.586745	-0.716668	-2.329882
C	3.818002	2.394900	1.583951	H	5.594403	-2.420985	-1.561921
C	4.190743	3.606959	0.709536	H	6.659326	-2.517785	0.689740
C	4.649013	2.314100	2.877998	H	7.797963	-2.618768	-0.661241
H	2.785871	2.570955	1.906981	H	7.689004	-1.142766	0.280377
H	3.579674	3.644280	-0.196939	H	5.798429	-0.430978	-3.032172
H	4.014248	4.525396	1.276202	H	7.122917	0.195319	-2.046190
H	5.240905	3.628663	0.399209	H	7.301961	-1.348632	-2.863459

5^{2+}-OS

C	-0.073786	-0.689970	-0.412868	H	-6.910003	-1.921187	-1.167500
C	1.132483	-1.302965	-0.772279	H	-7.885891	-2.658037	0.110910
C	1.092720	-2.501327	-1.502522	H	-7.826784	-0.911545	-0.043701
C	-0.121547	-3.071432	-1.859603	H	-5.537283	-1.768141	2.963094
C	-1.312121	-2.471677	-1.472581	H	-6.948640	-0.792437	2.540272
C	-1.303509	-1.272290	-0.743207	H	-7.080181	-2.542963	2.577366
H	-0.055765	0.211430	0.193202	C	-4.066301	2.879388	-0.034880
H	2.015554	-2.972914	-1.825056	C	-4.826609	3.274996	-1.318480
H	-0.140031	-3.983496	-2.445897	C	-2.747003	3.651704	0.057939
H	-2.254338	-2.920068	-1.771385	H	-4.657437	3.191523	0.838001
C	-2.573150	-0.647306	-0.335979	H	-5.791706	2.768176	-1.420824
C	-2.717112	0.759160	-0.319096	H	-5.009172	4.353042	-1.326021
C	-3.676374	-1.449427	0.037631	H	-4.229247	3.025094	-2.200808
C	-3.893211	1.372670	0.028747	H	-2.158589	3.347566	0.929259
H	-1.877801	1.369433	-0.631306	H	-2.140358	3.525192	-0.845322
C	-4.886283	-0.922040	0.415785	H	-2.960778	4.719423	0.151798
H	-3.552906	-2.527548	0.060705	C	5.867175	-2.017756	0.658057
C	-5.007333	0.521661	0.405249	C	6.316204	-1.902058	2.126737
C	2.427822	-0.712813	-0.394384	C	7.048264	-2.007509	-0.331164
C	2.612434	0.688348	-0.370397	H	5.411953	-3.009363	0.564105
C	3.520646	-1.543941	-0.057236	H	5.459978	-1.933267	2.806432
C	3.812481	1.274494	-0.051044	H	6.969343	-2.745048	2.367860
H	1.784392	1.328723	-0.658266	H	6.883183	-0.991236	2.348712
C	4.754043	-1.048583	0.286852	H	6.701838	-2.085212	-1.365566
H	3.371810	-2.618865	-0.037199	H	7.684415	-1.118073	-0.260214
C	4.913929	0.392416	0.283949	H	7.692162	-2.866784	-0.125359
N	-6.162220	1.086116	0.750374	C	3.932282	2.791287	-0.085431
H	-6.288406	2.089396	0.753958	C	4.882427	3.306381	-1.182851
H	-6.961459	0.529310	1.018399	C	4.214602	3.418707	1.292758
N	6.097323	0.915129	0.593484	H	2.933830	3.140136	-0.370880
H	6.888864	0.330673	0.822920	H	4.647009	2.858726	-2.152471
H	6.251227	1.913334	0.599338	H	4.770386	4.390199	-1.274165
C	-6.011955	-1.858623	0.828720	H	5.941967	3.116556	-0.979633
C	-7.221963	-1.821778	-0.124022	H	3.526415	3.036380	2.052109
C	-6.412611	-1.719666	2.309243	H	5.233927	3.253971	1.658629
H	-5.586588	-2.862866	0.728774	H	4.079520	4.501758	1.226844

5^{2+}-T

C	-0.074501	-0.704054	-0.405208	C	3.530867	-1.547608	-0.056281
C	1.133951	-1.327458	-0.744347	C	3.796695	1.273030	-0.050378
C	1.092690	-2.549516	-1.437839	H	1.763616	1.311760	-0.634819
C	-0.122031	-3.130012	-1.775872	C	4.762252	-1.041445	0.276361
C	-1.313216	-2.519542	-1.408233	H	3.393419	-2.623855	-0.033525
C	-1.306247	-1.296402	-0.715684	C	4.909656	0.400886	0.272408
H	-0.056555	0.213913	0.174890	N	-6.156574	1.107455	0.724668
H	2.014316	-3.031018	-1.748186	H	-6.273180	2.111874	0.726218
H	-0.140423	-4.059363	-2.334375	H	-6.963425	0.558309	0.985447
H	-2.254190	-2.977652	-1.695177	N	6.091100	0.933675	0.570232
C	-2.571461	-0.660592	-0.323187	H	6.889836	0.355977	0.791512
C	-2.703873	0.748202	-0.306550	H	6.236474	1.933099	0.575168
C	-3.688305	-1.451420	0.038126	C	-6.034462	-1.838115	0.807893
C	-3.877830	1.372218	0.026632	C	-7.234769	-1.791667	-0.156577
H	-1.857205	1.352305	-0.610404	C	-6.448073	-1.693176	2.284208
C	-4.896121	-0.912569	0.404303	H	-5.617537	-2.846456	0.713572
H	-3.576698	-2.530612	0.064878	H	-6.913641	-1.895905	-1.196803
C	-5.003958	0.532117	0.391622	H	-7.908842	-2.621189	0.073327
C	2.424898	-0.726833	-0.380535	H	-7.831709	-0.875632	-0.083763
C	2.598725	0.676886	-0.355724	H	-5.579578	-1.748844	2.946550

H	-6.977577	-0.760643	2.508793
H	-7.125909	-2.509746	2.547114
C	-4.036917	2.880505	-0.040299
C	-4.781874	3.281908	-1.330950
C	-2.711808	3.641261	0.064073
H	-4.633052	3.198530	0.827056
H	-5.750139	2.783102	-1.442254
H	-4.955484	4.361415	-1.340761
H	-4.178425	3.026579	-2.207576
H	-2.134264	3.333026	0.941237
H	-2.097946	3.508465	-0.833452
H	-2.916949	4.710948	0.154763
C	5.887376	-2.000661	0.637915
C	6.348618	-1.880279	2.102367
C	7.059288	-1.980771	-0.361982
H	5.440102	-2.996318	0.548543

H	5.498884	-1.919225	2.789777
H	7.011766	-2.717024	2.337873
H	6.908998	-0.964118	2.318984
H	6.704143	-2.061753	-1.393177
H	7.688608	-1.086028	-0.297115
H	7.712295	-2.834489	-0.161816
C	3.903146	2.790978	-0.086114
C	4.838167	3.314279	-1.192504
C	4.193137	3.420847	1.289318
H	2.899006	3.131253	-0.361936
H	4.597384	2.864518	-2.159841
H	4.715930	4.397089	-1.282733
H	5.901225	3.133710	-0.999554
H	3.515108	3.033016	2.054999
H	5.217057	3.264298	1.645788
H	4.048772	4.502786	1.224694

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Author Contributions

Y. Fang, T. Li, X. Chen, and Y. Qiu performed the chemical reactions and recorded the spectroscopic (NMR, CV, EPR, EA) data. Q. S. collected the UV/Vis absorption spectra and conducted the variable-temperature EPR spectra. C. Chen carried out the SQUID measurements. L. Zhang performed all the theoretical calculations. L. Wang and Y. Zhao conducted the X-ray diffraction studies. X. Wang conceived the project. X. Wang, Y. Su, and Y. Fang wrote the paper. All authors discussed the results and manuscript.