Supporting Information for

Magnetic Bistability in a Discrete Organic Radical

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Experimental Section

General. All manipulations were carried out under an Ar or N_2 atmosphere by using standard Schlenk or glove box techniques. Solvents were dried prior to use. Tetrabis(4-methoxyphenyl)-2,3,5,6-tetramethylbenzene-1,4-diamine **1** was synthesized by a method similar to that for the preparation of 1,5-bis(di-p-methoxyphenylamino)naphthalene.[S1] $Ag[Al(OR_{Me})_4]$ was prepared by the published procedure.[S2] 1,4-dibromotetramethylbenzene, di-*p*-tolylamine and $AgSbF_6$ were purchased from Alfa Aesar and used upon arrival. Cyclic voltammetry was performed on an IM6ex electrochemical workstation in CH_2Cl_2 at the scan rate of 100 mV/s with platinum as the working and counter electrodes, as solvent Ag/Ag^+ as the reference electrode and 0.2 M $^nBu_4NPF_6$ as the supporting electrolyte. The ^1H NMR and ^{13}C NMR spectra were recorded in solution of $CDCl_3$using a Bruker Ultra Shield 300 MHz spectrometer in ppm downfield from internal standard Me_4Si. Element analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. EPR spectra were obtained using Bruker EMX-10/12 X-band variable-temperature apparatus and were simulated with the software of WINEPR SimFonia. Magnetic measurements were performed using a Quantum Design SQUID VSM magnetometer with a field of 0.1 T. X-ray crystal structures were obtained by using Bruker D8 CMOS detectors. Crystal data and structure refinement for $\mathbf{1}^{2+}\bullet 2[Al(OR_{Me})_4]^-$ are listed in Table S1. CCDC 1479502 – 1479503 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Synthesis of neutral 1. A mixture of 1,4-dibromotetramethylbenzene (2.89 g, 9.9 mmol) , di-*p*-methoxyphenylamine(5.00 g, 21.80 mmol), $Pd(OAc)_2$ (0.05 g, 0.20 mmol), tri-*tert*-butylphosphine (0.20 mmol), sodium *tert*-butoxide (2.6 g, 27.7 mmol) in toluene (100 mL) was heated under nitrogen at 100℃ for 10 h. Upon cooling to room temperature, the reaction solution was taken up with Et_2O and washed with brine. The organic layer was dried with Na_2SO_4. After evaporation of the solvent, purification by column chromatography on silica gel using $CHCl_3$ afforded 1 (3.60 g, 63.82 %) as white solid; m.p. 217-219℃; ^1H NMR (300 MHz, $CDCl_3$) δ 6.91 (d, 8H), 6.79 (d, 8H), 3,80 (s, 12H), 2.01 (s, 12H); ^{13}C NMR (75MHz, $CDCl_3$) δ 153.2, 140.1, 135.5, 120.2, 114.6, 55.4, 15.4; UV-Vis (CH_2Cl_2): λ_{max} = 296 nm.

Synthesis of Dication Salt $\mathbf{1}^{2+}\bullet 2[Al(OR_{Me})_4]^-$. A solution of $AgSbF_6$ (0.181 g, 0.52 mmol) in CH_2Cl_2 (15 mL) was added dropwise to the mixture of **1** (0.148 g, 0.25 mmol) and $Li[Al(OR_{Me})_4]$ (0.397 g, 0.52 mmol) 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 concentrated and stored at around -30℃ for one day to afford blue crystals. Yield: 0.326 g, 61.97 %; m.p. 250-253 ^{o}C. UV-Vis (CH_2Cl_2): λ_{max} = 807 nm; elemental analysis calcd (%) for $C_{70}H_{64}Al_2F_{48}N_2O_{12}$: C 40.21, H 3.08, N 1.34; Found: C 39.72, H 3.05, N 1.47.

Table S1. Crystal data and structure refinement for $\mathbf{1}^{2+}$•2[$Al(OR_{Me})_4]^-$• $2CH_2Cl_2$.

	100 K	200 K
formula	$C_{72}H_{68}Al_2F_{48}Cl_4N_2O_{12}$	$C_{72}H_{68}Al_2F_{48}Cl_4N_2O_{12}$
Mr [g mol^{-1}]	2261.04	2261.04
crystal system	Monoclinic	Monoclinic
space group	*P*2(1)/c	*P*2(1)/c
Z	2	2
Temp. (K)	100(2)	200(2)
μ(mm^{-1})	0.310	0.302
a (Å)	10.0924(7)	10.2354(5)
b (Å)	22.1142(15)	22.4215(11)
c (Å)	20.0895(14)	20.0452(10)
α (°)		
β (°)	92.8778(19)	92.5728(16)
γ (°)		
V [Å^3]	4478.0(5)	4595.6(4)
*R*1 (I>2σ(I))	0.0492	0.0643
*wR*2 (all data)	0.1222	0.1740

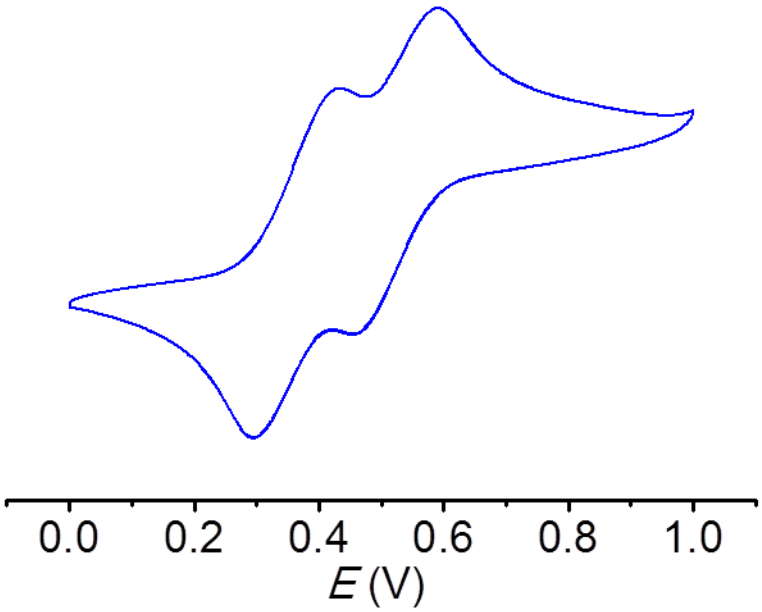

Figure S1. The cyclic voltammogram of **1** in CH_2Cl_2 at room temperature with Ag/Ag^+ as the reference electrode and 0.2 M $^nBu_4NPF_6$ as the supporting electrolyte. Scan rate: 100 mV/s.

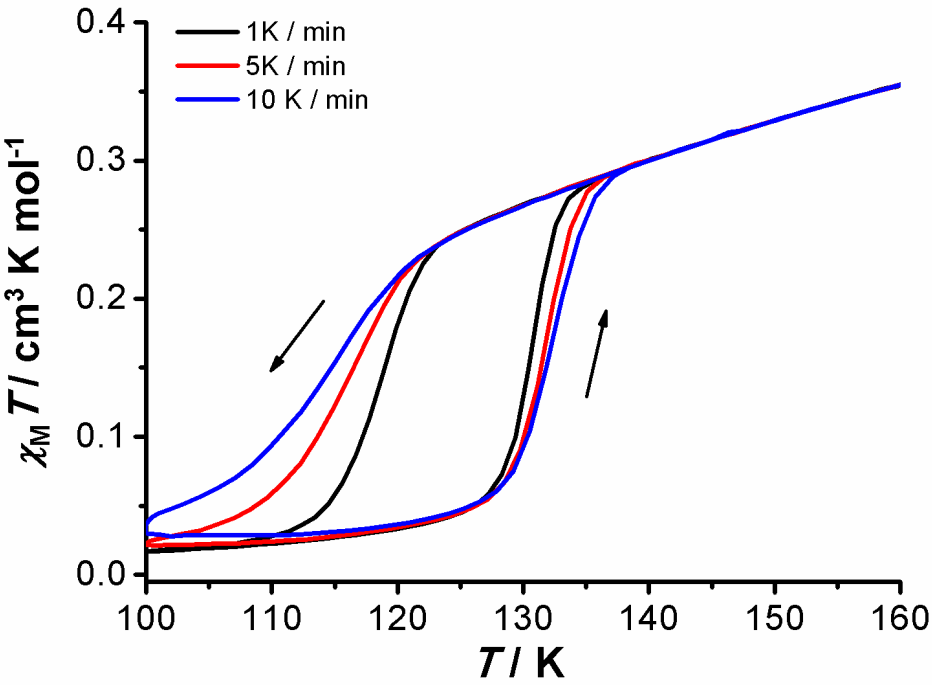

Figure S2. Temperature-dependent plots of $\chi_M T$ for the crystals of $\mathbf{1}^{2+}$ recorded in the sweep mode at different temperature sweep rates (1, 5 and 10 K min^{-1}).

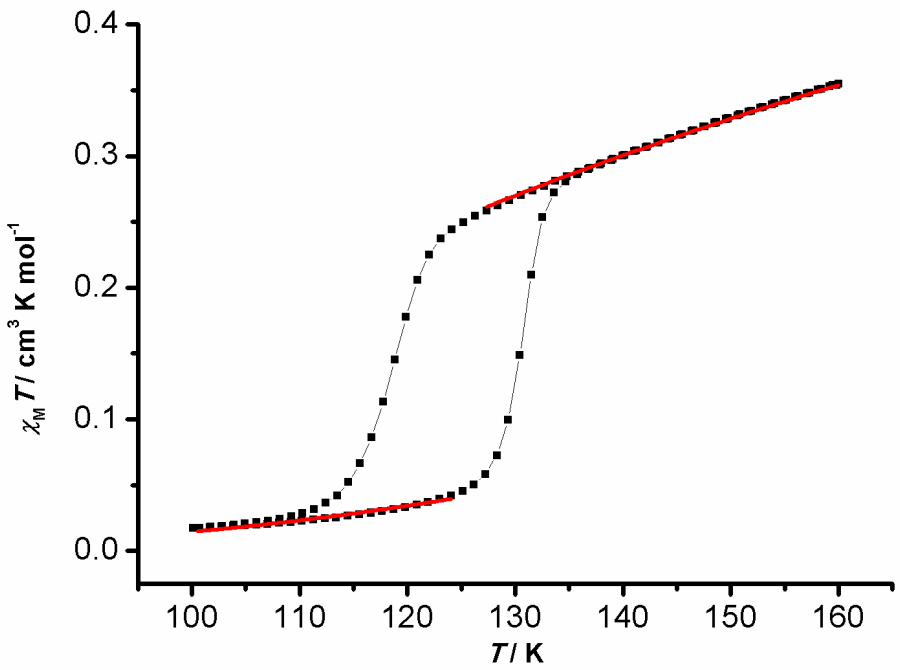

Figure S3. Temperature-dependent plots of $\chi_M T$ for the crystals of $\mathbf{1}^{2+}$ recorded in the sweep mode at the sweep rate of 1 K min^{-1} and the fitting plots (in red) via the Bleaney-Bowers equation.

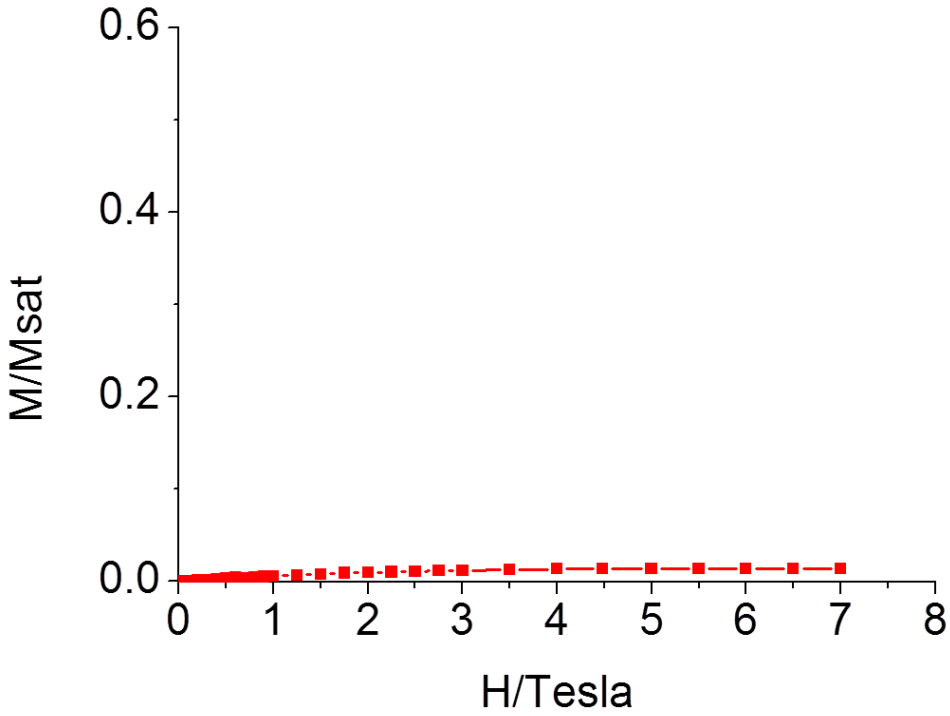

Figure S4. Plot of normalized magnetization, M/M_{sat} vs magnetic field, H of $\mathbf{1}^{2+}$ at T = 2 K.

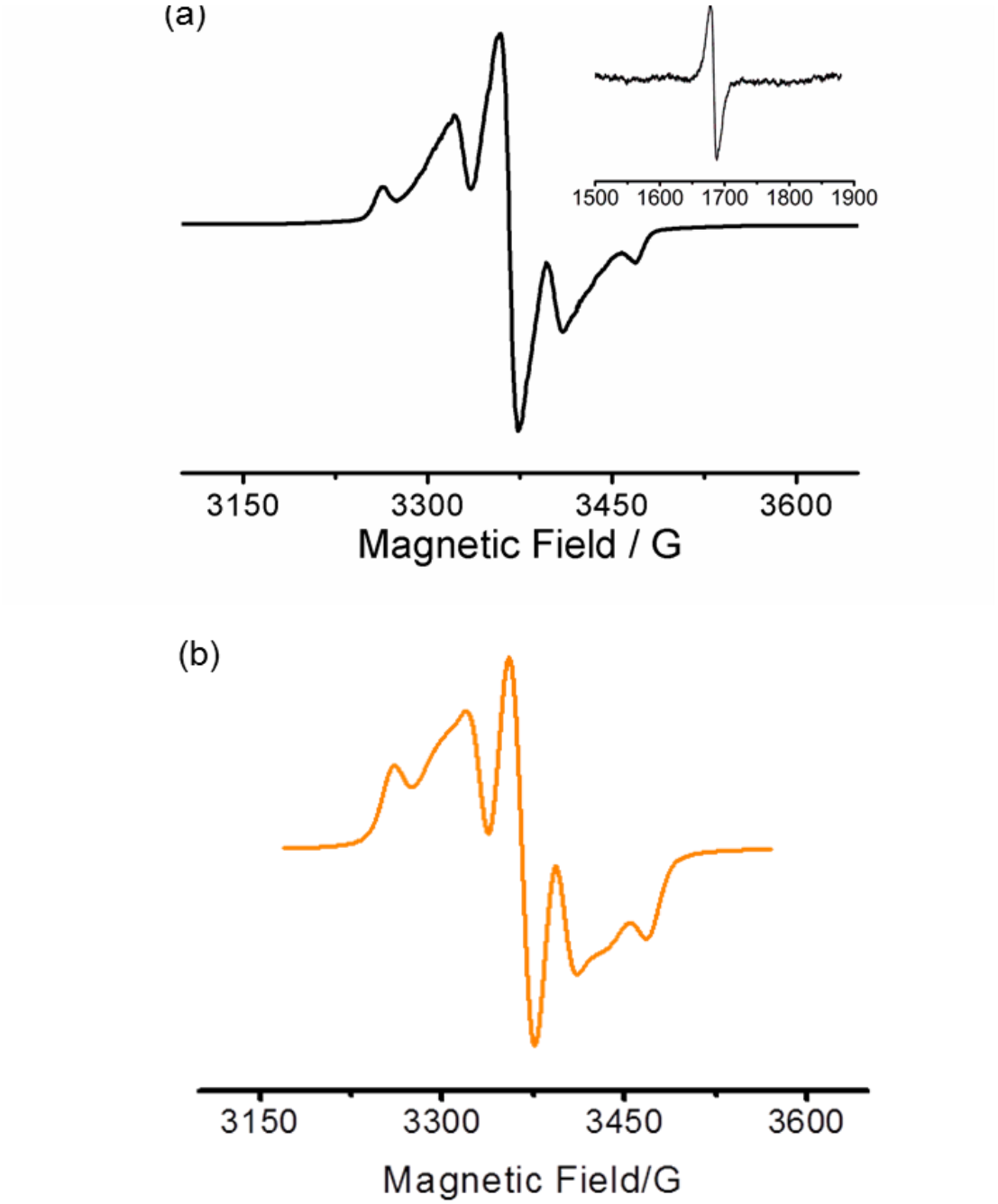

Figure S5. (a) The powder EPR spectrum of $\mathbf{1}^{2+}$•2[Al(OR$_{Me}$)$_4$]$^-$ at 100 K; (b) The simulated EPR spectrum with A_y (N) = 0.69 mT and E = 1.20 mT. The central line due to the mono-radical impurity is simulated with g = 2.0036.

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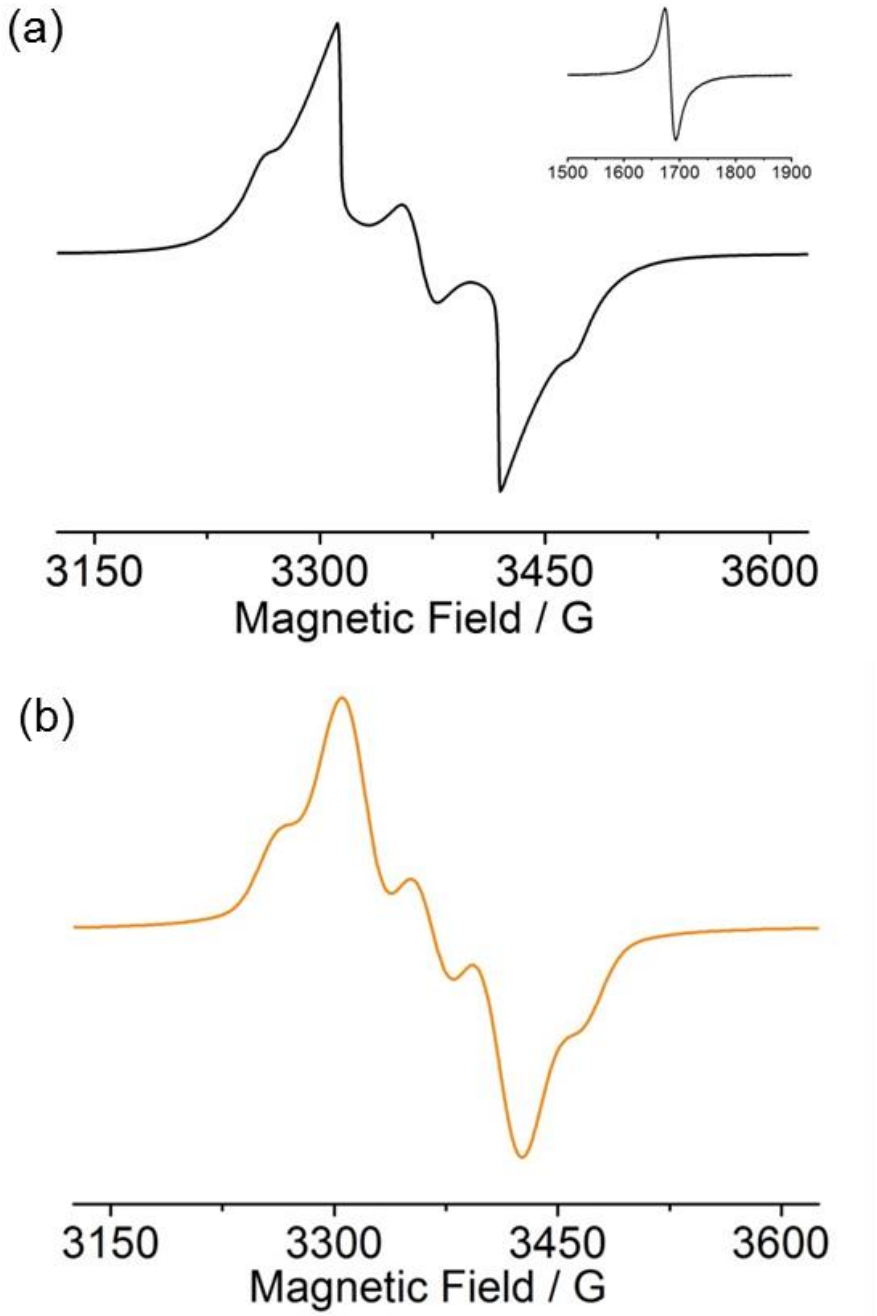

Figure S6. (a) The powder EPR spectrum of $\mathbf{1}^{2+}$•2[Al(OR$_{Me}$)$_4$]$^-$ at 200 K; (b) The simulated EPR spectrum. The central line due to the mono-radical impurity is simulated with g = 2.0037.

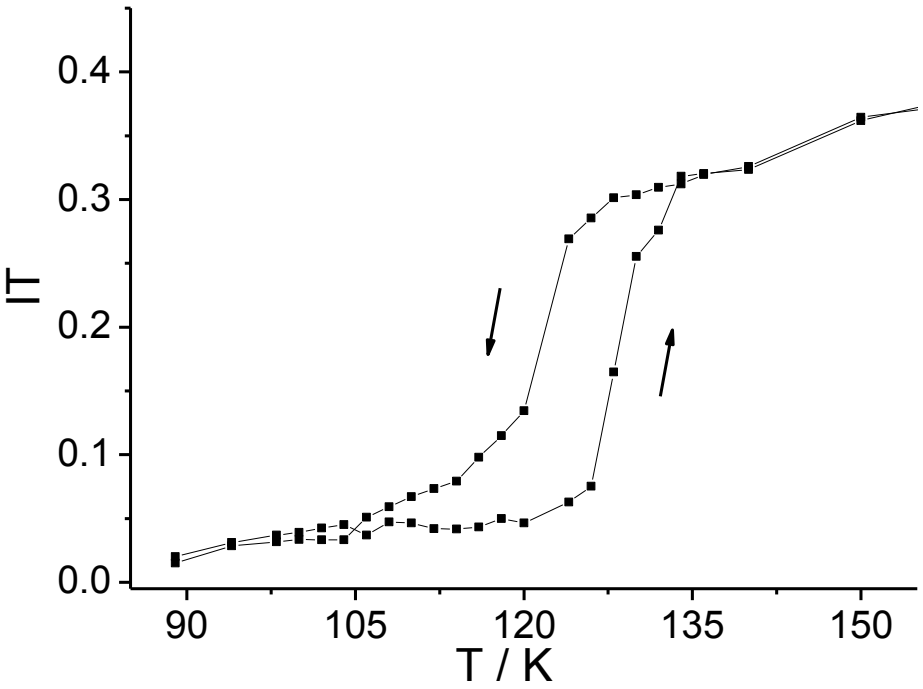

Figure S7. Plot of the product (*IT*) of the intensity for the $\Delta m_s = 2$ resonance and the temperature (*T*) vs. *T*. The values of *IT* are obtained by numerical double integration of the $\Delta m_s = 2$ region.

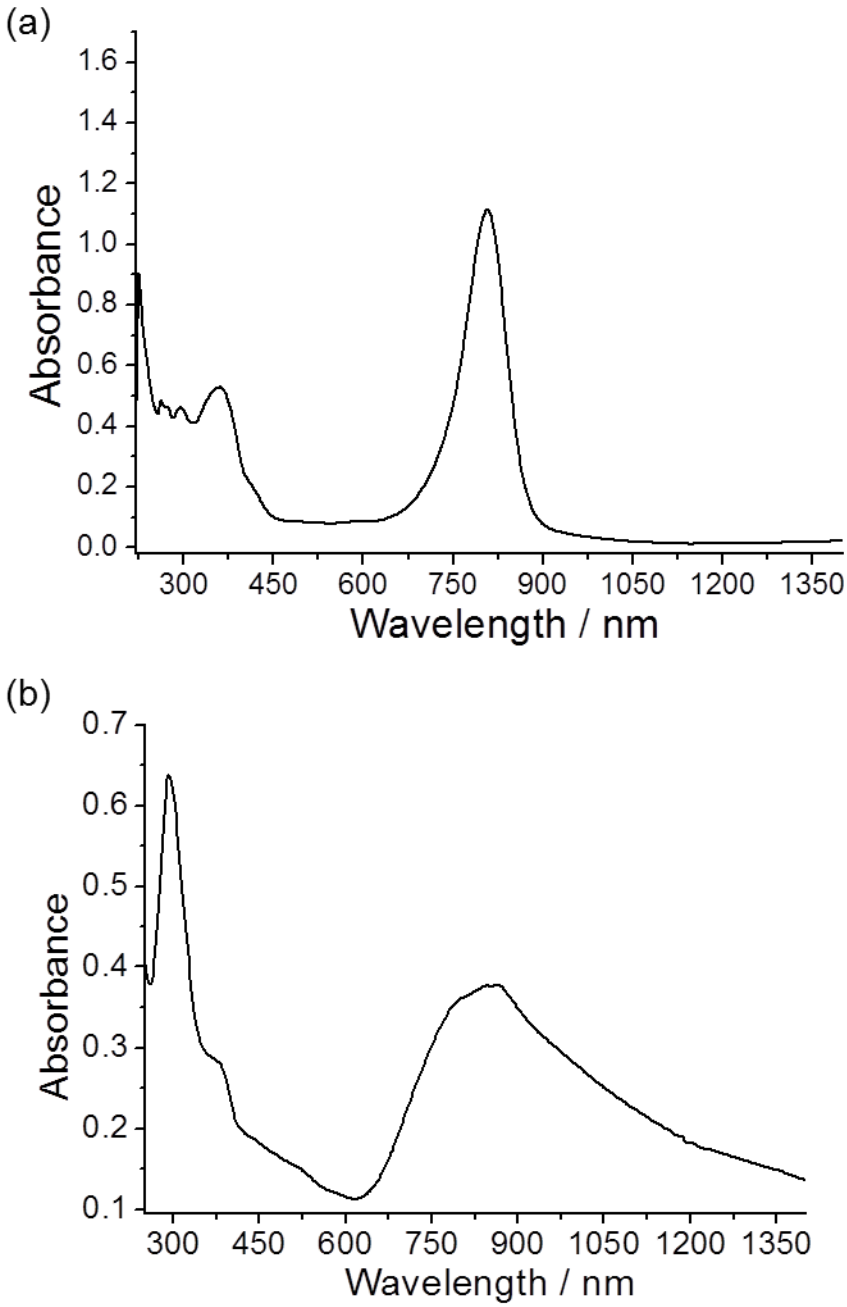

Figure S8. (a) Absorption spectrum of 1×10^{-4} M $\mathbf{1}^{2+}$ in CH_2Cl_2 at 25°C; (b) Absorption spectrum $\mathbf{1}^{2+}$ suspension in hexane upon sonication.

Quantum chemical calculations

All calculations were performed with the Gaussian 09 program suite.[S3] The symmetry-broken approach was applied for open-shell singlet calculations and spin contamination errors were corrected by approximate spin-projection method. All the geometry optimizations were carried out at the (U)B3LYP/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. Single point calculations using the HT and LT X-ray data of $\mathbf{1}^{2+}$ performed at the UB3LYP/6-311G(d,p) level.

Coordinates for optimized geometries.

1^{2+}-CS

N	-0.082472000	-0.026626000	2.810960000
C	0.255428000	-5.214420000	6.654642000
H	1.344005000	-5.104503000	6.614866000
H	-0.003235000	-6.248773000	6.876091000
H	-0.168421000	-4.553333000	7.417263000
C	-0.217408000	-3.734861000	4.820883000
C	0.483456000	-2.648467000	5.391293000
H	1.006400000	-2.760018000	6.333418000
C	0.530005000	-1.433900000	4.729758000
H	1.101833000	-0.617104000	5.157082000
C	-0.122231000	-1.259570000	3.488452000
C	-0.818052000	-2.353020000	2.920755000
H	-1.348607000	-2.223263000	1.983584000
C	-0.863196000	-3.566207000	3.572845000
H	-1.414428000	-4.405976000	3.163601000
C	0.615043000	5.918009000	5.246102000
H	1.691495000	5.723787000	5.197395000
H	0.408220000	6.659374000	6.016486000
H	0.246484000	6.274719000	4.278670000
C	-0.047268000	3.632724000	4.911750000
C	-0.785848000	2.531120000	5.410200000
H	-1.349038000	2.663753000	6.327754000
C	-0.801686000	1.334792000	4.730129000
H	-1.397219000	0.509739000	5.105750000
C	-0.077598000	1.189671000	3.519498000
C	0.648699000	2.291087000	3.021112000
H	1.230911000	2.180879000	2.112423000
C	0.667511000	3.498100000	3.702311000
H	1.255264000	4.320564000	3.312998000
C	-0.043111000	-0.011327000	1.392026000
C	-1.074563000	0.662443000	0.672259000
C	-1.029178000	0.674930000	-0.725497000
C	-2.278375000	1.245825000	1.380350000
H	-2.323069000	2.335200000	1.265640000

H	-2.289375000	1.024906000	2.444762000
H	-3.205868000	0.843779000	0.961100000
C	-2.166351000	1.293830000	-1.508635000
H	-3.127278000	1.112963000	-1.023306000
H	-2.235322000	0.893187000	-2.519434000
H	-2.050633000	2.381645000	-1.592323000
O	-0.328808000	-4.944874000	5.369004000
O	-0.093711000	4.737883000	5.655800000
N	0.082472000	0.026626000	-2.810960000
C	-0.255428000	5.214420000	-6.654642000
H	-1.344005000	5.104503000	-6.614866000
H	0.003235000	6.248773000	-6.876091000
H	0.168421000	4.553333000	-7.417263000
C	0.217408000	3.734861000	-4.820883000
C	-0.483456000	2.648467000	-5.391293000
H	-1.006400000	2.760018000	-6.333418000
C	-0.530005000	1.433900000	-4.729758000
H	-1.101833000	0.617104000	-5.157082000
C	0.122231000	1.259570000	-3.488452000
C	0.818052000	2.353020000	-2.920755000
H	1.348607000	2.223263000	-1.983584000
C	0.863196000	3.566207000	-3.572845000
H	1.414428000	4.405976000	-3.163601000
C	-0.615043000	-5.918009000	-5.246102000
H	-1.691495000	-5.723787000	-5.197395000
H	-0.408220000	-6.659374000	-6.016486000
H	-0.246484000	-6.274719000	-4.278670000
C	0.047268000	-3.632724000	-4.911750000
C	0.785848000	-2.531120000	-5.410200000
H	1.349038000	-2.663753000	-6.327754000
C	0.801686000	-1.334792000	-4.730129000
H	1.397219000	-0.509739000	-5.105750000
C	0.077598000	-1.189671000	-3.519498000
C	-0.648699000	-2.291087000	-3.021112000
H	-1.230911000	-2.180879000	-2.112423000
C	-0.667511000	-3.498100000	-3.702311000
H	-1.255264000	-4.320564000	-3.312998000

C	0.043111000	0.011327000	-1.392026000
C	1.074563000	-0.662443000	-0.672259000
C	1.029178000	-0.674930000	0.725497000
C	2.278375000	-1.245825000	-1.380350000
H	2.323069000	-2.335200000	-1.265640000
H	2.289375000	-1.024906000	-2.444762000
H	3.205868000	-0.843779000	-0.961100000
C	2.166351000	-1.293830000	1.508635000
H	3.127278000	-1.112963000	1.023306000
H	2.235322000	-0.893187000	2.519434000
H	2.050633000	-2.381645000	1.592323000
O	0.328808000	4.944874000	-5.369004000
O	0.093711000	-4.737883000	-5.655800000

1^{2+}-OS

N	-0.067553000	-0.028230000	2.829542000
C	0.075490000	-5.257008000	6.626541000
H	1.164666000	-5.146870000	6.633970000
H	-0.192182000	-6.294101000	6.822929000
H	-0.380642000	-4.605818000	7.378847000
C	-0.314306000	-3.754100000	4.792689000
C	0.362798000	-2.676601000	5.404490000
H	0.846788000	-2.799817000	6.365806000
C	0.440587000	-1.455052000	4.759595000
H	0.998352000	-0.647738000	5.221215000
C	-0.154139000	-1.262157000	3.489356000
C	-0.810044000	-2.356400000	2.872350000
H	-1.276033000	-2.226649000	1.902260000
C	-0.893597000	-3.571953000	3.513235000
H	-1.415326000	-4.410146000	3.063989000
C	0.753304000	5.937821000	5.171520000
H	1.825109000	5.738838000	5.070173000
H	0.588009000	6.684986000	5.946317000

H	0.337444000	6.289586000	4.221690000
C	0.072824000	3.650230000	4.890684000
C	-0.648507000	2.556698000	5.428336000
H	-1.178000000	2.700581000	6.364089000
C	-0.695438000	1.354074000	4.761772000
H	-1.283112000	0.538962000	5.169112000
C	-0.021544000	1.190345000	3.522385000
C	0.671670000	2.293271000	2.976591000
H	1.194844000	2.184120000	2.033276000
C	0.727274000	3.503015000	3.648111000
H	1.287885000	4.324380000	3.218432000
C	-0.031818000	-0.012345000	1.379443000
C	-1.168978000	0.444398000	0.682128000
C	-1.136073000	0.457717000	-0.727192000
C	-2.429023000	0.877023000	1.396254000
H	-2.616786000	1.948409000	1.254698000
H	-2.389871000	0.688113000	2.468045000
H	-3.304397000	0.350451000	1.001800000
C	-2.362452000	0.903826000	-1.490025000
H	-3.247107000	0.340187000	-1.174434000
H	-2.258712000	0.772820000	-2.565997000
H	-2.581382000	1.962069000	-1.303465000
O	-0.453796000	-4.969948000	5.320594000
O	0.061104000	4.763189000	5.624190000
N	0.067553000	0.028230000	-2.829542000
C	-0.075490000	5.257008000	-6.626541000
H	-1.164666000	5.146870000	-6.633970000
H	0.192182000	6.294101000	-6.822929000
H	0.380642000	4.605818000	-7.378847000
C	0.314306000	3.754100000	-4.792689000
C	-0.362798000	2.676601000	-5.404490000
H	-0.846788000	2.799817000	-6.365806000
C	-0.440587000	1.455052000	-4.759595000
H	-0.998352000	0.647738000	-5.221215000
C	0.154139000	1.262157000	-3.489356000
C	0.810044000	2.356400000	-2.872350000
H	1.276033000	2.226649000	-1.902260000

C	0.893597000	3.571953000	-3.513235000
H	1.415326000	4.410146000	-3.063989000
C	-0.753304000	-5.937821000	-5.171520000
H	-1.825109000	-5.738838000	-5.070173000
H	-0.588009000	-6.684986000	-5.946317000
H	-0.337444000	-6.289586000	-4.221690000
C	-0.072824000	-3.650230000	-4.890684000
C	0.648507000	-2.556698000	-5.428336000
H	1.178000000	-2.700581000	-6.364089000
C	0.695438000	-1.354074000	-4.761772000
H	1.283112000	-0.538962000	-5.169112000
C	0.021544000	-1.190345000	-3.522385000
C	-0.671670000	-2.293271000	-2.976591000
H	-1.194844000	-2.184120000	-2.033276000
C	-0.727274000	-3.503015000	-3.648111000
H	-1.287885000	-4.324380000	-3.218432000
C	0.031818000	0.012345000	-1.379443000
C	1.168978000	-0.444398000	-0.682128000
C	1.136073000	-0.457717000	0.727192000
C	2.429023000	-0.877023000	-1.396254000
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H	2.389871000	-0.688113000	-2.468045000
H	3.304397000	-0.350451000	-1.001800000
C	2.362452000	-0.903826000	1.490025000
H	3.247107000	-0.340187000	1.174434000
H	2.258712000	-0.772820000	2.565997000
H	2.581382000	-1.962069000	1.303465000
O	0.453796000	4.969948000	-5.320594000
O	-0.061104000	-4.763189000	-5.624190000

1^{2+}-T

N	-0.067743000	-0.028707000	2.830485000
C	0.059205000	-5.260430000	6.624244000
H	1.148356000	-5.150317000	6.634915000
H	-0.209075000	-6.297720000	6.818736000

H	-0.399091000	-4.609995000	7.375879000
C	-0.324607000	-3.755682000	4.790695000
C	0.350746000	-2.678901000	5.405432000
H	0.831819000	-2.802945000	6.368109000
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H	0.988057000	-0.650596000	5.225846000
C	-0.159069000	-1.262512000	3.489278000
C	-0.811628000	-2.356941000	2.868685000
H	-1.271704000	-2.227716000	1.895795000
C	-0.898461000	-3.572555000	3.508839000
H	-1.417566000	-4.410690000	3.056447000
C	0.767757000	5.937996000	5.166794000
H	1.838994000	5.738268000	5.061030000
H	0.606189000	6.685543000	5.942009000
H	0.348127000	6.289698000	4.218600000
C	0.084822000	3.650608000	4.889862000
C	-0.635791000	2.558080000	5.430234000
H	-1.162467000	2.702878000	6.367438000
C	-0.686132000	1.355234000	4.764341000
H	-1.273888000	0.541377000	5.173956000
C	-0.016633000	1.189855000	3.522574000
C	0.674364000	2.292684000	2.973383000
H	1.192005000	2.184005000	2.027050000
C	0.734026000	3.502313000	3.644598000
H	1.292711000	4.323379000	3.211838000
C	-0.031975000	-0.012817000	1.378365000
C	-1.177168000	0.421510000	0.682123000
C	-1.144088000	0.435372000	-0.728012000
C	-2.442703000	0.837565000	1.396295000
H	-2.648158000	1.904791000	1.248009000
H	-2.397693000	0.656852000	2.469362000
H	-3.310409000	0.294291000	1.007389000
C	-2.375890000	0.865297000	-1.491319000
H	-3.251409000	0.282844000	-1.184134000
H	-2.265583000	0.746442000	-2.568156000
H	-2.614735000	1.917582000	-1.295812000

O	-0.466249000	-4.971931000	5.317039000
O	0.076624000	4.763999000	5.622754000
N	0.067743000	0.028707000	-2.830485000
C	-0.059205000	5.260430000	-6.624244000
H	-1.148356000	5.150317000	-6.634915000
H	0.209075000	6.297720000	-6.818736000
H	0.399091000	4.609995000	-7.375879000
C	0.324607000	3.755682000	-4.790695000
C	-0.350746000	2.678901000	-5.405432000
H	-0.831819000	2.802945000	-6.368109000
C	-0.431070000	1.456927000	-4.761692000
H	-0.988057000	0.650596000	-5.225846000
C	0.159069000	1.262512000	-3.489278000
C	0.811628000	2.356941000	-2.868685000
H	1.271704000	2.227716000	-1.895795000
C	0.898461000	3.572555000	-3.508839000
H	1.417566000	4.410690000	-3.056447000
C	-0.767757000	-5.937996000	-5.166794000
H	-1.838994000	-5.738268000	-5.061030000
H	-0.606189000	-6.685543000	-5.942009000
H	-0.348127000	-6.289698000	-4.218600000
C	-0.084822000	-3.650608000	-4.889862000
C	0.635791000	-2.558080000	-5.430234000
H	1.162467000	-2.702878000	-6.367438000
C	0.686132000	-1.355234000	-4.764341000
H	1.273888000	-0.541377000	-5.173956000
C	0.016633000	-1.189855000	-3.522574000
C	-0.674364000	-2.292684000	-2.973383000
H	-1.192005000	-2.184005000	-2.027050000
C	-0.734026000	-3.502313000	-3.644598000
H	-1.292711000	-4.323379000	-3.211838000
C	0.031975000	0.012817000	-1.378365000
C	1.177168000	-0.421510000	-0.682123000
C	1.144088000	-0.435372000	0.728012000
C	2.442703000	-0.837565000	-1.396295000
H	2.648158000	-1.904791000	-1.248009000

H	2.397693000	-0.656852000	-2.469362000
H	3.310409000	-0.294291000	-1.007389000
C	2.375890000	-0.865297000	1.491319000
H	3.251409000	-0.282844000	1.184134000
H	2.265583000	-0.746442000	2.568156000
H	2.614735000	-1.917582000	1.295812000
O	0.466249000	4.971931000	-5.317039000
O	-0.076624000	-4.763999000	-5.622754000

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