Supporting Information

High-Spin Diradical Dication of Chiral π-Conjugated Double Helical Molecule.

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1. Experimental Section: Synthesis, Measurements, and Computations.

1.a General procedures and materials.

Throughout the following paragraphs labels "AO675" and alike correspond to sample or experiment codes directly traceable to the laboratory notebooks or raw data.

Dichloromethane (DCM) was obtained from solvent purification system (LC Technology Solutions). DCM for electrochemistry and for generation of radical cation, was in addition dried over calcium hydride (CaH_2), and then distilled to a Schlenk vessel, and subsequently degassed by repeated freeze-and-thaw procedure. Acetonitrile (MeCN) for generation of diradical dication was dried over CaH_2, then distilled to a Schlenk vessel, and subsequently degassed. Dibutyl phthalate (DBP) was obtained from commercial sources; prior to use, it was dried over calcium hydride (CaH_2), and then distilled under vacuum (~10 mTorr). Per-deuterated solvents for NMR spectroscopy were obtained from Cambridge Isotope Laboratories. All other commercially available chemicals were obtained from either Aldrich or Acros, unless indicated otherwise.

Column chromatography (0–20 psig pressure) was carried out on silica gel. Standard techniques for synthesis under inert atmosphere, using Schlenk glassware and argon-filled gloveboxes, were employed. A sample of conjoined [5]helicene **1**-C_{2h} (*meso* compound) was used from previous study.[S1] NMR spectra were obtained using commercial spectrometers (^{1}H, 700 MHz, 500 MHz, and 400 MHz) using chloroform-*d* ($CDCl_3$), benzene-d_6, or acetone-d_6 as solvent. The 500 and 700 MHz instruments were equipped with a cryoprobe. The chemical shift references were the peaks of the solvent with residual proton content (see: Figs. S37 – S45). Typical 1D FID was subjected to exponential multiplication with an exponent of 0.1 Hz (for ^{1}H) and 1.0 – 2.0 Hz (for ^{13}C). IR spectra were obtained using a commercial instrument, equipped with an ATR sampling accessory. MS analyses were carried out at local facilities for mass spectrometry.

1.b. Synthesis of conjoined [5]helicene 1-D_2.

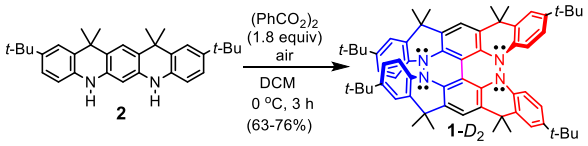


Table S1. Summary of preparation of **1**-D_2.

Run	S.M. (mg/mmol/equiv)	BPO (mg/mmol/equiv)	DCM (mL)	TM (mg, % yield)	Comment
CS-3-2-5	19.4/0.0429/1	18.7/0.0772/1.8	3	12.0, 63	Yellow solid; Fig. S37
CS-3-2-7	19.4/0.0429/1	18.7/0.0772/1.8	3	14.7, 76	Yellow solid; Figs. S38-S40
CS-3-2-15	19.4/0.0429/1	18.7/0.0772/1.8	3	12.3, 63	Yellow solid from 19.4 mg of brown crude mixture by treatment twice with MeOH; Figs. S41-S43.
CS-3-2-25	19.4/0.0429/1	18.7/0.0772/1.8	3	12.2, 63	Yellow solid by treatment with MeOH followed by short column; Fig. S44
CS-3-2-27	83.5/0.184/1	80.2/0.331/1.8	10	53.8, 64	Yellow solid by treatment with MeOH followed by short column; Fig. S45

General procedure (on the scale of the first four runs in Table S1):

To diamine (SM, 19.4 mg) in a vial, dichloromethane (DCM, 2 mL) was added, forming a pink suspension. A solution of benzoyl peroxide (BPO, 18.7 mg) in DCM (1 mL) was added to the suspension of SM. The resultant mixture was stirred at room temperature for 3 h. Subsequently, the reaction mixture (red brown solution) was extracted with phosphate buffer (pH ≈ 11, 2 × 5 mL) and DCM (2 × 5 mL). The resultant organic layer was dried over Na_2SO_4, and then concentrated in vacuo to give crude mixture; for representative ^{1}H NMR spectra of crude mixtures, see: Figs. S38, S39, S41, S42. The brown crude mixture was either purified by column chromatography (silica gel, 15% benzene in pentane) or treated with MeOH (and then, filtered through a short silica gel column), to obtain TM as a yellow solid (Figs. S37, S40, S43-S45).

1.c. Electrochemistry

Cyclic and square wave voltammetry of 1-*D*$_2$ in DCM at room temperature. Label: AO675. Voltammetry data for conjoined [5]helicene **1**-D_2 were obtained in a glovebag under argon gas atmosphere, using procedures described for other π-conjugated compounds.[S2-S4] (The supply gas was a commercial ultra-high purity argon, certified to contain <1 ppm of O_2 and <1 ppm of H_2O.) The custom-made electrochemical cell, all solid reagents, syringes, needles, etc. were extensively evacuated in Schlenk vessels (typical pressure ≤ 1 mTorr, temperature 20–70 °C), prior to the transfer to the glovebag. Dichloromethane (CH_2Cl_2) was obtained from commercial solvent purification system, then distilled from calcium hydride under nitrogen, and stored in the absence of light in a Schlenk vessel on a vacuum line; just prior to the use, the solvent was vacuum transferred as needed. Commercial potentiostat/galvanostat was used. Three electrodes were employed: quasi-reference (Ag-wire), counter (Pt-foil), and working (100-μm Pt-disk). The concentration of an electroactive solute was about 0.7 mM. Concentration of the tetrabutylammonium hexafluorophosphate supporting electrolyte ($[n\text{-}Bu_4N]^+[PF_6]^-$) was about 0.1 M. The solution volume was about 2.4 mL. After a series of cyclic voltammograms with potential increments of 2 – 4 mV, a small amount (ca. 8 drops) of solution of decamethylferrocene (ca. 0.7 mg of Cp^*_2Fe, loaded to a Schlenk vessel in a glovebox under an argon atmosphere in the supporting electrolyte, ca. 0.8 mL) was added to the cell, to provide reference potentials (–0.130 V vs. SCE for $Cp^*_2Fe/Cp^*_2Fe^+$ in

CH_2Cl_2).[S5,S6] Cyclic voltammograms with the scanning rates in the 20–500 mV/s range and several square wave voltammograms (frequency 4 and 10 Hz, pulse height 25 mV) were obtained. In another, initial experiment (label: AO658), ferrocene was used as potential reference (+0.46 V vs. SCE for Cp_2Fe/Cp_2Fe^+ in CH_2Cl_2);[S6] the first oxidation wave for **1**-D_2 was partially overlapped with the reference wave.

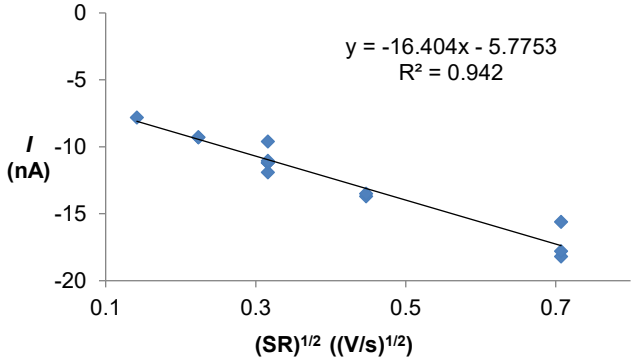


Fig. S1. Cyclic voltammetry of conjoined [5]helicene **1**-D_2 in DCM: plot of current (nA) vs. square root of scan rate ($(V/s)^{1.2}$) (CV labels: AO675C1–C13).

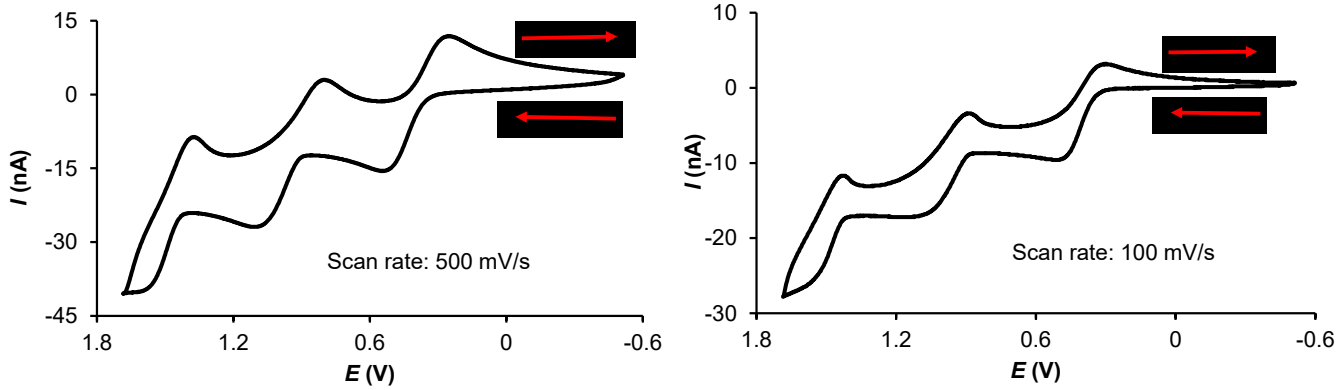


Fig. S2. Cyclic voltammetry of conjoined [5]helicene **1**-D_2 in DCM, showing the third wave corresponding to $E_3^0 \approx 1.53$ V (CV labels: AO675C12 and AO675C13).

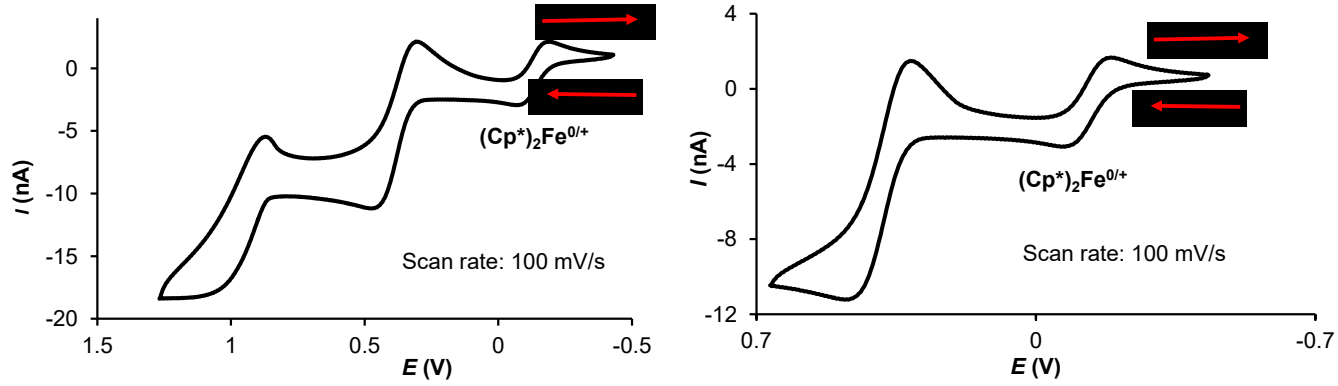


Fig. S3. Selected cyclic voltammograms of conjoined [5]helicene **1**-D_2 in DCM with reference Cp^*_2Fe (CV labels: AO675F14 and AO675F15).

1.d EPR, UV-vis-NIR, and ECD spectroscopy.

1.d1 General description and EPR microwave saturation plots. EPR spectra were obtained using Bruker CW EPR spectrometer (X-band EMXplus). For temperature control (400–95 K), EPR spectrometer was equipped with custom-made nitrogen flow system. Temperatures were calibrated using an additional thermocouple inserted to the EPR tube containing solvent (DBP). DPPH powder ($g = 2.0037$) was used as a *g*-value reference. Quantitative EPR spectroscopy for diradical dication in DBP was carried using tempone in DBP as a reference.[S7,S8] Average values of χT vs T were fit to the Bleaney–Bowers equation, using either one-parameter (J/k = exchange coupling constant) fit or a two-parameter fit with J/k and N, where N is weight correction factor.[S8]

EPR spectra were simulated using either Bruker Symphonia or EasySpin.[S9] Simulations for triplet state of diradical dication (using pepper of EasySpin) are presented in Figs. S14, S21, S24, and S26. Simulations for radical cation (using garlic of EasySpin) are presented in Figs. S5 and S8.

UV-vis-NIR spectra of neutral **1**-D_2, and its radical cation and diradical dication, were obtained using JASCO (model V-670) and Shimadzu (model UV-2401PC) spectrophotometers. Electronic circular dichroism (ECD) spectra were obtained using JASCO (model J-810) spectropolarimeters (one up to 700 nm and the other up to 900 nm).

Since at low temperatures required for quantitative EPR spectra obtained in the determination of singlet-triplet gap for diradical dication in DBP, slow electron spin relaxation rates may affect signal intensities, we have checked for microwave saturation at 117 K for both diradical dication and Tempone reference. In Fig. S4 below, absence of microwave saturation at 117 K is found down to attenuations of 25 dB and 28 dB (from 200 mW) for diradical dication and Tempone, respectively; therefore, the quantitative EPR can be carried out at attenuation of more than 30 dB – we have mostly used attenuation of 40 dB. Similarly, for different samples of diradical dication in DBP, absence of saturation at 129 K in the 30 – 55 dB range was found (Fig. S21).

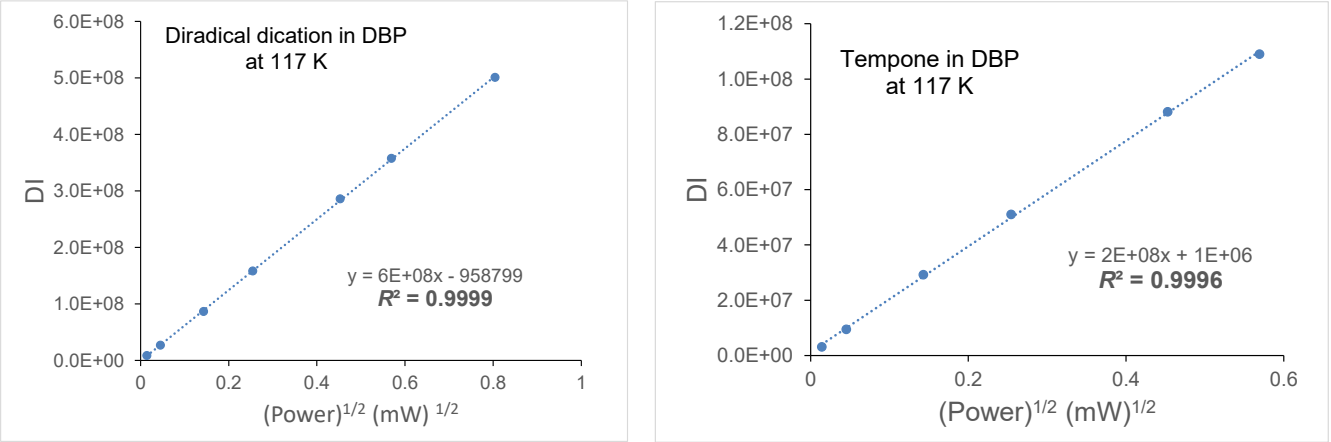


Fig. S4. Plots of EPR double integrated signal intensity (DI) versus the square root of microwave power in DBP at 117 K. Microwave power attenuation ranges were: for 0.56 mM diradical dication (sample label: HZ1015), 25 – 60 dB (EPR labels: HZ1015r21-r42) and for 5.08 mM Tempone, 28 – 60 dB (EPR labels: HZ1015r43-r64).

1.d2 Generation of radical cation $1^{\bullet+}BF_4^-$ via oxidation of 1-D_2 with $AgBF_4$ in DCM: EPR and UV-vis-NIR spectra. To the starting material **1**-D_2 (4.2 mg, 4.67 μmol, CS-2-2-6pL) in custom-made Schlenk vessel,[S2] evacuated on vacuum line at room temperature overnight, $AgBF_4$ in dichloromethane (0.41 mL, 0.0149 M) was added to the vessel; color of the reaction mixture immediately changed to dark purple. After stirring at room temperature for 2 h, the reaction mixture was filtered with dichloromethane and dried under the high vacuum overnight. Dark purple crude (5.5 mg) was obtained. Subsequently, the curde mixture was dissolved in DCM (0.584 mM) and transferred to a 4-mm EPR tube. EPR spectra were obtained at 294 K (Figure S5, top panel). Using tempone in DCM (1.091 mM) as reference, spin concentration was determined as 82% at 294 K (EPR labels: CS294r1-r10). The sample solution was diluted to 0.295 mM and transferred to a UV cuvette (1-cm). Dichloromethane was prepared in another UV cuvette (1-cm). UV-vis-NIR spectra were obtained (Fig. S5, middle panel). Following UV-vis-NIR experiments, solution in UV cuvette was transferred back to a new 4 mm EPR tube. Using the same reference, the spin concentration was determined as 80% at 294 K (Fig. S5, bottom panel, EPR labels: CS296r1-r10).

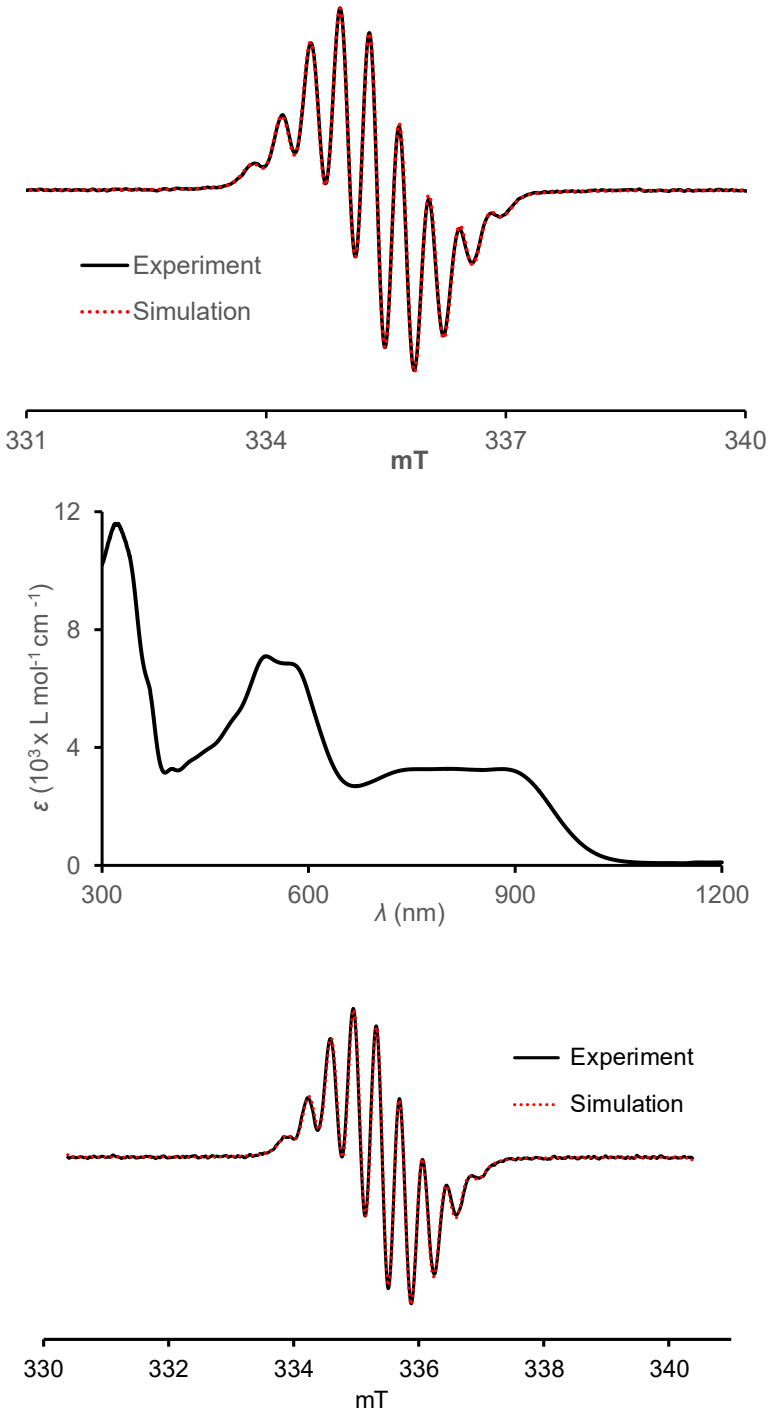


Fig. S5. Enlarged Figure 4 in the main text with additional details: EPR and UV-vis-NIR spectra of radical cation $\mathbf{1}^{\bullet+}BF_4^-$ in DCM at room temperature. Top panel: EPR (ν = 9.4058 GHz, label: CS294r1) spectrum of 0.58 mM $\mathbf{1}^{\bullet+}BF_4^-$ prior to dilution for UV-vis-NIR spectra; spin concentration is ~82%. Middle panel: UV-vis-NIR absorption spectrum (UV label: CS2294-1200nm) of 0.30 mM $\mathbf{1}^{\bullet+}BF_4^-$. Bottom panel: EPR (ν = 9.4059 GHz, label: CS296r1) spectrum of 0.30 mM $\mathbf{1}^{\bullet+}BF_4^-$ following UV-vis-NIR spectra; spin concentration is ~80%. Simulation (garlic, EasySpin, rmsd = 0.288): $A(^{14}N)$ = 9.984 MHz, g = 2.0029, line-width = 0.207 mT (Gaussian) and 0.109 mT (Lorentzian).

1.d3 EPR and UV-vis-NIR spectral monitoring: generation of radical cation $1^{\bullet+}BF_4^-$ using $[Th]^{\bullet+}[BF_4]^-$ in DCM.

Table S2. Summary of preparation of radical cation $\mathbf{1}^{\bullet+}BF_4^-$ using $[Th]^{\bullet+}[BF_4]^-$ in DCM.

run no	sample label	**1-*D*₂** (mg)	Initial concentration of **1-*D*₂** (mM)[a]	Figures and comments
1	AO1035	0.80	1.20	The best run: vis-NIR spectra (Fig. S7), EPR (with simulation), UV-vis-NIR, no change in spin conc. after 24 h at rt (Fig. S8); quench with Cp^*_2Fe, ^1H NMR (Fig. S9).
2	AO1033	0.83	0.87	First addition of $[Th]^{\bullet+}[BF_4]^-$ gave radical cation with an admixture of diradical dication; spin conc. of 96%.
3	AO688	0.80	1.96	No spin concentrations; 2nd addition of $[Th]^{\bullet+}[BF_4]^-$ gave a mixture of radical cation and diradical dication: Fig. S10; quench with Cp^*_2Fe, ^1H NMR (Fig. S11).

[a] Based on extinction coefficient for the λ = 407 nm band of **1**-D_2 in DCM (Figure S6) and initial UV-vis spectra of **1**-D_2 that were obtained just before addition of $[Th]^{\bullet+}[BF_4]^-$ in DCM (UV-vis labels: AO688u1 and u2, AO1033u1 and u2, AO1035u1 and u2).

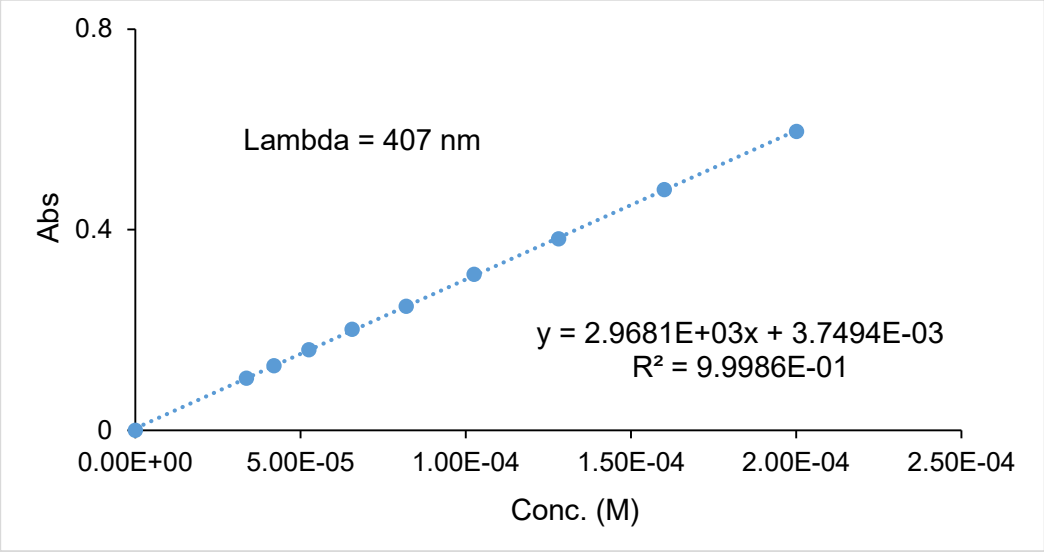


Fig. S6. Determination of molar extinction coefficient for conjoined [5]helicene **1**-D_2 in DCM.

Radical cation $1^{\bullet+}BF_4^-$ generated using $[Th]^{\bullet+}[BF_4]^-$: sample label: AO1035. Conjoined [5]helicene **1**-D_2 (KS1242-1, MW = 899.3, 0.80 mg, 0.89 μmol) and a small teflon-coated magnetic bar were placed into a home-made Schlenk vessel (4-mm quartz EPR sample tube, 1-mm pathway UV-vis cell and Schlenk compartment for mixing of reagents)[S2,S10] equipped with high-vacuum PTFE stopcocks. The Schlenk was dried under high vacuum at 70 °C for overnight. Dichloromethane (DCM) was vacuum transferred to the UV-vis cell. The baseline for UV-vis-NIR spectra was obtained. Subsequently, total volume of 0.72 mL of DCM (volume estimate based on weight of **1**-D_2 and its UV-vis spectrum) was

vacuum transferred to the Schlenk compartment. The solution of **1**-D_2 was stirred briefly at r.t. to obtain a clear yellow solution. The solution was decanted to the UV-vis-NIR cell and UV-vis-NIR absorption spectra were taken (label: AO1035u1-u2), providing initial concentration estimate of **1**-D_2 as 1.23 mM (Fig. S6). Subsequently, series of background EPR spectra, together with Tempone in DCM, were obtained; no detectable EPR signal from sample containing 1.23 mM **1**-D_2 was observed. $[Th]^{\bullet+}[BF_4]^-$ was weighed inside N_2-glovebag and transferred to a Schlenk vessel. The vessel was attached to high-vacuum line and evacuated for 15 min. DCM was added to the Schlenk vessel by vacuum transfer to produce a deep purple solution. The first small portion of solution of $[Th]^{\bullet+}[BF_4]^-$ (0.11 mL) was then added to the solution of conjoined [5]helicene **1**-D_2 to produce the purple solution. The reaction mixture was consecutively decanted to the UV-vis-NIR cell and the EPR tube, respectively. The vis-NIR and EPR spectra were consecutively taken (e.g., vis-NIR in Fig. S7); spin concentration of this sample was 43%; peaks corresponding to unreacted **1**-D_2 could be observed in the UV-vis-NIR spectra. Additional solution of $[Th]^{\bullet+}[BF_4]^-$ (0.11 mL) was added to the Schlenk vessel and the consecutive EPR and vis-NIR spectra were recorded (Figs. S7 and S8). The vessel was attached to high vacuum line and evacuated briefly. Dichloromethane was added by vacuum transfer to maintain the concentration of the solution. EPR spectra, taken at 150 K (A1036r34-r36), showed a single broad signal with peak-to-peak linewidth of 1.41 mT.

Following spectroscopic monitoring experiments, decamethylferrocene (Cp^*_2Fe, 0.38 mg, 1.157 μmol) was added to the reaction mixture to produce the yellow solution; the EPR and UV-vis-NIR spectra showed absence of the radical cation of conjoined [5]helicene. The reaction mixture was transferred to a vial and evaporated under nitrogen flow. The crude mixture was evacuated under high vacuum for overnight to produce 1.06 mg of green solid. The ^{1}H NMR (700 MHz, acetone-d_6, AO-10-35-crd) spectrum showed the conjoined [5]helicene **1**-D_2 as a major product (Figure S9).

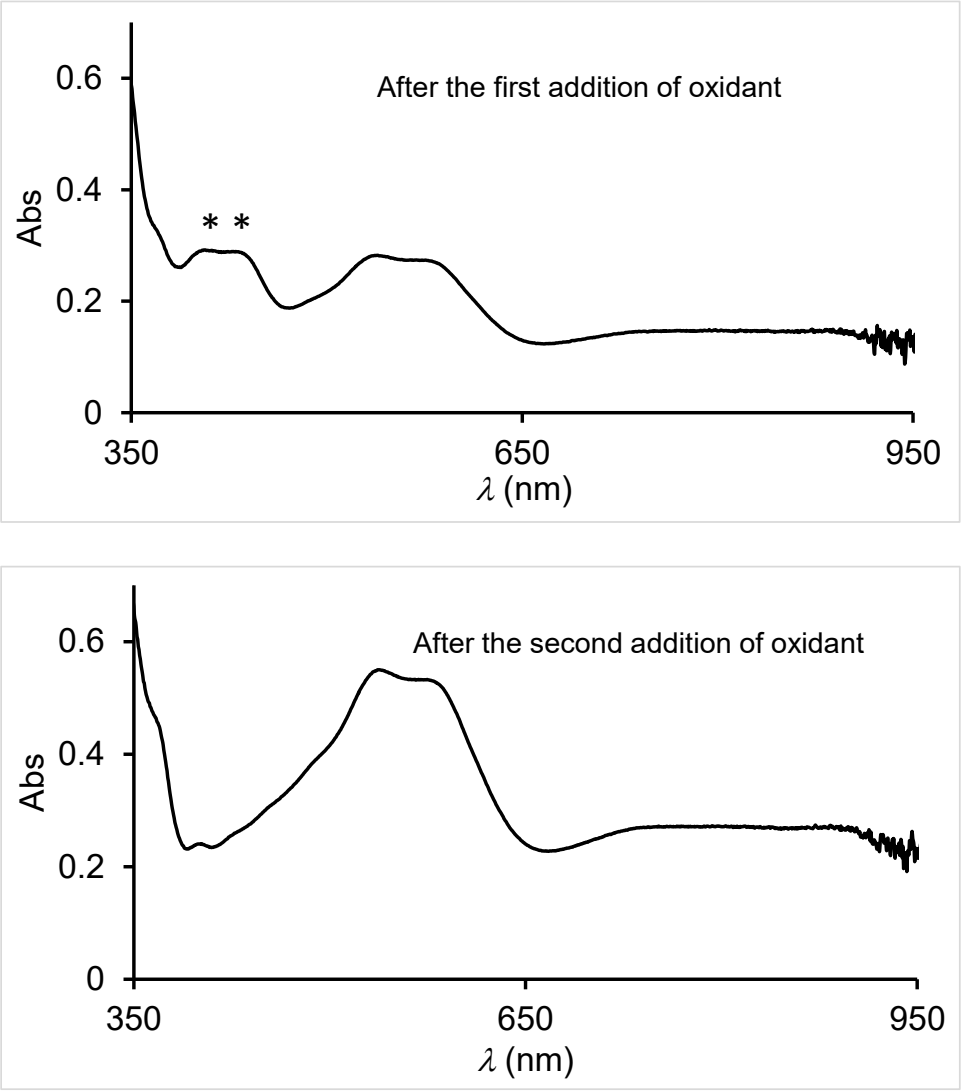


Fig. S7. Vis-NIR absorption spectra (vis_NIR labels: AO1035u4 and AO1035u8) at ambient temperature obtained during oxidation of **1**-D_2 with $[Th]^{\bullet+}[BF_4]^-$ showing radical cation $\mathbf{1}^{\bullet+}BF_4^-$. EPR spin concentrations of 43% and 98% were measured for these samples. For the second sample, EPR spectrum and replotted vis-NIR spectrum are shown in the next figure (Fig. S8). In the vis-NIR spectrum of first sample (top panel), asterisks (*) indicate peaks from starting material **1**-D_2.

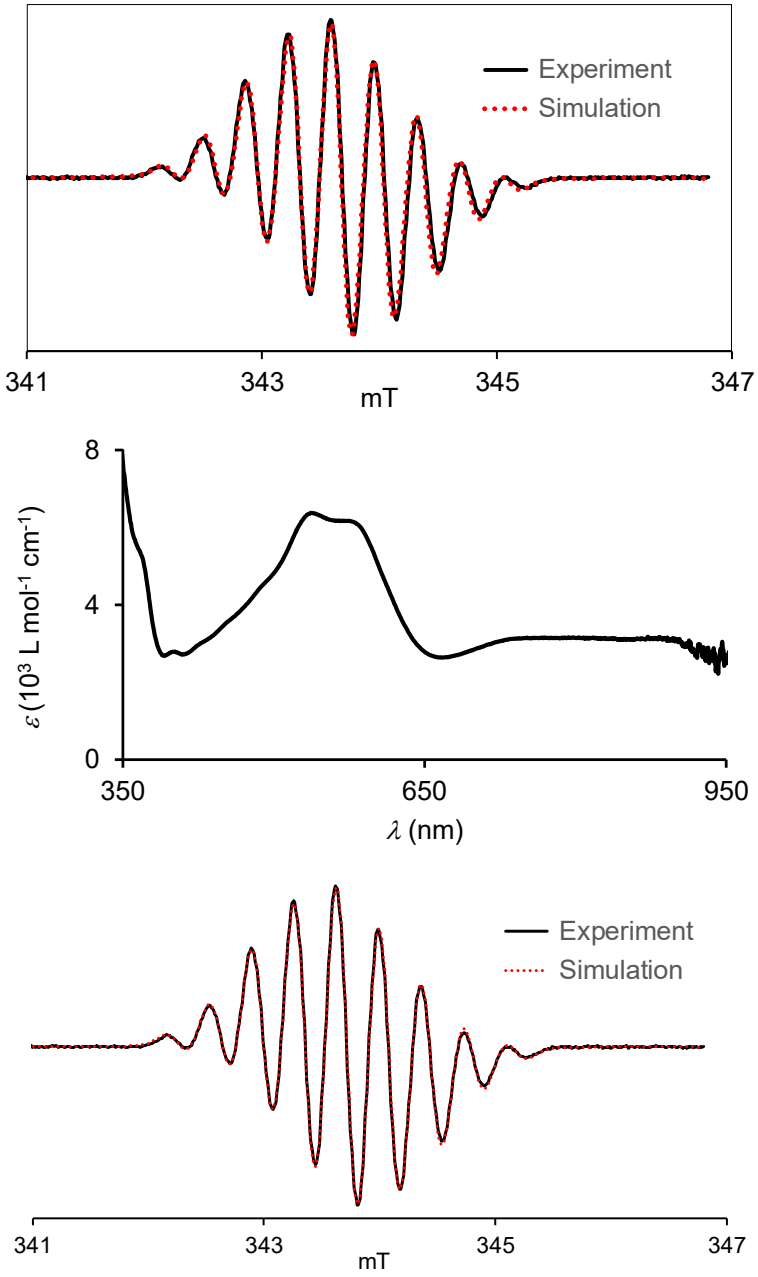


Fig. S8. Consecutive EPR and vis-NIR absorption spectra: oxidation of **1**-D_2 with [Th]$^{\bullet+}$[BF_4]$^-$ showing radical cation **1**$^{\bullet+}BF_4^-$ (sample label: AO1035). Top panel: EPR (ν = 9.6356 GHz, EPR label: AO1035r23) spectrum (spin conc. of 98%) prior to vis-NIR spectrum; simulation (Garlic, EasySpin, rmsd = 0.352): $A(^{14}N)$ = 10.04 MHz, g = 2.0030, line-width = 0.144 mT (Gaussian) and 0.078 mT (Lorentzian). Middle panel: vis-NIR absorption spectrum (vis_NIR label: AO1035u8) at ambient temperature: bands at λ_{max} = 538, 567, 744, 884 nm have the extinction coefficients: $\varepsilon_{538} = 6.4 \times 10^3$, $\varepsilon_{567} = 6.2 \times 10^3$, $\varepsilon_{744} = 3.1 \times 10^3$, and $\varepsilon_{884} = 3.2 \times 10^3$ L mol^{-1} cm^{-1}. Bottom panel: EPR (ν = 9.6359 GHz, EPR label: AO1035r26) spectrum following vis-NIR spectrum, obtained after 24 h at rt; spin conc. = 99%; simulation (Garlic, EasySpin, rmsd = 0.200): $A(^{14}N)$ = 10.20 MHz, g = 2.0029, line-width = 0.192 mT (Gaussian) and 0.043 mT (Lorentzian).

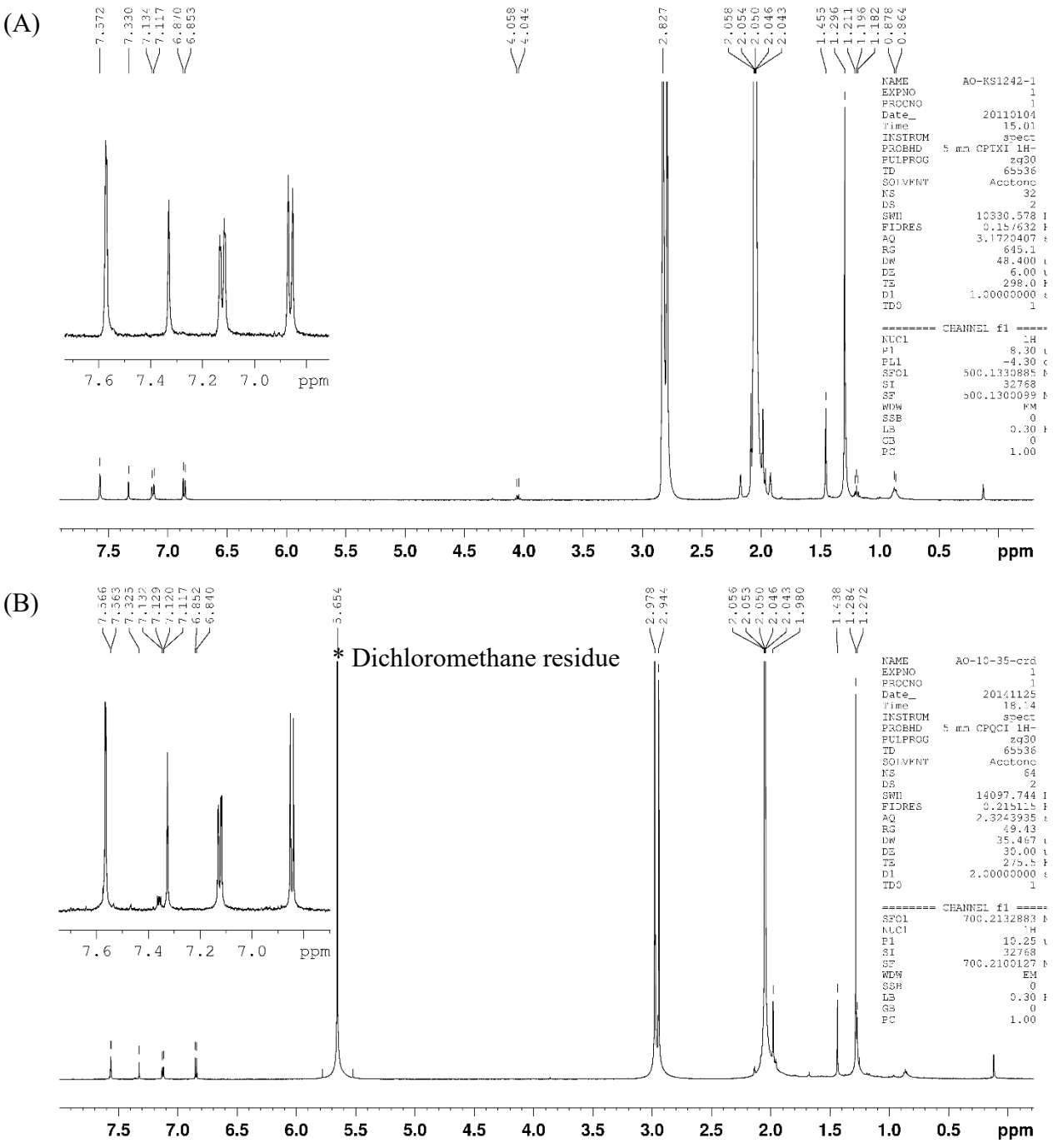


Fig. S9. (A) ^{1}H NMR spectrum (500 MHz, acetone-d_6, label: AO-KS1242-1) of conjoined [5]helicene **1**-D_2. (B) ^{1}H NMR spectrum (700 MHz, acetone-d_6, label: AO-10-35-crd) of the crude sample obtained after addition of Cp*$_2$Fe.

Radical cation $\mathbf{1}^{\bullet+}BF_4^-$ generated using $[Th]^{\bullet+}[BF_4]^-$: sample label, AO688. Conjoined [5]helicene **1**-D_2 (KS1242-1, MW = 899.3, 0.80 mg, 0.89 μmol) and a small teflon-coated magnetic bar were placed into a home-made Schlenk vessel (4-mm quartz EPR sample tube, 1-mm pathway UV-vis cell and Schlenk compartment for mixing of reagents)[S2,S10] equipped with high-vacuum PTFE stopcocks. The Schlenk vessel was dried under high vacuum at 70 °C for overnight. Dichloromethane was vacuum transferred to the UV-vis-NIR cell. The baseline for UV-vis-NIR spectra was obtained. Subsequently, total volume of 0.45 mL dichloromethane (volume estimate based on weight and UV-vis spectrum of **1**-D_2) was vacuum transferred to the Schlenk compartment. The solution of conjoined amine was stirred briefly at r.t. to obtain a clear yellow solution. The solution was decanted to the UV-vis-NIR cell and UV-vis-NIR spectra were taken (AO688u1-3), providing initial concentration estimate of **1**-D_2 as 1.96 mM (Fig. S6). $[Th]^{\bullet+}[BF_4]^-$ was weighed inside argon-filled Vacuum Atmospheres glovebox and transferred to a Schlenk vessel inside glovebox. The vessel was transferred from the glovebox to high-vacuum line and then dichloromethane was vacuum transferred. This first portion of solution of $[thianthrene]^{\bullet+}[BF_4]^-$ (0.33 mL, ~1 equiv) was added to produce the purple solution. The reaction solution was consecutively decanted to the UV-vis-NIR cell and the EPR tube. The UV-vis-NIR and EPR spectra were consecutively taken. Additional solution of $[thianthrene]^{\bullet+}[BF_4]^-$ (~1+ equiv) was added to the Schlenk vessel and the UV-vis-NIR and EPR spectra were recorded.

Following spectroscopic monitoring experiments, decamethylferrocene (Cp^*_2Fe, 0.37 mg, 1.13 μmol, 1.3 equiv) was added to the reaction mixture to produce the yellow solution and the UV-vis-NIR and EPR spectra were consecutively recorded, revealing absence of the radical cation. The reaction mixture was transferred to a vial and evaporated under nitrogen flow. The crude mixture was evacuated under high vacuum for overnight to produce yellow solid (1.6 mg). The ^1H NMR (500 MHz, acetone-d_6, AO-6-88-crd) spectrum showed the conjoined [5]helicene **1**-D_2 and excess of thianthrene.

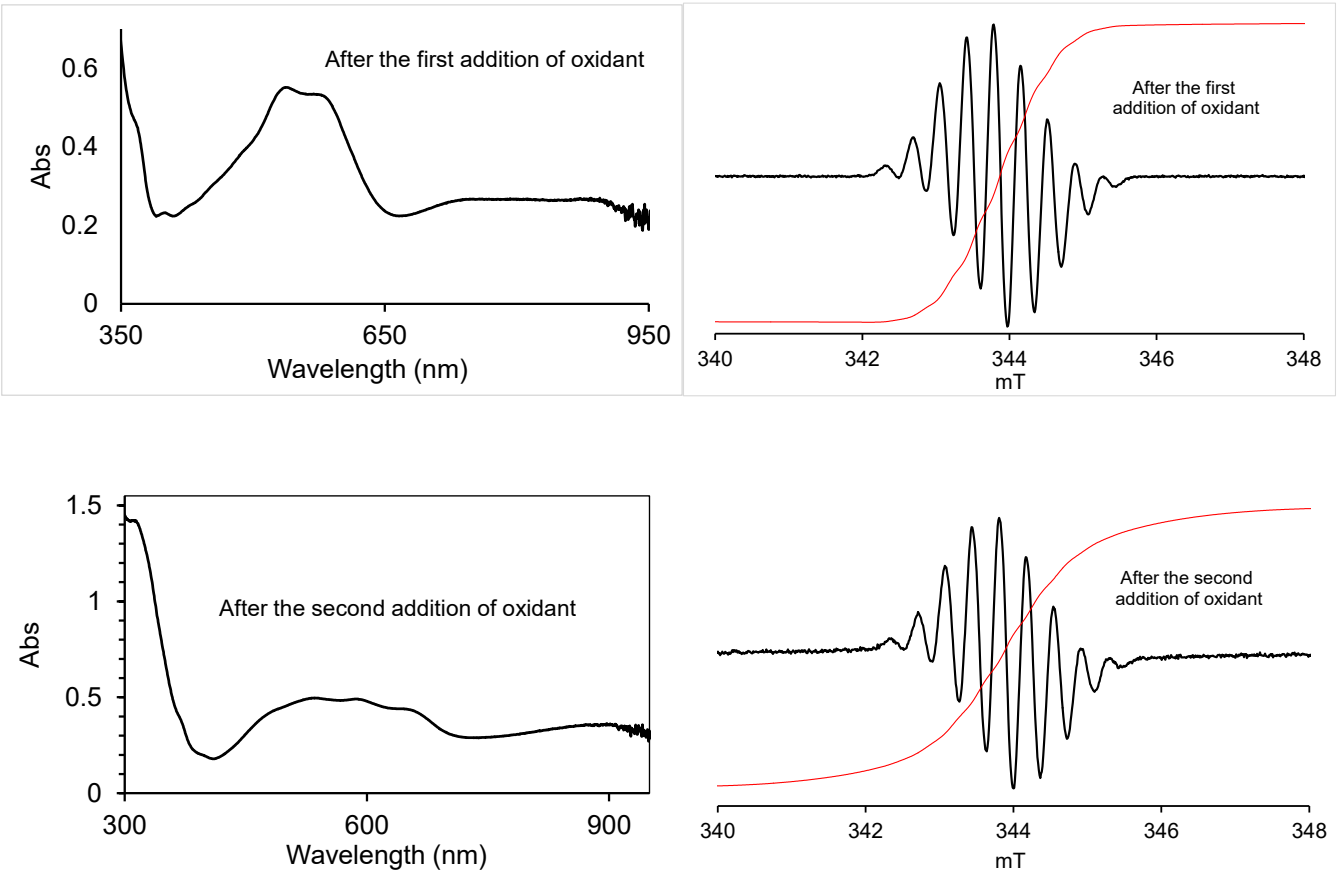


Fig. S10. Consecutive EPR (ν = 9.6356 GHz, EPR label: AO1035r23, sample label: AO1035) and vis-NIR spectra (vis_NIR label: AO1035u8) at ambient temperature in DCM obtained during oxidation of **1**-D_2 with $[Th]^{\bullet+}[BF_4]^-$ (first addition of ~1 equiv and second addition of ~1+ equiv). Top panels: spectra showing radical cation $\mathbf{1}^{\bullet+}BF_4^-$. Bottom panels: spectra showing a mixture of radical cation $\mathbf{1}^{\bullet+}BF_4^-$ and diradical dication $\mathbf{1}^{2\bullet2+}2BF_4^-$; in the EPR spectrum at room temperature in DCM, only radical cation can be seen as the triplet state of the diradical dication is very likely broadened to the baseline at these conditions, e.g., compare double integration lines (in red) in the two EPR spectra.

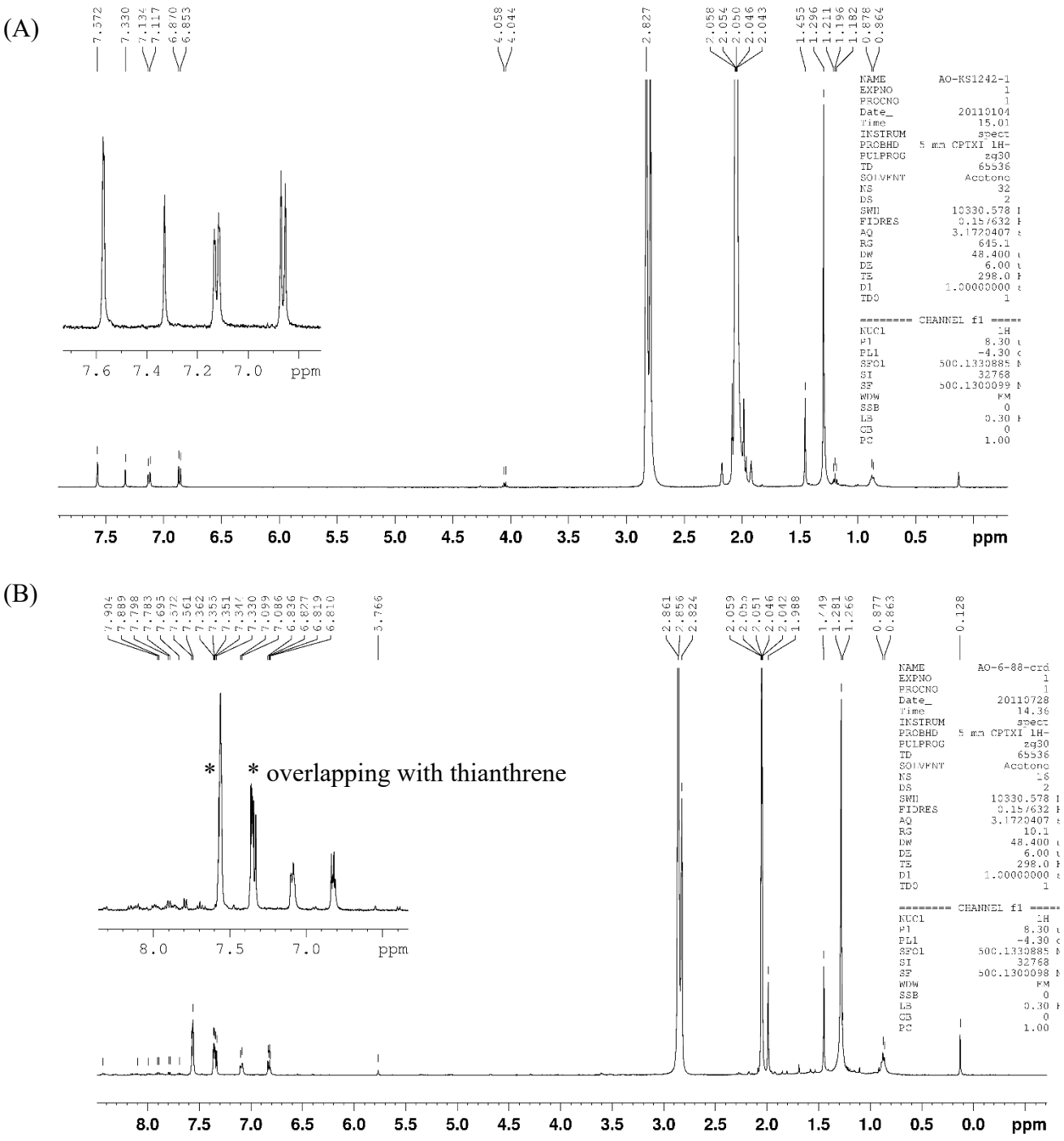


Fig. S11. (A) ^{1}H NMR spectrum (500 MHz, acetone-d_6, label: AO-KS1242-1) of conjoined [5]helicene **1**-D_2. (B) ^{1}H NMR spectrum (500 MHz, acetone-d_6, label: AO-6-88-crd) of the crude sample obtained after adding Cp*$_2$Fe.

1.d4 Preparation of diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ by oxidation of *rac*-1-D_2 using $[NO]^+[SbF_6]^-$.

Table S3. Summary of preparation of diradical dication $\mathbf{1}^{2\bullet 2+}2SbF_6^-$ using $[NO]^+[SbF_6]^-$ in DBP.

run no	sample label	**1**-D_2 (mg)	$[NO]^+[SbF_6]^-$ (equiv)	Figures and comments	Recovered **1**-D_2 (mg, %)
1	HZ1164	0.34	(3.8)+(3.2)	Initial χT = 0.872 ± 0.004 at 117 K; quantitative EPR (105 – 330 K), giving $2J$ = 145 K (Fig. S12); EPR, stability on air (Fig. S13); EPR (with simulation), UV-vis-NIR, EPR (Fig. S14); quench with Cp^*_2Fe, ^1H NMR (Fig. S15).	0.29, 85%
2	HZ1015	0.25	3+(1.6)	Quantitative EPR (105 – 340 K, Fig. S16), quantitative EPR spectra at 295 K following annealing at 340 K for 10 – 120 min (Fig. S17), EPR, UV-vis-NIR, EPR (Fig. S18); quench with Cp^*_2Fe, ^1H NMR and ESI MS (Figs. S19&20).	0.24, 96%
3	HZ1001	0.29	(2.2)+2+4	EPR spectrum (with simulation) and power saturation plot (Fig. S21); quench with Cp^*_2Fe, ^1H NMR and ESI MS (Figs. S22&23).	0.24, 83%
4	CS332	0.47	5.6	EPR spectra of 1.10 mM diradical dication (Fig. S24); determination of half-life = 16 days on air at room temperature (Fig. S25).	-
5	CS374	0.31	5.5	Quantitative EPR (117 – 196 K) spectra giving $2J$ = 157 ± 7 K (Fig. S26); quench with Cp^*_2Fe, ^1H NMR and ESI MS (Figs.S27&S28).	0.29, 94%

Diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ generated using $[NO]^+[SbF_6]^-$ in DBP: sample label, HZ1164. To the starting material **1**-D_2 (0.34 mg, 0.38 μmol, CS0188 & CS0192) in a custom-made Schlenk vessel with 4-mm EPR tube,[S2] evacuated on vacuum line at room temperature for several days, distilled dibutyl phthalate (DBP, ~100 μL) was added under argon flow to obtain a yellow solution. Subsequently, the solution was cooled to −30 ºC by ethanol-liquid nitrogen bath, and the oxidant, $NOSbF_6$, in distilled DBP (60 μL, 3.8 equiv, 6.4 mg/1.0 mL) was added under flow of argon. The reaction mixture was mixed with stir bar at −30 ºC and evacuated until vacuum build up inside the vessel (pressure = 0.9 mTorr). During this process the color of the reaction mixture changed from yellow to dark blue-purple. EPR spectrum was obtained at 243 K (label: HZ1164r1), showing diradical with a significant admixture of monoradical.

Subsequently, an additional amount of oxidant was added (50 μL, 3.2 equiv, 6.4 mg/1.0 mL) under flow of argon at −30 ºC. As before, the reaction mixture was mixed with stir bar at −30 ºC and evacuated until vacuum build up inside the vessel (pressure = 0.9 mTorr). EPR spectra were obtained at 243 K and 295 K (EPR labels: HZ1164r2-r8), showing still a small admixture of monoradical. Then, the reaction mixture was evacuated for 30 min at rt, and subsequently EPR spectra were obtained (EPR label: HZ1164r9 and r10). The the reaction mixture was evacuated again for 10 min at rt, and then EPR spectra at 243 K and 140 K were obtained (EPR label: HZ1164r11-r15), showing absence of monoradical. The dark blue-purple solution was stored in liquid nitrogen.

Subsequently, the EPR tube was attached to the vacuum line. The reaction mixture was diluted by distilled dibutyl phthalate (200 μL). The dark blue mixture was mixed at –20 ºC thoroughly until homogeneous solution was obtained, and then evacuated to build up pressure of 0.9 mTorr inside the

vessel at –20 ºC. EPR spectra of the dark blue-purple solution (total height 6.20 cm, 0.816 mM) were obtained at 117 K, together with spectra for Tempone reference in DBP (1.005 mM) (EPR label: HZ1164r16-r40); the initial $\chi T = 0.872 \pm 0.004$ ($n = 6$) at 117 K was obtained. The dark blue solution was stored in liquid nitrogen.

Subsequently, quantitative EPR spectra (sample: HZ1164, 0.816 mM) at variable temperature were obtained in the 105 – 330 K range (Figure S12, top and bottom panels) using 1.005 mM TEMPONE in dibutyl phthalate as reference.

Subsequently, quantitative EPR spectra (sample: HZ1164, 0.816 mM) at room temperature, following annealing of the smaple on air at room temperature for 0 – 2 h were obtained (Figure S13).

For diradical dication (sample: HZ1164, 0.816 mM), EPR spectra were obtained at 117 K to re-check the spin concentration (EPR labels: CS291r1-r11). Using Tempone in DBP (0.975 mM) as reference, the spin concentration was 245% ($\chi T = 0.918 \pm 0.009$ ($n = 2$)). Subsequently, the solution was diluted to 0.301 mM with DBP under flow of argon. Then this solution was transferred to a custom-made Schlenk vessel with 2 mm UV cuvette under flow of argon. In another similar custom-made Schlenk vessel with 2 mm UV cuvette, DBP was prepared as reference. UV-vis-NIR spectra were obtained with these 2 cells (Figure S14). After finishing UV-vis-NIR experiments, diradical dication solution in UV cuvette was transferred back to a new 4 mm EPR tube under argon flow. Sample was frozen in the liquid nitrogen.

On the next day, the spin concentration of diradical dication solution was measured again (Figure S14). Using the same reference (tempone in DBP, 0.975 mM), the spin concentration was 237%, $\chi T = 0.891 \pm 0.016$ ($n = 2$), at 117 K (EPR labels: CS293r1-r9).

Finally, the EPR tube was attached to the vacuum line, the reaction was quenched by addition of bis(pentamethylcyclopentadienyl)iron(II) in DCM (1.34 mg, 10 eq). The color changed from blue-purple to yellow. The solution was transferred to a vial and evaporated by N_2, which was purified by column chromatography (regular silica gel, pentane/DCM, 5:1) in with exclusion of light, and then analytical TLC plate to obtain a yellow powder (0.29 mg, 85% recovery). ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: HZ1164 reduced by CS-plate) data of sample showed the starting material (Figure S15).

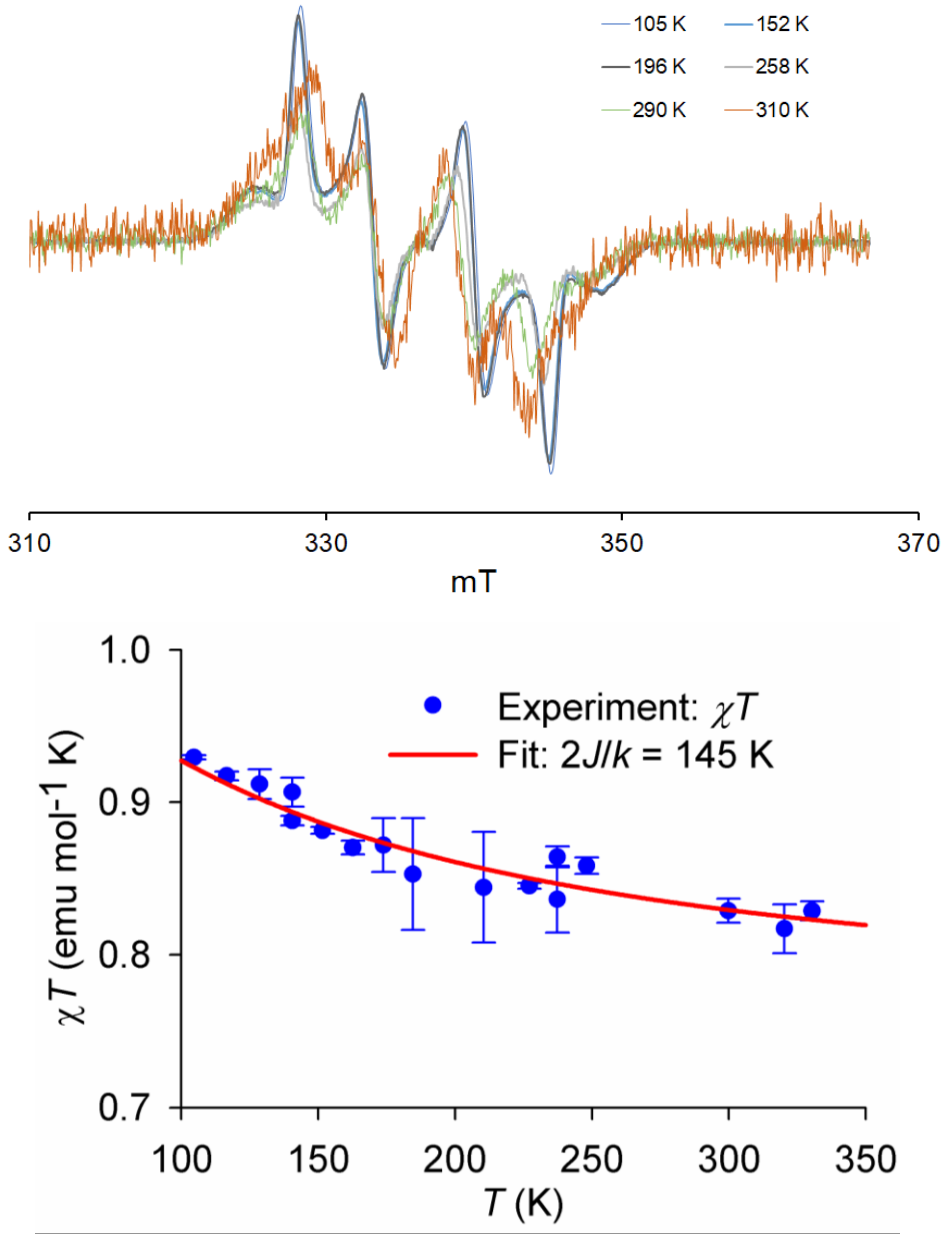


Fig. S12. Top panel: selected EPR spectra of 0.82 mM diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ (sample label: HZ1164) in DBP in the 105 – 310 K temperature range. Bottom panel (same graphic as in Figure 6, main text): quantitative EPR spectroscopy of 0.82 mM diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ in DBP (sample label: HZ1164) with 1.00 mM TEMPONE in DBP as a reference: experimental values of χT (mean ± SE), the product of paramagnetic susceptibility (χ) and T in the T = 105 – 330 K range; final numerical fit with no weighing and one variable parameter, $2J/k$ = 145 ± 4 K (mean ± SE). The raw average values of χT vs T were fit to the Bleaney–Bowers equation with two variable parameters, J/k = exchange coupling constant and N = weighing correction (parameter dependence = 0.989). Then, the value of N = 0.9695 was used to correct the experimental values of χT. Subsequently one-parameter (J/k) fit of corrected χT vs T to the Bleaney–Bowers equation gave J/k = 72.5 ± 2 K (mean ± SE).

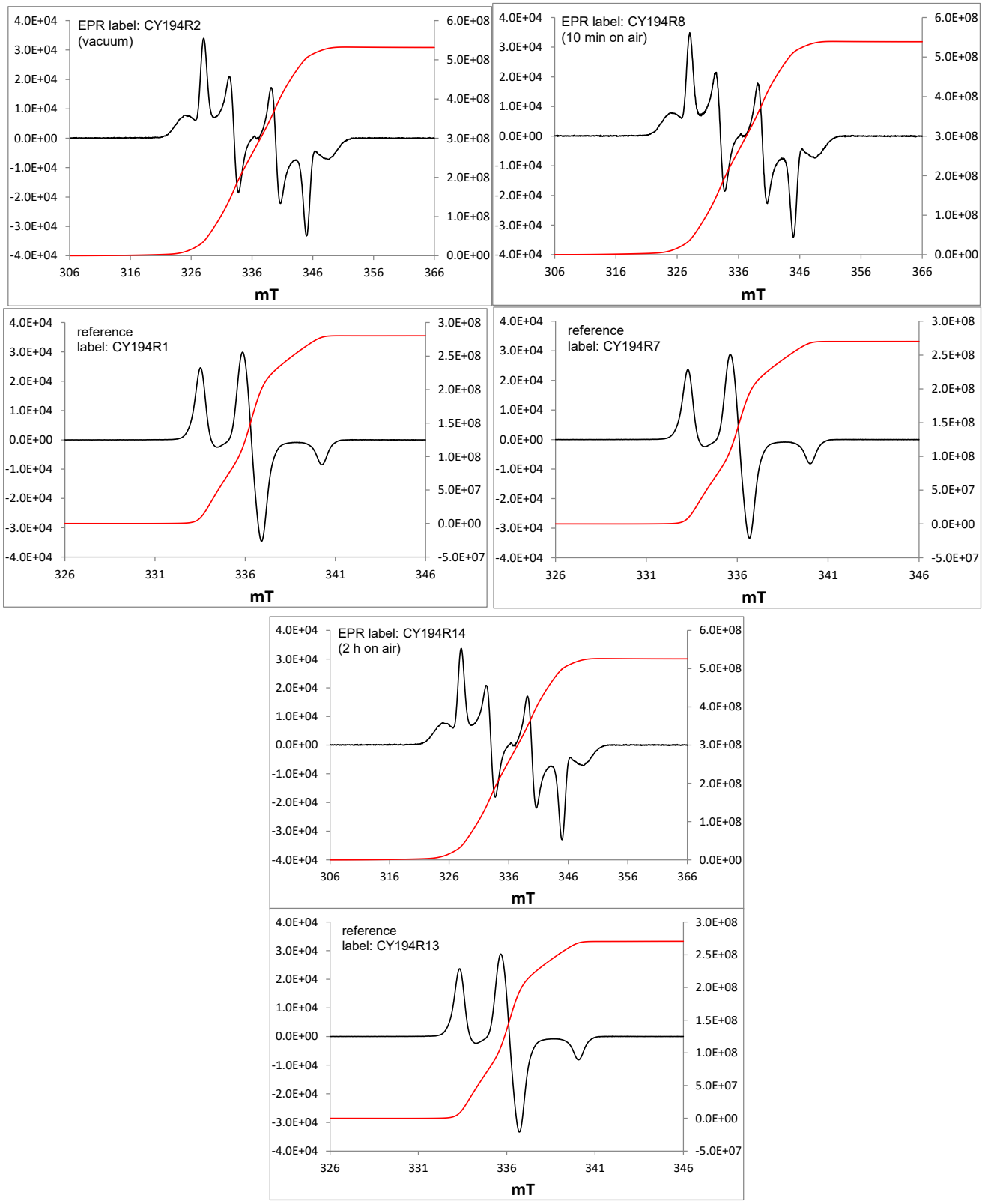


Fig. S13. EPR spectra of 0.82 mM diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ (sample label: HZ1164) and Tempone reference in DBP at 117 K, demonstrating stability of $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ in DBP, upon exposure to air for 2 h at room temperature.

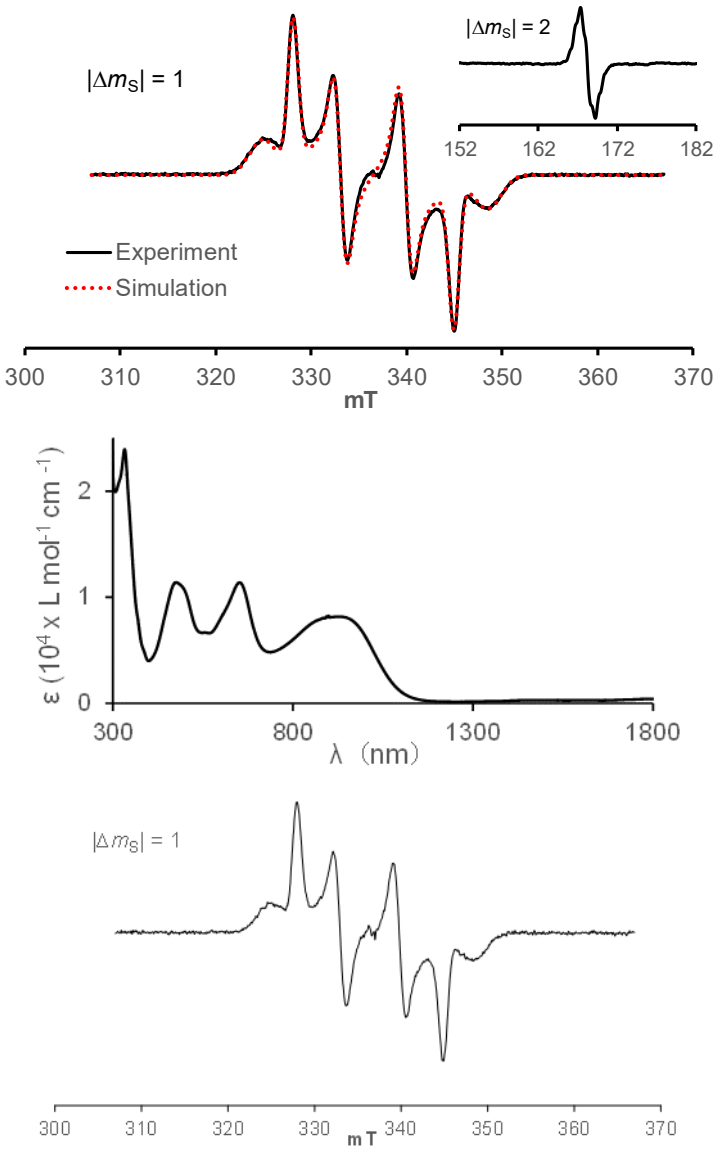


Fig. S14. Enlarged Figure 4 in the main text with additional details: EPR spectra at 117 K prior (top panel) and following (bottom panel) the UV-vis-NIR spectrum at room temperature. Top panel: EPR (ν = 9.4387 GHz, EPR label: CS291R4, sample label: HZ1164) spectrum (inset: the $|\Delta m_s| = 2$ transition) with simulation, shown in the main text (Figure 5), obtained during oxidation of **1**-D_2 with $[NO]^+[SbF_6]^-$ in dibutyl phthalate (DBP) showing 0.82 mM diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$. EPR spin counting at T = 117 K (vs. Tempone in DBP), prior to UV-vis-NIR spectrum, showed $\chi T \approx 0.92$ emu mol^{-1} K. Spectral simulation of the $|\Delta m_s| = 1$ region: $|D/hc| = 1.11 \times 10^{-2}$ cm^{-1}, $|E/hc| = 1.56 \times 10^{-3}$ cm^{-1}, $|A_{zz}/hc|/2 = 7.3 \times 10^{-4}$ cm^{-1}, $g_{xx} = 2.0036$, $g_{yy} = 2.0035$, $g_{zz} = 2.0025$; H-strain (MHz): $H_x = 30.84$, $H_y = 28.07$, $H_z = 11.78$; g-strain: $g_x = 0.0019$, $g_y = 0.0021$, $g_z = 0.0020$; D-strain (MHz): $D = 2.421$, $E = 0.387$. Middle panel: repeat UV-vis-NIR spectrum of the identical sample of diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ (sample label: HZ1164) after dilution of its solution with DBP to 0.30 mM. Bottom panel: EPR spectrum (ν = 9.4355 GHz, EPR label: CS293R1, sample label: HZ1164)) of 0.30 mM $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ in DBP following the UV-vis-NIR spectrum. EPR spin counting at T = 117 K showed $\chi T \approx 0.89$ emu mol^{-1} K.

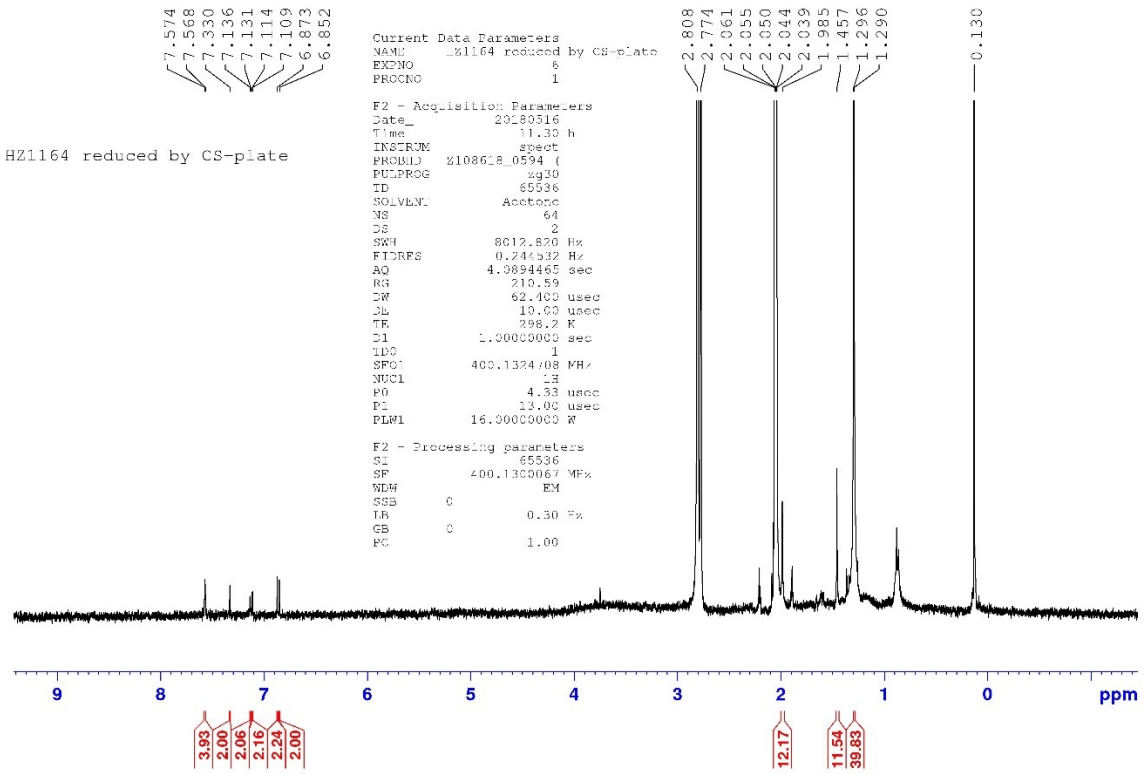


Fig. S15. ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: HZ1164 reduced by CS-plate) of the sample obtained after quench of diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ in DBP, using Cp^*_2Fe, and purification. The spectrum is identical to that of starting material **1**-D_2.

Diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ generated using $[NO]^+[SbF_6]^-$ in DBP: sample label, HZ1015. To the starting material **1**-D_2 (0.25 mg, 0.28 μmol, PB4_68B-tl) in custom-made Schlenk vessel with 4-mm EPR tube,[S2] evacuated on vacuum line at room temperature for several days, distilled dibutyl phthalate (DBP, ~10 μL) was added under argon flow to get a yellow solution. Subsequently, the solution was cooled to −30 ºC by ethanol-liquid nitrogen bath, and the oxidant $NOSbF_6$ in distilled DBP (30 μL, 3 equiv, 13.6 mg/1.8 mL) was added under flow of argon. The reaction mixture was mixed with stir bar at −30 ºC and evacuated until vacuum build up inside the vessel (pressure = 0.9 mTorr). During this process the color of the reaction mixture changed from yellow to green and finally dark blue-purple. EPR spectra were obtained at 240 K and 129 K (label: HZ1015r1 and r5 at 240 K; HZ1015r4 and r6 at 129 K). The dark blue solution was stored in liquid nitrogen.

Subsequently, the EPR tube was attached to the vacuum line, more oxidant was added under argon flow (16 μL, 1.6 eq), mixed with stir bar at −30 °C and evacuated until vacuum build up inside the vessel (pressure = 0.9 mTorr). EPR spectra were obtained at 240 K and 129 K (label: HZ1015r7 at 240 K; HZ1015r8 at 129 K), showing pure diradical.

Subsequently, the EPR tube was attached to the vacuum line. The reaction mixture was diluted by distilled dibutyl phthalate (350 μL). The dark blue mixture was mixed at –30 °C for 2 h until get homogeneous solution (very difficult to mix because the solvent is viscous), and then evacuated to build up pressure of 0.9 mTorr inside the vessel. EPR spectra of the dark blue-purple solution (total height 6.65 cm, 0.559 mM) were obtained at 240 K and 129 K (label: HZ1015r9 at 240 K; HZ1015r12 at 129 K). The dark blue-purple solution was stored in liquid nitrogen.

Subsequently, EPR spectra at different power levels were obtained at 117 K (label: HZ1015r21-r42) using TEMPONE in dibutyl phthalate as reference (conc.=5.081 mM, label: HZ1015r43-r64) (Figure S5). Magnetic susceptibility was determined at 117 K, using EPR spin counting (label: HZ1015r65-r66, r69-r70, r73-r74, r77-r78, r81-r82, r85-r86) employing TEMPONE in dibutyl phthalate as reference (conc.=5.081 mM, label: HZ1015r67-r68, r71-r72, r75-r76, r79-r80, r83-r84, r87-r88). The dark blue-purple solution was stored in liquid nitrogen.

Subsequently, EPR spectra at variable temperature were obtained at 105 - 295 K (Figure S16, top and bottom panels) (label: HZ1015r93-r94, r97-r98, r101-r102 at 295 K; HZ1015r106-r107, r110-r111, r114-r115 at 279 K; HZ1015r118-r119, r122-r123, r126-r127 at 258 K; HZ1015r130-r131, r134-r135, r138-r139 at 237 K; HZ1015r142-r143, r146-r147, r150-r151 at 216 K; HZ1015r154-r155, r158-r159, r162-r163 at 196 K; HZ1015r178-r179, r182-r183, r186-r187 at 174 K; HZ1015r190-r191, r194-r195, r198-r199 at 152 K; HZ1015r202-r203, r206-r207, r210-r211 at 141 K; HZ1015r214-r215, r218-r219, r222-r223 at 129 K; HZ1015r226-r227, r230-r231, r234-r235 at 117 K; HZ1015r238-r239, r242-r243, r246-r247 at 105 K) using TEMPONE in dibutyl phthalate as reference (conc.=5.081 mM, label: HZ1015r95-r96, r99-r100, r103-r104 at 295 K; HZ1015r108-r109, r112-r113, r116-r117 at 279 K; HZ1015r120-r121, r124-r125, r128-r129 at 258 K; HZ1015r132-r133, r136-r137, r140-r141 at 237 K; HZ1015r144-r145, r148-r149, r152-r153 at 216 K; HZ1015r156-r157, r160-r161, r164-r165 at 196 K;

HZ1015r180-r181, r184-r185, r188-r189 at 174 K; HZ1015r192-r193, r196-r197, r200-r201 at 152 K; HZ1015r204-r205, r208-r209, r212-r213 at 141 K; HZ1015r216-r217, r220-r221, r224-r225 at 129 K; HZ1015r228-r229, r232-r233, r236-r237 at 117 K; HZ1015r240-r241, r244-r245, r248-r249 at 105 K). The dark blue-purple solution was stored in liquid nitrogen. Subsequently, the sample of was consecutively annealed at 340 K for 0, 10, 30, 60, 120 min (total time). The EPR was taken at 295 K after each annealing (label: HZ1015r265, r267, r269, r271, r273) using TEMPONE in dibutyl phthalate as reference (conc.=5.081 mM, label: HZ1015r266, r268, r270, r272, r274) (Figure S17). The dark blue-purple solution was stored in liquid nitrogen. Subsequently, EPR spectra at higher temperature were obtained, 295 K to 340 K (label: HZ1015r275-r276, r279-r280, r283-r284 at 295 K; HZ1015r287-r288, r291-r292, r295-r296 at 305 K; HZ1015r299-r300, r303-r304, r307-r308 at 320 K; HZ1015r311-r312 at 340 K) using TEMPONE in dibutyl phthalate as reference (conc.=5.081 mM, label: HZ1015r277-r278, r281-r282, r285-r286 at 295 K; HZ1015r289-r290, r293-r294, r297-r298 at 305 K; HZ1015r301-r302, r305-r306, r309-r310 at 320 K). The dark blue-purple solution was stored in liquid nitrogen.

Subsequently, the dark blue solution was transferred to customed Schlenk vessel with UV-vis-NIR cuvette (2-mm path-length) under argon flow. UV-vis-NIR spectra were obtained (label: HZ1015UV7, HZ1015UV8, HZ1015UV9, HZ1015UV10, HZ1015UV11). Then the dark blue-purple solution was transferred back to a clean customed Schlenk vessel with 4-mm EPR tube. EPR spectra were obtained at 129 K (label: HZ1015r330-r331, r334-r335, r338-r339, r342-r343, r346-r347) using TEMPONE in dibutyl phthalate as reference (conc. = 5.081 mM, label: HZ1015332-r333, r336-r337, r340-r341, r344-r345, r348-r349) (Fig. S18).

Finally, the EPR tube was attached to the vacuum line, the reaction was quenched by addition of bis(pentamethylcyclopentadienyl)iron(II) in DCM (0.92 mg, 10 eq). The color changed from dark blue-purple to yellow. The solution was transferred to a vial and evaporated by N_2 to give HZ1015crude, which was purified by column chromatography (regular silica gel, pentane/DCM, 5:1) without light to get a yellow powder (0.24 mg (96%), HZ1015COL). ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: HZ1015COL-400) and ESI-MS (0.1% of trifluoroacetic acid in dichloromethane, label: HZ1015COL) data of the sample showed the starting material **1**-D_2 (Figs. S19 and S20).

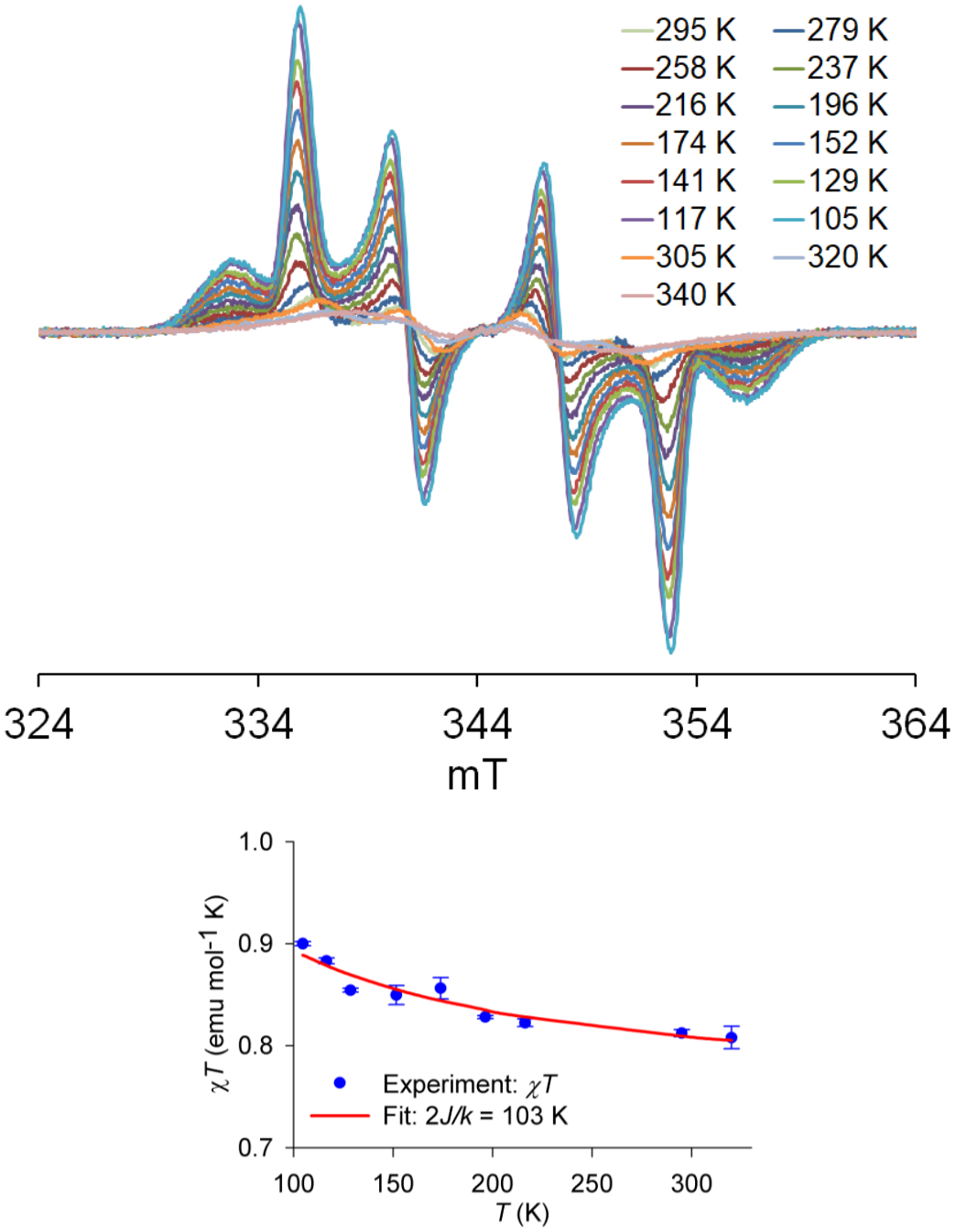


Fig. S16. Top panel: EPR spectra of 0.56 mM diradical dication $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ (sample label: HZ1015) in DBP in the 105 – 340 K temperature range (EPR labels: HZ1015r93, r106, r118, r130, r142, r154, r178, r190, r202, r214, r226, r238, r287, r299, r311). Bottom panel: repeat quantitative EPR spectroscopy of diradical dication $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ in DBP (sample label: HZ1015) with TEMPONE in DBP as a reference: experimental values of χT (mean ± SE), the product of paramagnetic susceptibility (χ) and T in the T = 105 – 320 K range and numerical two-parameter fit with the variable parameters, $2J/k$ = 103 ± 21 K and N = 0.8403 ± 0.017 (mean ± SE), and parameter dependence of 0.963. After scaling χT with N = 0.8403, one-parameter fit gave $2J/k$ = 103 ± 4 K.

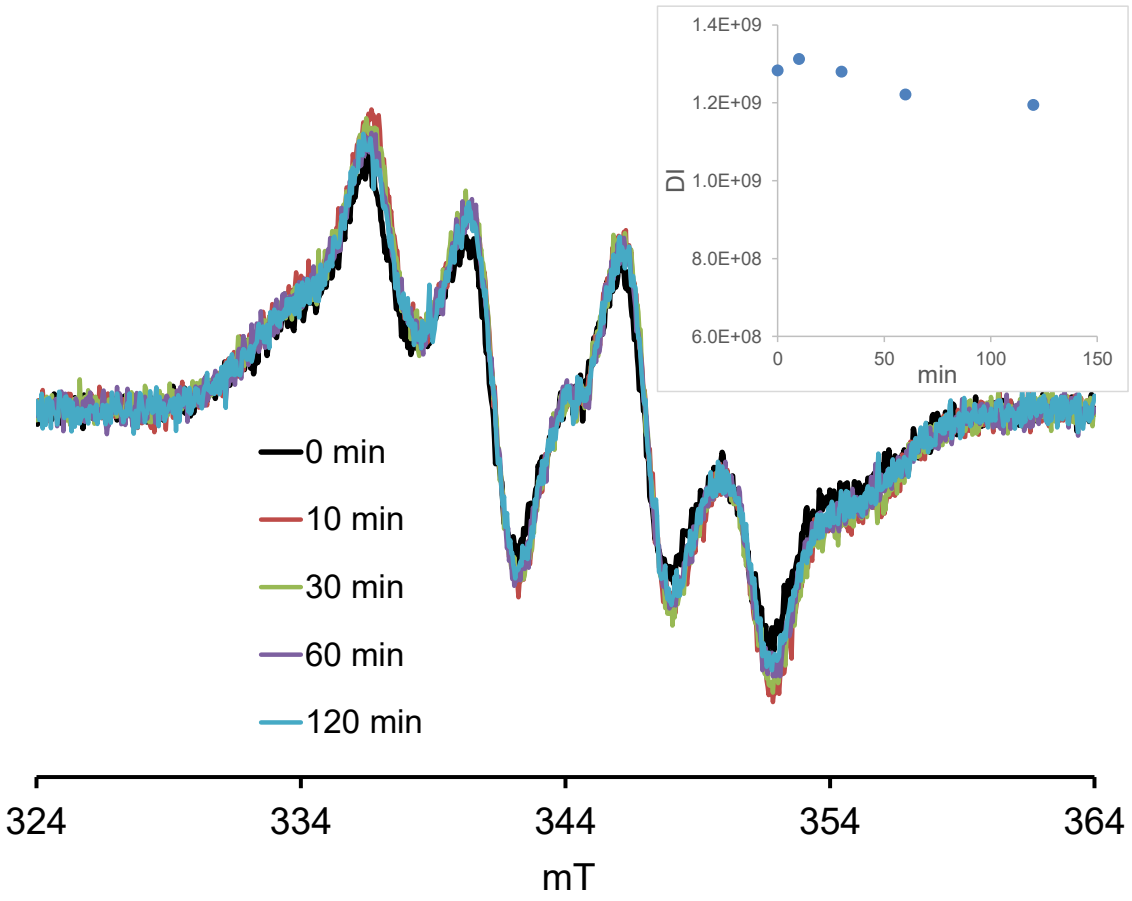


Fig. S17. EPR spectra of 0.56 mM diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ (sample label: HZ1015) in DBP at 295 K, including Tempone reference, following annealing at 340 K for 10 – 120 min (total time); EPR labels: HZ1015r265, r267, r269, r271, and r273. Inset plot shows dependence of double integrated spectral intensity vs time (at 340 K).

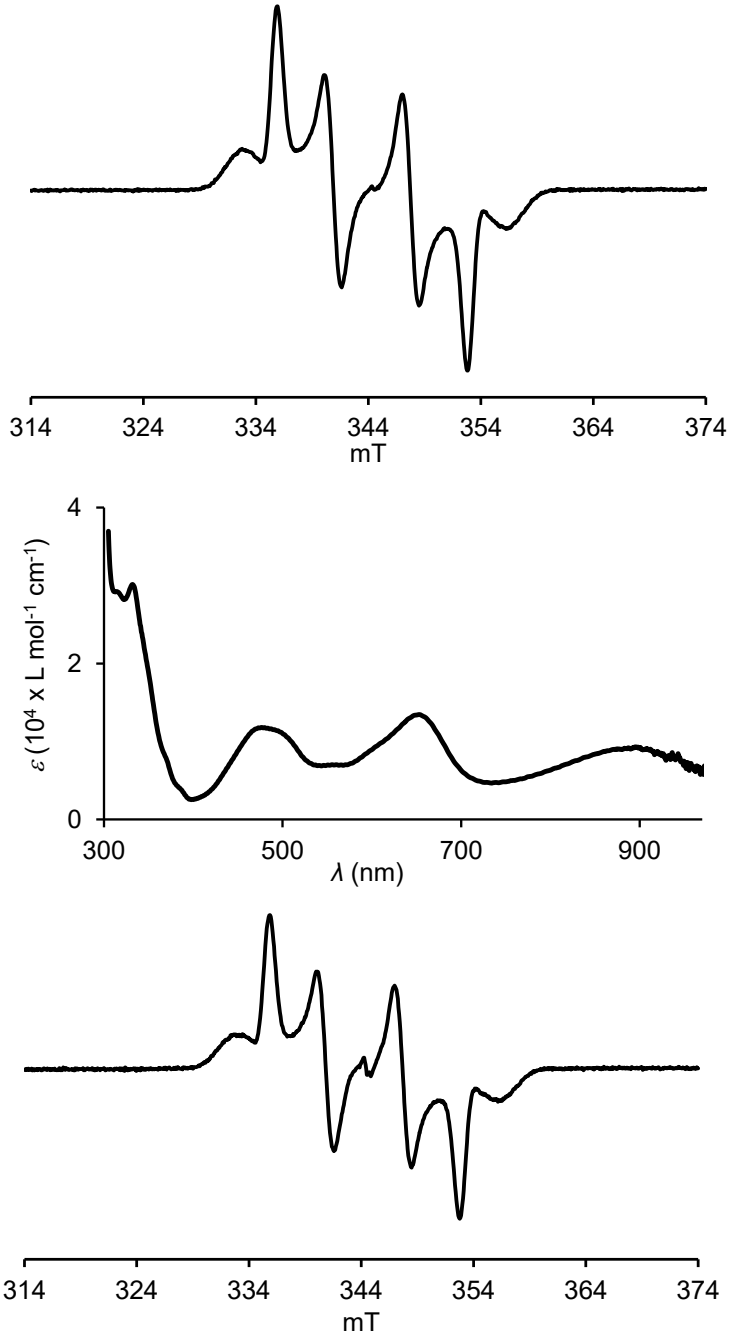


Fig. S18. EPR (X-band) and UV-vis-NIR spectra of diradical dication $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ (sample label: HZ1015) obtained during oxidation of **1**-D_2 with $[NO]^+[SbF_6]^-$ in dibutyl phthalate (DBP). Top panel: EPR spectrum of 0.56 mM $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ in DBP at 117 K prior to UV-vis-NIR spectrum (EPR label: HZ1015r264). Middle panel: UV-vis-NIR spectrum of 0.56 mM $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ in DBP at room temperature (UV-vis-NIR label: HZ1015uv7-uv11): bands at λ_{max} = 332, 477, 653, and 929 nm have the following extinction coefficients: $\varepsilon_{332} = 3.0 \times 10^4$, $\varepsilon_{477} = 1.2 \times 10^4$, $\varepsilon_{653} = 1.3 \times 10^4$, and $\varepsilon_{929} = 8.3 \times 10^3$ L mol^{-1} cm^{-1}. Bottom panel: EPR spectrum of 0.56 mM $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ in DBP at 129 K following the UV-vis-NIR spectrum (EPR label: HZ1015r329).

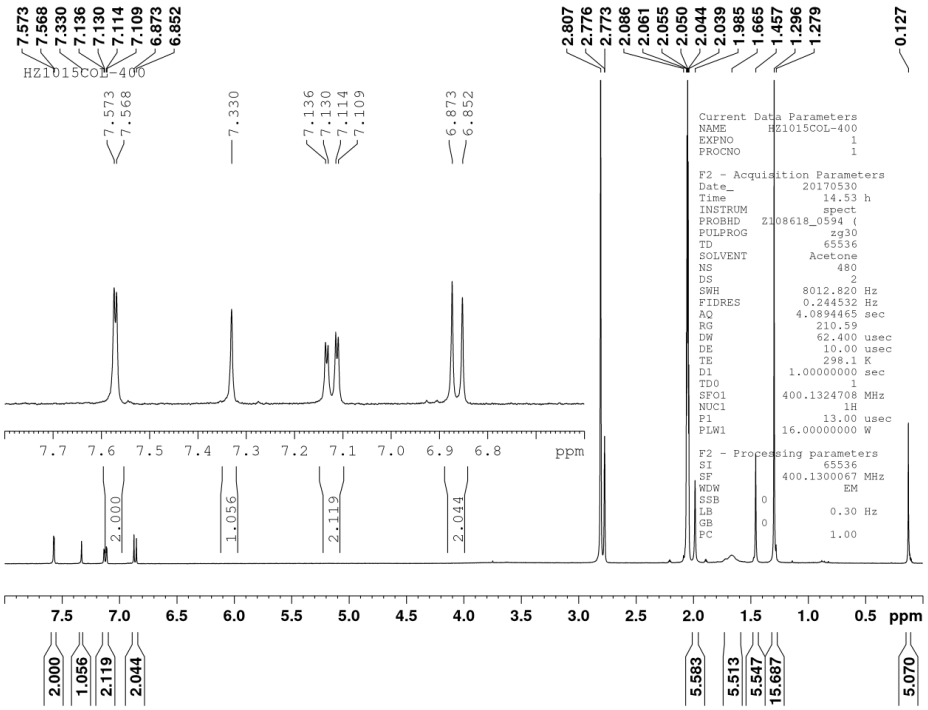


Fig. S19. ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: HZ1015COL-400) of the sample obtained after quench of diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ in DBP, using Cp^*_2Fe, and purification. The spectrum is identical to that of starting material **1**-D_2.

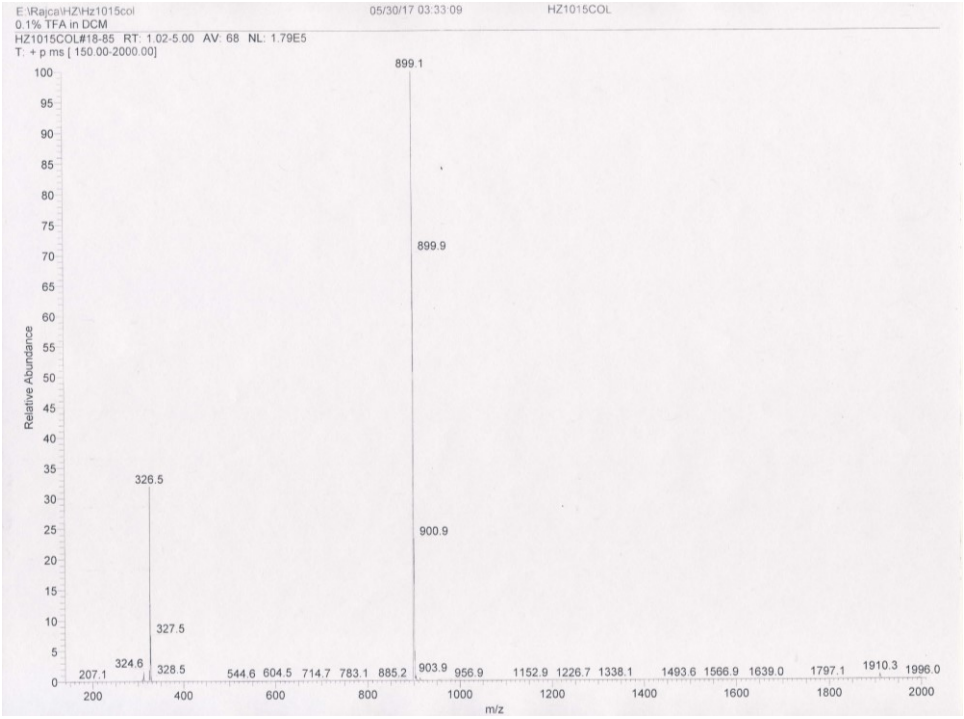


Fig. S20. LRMS spectrum (0.1% TFA in DCM, label: HZ1015COL) of the sample obtained after quench of diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ in DBP and purification. The spectrum is consistent with the starting material **1**-D_2.

Diradical dication $1^{2\bullet2+}$ $2SbF_6^-$ generated using $[NO]^+[SbF_6]^-$ in DBP/DCM/MeCN: sample label, HZ1001. To the starting material **1**-D_2 (0.29 mg, 0.32 μmol, PB4_68B-tl) in a custom-made Schlenk vessel with 4-mm EPR tube,[S2] evacuated on vacuum line at room temperature overnight, anhydrous dichloromethane (~10 μL) was added by vacuum transfer to get a yellow solution. Subsequently, the solution was cooled to −40 ºC by ethanol-liquid nitrogen bath, and the oxidant $NOSbF_6$ in anhydrous CH_3CN (24 μL, 2.2 eq, 4.7 mg/0.6 mL) was added under flow of argon. The reaction mixture was mixed with stir bar at −40 ºC and degassed until vacuum build up in the vessel; the color of the reaction mixture changed from yellow to dark-purple blue. EPR spectra were obtained at 230 K and 129 K (label: HZ1001r1-r6 at 230 K, r8-r9 at 129 K) using TEMPONE in DCM as reference (conc.=1.2043 mM, label: HZ1001r11-r12 at 129 K); the spectra showed the presence of monoradical only. The spin concentration determined at 129 K was about 65%. The dark blue-purple solution was stored in liquid nitrogen.

Subsequently, the EPR tube was attached to the vacuum line, more $NOSbF_6$ in CH_3CN (22 μL, 2 eq) and distilled dibutyl phthalate (140 μL) were added under argon flow, the solution was mixed with stir bar at −30 ºC and degassed until vacuum build up in the vessel. EPR spectra at different power levels were obtained at 129 K (label: HZ1001r16-r23, r30-r33) using TEMPONE in DCM as reference (conc.=1.2043 mM, label: HZ1001r24-r29). The samples possessed spin concentration of about 120 – 130% and the spectra showed presence of triplet diradical with an significant admixture of $S = ½$ monoradical. The dark blue solution was stored in liquid nitrogen.

Subsequently, the EPR tube was attached to the vacuum line, the reaction mixture was diluted by distilled dibutyl phthalate (250 μL). The dark blue mixture was mixed at –30 ºC until homogeneous solution was obtained, and then evacuated well until vacuum build up in the vessel. EPR spectra at 240 K were obtained (label: HZ1001r34-r35). EPR spectra at different power levels were obtained at 129 K (label: HZ1001r38-r43) using TEMPONE in dibutyl phthalate as reference (conc.=1.557 mM, label: HZ1001r44-r49). The spectra showed somewhat decreased amount of monoradical and increased spin concentration of about 150 – 160%. The dark blue solution was stored in liquid nitrogen.

Subsequently, the EPR tube was attached to the vacuum line, third portion of $NOSbF_6$ in CH_3CN (44 μL, 4 eq) was added under argon flow, the solution was mixed with stir bar at −30 ºC and degassed

well until vacuum build up in the vessel (total height 7.0 cm, 0.6104 mM). EPR spectra at 240 K were obtained (label: HZ1001r51-r52). EPR spectra at different power levels were obtained at 129 K (label: HZ1001r55-r60) using TEMPONE in dibutyl phthalate as reference (conc.=1.557 mM, label: HZ1001r61-r66) (Figure S21); spin concentration is more than 200%. The dark blue-purple solution was stored in liquid nitrogen. Subsequently, EPR spectra with high S/N at 112 and 117 K (HZ1001r67-r72) were obtained (Fig. S21).

Attempts to obtain quantitative EPR data at variable temperaures (105 K to 300 K) failed: (label: HZ1001r73-r74, r77-r78, r81-r82 at 105 K; HZ1001r85-r86, r89-r90, r93-r94 at 112 K; HZ1001r97-r98, r101-r102, r105-r106 at 117 K; HZ1001r109-r110, r113-r114, r117-r118 at 123 K; HZ1001r121-r122, r125-r126, r129-r130 at 129 K; HZ1001r133-r134, r137-r138, r141-r142 at 141 K; HZ1001r145-r146, r149-r150, r153-r154 at 159 K; HZ1001r157-r158, r161-r162, r165-r166 at 174 K; HZ1001r169-r170, r173-r174, r177-r178 at 196 K; HZ1001r181-r182, r185-r186, r189-r190 at 227 K; HZ1001r205-r207, r210-r211, r214-r215 at 258 K; HZ1001r218-r219 at 300 K) using TEMPONE in dibutyl phthalate as reference (conc.=1.5567 mM, label: HZ1001r75-r76, r79-r80, r83-r84 at 105 K; HZ1001r87-r88, r91-r92, r95-r96 at 112 K; HZ1001r99-r100, r103-r104, r107-r108 at 117 K; HZ1001r111-r112, r115-r116, r119-r120 at 123 K; HZ1001r123-r124, r127-r128, r131-r132 at 129 K; HZ1001r135-r136, r139-r140, r143-r144 at 141 K; HZ1001r147-r148, r151-r152, r155-r156 at 159 K; HZ1001r159-r160, r163-r164, r167-r168 at 174 K; HZ1001r171-r172, r175-r176, r179-r180 at 196 K; HZ1001r183-r184, r187-r188, r191-r192 at 227 K; HZ1001r208-r209, r212-r213, r216-r217 at 258 K; HZ1001r220-r221 at 300 K). The data were not useful because of drop-off in Q-values at higher temperatures for the sample of diradical dication, caused most likely by residual DCM/MeCN present in DBP; e.g., while at $T < 160$ K, Q-values for the sampel and for Tempone reference (in pure DBP) were about the same ($Q = 3200 \pm 100$ in a double mode cavity), at $T = 227$ K, Q = 1400 and 3100 were measured for the sample and for the reference. Consequently, χT values at near 300 K were by a factor of 3 – 4 smaller than those at near 100 K, i.e., the excessive drop-off at higher temperatures was an artefact due to the Q-values. The dark blue-purple solution was stored in liquid nitrogen.

Finally, the EPR tube was attached to the vacuum line, the reaction was quenched by addition of bis(pentamethylcyclopentadienyl)iron(II) in DCM (1.78 mg, 17 eq). The color changed from dark blue-purple to yellow. The solution was transferred to a vial and evaporated by N_2 gas to give HZ1001crude, which was purified by column chromatography (regular silica gel, pentane/DCM, 5:1) with exclusion of light, to obtain a yellow powder (0.24 mg, HZ1001COL). ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: HZ1001COL-400) and ESI-MS (0.1% of trifluoroacetic acid in dichloromethane, label: HZ1001COL) data of the sample showed the starting material **1**-D_2 (Figs. S22 and S23).

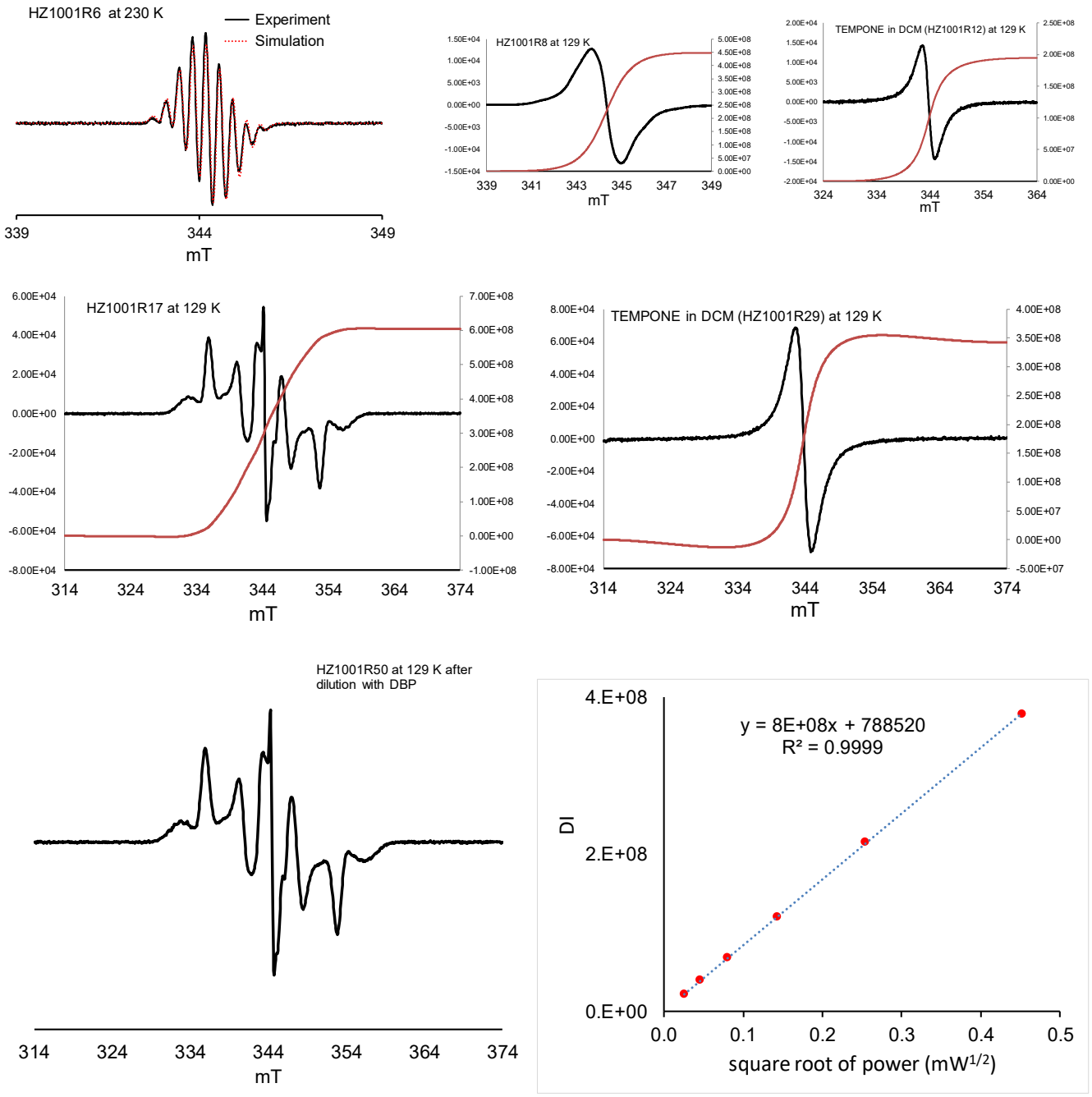
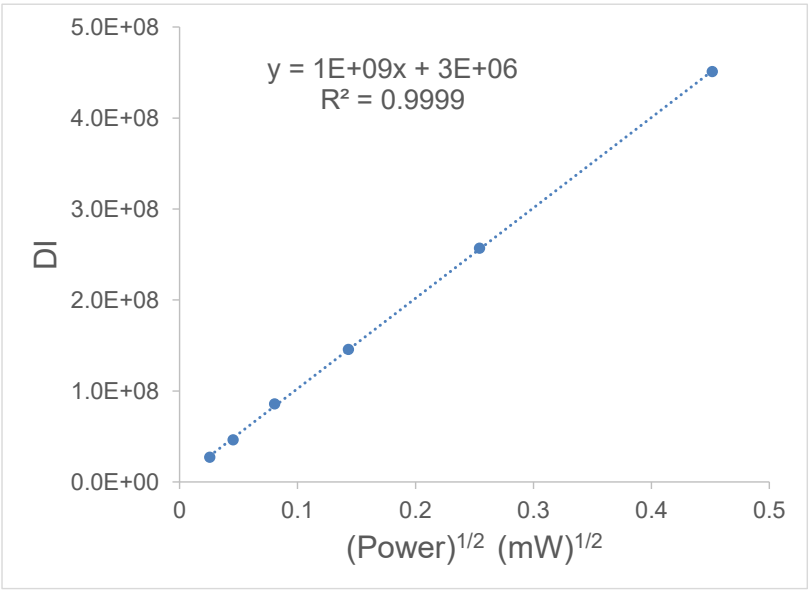


Fig. S21. EPR spectroscopic follow up of oxidation of **1**-D_2 in DCM/MeCN/DBP. Top panel: EPR spectra in DCM/MeCN at 230 and 129 K after initial addition of $NOSbF_6$ (2.2 equiv) in MeCN; spin concentration at 129 K is 65%; ; simulation (Garlic, EasySpin, rmsd = 1.110) for spectrum at 230 K: $A(^{14}N)$ = 10.02 MHz, g = 2.0029, line-width = 0.216 mT (Gaussian) and 0.038 mT (Lorentzian). Middle panel: the spectra in DCM/MeCN/DBP at 129 K after the second addition of $NOSbF_6$ (2 equiv) in MeCN; spin concentration at 129 K is 120 – 130 %. Bottom panel: the spectra DCM/MeCN/DBP at 129 K after dilution with DBP: spin concentration at 129 K is 150 – 160 %, the plot of EPR double integrated signal intensity (DI) versus the square root of microwave power (MW attn. 30 – 55 dB) in DBP/DCM/MeCN at 129 K for samples after dilution with DBP. **Fig. S21 is continued on the next page.**



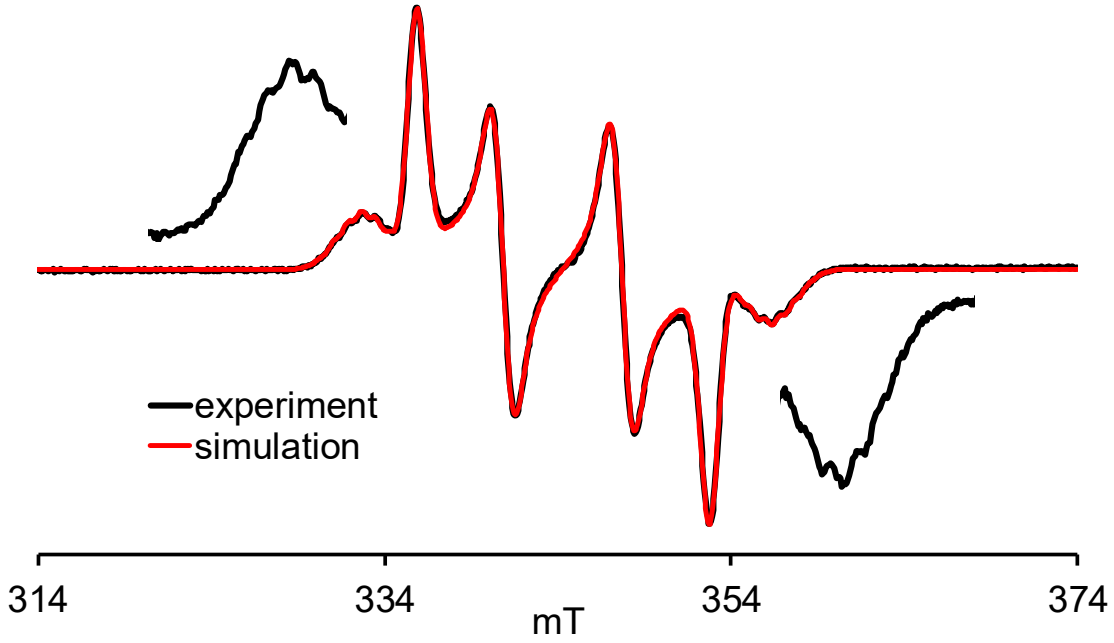


Fig. S21 (contd.). EPR spectra at following 3rd addition of $NOSbF_6$ (2.2 equiv) in MeCN; spin concentration is 200+%. Top panel: plot of EPR double integrated signal intensity (DI) versus the square root of microwave power in DBP/DCM/MeCN at 129 K. Microwave power attenuation ranges for 0.61 mM diradical dication (sample label: HZ1001), 30 – 55 dB (EPR labels: HZ1001r55-r60). Bottom panel: EPR (ν = 9.6532 GHz, 64 scans, EPR label: HZ1001r67, sample label: HZ1001) spectrum (insets: expansions of the *z*-lines) with simulation, obtained during oxidation of **1**-D_2 with $[NO]^+[SbF_6]^-$ in DBP/DCM/MeCN showing 0.61 mM diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ at 112 K. Spectral simulation, obtained using EasySpin, of the $|\Delta m_s| = 1$ region: $|D/hc| = 1.107 \times 10^{-2}$ cm^{-1}, $|E/hc| = 1.566 \times 10^{-3}$ cm^{-1}, $|A_{zz}/hc|/2 = 7.3 \times 10^{-4}$ cm^{-1}, $g_{xx} = 2.0030$, $g_{yy} = 2.0030$, $g_{zz} = 2.0019$; line width, lwpp = 0.585 mT; *H*-strain (MHz): $H_x = 31.01$, $H_y = 28.19$, $H_z = 11.78$.

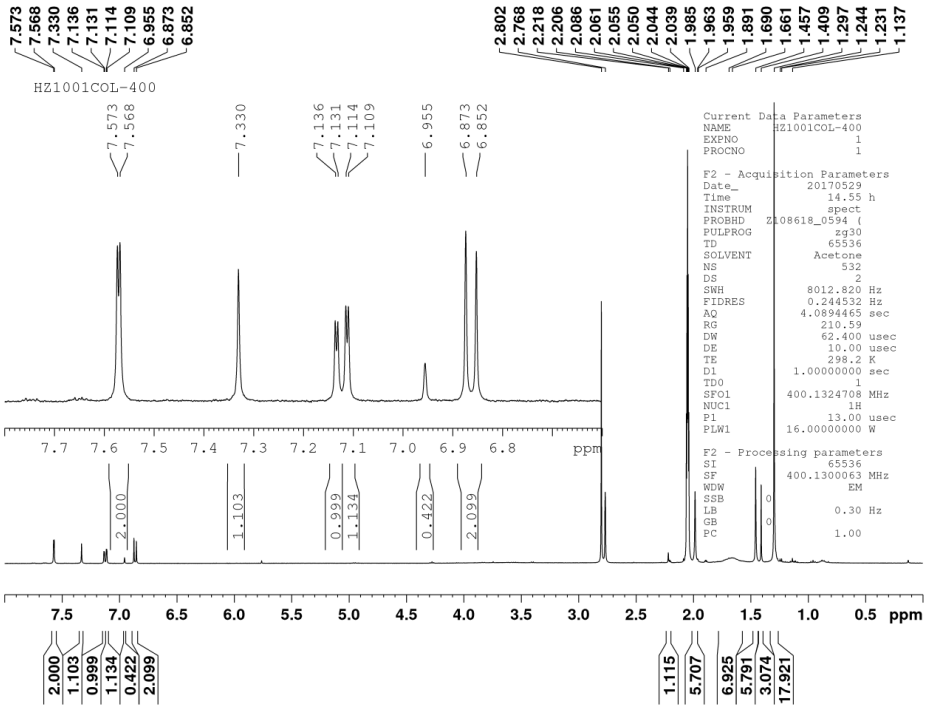


Fig. S22. ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: HZ1001COL-400) of the sample obtained after quench of diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ in DBP, using Cp^*_2Fe, and purification. The spectrum is identical to that of starting material **1**-D_2.

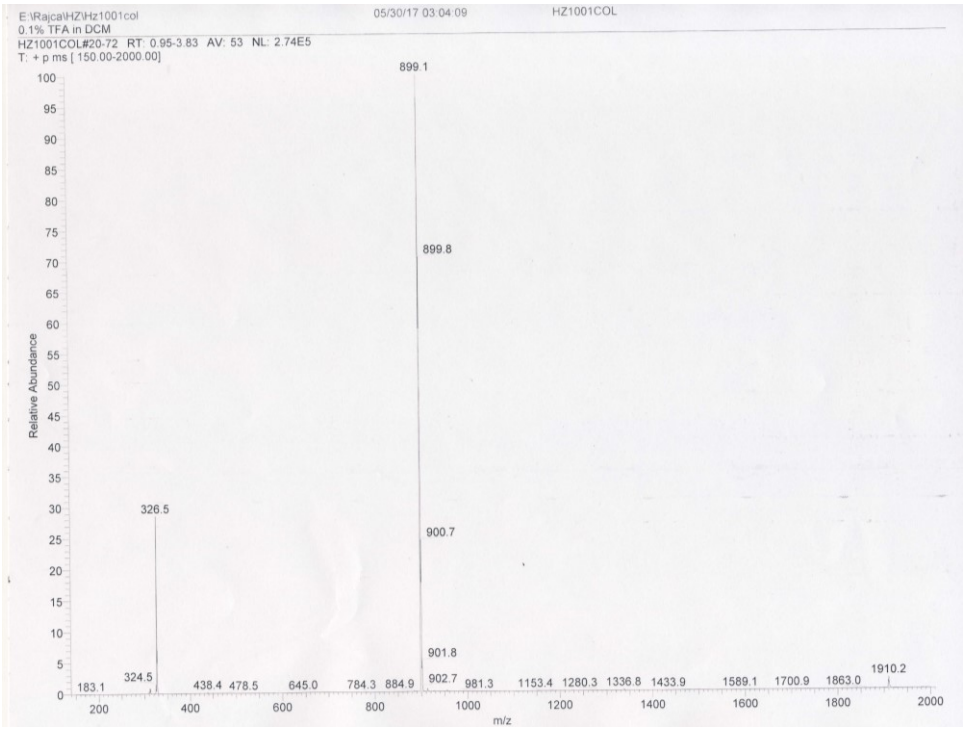


Fig. S23. LRMS spectrum (0.1% TFA in DCM, label: HZ1001COL) of the sample obtained after quench of diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ in DBP and purification. The spectrum is consistent with the starting material **1**-D_2.

Diradical dication $1^{2\bullet 2+}$ $2SbF_6^-$ generated using $[NO]^+[SbF_6]^-$ in DBP: sample label, CS332.

To the starting material **1**-D_2 (0.47 mg, 0.523 μmol, sample label: CS-3-2-25p) in a custom-made Schlenk vessel with 4-mm EPR tube,[S2] evacuated on vacuum line at room temperature for several days, distilled dibutyl phthalate (DBP, ~100 μL) was added under argon flow to get a yellow solution. Subsequently, the solution was cooled to −30° C by ethanol-liquid nitrogen bath, and the oxidant $NOSbF_6$ in distilled DBP (125 μL, 5.6 equiv, 11.8 mg/1.897 mL) was added under flow of argon. The reaction mixture was mixed with stir bar at −30°C and evacuated 2 hours until vacuum build up inside the vessel (pressure = 1.6 mTorr). During this process the color of the reaction mixture changed from yellow to dark blue. EPR spectra was obtained at 240 K (label:CS332R1). Subsequently, the EPR tube was attached to the vacuum line. The reaction mixture was diluted by distilled dibutyl phthalate (~200 μL). The dark blue mixture was mixed at –30 °C for 40 mins until get homogeneous solution (very difficult to mix because the solvent is viscous), and then evacuated to build up pressure of 1.6 mTorr inside the vessel. EPR spectra was obtained at 240 K (label: CS322R2). Then the dark blue mixture was mixed at RT for another 1 hour and EPR spectra was obtain at 240 K (label: CS322R3). The dark blue solution was stored in liquid nitrogen. Prior to air-stability measurements, EPR spectrum of 1.10 mM diradical dication was obtained at 105 K (Fig. S24).

Air-stability. Magnetic susceptibility, χT, was measured at 117 K by alternating measurements for the sample and for the reference (1.17 mM tempone in DBP) three times. Subsequently, the EPR sample tube was warmed up to room temperature and the tube was open to air for specified period of time (30 min – 12 h, with total time on air equal to 48 h). The solution of diradical dication was mixed with a stirbar, while the tube was open to air. Then, the tube was connected to a vaccum line and the solution was pumped for ca. 5 min, until attaining pressure of ca. 2 mTorr. Magnetic susceptibility was measured at 117 K as described above. This process was repeated for more than a dozen times (Fig. S25). The sample and reference tubes were stored in liquid nitrogen after every measurement.

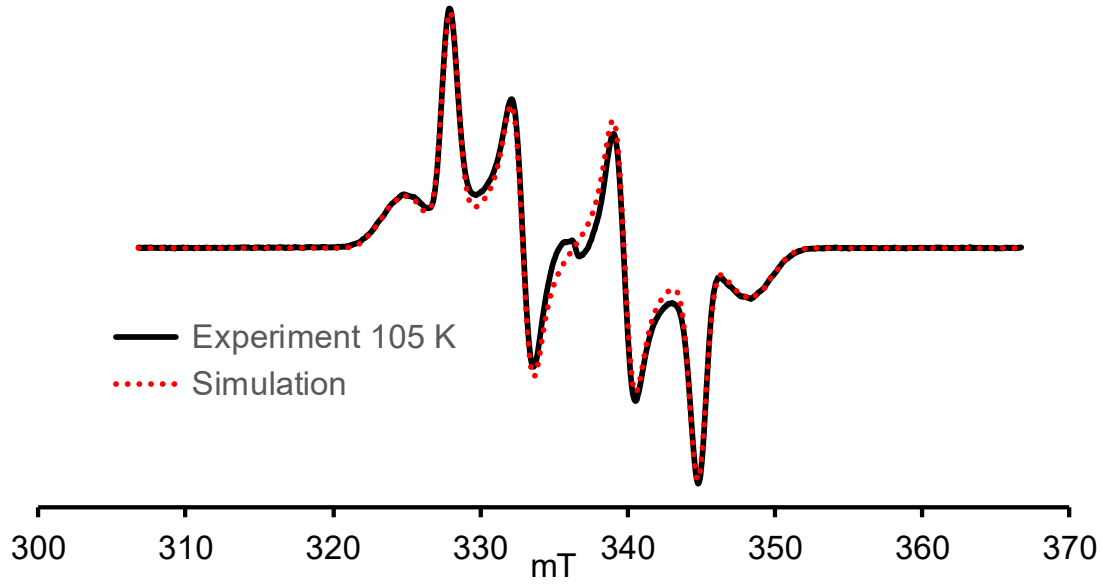


Fig. S24. EPR (ν = 9.4353 GHz, EPR label: CS349R1, sample label: CS332) spectrum of 1.10 mM diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ in DBP at 105 K (inset: the $|\Delta m_s| = 2$ transition) with simulation, prior to air stability measurements, obtained during oxidation of **1**-D_2 with $[NO]^+[SbF_6]^-$. EPR spin counting at T = 105 K (vs. Tempone in DBP) showed $\chi T \approx 0.90$ emu mol^{-1} K. Spectral simulation, obtained using EasySpin, of the $|\Delta m_s| = 1$ region: $|D/hc| = 1.107 \times 10^{-2}$ cm^{-1}, $|E/hc| = 1.556 \times 10^{-3}$ cm^{-1}, $|A_{zz}/hc|/2 = 7.4 \times 10^{-4}$ cm^{-1}, $g_{xx} = 2.0039$, $g_{yy} = 2.0039$, $g_{zz} = 2.0029$; H-strain (MHz): $H_x = 39.58$, $H_y = 36.53$, $H_z = 21.78$.

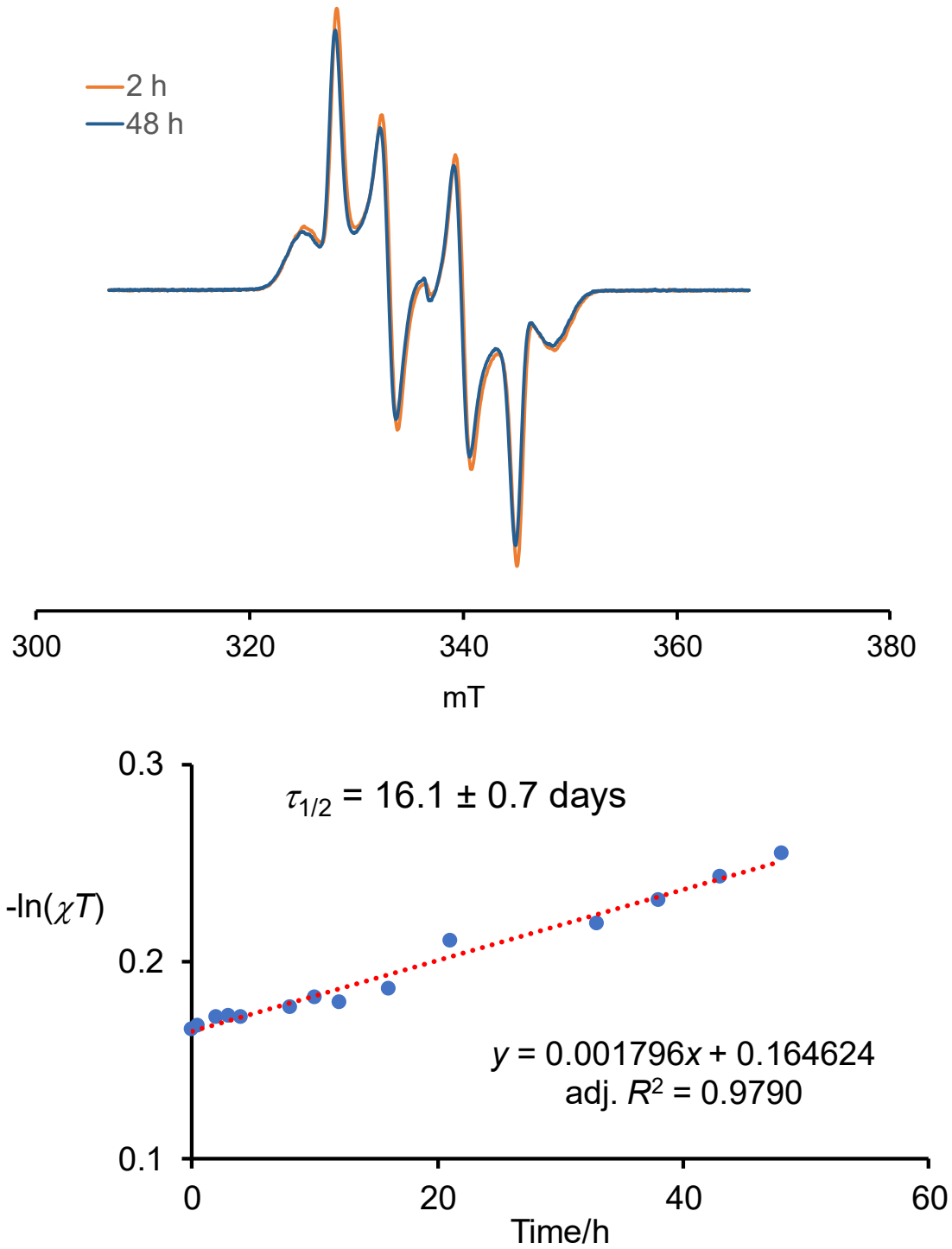


Fig. S25. Determination of half-life for diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ in DBP at ambient conditions by quantitative EPR spectroscopy (sample label: CS332). Top plot: examples of EPR spectra at 117 K after exposure of diradical dication to air at room temperature for 2 h and 48 h. Bottom plot: quantitative EPR spectroscopy of 1.10 mM diradical dication $\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ in DBP: plot of ln(χT) versus time (0 – 48 h), where time corresponds to exposure to ambient conditions and values of χT are measured at 117 K; first-order rate constant was k = 0.001696 ± 0.0000729 h^{-1} (mean ± SE).

Diradical dication $1^{2\bullet 2+}$ $2SbF_6^-$ generated using $[NO]^+[SbF_6]^-$ in DBP: sample label, CS374.

To the starting material **1**-D_2 (0.31 mg, 0.35 μmol, cs-3-2-25p) in custom-made Schlenk vessel with 4-mm EPR tube,[S2] evacuated on vacuum line at room temperature for several days, distilled dibutyl phthalate (DBP, ~100 μL) was added under argon flow to get a yellow solution. Subsequently, the solution was cooled to −30ºC by ethanol-liquid nitrogen bath, and the oxidant $NOSbF_6$ in distilled DBP (75 μL, 5.5 equiv, 6.819 mg/mL) was added under flow of argon. The reaction mixture was mixed with stir bar at −30 ºC and evacuated until vacuum build up inside the vessel (pressure = 1.9 mTorr). During this process the color of the reaction mixture changed from yellow to green and finally dark blue-purple. EPR spectra were obtained at 240 K (label:CS374R1). Subsequently, the EPR tube was attached to the vacuum line. The reaction mixture was diluted by distilled dibutyl phthalate (~300 μL). The dark blue mixture was mixed at –30 ºC for 1 h until get homogeneous solution (very difficult to mix because the solvent is viscous), and then evacuated to build up pressure of 1.9 mTorr inside the vessel. EPR spectra of the dark blue-purple solution (total height 8.80 cm, 0.84 mM) were obtained at 240 K (label:CS374R2). The dark blue solution was stored in liquid nitrogen.

Subsequently, EPR spectra at variable temperature were obtained (120 K to 200 K) to calculate experimental χT. TEMPONE in dibutyl phthalate as reference (conc.=1.17 mM).

Finally, the EPR tube was attached to the vacuum line. The sample was quenched by addition of bis(pentamethylcyclopentadienyl)iron(II) (Cp^*_2Fe) in DCM (1.34 mg, 10 eq). The color changed from blue-purple to yellow. The solution was transferred to a vial and evaporated by N_2, which was purified by column chromatography (regular silica gel, pentane/DCM=5/1) without light to get a yellow powder (0.29 mg, 94%). ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: CS374_reduced) and ESI-MS (0.1% of trifluoroacetic acid in dichloromethane, label CS374 reduced) showed the starting material **1**-D_2.

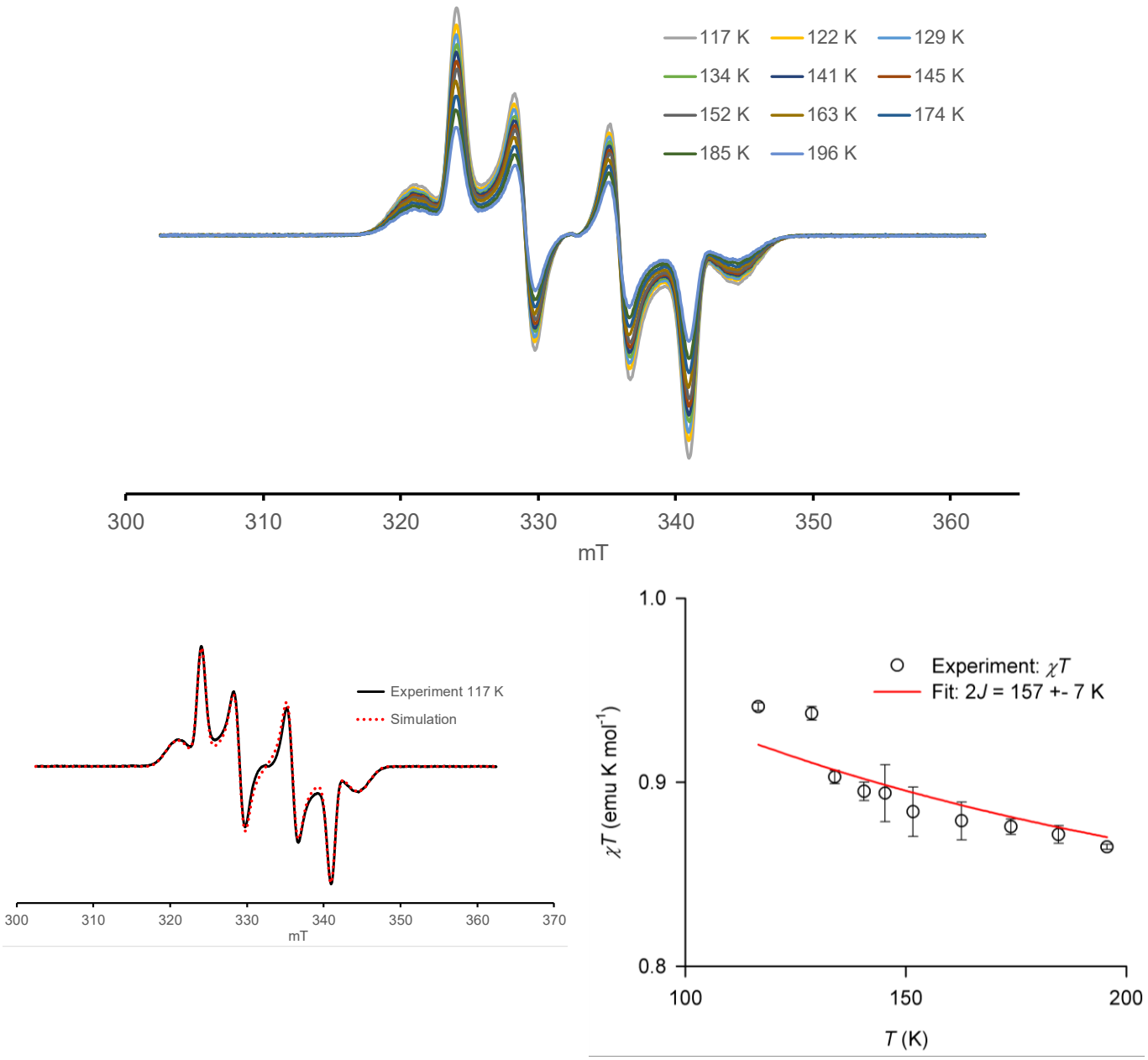


Fig. S26. Top panel: selected EPR spectra of 0.84 mM diradical dication $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ (sample label: CS374) in DBP in the 117 – 196 K temperature range. Bottom left panel: EPR spectrum of 0.84 mM diradical dication $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ at 117 K (sample label: CS374, spectrum label: CS426R13) with spectral simulation, obtained using EasySpin, of the $|\Delta m_s| = 1$ region: $|D/hc| = 1.108 \times 10^{-2}$ cm^{-1}, $|E/hc| = 1.560 \times 10^{-3}$ cm^{-1}, $|A_{zz}/hc|/2 = 7.3 \times 10^{-4}$ cm^{-1}, $g_{xx} = 2.0038$, $g_{yy} = 2.0037$, $g_{zz} = 2.0027$; H-strain (MHz): $H_x = 39.60$, $H_y = 36.55$, $H_z = 21.77$. Bottom right panel: repeat quantitative EPR spectroscopy of 0.84 mM diradical dication $\mathbf{1}^{\mathbf{2\cdot 2+}}$ $2SbF_6^-$ in DBP (sample label: CS374) with 1.17 mM TEMPONE in DBP as a reference: experimental values of χT (mean ± SE), the product of paramagnetic susceptibility (χ) and T in the $T = 117 – 196$ K range; final numerical fit with no weighing and one variable parameter, $2J/k = 157 \pm 7$ K (mean ± SE), after scaling the χT data with a weight factor of $N = 0.90$.

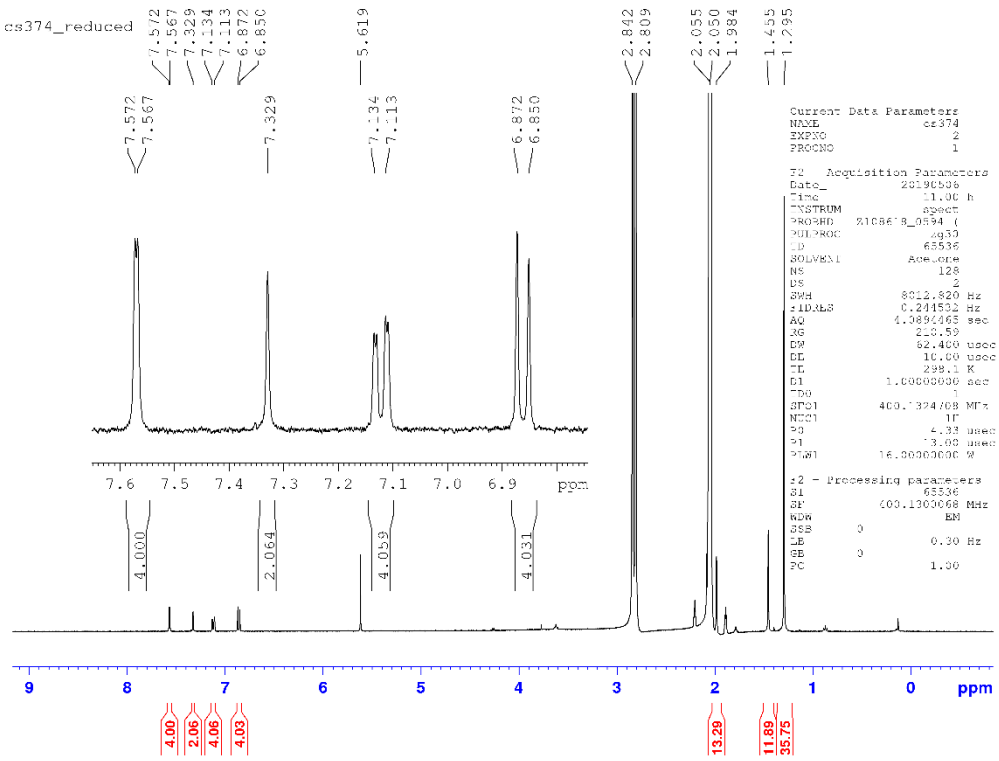


Fig. S27. ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: CS374_reduced) of the sample obtained after quench of diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ with Cp^*_2Fe, followed by purification. The spectrum shows the starting material **1-D_2**.

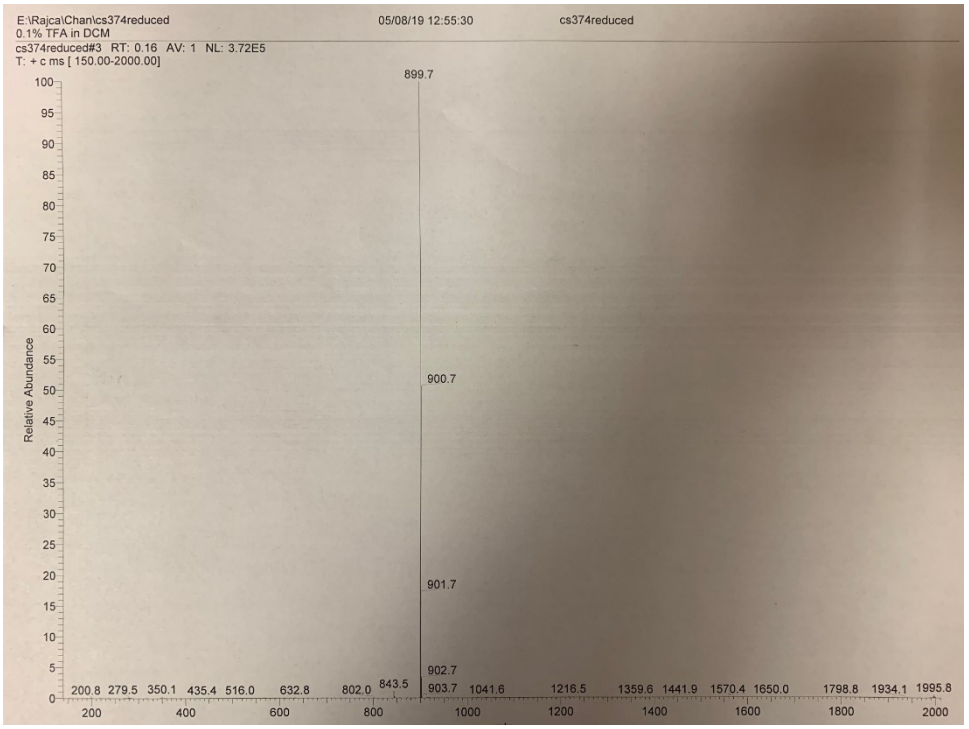


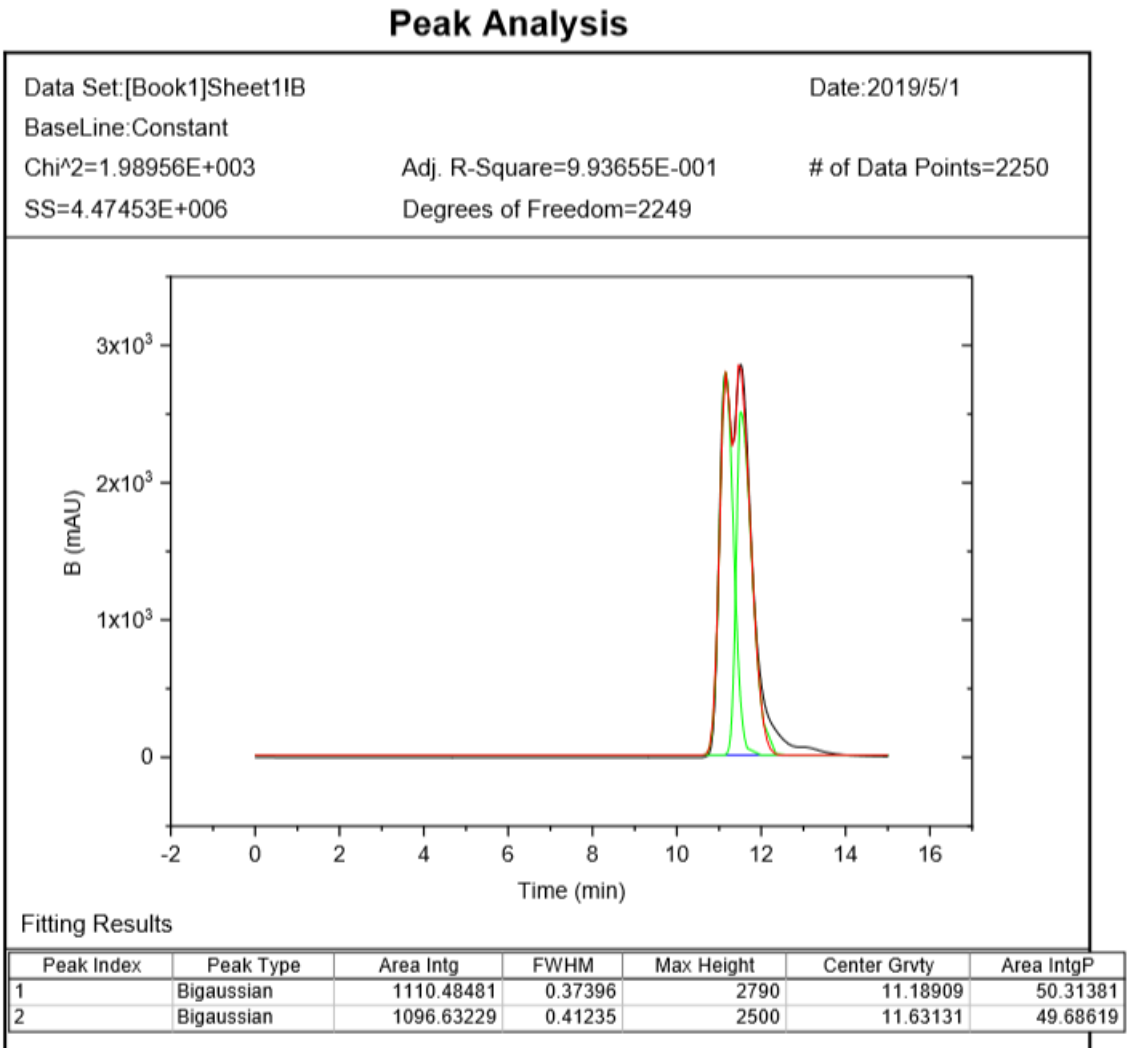
Fig. S28. ESI-MS (0.1% TFA in DCM, label: CS374reduced) of the sample obtained after quench of diradical dication $\mathbf{1}^{2\cdot 2+}$ $2SbF_6^-$ with Cp^*_2Fe, followed by purification.

1.d5 Resolution of 1-D_2: ECD spectroscopy.

HPLC (Agilent Technologies 1260 Infinity), equipped with Daicel CHIRALPAK AD-H column (0.46 cm ϕ x 25 cm), is used to resolve racemic **1**-D_2. Before running the sample, the column has been equilibriated with hexane (HPLC grade) overnight at 12 °C. HPLC trace for racemic **1**-D_2 shows two partially resolved peaks, with the 50:50 integrated ratio (Fig. S29). Two enantiomerically enriched compounds were obtained: *P*,*P*-**1**-D_2, 0.82 mg (Fig. S30, label: cs-3-2-27p1) and *M*,*M*-**1**-D_2, 0.90 mg (Fig. S30, label: cs-3-2-27p3); the respective %ee values were determined to 61.3% and 41.7% by Bigaussian fits (Eqs. S1A&B). The fitting was carried out using Origin software.

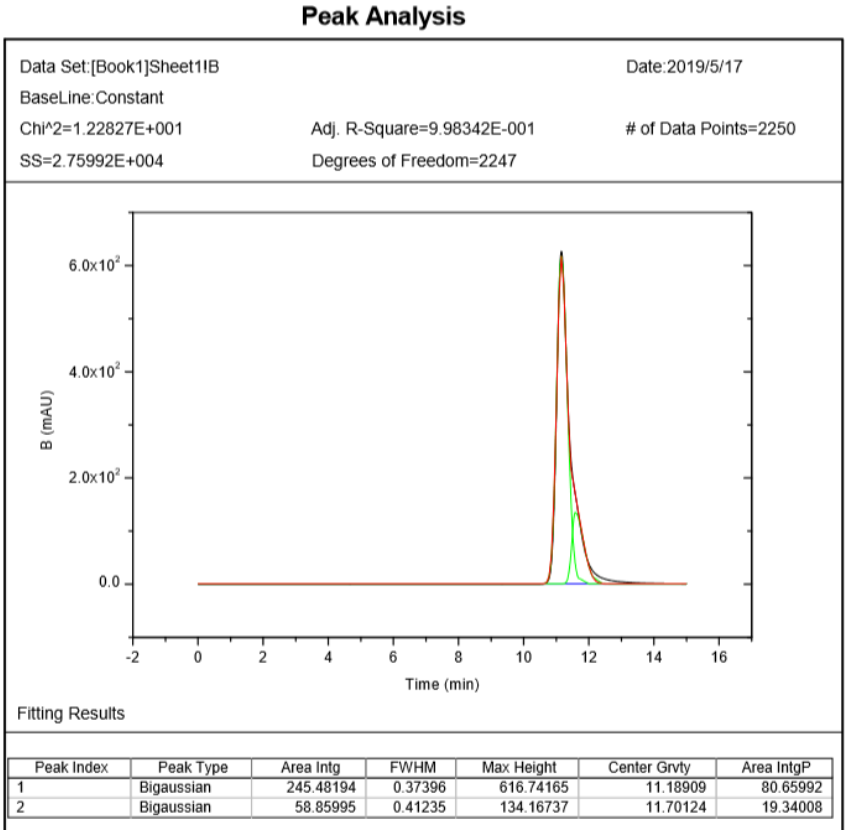
$$y = y_0 + He^{-0.5\left(\frac{x-x_c}{w1}\right)^2} \quad (x < x_c) \qquad \text{(S1A)}$$

$$y = y_0 + He^{-0.5\left(\frac{x-x_c}{w2}\right)^2} \quad (x > x_c) \qquad \text{(S1B)}$$

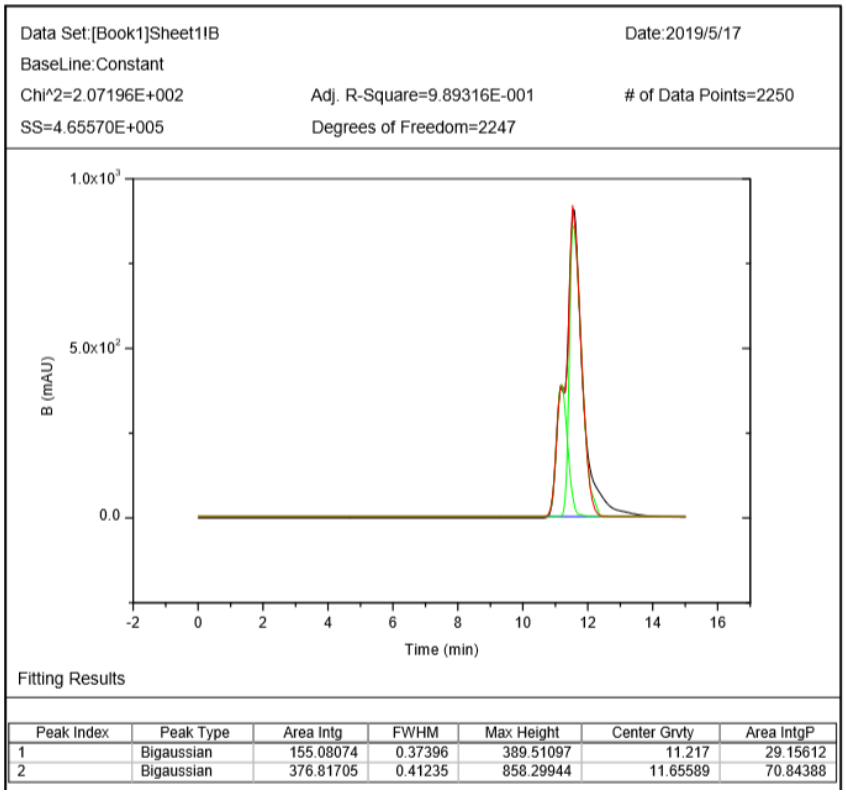


Peak Index	Peak Type	Area Intg	FWHM	Max Height	Center Grvty	Area IntgP
1	Bigaussian	1110.48481	0.37396	2790	11.18909	50.31381
2	Bigaussian	1096.63229	0.41235	2500	11.63131	49.68619

Fig. S29. Chiral HPLC (100% hexane, 0.3 mL/min, 12 °C) for racemic **1**-D_2. Bigaussian fit is shown.



Peak Index	Peak Type	Area Intg	FWHM	Max Height	Center Grvty	Area IntgP
1	Bigaussian	245.48194	0.37396	616.74165	11.18909	80.65992
2	Bigaussian	58.85995	0.41235	134.16737	11.70124	19.34008



Peak Index	Peak Type	Area Intg	FWHM	Max Height	Center Grvty	Area IntgP
1	Bigaussian	155.08074	0.37396	389.51097	11.217	29.15612
2	Bigaussian	376.81705	0.41235	858.29944	11.65589	70.84388

Fig. S30. Chiral HPLC (100% hexane, 0.3 mL/min, 12 °C) for for enantiomerically enriched **1**-D_2 with bigaussian fits shown; top panel: *P*,*P*-**1**-D_2 (%ee = 61.3%), bottom panel: *M*,*M*-**1**-D_2 (%ee = 41.7%).

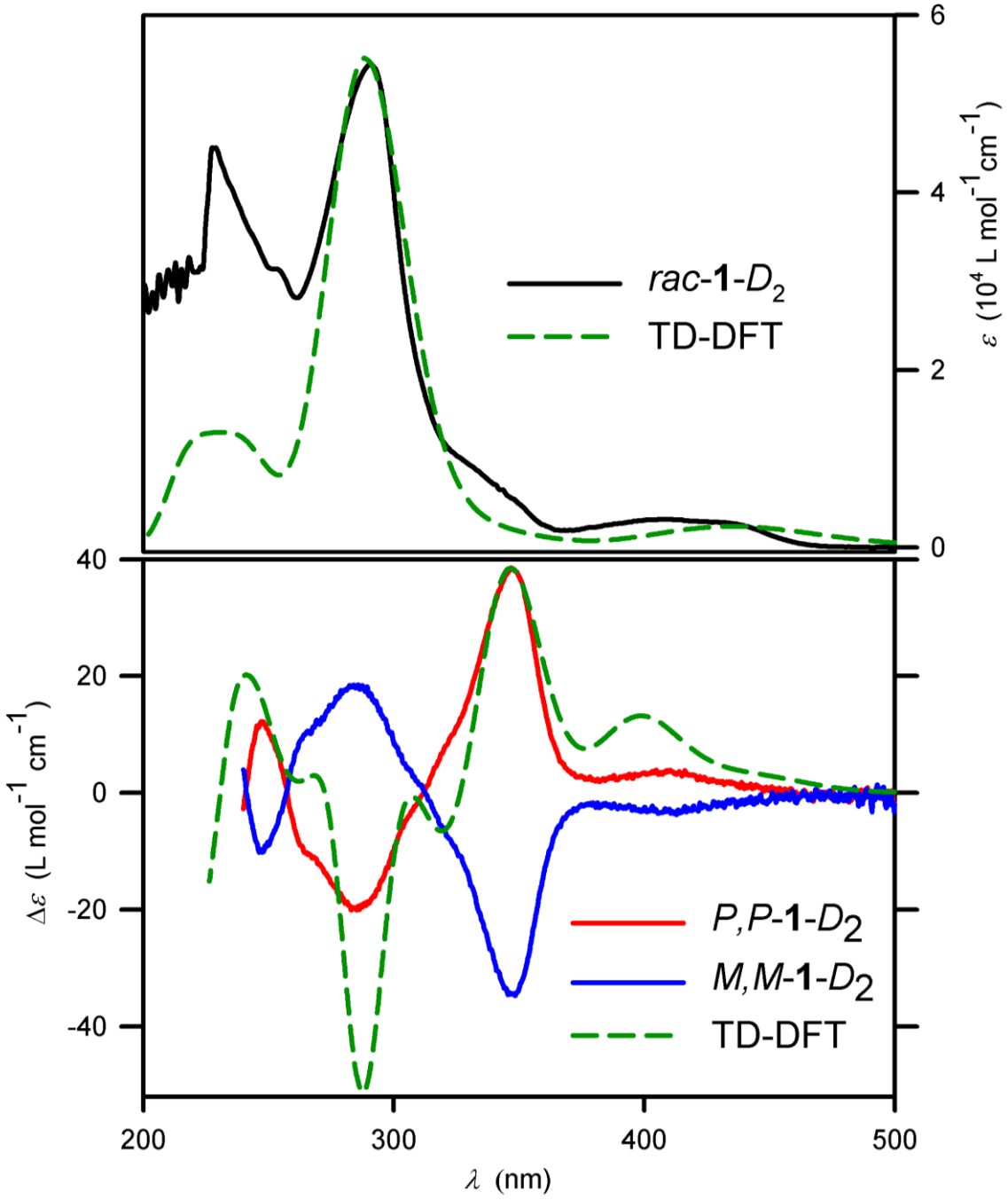


Fig. S31. UV-vis absorption and ECD spectra for racemic and enantiomerically enriched **1**-D_2. Experimental ECD spectra are scaled by the ee. TD-DFT computed spectra for *P*,*P*-**1**-D_2 are shown using dashed green lines. Computed UV-vis and ECD spectra are convoluted with Gaussian lines (line width of 0.25 eV for UV-vis and 0.15 eV for ECD) and shifted by -0.60 and -0.65 eV, respectively; in each case, the spectra are scaled vertically to obtain reasonable fit to the experimental data. UV-vis, DCM, λ_{max}/nm (ε_{max}/L mol^{-1} cm^{-1}) for *rac*-**1**-D_2: 229 (4.5×10^4), 291 (5.5×10^4), 407 (3.2×10^3). ECD, DCM, λ_{max}/nm ($\Delta\varepsilon_{max}$/L mol^{-1} cm^{-1}) for *P*,*P*-**1**-D_2: 247 (12.4), 285 (–20.3), 348 (38.8), 410 (4.0).

1.d6 Preparation of chiral diradical dication $1^{2\bullet2+}$ $2SbF_6^-$ via oxidation of enantiomerically enriched 1-D_2 using $[NO]^+[SbF_6]^-$ in DBP: ECD spectroscopy.

Table S4. Summary of preparation of chiral diradical dication $\mathbf{1}^{2\bullet2+}2SbF_6^-$ using $[NO]^+[SbF_6]^-$ in DBP.

run no	sample label	**1**-D_2 (mg)	SM label (chirality, ee%)	$[NO]^+[SbF_6]^-$ (equiv)	Figures and comments	Recovered **1**-D_2 (mg, %)
1	CS437_Dirad Dicat	0.10	CS32-27P1 (*P*,*P*, 61.3%)	8	Initial χT = 0.79 ± 0.02 at 117 K by quantitative EPR (Fig. S32); UV-vis-NIR, ECD spectra showing that the diradical dication is configurationally stable on the scale of day at rt (Fig. S32); quantitative EPR with χT = 0.78 ± 0.01 at 117 K (Fig. S32); quench with Cp^*_2Fe, ^{1}H NMR (Fig. S34).	~0.08, ~80%
2	CS441_Dirad Dicat	0.033[a]	CS32-27P1 (*P*,*P*, 61.3%)	~10	Initial χT = 0.82 ± 0.04 at 117 K by quantitative EPR (Fig. S33); UV-vis-NIR, ECD spectra showing that the diradical dication is configurationally stable on the scale of day at rt (Fig. S33); quantitative EPR with χT = 0.80 ± 0.04 at 117 K (Fig. S33)	-
3	CS439_Dirad Dicat	0.11	CS32-27P3 (*M*,*M*, 41.7%)	6	Initial χT = 0.84 ± 0.01 at 117 K by quantitative EPR (Fig. S35); UV-vis-NIR, ECD spectra showing that the diradical dication is configurationally stable on the scale of 2 days at rt (Fig. S35); quantitative EPR with χT = 0.82 ± 0.02 at 117 K (Fig. S35); quench with Cp^*_2Fe, ^{1}H NMR (Fig. S36).	~0.10, ~90%

[a] Weight estimated based upon UV-vis-NIR spectrum.

Estimate of barrier for racemization of *M*,*M*-$\mathbf{1}^{2\bullet2+}$ $2SbF_6^-$ in DBP at room temperature.

Rate constant (k_1) for racemization was computed from equation S2, where

$$\ln\{[1+(M/P)]/[1-(K'*M/P)]\} = (1+K')*k_1*t + C, \quad \text{(S2)}$$

where $K' = 1/K = k_2/k_1$; we have assumed that $k_1 = k_2$, i.e., $K' = 1$; the constant of integration C: $C = \ln\{[1+(M0/P0)]/[1-(K'*M0/P0)]\}$, where M0 and P0 are starting concentrations of M and P.

Diradical dication *P*,*P*-$\mathbf{1}^{2\bullet2+}$ $2SbF_6^-$ generated using $[NO]^+[SbF_6]^-$ in DBP: sample label, CS437_DiradDicat. Chiral diradical dication *P*,*P*-$\mathbf{1}^{2\bullet2+}$ $2SbF_6^-$ (sample label: CS437_DiradDicat) was prepared from the starting material *P*,*P*-**1**-D_2 (0.10 mg, 0.11 μmol, %ee = 61.3%, sample label: CS32-27P1) in a custom-made Schlenk vessel with 4-mm EPR tube, as described for racemic compound. Distilled dibutyl phthalate (DBP, ~100 μL) and the oxidant $NOSbF_6$ in distilled DBP (33μL, 8 equiv, 7.960 mg/mL) were used; following dilution with DBP (~400 μL), quantitative EPR spectroscopy at 117 K indicated χT = 0.79 emu K mol^{-1}; as EPR spectra show almost pure triplet state with negligible doublet impurity (Fig. S32), this relatively low value of χT must reflect weighing error of 0.10 mg of

starting material. Spin concentrations were obtained with TEMPONE in dibutyl phthalate as reference (conc. = 1.17 mM). The sample was kept in liquid nitrogen.

Next day, the sample was warmed up to room temperature and the dark purple/blue solution was transferred with syringe to a custom-made Schlenk vessel with UV-vis-NIR cuvette (1-mm path) under argon flow, to obtin UV-vis-NIR absorption spectra. Then the Schlenk vessel was kept on the high vacuum line at room temperature without light. Afer 24 h, ECD spectra (300–500 nm) were measured. After another 23 h, at room temperature, repeat ECD spectra (300-500 nm) were measured (Fig. S32). Then, another rset of ECD spectra (500-900 nm) was obtained. Subsequently, the dark purple/blue solution was transferred back to the same custom-made Schlenk vessel with 4-mm EPR tube. EPR spectra were obtained at 117 K (label: CS438R1, R3 and R5) using TEMPONE in DBP as reference to obtain spin concentration; value of χT = 0.78 emu K mol^{-1} was practically unchanged (Fig. S32).

Finally, the EPR tube was attached to the vacuum line, the reaction was quenched by addition of bis(pentamethylcyclopentadienyl)iron(II) in DCM (0.37 mg, 10 eq). The color changed from dark blue-purple to yellow. The solution was transferred to a vial and evaporated by N_2 to give yellow oil crude, which was purified by column chromatography (regular silica gel, pentane/DCM, 5:1) without light to get a yellow solid (~0.08 mg, ~80%, sample label: CS437_DiradDicat_Reduced), corresponding to starting material **1**-D_2, based on ^{1}H NMR spectrum (Fig. S34).

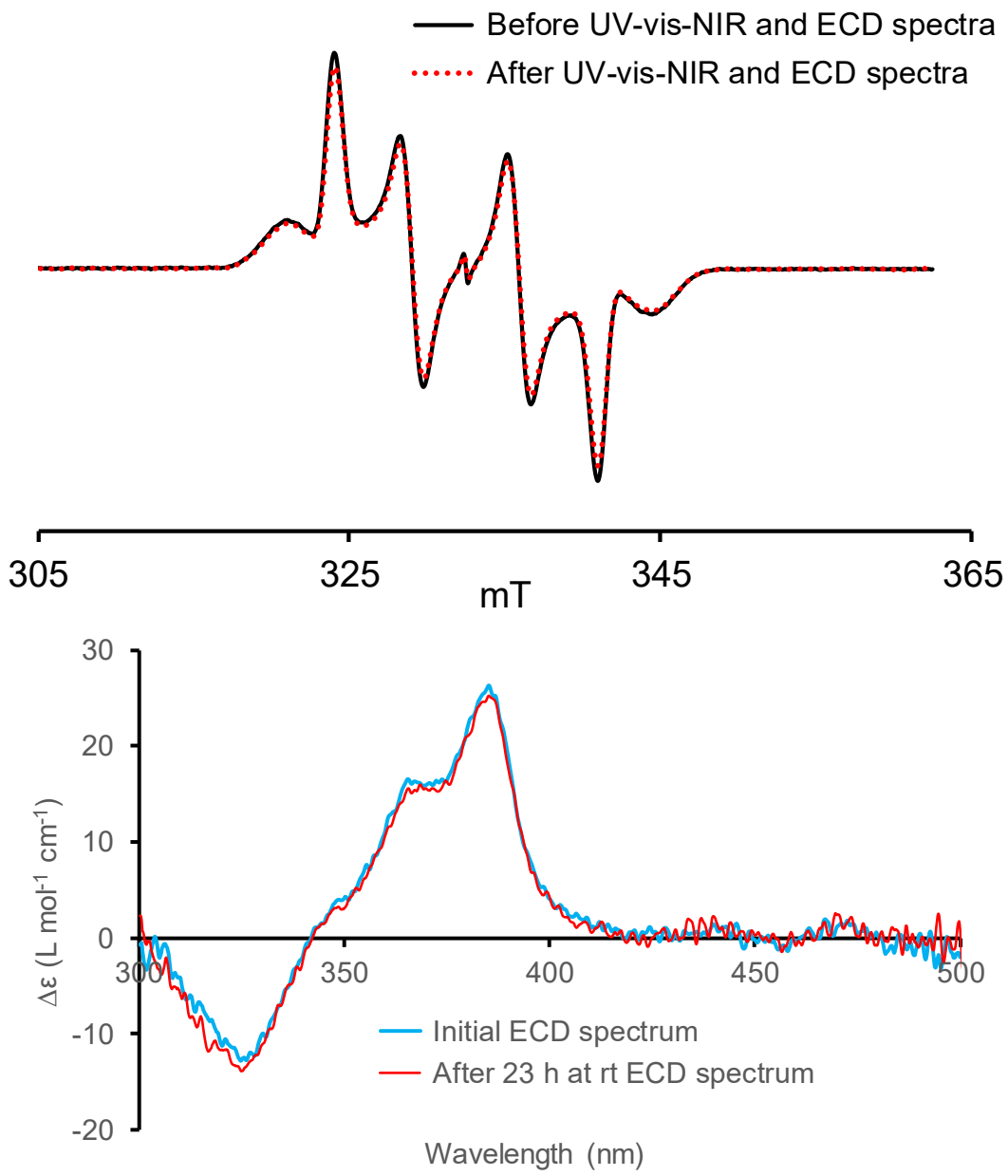


Fig. S32. Initial ECD/UV-vis-NIR/EPR spectroscopy experiment for diradical dication *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$. Top panel: EPR spectra before (ν = 9.3256 GHz, sample label: CS437_DiradDicat, spectrum label: CS437R6) and after (ν = 9.3262 GHz, spectrum label: CS438R5) UV-vis-NIR and ECD spectra for dication *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$; the respective values of χT = 0.79 ± 0.02 and 0.78 ± 0.01 emu K mol^{-1} also show practically no change. Bottom panel: ECD spectra for *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ (sample label: CS437_DiradDicat) taken 23 h apart after storing the sample at room temperature; the data shows configurational stability of *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ on the time scale of day at room temperature, e.g., rmsd for the the two ECD spectra in the 300-450 nm region is 0.991 L mol^{-1} cm^{-1}. ECD (initial), DBP, λ_{max}/nm ($\Delta\varepsilon_{max}$/L mol^{-1} cm^{-1}) for *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$: 327 (–13.4), 369 sh (16.4), 385 (26.4). ECD (after 23 h at rt), DBP, λ_{max}/nm ($\Delta\varepsilon_{max}$/L mol^{-1} cm^{-1}) for *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$: 327 (–13.5), 369 sh (16.1), 385 (25.5).

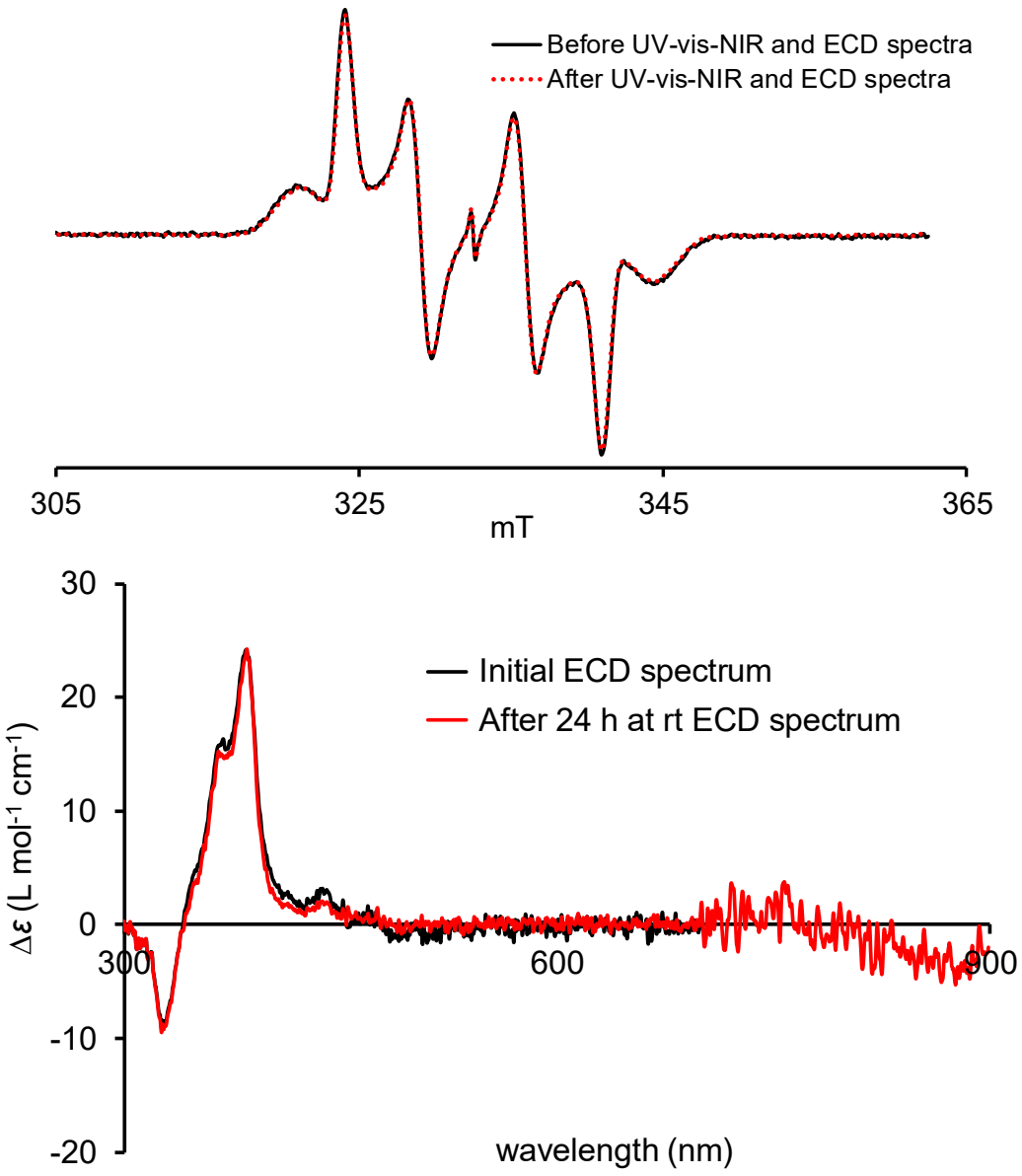


Fig. S33. Repeat ECD/UV-vis-NIR/EPR spectroscopy experiment for diradical dication *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$. Top panel: EPR spectra before (ν = 9.3263 GHz, sample label: CS441_DiradDicat, spectrum label: CS441R5) and after (ν = 9.3262 GHz, spectrum label: CS442R5) UV-vis-NIR and ECD spectra for diradical dication *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$; the respective values of χT = 0.82 ± 0.04 and 0.80 ± 0.04 emu K mol^{-1} also show practically no change. Bottom panel: ECD spectra for *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ (sample label: CS441_DiradDicat) taken 24 h apart after storing the sample at room temperature; the data shows configurational stability of *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ on the time scale of day at room temperature, e.g., rmsd for the the two ECD spectra in the 300-450 nm region is 0.833 L mol^{-1} cm^{-1}. ECD (initial), DBP, λ_{max}/nm ($\Delta\varepsilon_{max}$/L mol^{-1} cm^{-1}) for *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$: 327 (–8.9), 369 sh (16.3), 385 (24.2), 440 (3.0). ECD (after 24 h at rt), DBP, λ_{max}/nm ($\Delta\varepsilon_{max}$/L mol^{-1} cm^{-1}) for *P,P*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$: 326 (–9.5), 367 sh (15.0), 385 (24.2), 440 (2.0), 876.4 (–5.3).

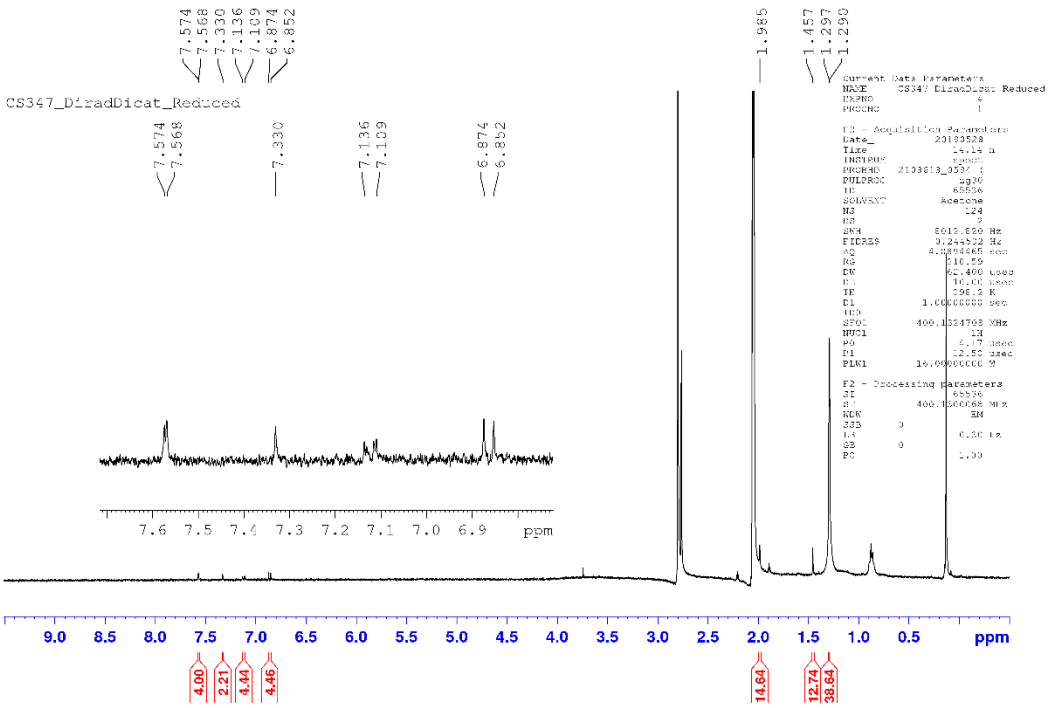


Fig. S34. ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: CS437_reduced) of the sample obtained after quench of diradical dication *P,P*-**1**$^{2\bullet 2+}$ 2SbF_6^- with Cp*$_2$Fe, followed by purification. The spectrum shows the starting material **1**-D_2**.**

Diradical dication *M,M*-1$^{2\bullet 2+}$ 2SbF_6^- generated using [NO]$^+$[SbF_6]$^-$ in DBP: sample label, CS439_DiradDicat. Chiral diradical dication *M,M*-**1**$^{2\bullet 2+}$ 2SbF_6^- was prepared from the starting material *M,M*-**1**-D_2 (0.11 mg, 0.12 μmol, %ee = 41.7%, sample label: CS32-27P3) in a custom-made Schlenk vessel with 4-mm EPR tube, as described for racemic compound. Distilled dibutyl phthalate (DBP, ~500 μL) and the oxidant $NOSbF_6$ in distilled DBP (36 μL, 6 equiv, 5.430 mg/mL) were used to prepare a dilute, 0.227 mM sample of diradical dication (total height of solution: 7.90 cm); quantitative EPR spectroscopy at 117 K indicated χT = 0.84 ± 0.01 emu K mol^{-1} (label: CS439R1, R3 and R5); as EPR spectra show almost pure triplet state with negligible doublet impurity (Fig. S35), this relatively low value of χT must reflect weighing error of 0.11 mg of starting material. Spin concentrations were obtained with TEMPONE in dibutyl phthalate as reference (conc. = 1.17 mM). The sample was kept in liquid nitrogen.

Next day, the sample was warmed up to room temperature and the dark purple/blue solution was diluted with DBP (total height of solution: 13.10 cm) to obtain 0.137 mM solution of diradical dication. The diluted solution was transferred with syringe to a custom-made Schlenk vessel with UV-vis-NIR cuvette (2-mm path) under argon flow, to obtain ECD (300 – 700 nm) and UV-vis-NIR absorption spectra. Then, the Schlenk vessel was kept on the high vacuum line at room temperature without light. Afer 24 h, another two sets of ECD spectra (300–700 nm and 500–900 nm) were measured. After additional 24 h at room temperature (total of 48 h at rt), re-repeat ECD spectra (300–700 nm) were measured (Fig. S35). Subsequently, the dark purple/blue solution was transferred back to the same custom-made Schlenk vessel with 4-mm EPR tube. EPR spectra were obtained at 117 K (label:

CS440R1, R3 and R5) using TEMPONE in DBP as reference to obtain spin concentration; value of χT = 0.82 ± 0.02 emu K mol^{-1} was practically unchanged (Fig. S35).

Finally, the EPR tube was attached to the vacuum line, the reaction was quenched by addition of bis(pentamethylcyclopentadienyl)iron(II) in DCM (0.38 mg, 10 eq). The color changed from dark blue-purple to yellow. The solution was transferred to a vial and evaporated by N_2 gas to give yellow oil crude, which was purified by column chromatography (regular silica gel, pentane/DCM = 5:1) without light to get a yellow solid (~0.1 mg, label: CS439_DiradDicat_Reduced).

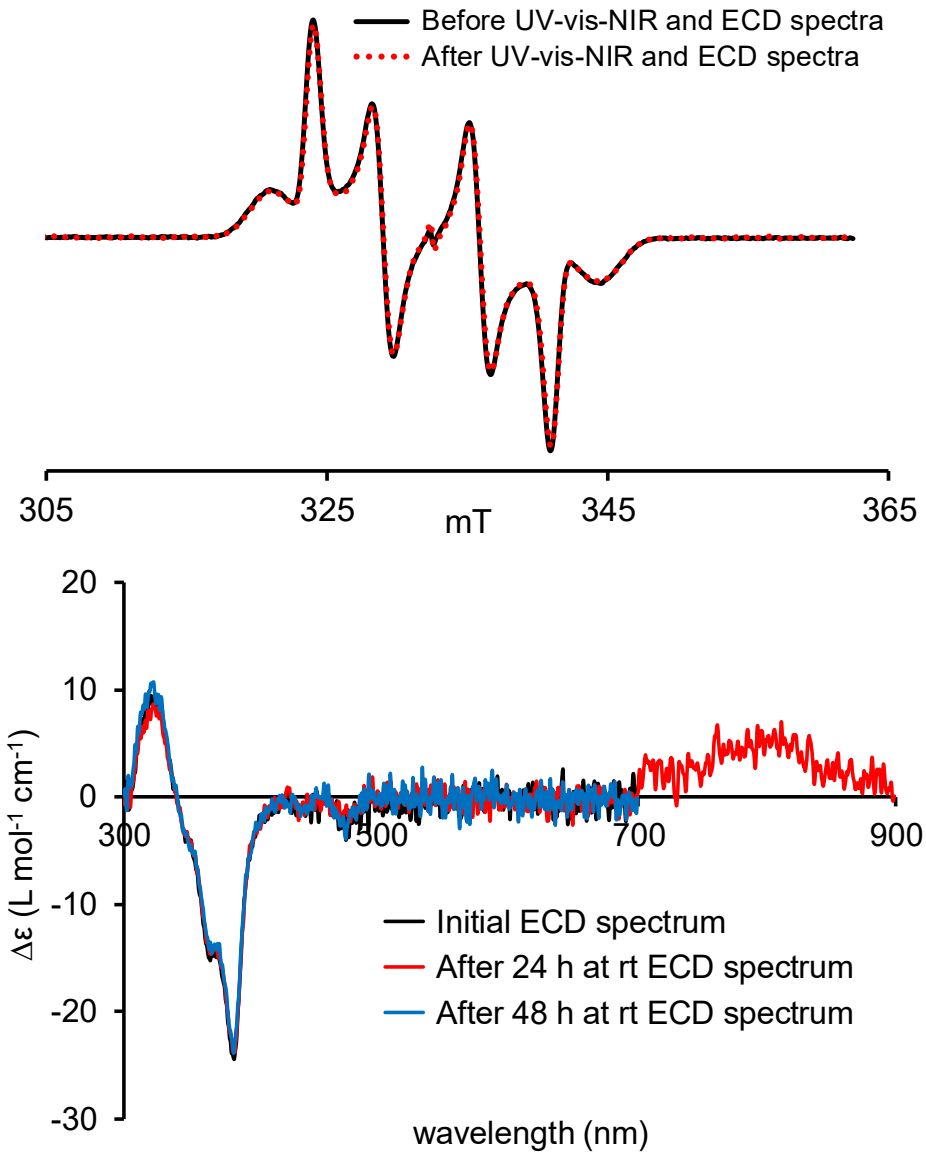


Fig. S35. ECD/UV-vis-NIR/EPR spectroscopy experiment for diradical dication *M,M*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$. Top panel: EPR spectra before (ν = 9.3251 GHz, sample label: CS439_DiradDicat, spectrum label: CS439R5) and after (ν = 9.3262 GHz, spectrum label: CS440R5) UV-vis-NIR and ECD spectra for diradical dication *M,M*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$; the respective values of χT = 0.84 ± 0.01 and 0.82 ± 0.02 emu K mol^{-1} also show practically no change. Bottom panel: Same data as shown in Figure 11 (bottom panel); ECD spectra for *M,M*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ (sample label: CS441_DiradDicat) taken after 24 and 48 h while the sample is kept at room temperature; the data shows configurational stability of *M,M*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$ on the time scale of 2 days at room temperature, e.g., rmsd for the the ECD spectra in the 300-450 nm region is 0.87 and 1.00 L mol^{-1} cm^{-1}, after 24 and 48 h at rt, respectively. ECD (initial), DBP, λ_{max}/nm ($\Delta\varepsilon_{max}$/L mol^{-1} cm^{-1}) for *M,M*-$\mathbf{1}^{2\bullet 2+}$ $2SbF_6^-$: 321 (9.5), 367 sh (–15.3), 385 (–24.5), 472 (–4.0); after 24 h at rt: 323 (8.7), 368 sh (–14.7), 386 (–23.8), 811 (7.0); after 48 h at rt: 323 (10.7), 368 sh (–14.6), 385 (–23.9), 472 (–3.9). Barrier for racemization of >27 kcal mol^{-1} was determined based on the rate constant obtained from Eq. S2 and estimating <1 % loss of %ee over 48 h at room temperature (294 K).

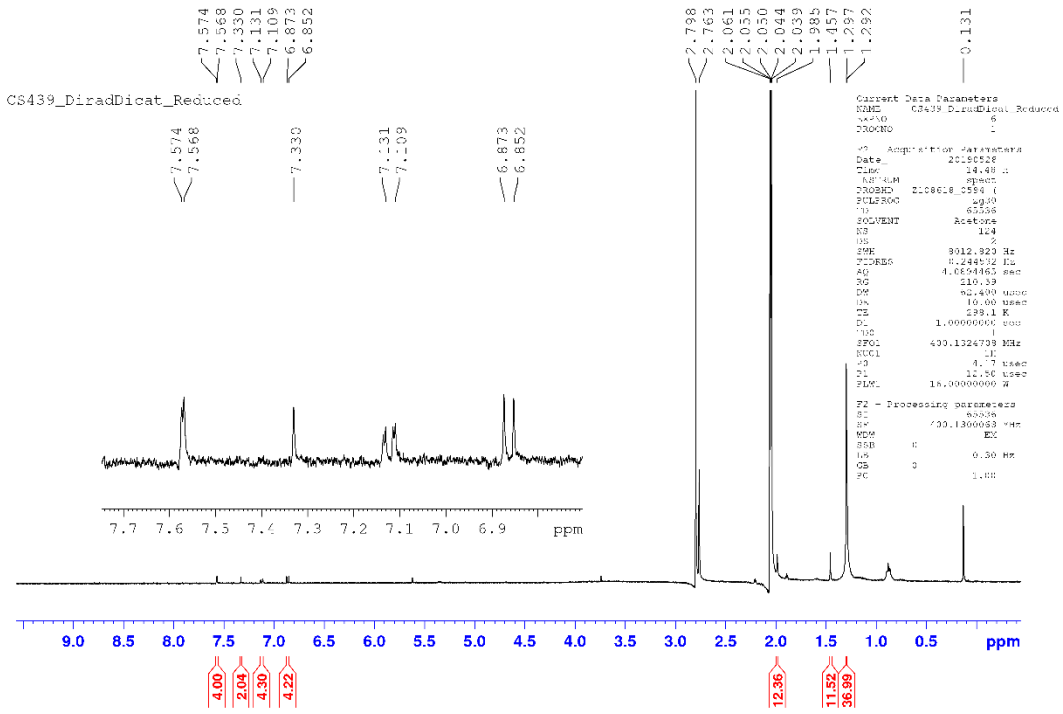


Fig. S36. ^{1}H NMR spectrum (400 MHz, acetone-d_6, label: CS439_reduced) of the sample obtained after quench of diradical dication *M,M*-**1**$^{2\bullet 2+}$ $2SbF_6^-$ with Cp*$_2$Fe, followed by purification. The spectrum shows the starting material **1**-D_2.

1.e DFT calculations.

Geometry optimizations and frequency calculations were performed using the Gaussian 09 and Gaussian 16 program packages[S11] running on a 4-cpu or 16-cpu workstation under Linux operating system.

Geometries were fully optimized for neutral conjoined [5]helicenes, radical cations, and dications at the B3LYP/6-31G(d) and UB3LYP/6-31G(d) level of theory in the gas phase and at the B3LYP/6-31G(d)/IEF-PCM-UFF and UB3LYP/6-31G(d)/IEF-PCM-UFF level of theory, using solvent model for dichloromethane. Geometry optimizations were carried out by constraining molecular symmetry to either to D_2 or C_{2h} point group of symmetry for minima (zero imaginary frequencies) and to C_1 point group of symmetry for transition states (one imaginary frequency). IRC computations followed by geometry optimizations show that C_1-symmetric transition states are indeed correct transition states connecting D_2- and C_{2h}-symmetric minima (Tables S14 and S15). Except for geometry optimization of the neutral D_2-symmetric conjoined [5]helicene in the gas phase and some of the broken symmetry singlet states for diradical dications, all other optimized geometries have RMS forces in Cartesian coordinates less than 7×10^{-6} a.u. (and significantly lower in internal coordinates) that is typically better than the "tight" criterion for RMS forces in geometry optimization in Gaussian 09. All broken-symmetry wavefunctions that were tested for stability (stable=opt) were found to be stable by Gaussian 09 criteria. The results are summarized in Tables S5 – S16.

Using the B3LYP/6-31G(d)/IEF-PCM-UFF geometries, the time-dependent density functional response theory (TD-DFT) calculations at the CAM-B3LYP/6-31G(d)/IEF-PCM-UFF level of theory provided excitation energies, oscillator strengths (*f*), rotatory strengths *R* in the dipole velocity form (R_{vel}) and dipole length form (R_{len}) for electronic transitions. For computed UV-vis absorption and ECD spectra, the electronic UV-vis data (*f*) and ECD data in the Gaussian 09 output files were converted to stick spectra in the text file format and then convoluted with the Gaussian functions with half-width of 0.25 and 0.15 eV (for **1**-D_2), respectively, using graphical user interface Gabedit (version 2.5.0).[S12] The resultant UV and ECD spectra of **1**-D_2 were re-plotted with the wavelength (nm) axis using SigmaPlot program, with horizontal axes shifted by -0.60 and -0.65 eV, respectively. Vertical axes were scaled to

fit the experimental spectra. Computed spectra for **1**-D_2 are plotted in Fig. S31. For calculation of electronic absorption and ECD spectra, up to 40 excited states were computed.

The singlet-triplet energy gaps (ΔE_{ST}) between the triplet ground states and the first open-shell singlet excited states for diradical dications were calculated using UB3LYP and UM06-2X wave functions. The value of ΔE_{ST} was obtained by correcting the calculated energy gap (ΔE_U) for spin contamination, using eq. S3.[S13-S15] In particular, the open-shell singlet excited states, which were calculated using broken-symmetry formalism, had a significant spin contamination as indicated by the mean values of S^2 operator, $\langle S^2_{BS}\rangle \approx 1.0$, while the triplet ground states had $\langle S^2_T\rangle \approx 2.0$ which is close to the expected value of $S(S + 1) = 2$. In eq. S3, it is assumed that the spin contamination of this singlet state originates from the triplet ground state only. The values of ΔE_{ST} obtained using eq. S3 usually overestimate the actual singlet-triplet gaps for triplet ground state diradicals.[S16,S17] The calculated energy gaps, ΔE_{ST}, are summarized in Tables S5, S6, and S8.

$$\Delta E_{ST} = \Delta E_U[\langle S^2_T\rangle/(\langle S^2_T\rangle - \langle S^2_{BS}\rangle)] \quad \text{(S3)}$$

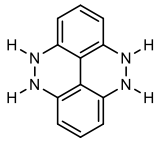
Spin density surfaces for radicals were calculated at the UB3LYP/6-31G(d) level. Cube files were obtained using "medium" setting in Gaussian 09 or 16, and surfaces were plotted with isodensity of 0.002, 0.003, or 0.006 electron/Bohr^3 (Tables 12BC, S13, S15, and Figure 10 main text). Orbital plots were obtained using cube files with "coarse" setting in Gaussian 09, and surfaces were plotted with isodensity 0.02.

Table S5. Summary table with relative energies (ΔE in kcal mol^{-1}), including barriers for ring inversion (racemization) for **1**-D_2, **1**-C_{2h}, and the corresponding radical cations and diradical dications. Singlet-triplet energy gaps (ΔE_{ST} in kcal mol^{-1}, Eq. S3) for diradical dications.[a]

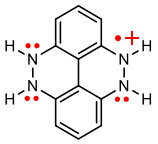
DFT	Medium	Crit. point	Compd.	State	ΔE	ΔE_{ST}
B3LYP	gas phase	min	**1**-C_{2h}	^1A_g	0.00	-
		min	**1**-D_2	^1A	1.08	-
		TS	**1**-C_1	^1A	43.12	-
B3LYP	DCM	min	**1**-C_{2h}	^1A_g	0.00	-
		min	**1**-D_2	^1A	1.08	-
M06-2X	DCM	min	**1**-C_{2h}	^1A_g	0.00	-
		min	**1**-D_2	^1A	1.28	-
		TS	**1**-C_1	^1A	45.03	-
UB3LYP	gas phase	min	$\mathbf{1}^{\bullet+}$-C_{2h}	^2A_g	0.00	-
		min	$\mathbf{1}^{\cdot+}$-D_2	$^2B_3$	0.14	-
		TS	$\mathbf{1}^{\bullet+}$-C_1	^2A	38.14	-
UB3LYP	DCM	min	$\mathbf{1}^{\bullet+}$-C_{2h}	^2A_g	0.00	-
		min	$\mathbf{1}^{\cdot+}$-D_2	$^2B_3$	0.12	-
		TS	$\mathbf{1}^{\bullet+}$-C_1	^2A	37.69	-
UB3LYP	gas phase	min	$\mathbf{1}^{2\bullet2+}$-D_2	$^3B_3$	0.00	0.00
		min	$\mathbf{1}^{2\bullet2+}$-D_2	BS[b]	-	0.59
		min	$\mathbf{1}^{2\bullet2+}$-C_{2h}	^3A_u	0.51	0.00
		min	$\mathbf{1}^{2\bullet2+}$-C_{2h}	BS[b]	-	0.95
		TS	$\mathbf{1}^{2\bullet2+}$-C_1	^3A	35.61	0.00
		TS	$\mathbf{1}^{2\bullet2+}$-C_1	BS[b]	-	0.81
UB3LYP	DCM	min	$\mathbf{1}^{2\bullet2+}$-D_2	$^3B_3$	0.00	0.00
		min	$\mathbf{1}^{2\bullet2+}$-D_2	BS[b]	-	0.71
		min	$\mathbf{1}^{2\bullet2+}$-C_{2h}	^3A_u	0.42	0.00
		min	$\mathbf{1}^{2\bullet2+}$-C_{2h}	BS[b]	-	1.08
		TS	$\mathbf{1}^{2\bullet2+}$-C_1	^3A	35.45	-
UM06-2X	DCM	min	$\mathbf{1}^{2\bullet2+}$-D_2	$^3B_3$	0.00	0.00
		min	$\mathbf{1}^{2\bullet2+}$-D_2	BS[b]	-	1.12
		min	$\mathbf{1}^{2\bullet2+}$-C_{2h}	^3A_u	0.30	0.00
		min	$\mathbf{1}^{2\bullet2+}$-C_{2h}	BS[b]	-	0.81
		TS	$\mathbf{1}^{2\bullet2+}$-C_1	^3A	37.96	-

[a] All computations are carried out using 6-31G(d) basis set. [b] BS corresponds to broken-symmetry singlet.

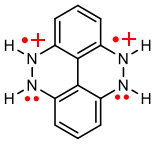
Table S6. Model simplified bishydrazines **1a** and the corresponding radical cations and diradical dications. The B3LYP/6-31G(d)+ZPVE and UB3LYP/6-31G(d)+ZPVE energies in the gas phase ($E°$ + ZPVE, hartree), and UB3LYP/6-31G(d)/IEF-PCM-UFF+ZPVE energies ($E°$ + ZPVE, hartree) in dichloromethane (DCM) and in water, zero point vibrational energies (hartree), lowest vibrational frequencies (cm^{-1}), RMS gradient norms (a.u.), and relative energies (ΔE, kcal mol^{-1}) at the optimized geometries for charge/spin species. All computations listed in this Table were carried out with keyword int=(grid=ultrafine).[a]



1a



1a$^{\bullet+}$



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

Compd.	Charge spin	Medium	Point on PES[b]	Point group	El. State	$<S^2>$	$E°$	ZPVE	$E°$ + ZPVE	RMS gradient norm[b] ($\times 10^{-6}$)	Lowest vibrational frequencies	μ	ΔE
1a	0,0	gas ph.	Min	C_{2h}	^1A_g	0	–682.23555507	0.206388	–682.029167	2.09	55.3, 106.0, 186.6	0.00	0.00
1a	0,0	gas ph.	Min	D_2	^1A	0	–682.23042511	0.206441	–682.023984	0.05	78.8, 80.9, 131.2	0.00	3.25
1a$^{\bullet+}$	1,1/2	gas ph.	Min	C_{2h}	^2A_g	0.7625	–682.01589102	0.205673	–681.810218	0.45	73.9, 88.2, 123.1	0.00	0.00
1a$^{\bullet+}$	1,1/2	gas ph.	Min	D_2	$^2B_2$	0.7627	–682.01614022	0.205964	–681.810176	0.52	88.2, 110.2, 124.4	0.00	0.03
1a$^{\bullet+}$	1,1/2	gas ph.	2 imag. freqs.	D_{2h}	$^2B_{2g}$	0.7643	–682.010002820	0.203229	–681.806774	5.22	***i456.7, i451.1,*** 55.0, 121.1	0.00	2.16
1a$^{\bullet+}$	1,1/2	DCM	Min	C_2	^2A	0.7582	–682.081811294	0.205948	–681.875863	3.18	21.4, 88.2, 96.9	4.66	0.00
1a$^{\bullet+}$	1,1/2	DCM	TS	D_2	$^2B_2$	0.7640	–682.08082567	0.206018	–681.874808	0.44	***i360.4,*** 86.5, 135.3	0.00	0.66
1a$^{\bullet+}$	1,1/2	DCM	TS	C_{2h}	^2A_g	0.7638	–682.080345619	0.205628	–681.874718	0.62	***i384.3,*** 87.2, 124.7	0.00	0.72
1a$^{\bullet+}$	1,1/2	water	Min	C_2	^2A	0.7583	–682.090133432	0.206371	–681.883762	1.70	86.9, 93.1, 154.0	5.03	0.00
1a$^{\bullet+}$	1,1/2	water	TS	D_2	$^2B_2$	0.7643	–682.088533760	0.205626	–681.882908	1.99	***i411.7,*** 83.3, 132.6	0.00	0.54
1a$^{\bullet+}$	1,1/2	water	TS	C_{2h}	^2A_g	0.7641	–682.088149211	0.205354	–681.882795	2.53	***i422.9,*** 87.1, 125.6	0.00	0.61
1a$^{2\bullet 2+}$	2,1	gas ph.	Min	D_{2h}	Triplet-$^3B_{2u}$	2.0283	–681.657433460	0.206544	–681.450889	0.75	95.4, 133.4, 208.6	0.00	0.00
1a$^{2\bullet 2+}$	2,0	gas ph.	Min	D_{2h}	*BSsinglet	0.9634	–681.65368958	0.206168	–681.447522	0.90	92.9, 129.3, 193.2	0.00	**4.02**[c]
1a$^{2\bullet 2+}$	2,1	water	Min	D_{2h}	Triplet-$^3B_{2u}$	2.0304	–681.916530887	0.207416	–681.709114	3.92	100.9, 117.8, 223.6	0.00	0.00
1a$^{2\bullet 2+}$	2,0	water	Min	D_{2h}	BSsinglet	0.9293	–681.913421268	0.207147	–681.706275	6.18	99.6, 117.6, 214.4	0.00	**3.29**[c]

[a]1 Hartree = 627.51 kcal mol^{-1}. [b]In Cartesian coordinates. [c]ΔE_{ST}, Eq. S3 *Wavefunction was tested for stability (stable=opt) and was found to be stable.

Table S7. Conjoined [5]helicenes: D_2-symmetric (*P,P*)-**1**-D_2, C_{2h}-symmetric (*meso*) (*P,M*)-**1**-C_{2h}, C_1-symmetric transition state TS-(*P*)-**1**-C_1, and the corresponding radical cations. The B3LYP/6-31G(d)+ZPVE and UB3LYP/6-31G(d)+ZPVE energies in the gas phase ($E°$ + ZPVE, hartree) and the B3LYP/6-31G(d)/IEF-PCM-UFF+ZPVE, M06-2X/6-31G(d)/IEF-PCM-UFF+ZPVE, and UB3LYP/6-31G(d)/IEF-PCM-UFF+ZPVE energies ($E°$ + ZPVE, hartree) in dichloromethane (DCM), zero point vibrational energies (ZPVE, hartree), lowest vibrational frequencies (cm^{-1}), RMS gradient norms (a.u.), and relative energies (ΔE, kcal mol^{-1}) at the optimized geometries for each state. Transition states for racemization of conjoined [5]helicenes possess C_1 point group of symmetry.[a]

Charge, spin	DFT	Medium	Point on PES	Point group (state)	Electronic state	$<S^2>$	$E°$	ZPVE	$E°$ + ZPVE	RMS gradient norm[b] ($\times 10^{-6}$)	Lowest vibrational frequencies[c]	μ	ΔE
0,0	B3LYP	gas ph.	Min	C_{2h}	^1A_g	0	–2702.42829142	1.234401	–2701.193891	2.62	13.2, 14.3, 18.4	0.00	0.00
0,0	B3LYP	gas ph.	Min	D_2	^1A	0	–2702.42652661	1.234362	–2701.192164	8.98	14.1, 14.7, 20.2	0.00	1.08
0.0	B3LYP	gas ph.	TS	C_1	^1A	0	–2702.35839345	1.233226	–2701.125167	0.75	***i52.3***, 14.3, 16.7	1.66	***43.12***
0,0	B3LYP	DCM	Min	C_{2h}	^1A_g	0	–2702.43631751	1.233152	–2701.203165	4.08	13.2, 14.6, 18.3	0.00	0.00
0,0	B3LYP	DCM	Min	D_2	^1A	0	–2702.43460513	1.233163	–2701.201442	0.11	13.9, 14.5, 20.0	0.00	1.08
0,0	UM06-2X[e]	DCM	Min	C_{2h}	^1A_g	0	–2701.31593887	1.246179	–2700.069760	0.24	13.7, 15.7, 19.4	0.00	0.00
0,0	UM06-2X[e]	DCM	Min	D_2	^1A	0	–2701.31393953	1.246215	–2700.067725	0.09	14.7, 15.0, 22.2	0.00	1.28
0,0	UM06-2X[e]	DCM	TS[d]	C_1	^1A	0	–2701.24305214	1.245059	–2699.997993	0.27	***i34.3***, 14.6, 17.5	2.09	***45.03***
1,1/2	UB3LYP	gas ph.	Min	C_{2h}	^2A_g	0.7601	–2702.23154745	1.235038	–2700.996509	3.86	13.3, 14.0, 19.0	0.00	0.00
1,1/2	UB3LYP	gas ph.	Min	D_2	$^2B_3$	0.7601	–2702.23141674	1.234683	–2700.996733	2.27	12.7, 13.9, 17.5	0.00	0.14
1,1/2	UB3LYP	gas ph.	TS	C_1	^2A	0.7598	–2702.16975043	1.234021	–2700.935729	1.83	***i60.9***, 15.1, 16.6	5.25	***38.14***
1,1/2	UB3LYP	gas ph.	2 imag. freqs.	C_{2h}	^2B_g	0.7667	–2702.07993638	1.230917	–2700.849019	0.71	***i101.8, i96.4,*** 9.8, 15.0	0.00	92.55
1,1/2	UB3LYP	DCM	Min	C_{2h}	^2A_g	0.7599	–2702.27058593	1.233896	–2701.036690	4.50	7.9, 14.2, 19.7	0.00	0.00
1,1/2	UB3LYP	DCM	Min	D_2	$^2B_3$	0.7599	–2702.27048330	1.234025	–2701.036459	0.36	11.6, 14.3, 14.5	0.00	0.12
1,1/2	UB3LYP	DCM	TS	C_1	^2A	0.7586	–2702.21029074	1.233664	–2700.976626	2.91	***i45.7***, 16.1, 17.8	8.04	***37.69***

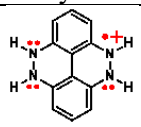
[a] 1 Hartree = 627.51 kcal mol^{-1}. [b] In Cartesian coordinates. [c] All calculated structures, indicated as "Min", correspond to minima on the potential energy surface (PES, zero imaginary vibrational frequencies); structures, indicated as "TS", correspond to transition states on the PES (one imaginary vibrational frequency) and structures indicated as "2 imag. freqs" correspond to stationary points at the PES with two imaginary vibrational frequencies. [d] Following IRC starting from the TS, optimization of one of the structures gave C_{2h}-symmetric double helicene (see: Table S14 below). [e] int=(grid=ultrafine) G09 keyword was used.

Table S8. Diradical dications of conjoined [5]helicenes: D_2-symmetric (*P,P*)-**1**$^{2.2+}$-D_2, C_{2h}-symmetric (*meso*) (*P,M*)-**1**$^{2.2+}$-C_{2h}, and C_1-symmetric transition state TS-(*P*)-**1**$^{2.2+}$-C_1: UB3LYP/6-31G(d)+ZPVE (in the gas phase) and UB3LYP/6-31G(d)/IEF-PCM-UFF+ZPVE (in DCM), and UM06-2X/6-31G(d)/IEF-PCM-UFF+ZPVE (in DCM) energies (hartree), zero point vibrational energies (hartree), lowest vibrational frequencies (cm^{-1}), RMS gradient norms (a.u.) in Cartesian coordinates, relative energies for triplet states (kcal mol^{-1}), and S-T splittings (ΔE_{ST} in kcal mol^{-1}, Eq. S3). Two racemic transition states for racemization of conjoined [5]helicenes [D_2-(*P,P*) to C_{2h}-(*P,M*) to D_2-(*M,M*)] possess C_1 point group of symmetry. All computations listed in this Table were carried out with keyword int=(grid=ultrafine).[a]

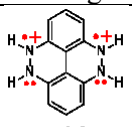
	DFT	Medium	Point on PES	State	Geometry	Spin densities	*E*° (gas phase)	ZPVE	*E*° + ZPVE	$\langle S^2\rangle$	RMS gradient norm (×10^{-6})[b]	Lowest vibrational frequencies	Rel. triplet energy (kcal mol^{-1})	ΔE_U (S-T)	ΔE_{ST}
1$^{2.2+}$-D_2	UB3LYP	Gas ph.	Min	*Triplet-$^3B_3$	triplet	N1=N2=N48=N49=+0.247	–2701.93771786	1.234754	–2700.702964	2.0205	0.04	12.7, 13.8, 20.9	**0.00**	0.00	**0.00**
				BS-singlet	triplet	N1=+0.244 N2=-0.244 N48=-0.244 N49=+0.244	–2701.93710255	-	-	0.9840	-	-	-	0.39	**0.75**
				*BS-singlet	BS-singlet	N1=+0.242 N2=-0.242 N48=-0.242 N49=+0.242	–2701.93719348	1.234717	–2700.702476	0.9753	1.54	12.9, 13.8, 20.9	-	0.31	**0.59**
1$^{2.2+}$-C_{2h}	UB3LYP	Gas ph.	Min	Triplet-^3A_u	triplet	N1=N2=N48=N49=+0.242	–2701.93695236	1.234807	–2700.702145	2.0201	4.34	13.3, 14.5, 19.7	**0.51**	0.00	**0.00**
				BS-singlet	triplet	N1=+0.241 N2=-0.241 N48=-0.241 N49=+0.241	–2701.93607115	-	-	0.9943	-	-	-	0.55	**1.09**
				*BS-singlet	BS-singlet	N1=+0.240 N2=-0.240 N48=-0.240 N49=+0.240	–2701.93612640	1.234751	–2700.701376	0.9899	9.68	13.6, 14.6, 19.7	-	0.48	**0.95**
1$^{2.2+}$-C_1	UB3LYP	Gas ph.	TS[c]	Triplet-^3A	triplet	N1=+0.295 N2=+0.227 N30=+0.264 N31=+0.301	–2701.87955672	1.233775	–2700.645781	2.0214	0.52	***i55.5***, 12.8, 16.2	**35.61**	0.00	**0.00**
				*BS-singlet	BS-singlet	N1=–0.289 N2=+0.223 N30=+0.258 N31=–0.296	–2701.87881227	1.233700	–2700.645112	0.9763	0.90	***i56.8***, 13.0, 16.3	-	0.42	**0.81**
				**singlet	singlet	N1=N2=N30=N31=0.000	–2701.86866592	1.233848	–2700.634818	0.0000	4.61	***i61.0***, 14.1, 16.2	41.77	6.88	**6.88**
1$^{2.2+}$-D_2	UB3LYP	DCM	Min	Triplet-$^3B_3$	triplet	N1=N2=N48=N49=+0.253	–2702.07978422	1.235408	–2700.844376	2.0207	0.03	13.8, 15.6, 21.0	**0.00**	0.00	**0.00**
				BS-singlet	triplet	N1=+0.250 N2=–0.250 N48=–0.250 N49=+0.250	–2702.07909951	-	-	0.9768	-	-	–	0.43	**0.83**
				BS-singlet	BS-singlet	N1=+0.247 N2=–0.247 N48=–0.247 N49=+0.247	–2702.07912348	1.235334	–2700.843790	0.9728	3.01	11.9, 15.7, 19.5	–	0.37	**0.71**
1$^{2.2+}$-C_{2h}	UB3LYP	DCM	Min	Triplet-^3A_u	triplet	N1=N2=N48=N49=+0.248	–2702.07901795	1.235311	–2700.843707	2.0204	4.28	13.4, 15.2, 19.6	**0.42**	0.00	**0.00**
				BS-singlet	triplet	N1=+0.247 N2=-0.247 N48=-0.247 N49=+0.247	–2702.07800529	-	-	0.9916	-	-	–	0.55	**1.25**
				BS-singlet	BS-singlet	N1=+0.245 N2=-0.245 N48=-0.245 N49=+0.245	–2702.07806999	1.235246	–2700.842824	0.9858	6.55	13.2, 15.1, 19.3	–	0.64	**1.08**
1$^{2.2+}$-C_1	UB3LYP	DCM	TS	triplet	triplet	N1=+0.300 N2=+0.300 N30=+0.271 N31=+0.304	–2702.02216239	1.234283	–2700.787879	2.0219	0.45	***i64.3***, 8.3, 15.6	**35.45**	-	-
1$^{2.2+}$-D_2	UM06-2X	DCM	Min	Triplet-$^3B_3$	triplet	N1=N2=N48=N49=+0.283	–2700.93063140	1.247812	–2699.682820	2.0242	0.04	9.4, 12.0, 21.5	**0.00**	0.00	**0.00**
				BS-singlet	BS-singlet	N1=+0.280 N2=–0.280 N48=–0.280 N49=+0.280	–2700.92991286	1.247994	–2699.681919	0.9994	0.24	10.7, 13.1, 22.1	–	0.57	**1.12**
1$^{2.2+}$-C_{2h}	UM06-2X	DCM	Min	Triplet-^3A_u	triplet	N1=N2=N48=N49=+0.279	–2700.93006467	1.247725	–2699.682340	2.0242	1.40	13.9, 15.8, 20.7	**0.30**	0.00	**0.00**
				BS-singlet	BS-singlet	N1=+0.278 N2=–0.278 N48=-0.278 N49=+0.278	–2700.92912184	1.247428	–2699.681694	1.0049	1.73	13.8, 15.3, 20.1	-	0.41	**0.81**
1$^{2.2+}$-C_1	UM06-2X	DCM	TS	triplet	triplet	N1=+0.330 N2=+0.255 N30=+0.304 N31=+0.335	–2700.8694201	1.247100	-2699.622320	2.0253	1.43	***i40.9***, 12.3, 17.9	**37.96**	-	-

[a] 1 Hartree = 627.51 kcal mol^{-1}. [b] In Cartesian coordinates. * Wavefunction was tested for stability (stable=opt) and was found to be stable. **For transition state **1**$^{2.2+}$-C_1 in the gas phase, singlet ($\langle S^2\rangle$ = 0.0000) wavefunction was found to be unstable; upon reoptimization of the wavefunction and geometry, BSsinglet wavefunction ($\langle S^2\rangle$ = 0.9763), which was found to be stable, was obtained. [c] Following IRC starting from the TS, optimization of one of the structures gave C_{2h}-symmetric double helicene (see: Table S15 below)

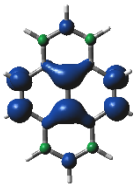
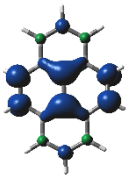
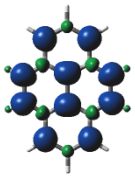
Table S9. Spin densities, positive (blue) and negative (green) spin densities shown at the isodensity level of 0.003 electron/Bohr^3 and determining molecular orbital configurations for radical cations **1a**$^{\bullet+}$-C_{2h} and -D_2, and diradical dication **1a**$^{2\bullet2+}$-D_{2h} of model bishydrazine **1a** at the UB3LYP/6-31G(d) level in the gas phase.[a]



1a$^{\bullet+}$



1a$^{2\bullet2+}$

1a$^{\bullet+}$-C_{2h} (gas phase)		**1a**$^{\bullet+}$-D_2 (gas phase)		**1a**$^{2\bullet2+}$-D_{2h} (triplet, gas phase)	
					
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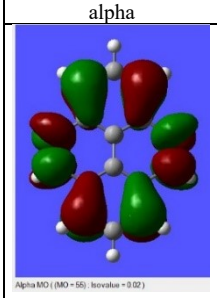
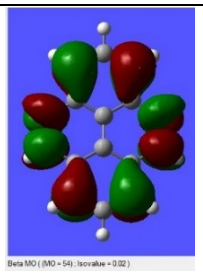
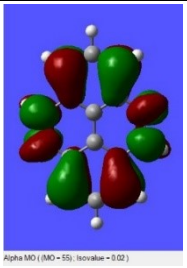
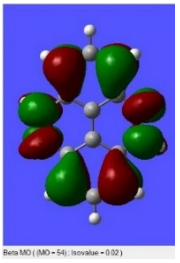
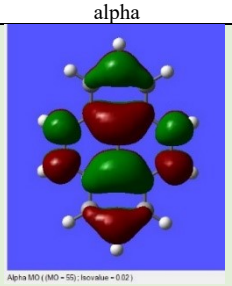
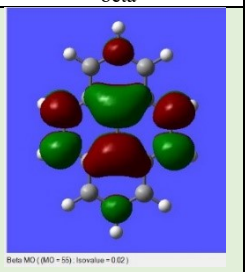
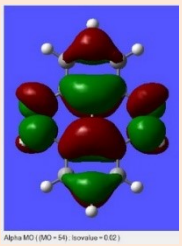
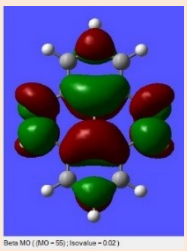
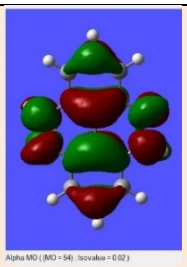
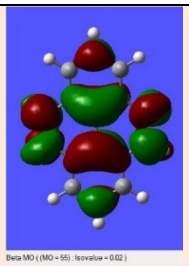
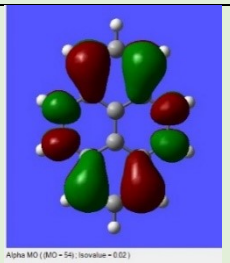
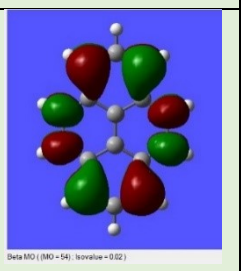
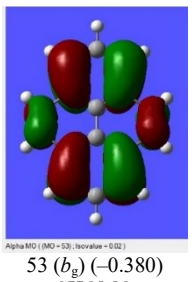
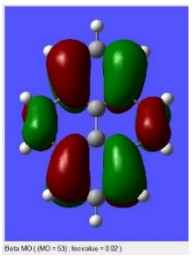
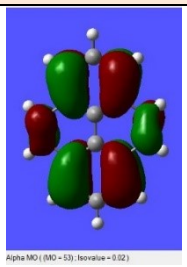
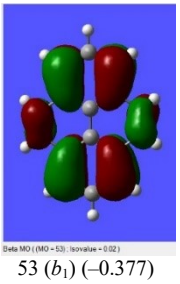
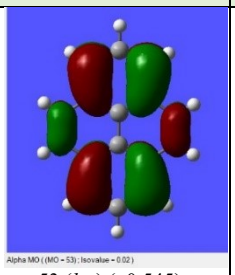
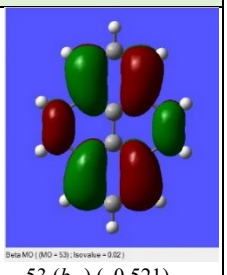
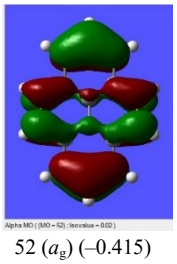
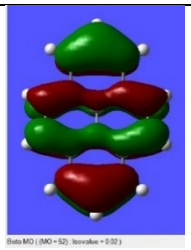
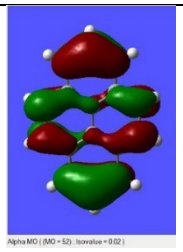
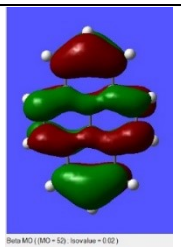
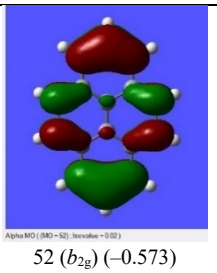
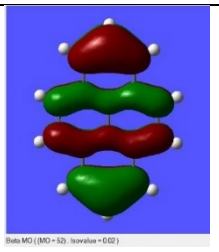
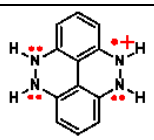
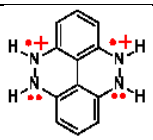
					
55 (a_u) (–0.3244) HOMO	54 (a_u) (–0.3093) HOMO	55 (a) (–0.3252) HOMO	54 (a) (–0.3097) HOMO	55 (b_{2g}) (–0.4799) SOMO	55 (b_{2g}) (–0.3956) LUMO
					
54 (a_g) (–0.3255) SOMO	55 (a_g) (–0.2611) LUMO	54 (b_2) (–0.3260) SOMO	55 (b_2) (–0.2615) LUMO	54 (a_u) (–0.4888) SOMO	54 (a_u) (–0.4107) LUMO
					
53 (b_g) (–0.380) SHOMO	53 (b_g) (–0.376) SHOMO	53 (b_1) (–0.380) SHOMO	53 (b_1) (–0.377) SHOMO	53 (b_{1g}) (–0.545) HOMO	53 (b_{1g}) (–0.521) HOMO
					
52 (a_g) (–0.415) S2HOMO	52 (a_g) (–0.402) S2HOMO	52 (b_2) (–0.414) S2HOMO	52 (b_2) (–0.402) S2HOMO	52 (b_{2g}) (–0.573) SHOMO	52 (b_{2g}) (–0.547) SHOMO

[a] MO number (symmetry label) (energy in a.u.) and frontier MO label are given for each MO.

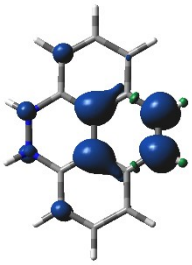
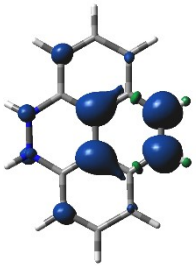
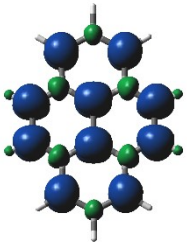
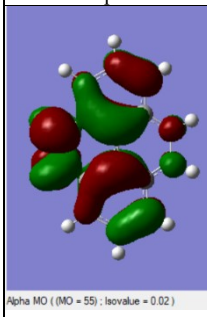
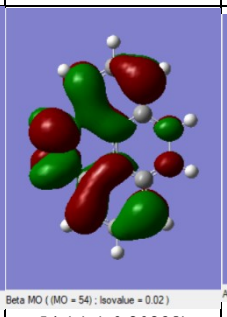
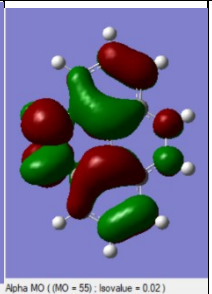
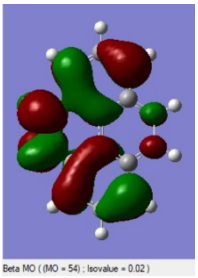
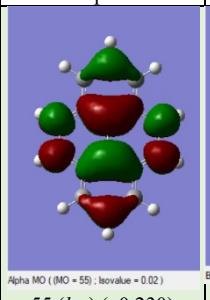
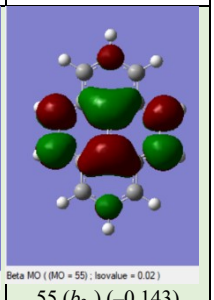
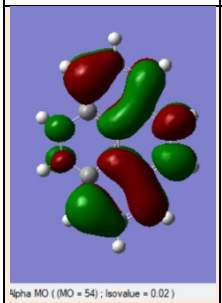
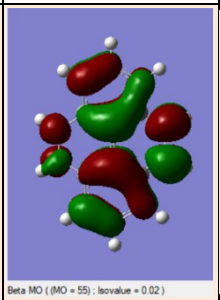
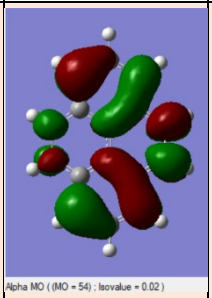
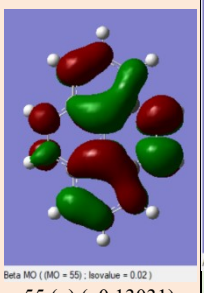
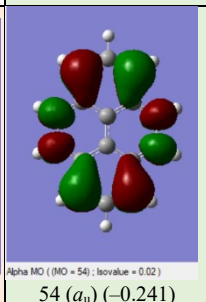
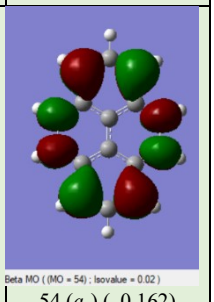
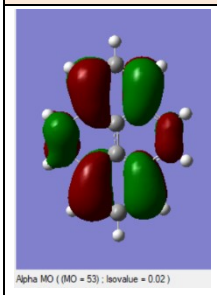
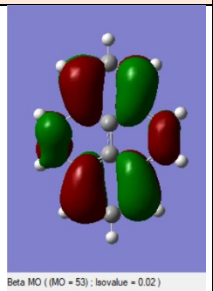
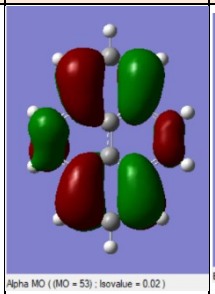
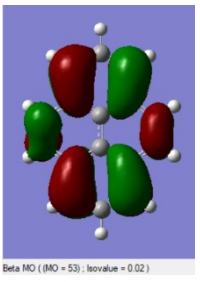
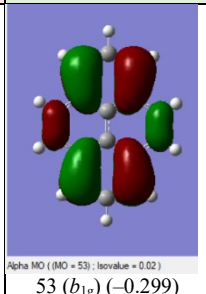
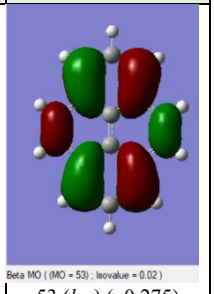
Table S10. Spin densities, positive (blue) and negative (green) spin densities shown at the isodensity level of 0.003 electron/Bohr^3 and determining molecular orbital configurations for radical cations **1a**$^{\bullet+}$-C_2 of model bishydrazine **1a** at the UB3LYP/6-31G(d)/IEF-PCM-UFF level in DCM and in water, and for triplet ground state of diradical dication **1a**$^{2\bullet2+}$-D_{2h} in water.[a]



1a$^{\bullet+}$

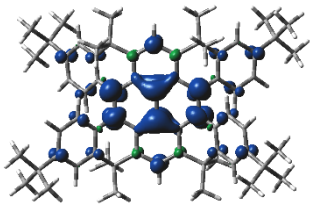
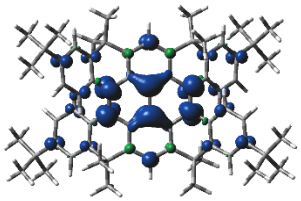
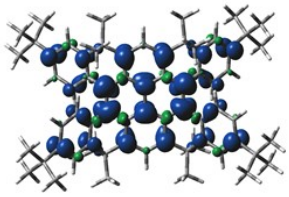
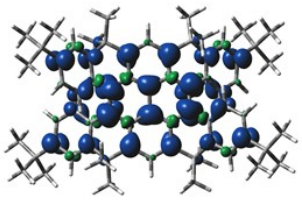
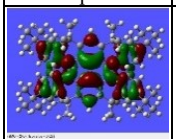
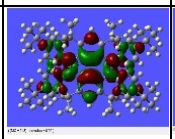
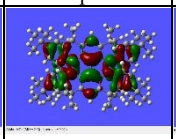
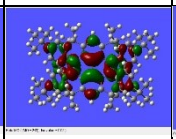
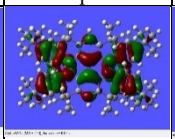
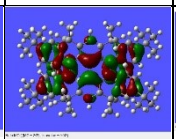
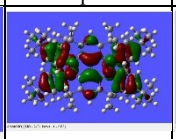
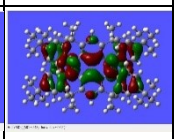
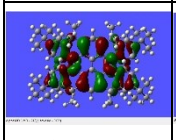
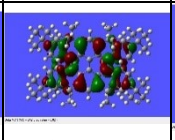
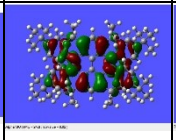
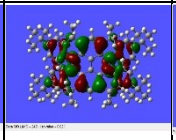
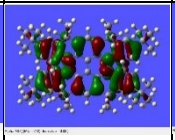
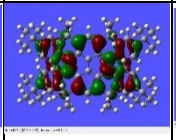
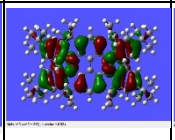
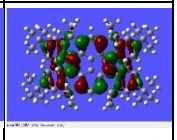
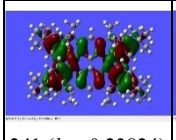
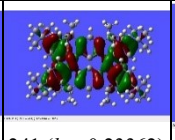
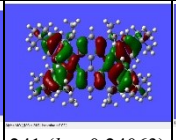
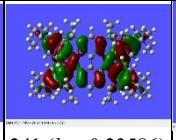
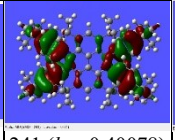
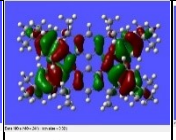
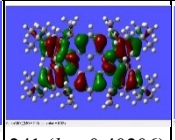
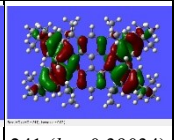


1a$^{2\bullet2+}$

1a$^{\bullet+}$-C_2 (DCM)		**1a**$^{\bullet+}$-C_2 (water)		**1a**$^{2\bullet2+}$-D_{2h} (triplet, water)	
					
alpha	beta	alpha	beta	alpha	beta
					
55 (*a*) (–0.20852) HOMO	54 (*a*) (–0.20298) HOMO	55 (*a*) (–0.19744) HOMO	54 (*a*) (–0.19239) HOMO	55 (b_{2g}) (–0.230) SOMO	55 (b_{2g}) (–0.143) LUMO
					
54 (*a*) (–0.21810) SOMO	55 (*a*) (–0.14268) LUMO	54 (*a*) (–0.20650) SOMO	55 (*a*) (–0.13031) LUMO	54 (a_u) (–0.241) SOMO	54 (a_u) (–0.162) LUMO
					
53 (*b*) (–0.27250) SHOMO	53 (*b*) (–0.26540) SHOMO	53 (*b*) (–0.26144) SHOMO	53 (*b*) (–0.25406) SHOMO	53 (b_{1g}) (–0.299) HOMO	53 (b_{1g}) (–0.275) HOMO

[a] Spin density maps, and MO number (symmetry label) (energy in a.u.) and frontier MO label are given for each MO.

Table S11. Spin densities, positive (blue) and negative (green) spin densities shown at the isodensity level of 0.002 electron/Bohr^3, and determining molecular orbital configurations for radical cations C_{2h}- and D_2-**1**$^{\bullet+}$ at the UB3LYP/6-31G(d)/IEF-PCM-UFF level in dichloromethane (DCM) and for triplet states of diradical dications C_{2h}- and D_2-**1**$^{2\bullet2+}$ at the UB3LYP/6-31G(d) level in the gas phase.[a]

Radical cation				Diradical dication (triplet)			
C_{2h} in DCM		D_2 in DCM		C_{2h} in the gas phase		D_2 in the gas phase	
							
alpha	beta	alpha	beta	alpha	beta	alpha	beta
							
243 (a_g, -0.20663) SOMO	243 (a_g, -0.16110) LUMO	243 (b_3, -0.20462) SOMO	243 (b_3, -0.15929) LUMO	243 (a_g, -0.37583) SOMO	243 (a_g, -0.31840) LUMO	243 (b_3, -0.37434) SOMO	243 (b_3, -0.31644) LUMO
							
242 (a_u, -0.20934) HOMO	242 (a_u, -0.19591) HOMO	242 (a, -0.20949) HOMO	242 (a, -0.19533) HOMO	242 (a_u, -0.37976) SOMO	242 (a_u, -0.32623) LUMO	242 (a, -0.37979) SOMO	242 (a, -0.32529) LUMO
							
241 (b_g, -0.23824) SHOMO	241 (b_g, -0.23362) SHOMO	241 (b_1, -0.24063) SHOMO	241 (b_1, -0.23586) SHOMO	241 (b_g, -0.40078) HOMO	241 (b_g, -0.38872) HOMO	241 (b_1, -0.40206) HOMO	241 (b_1, -0.39034) HOMO

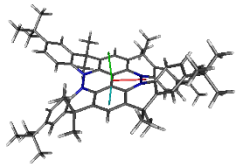
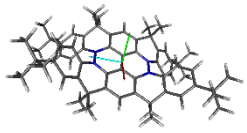
[a] Spin density maps, and MO number (symmetry label) (energy in a.u.) and frontier MO label are given for each MO.

Table S12. Selected bond lengths (Å) in conjoined [5]helicenes: D_2-symmetric (*P,P*)-**1**-D_2, C_{2h}-symmetric (*meso*) (*P,M*)-**1**-C_{2h}, the corresponding radical cations and diradical dications computed at the B3LYP/6-31G(d)+ZPVE (gas phase) and B3LYP/6-31G(d)/IEF-PCM-UFF +ZPVE (DCM) levels of theory.

Compound	Bond length (Å)			
	Gas Phase		DCM	
	C23-C46[a]	N1-N49	C23-C46[a]	N1-N49
(*P,P*)-**1**-D_2	1.446	1.420	1.446	1.420
(*P,M*)-**1**-C_{2h}	1.448	1.419	1.448	1.419
(*P,P*)-$\mathbf{1}^{\cdot+}$-D_2	1.421	1.399	1.420	1.398
(*P,M*)-$\mathbf{1}^{\cdot+}$-C_{2h}	1.423	1.397	1.421	1.396
(*P,P*)-$\mathbf{1}^{2.2+}$-D_2 triplet	1.422	1.381	1.419	1.378
(*P,M*)-$\mathbf{1}^{2.2+}$-C_{2h} triplet	1.423	1.381	1.420	1.378
(*P,P*)-$\mathbf{1}^{2.2+}$-D_2 BS singlet	1.418	1.381	1.414	1.378
(*P,M*)-$\mathbf{1}^{2.2+}$-C_{2h} BS singlet	1.420	1.380	1.416	1.378

[a] Center C-C bond.

Table S13. B3LYP/EPR-II *D*-tensors and largest component of the ^{14}N *A*-tensors for triplet states of diradical dications. Coordinates *x*, *y*, *z* define molecule orientation in ORCA.[a]

			D-tensor (cm^{-1})				*A*$_{ZZ}$ (MHz)			
Diradical dication	*D* (cm^{-1})	*E* (cm^{-1})		D_{YY}	D_{XX}	D_{ZZ}	N1	N2	N3	N4
	+0.01316	+0.00367		–0.00806	+0.00072	+0.00877	+20.899	+20.899	+20.899	+20.899
			x	-1.0000	0.0000	0.0000	-0.2860	-0.2860	+0.2860	+0.2860
			y	0.0000	0.0000	+1.0000	+0.9160	+0.9160	+0.9160	+0.9160
(*P,P*)-$\mathbf{1}^{2.2+}$-D_2			z	0.0000	+1.0000	0.0000	-0.2860	+0.2860	+0.2860	-0.2860
				D-tensor (cm^{-1})			*A*$_{ZZ}$ (MHz)			
Diradical dication	*D* (cm^{-1})	*E* (cm^{-1})		D_{YY}	D_{XX}	D_{ZZ}	N1	N2	N3	N4
	+0.01354	+0.00375		-0.00826	-0.00077	+0.00903	+20.602	+20.602	+20.602	+20.602
			x	0.0000	+0.8915	+0.4530	-0.2065	-0.2065	-0.2065	-0.2065
			y	0.0000	-0.4530	+0.8915	-0.9331	-0.9331	-0.9331	-0.9331
(*P,M*)-$\mathbf{1}^{2.2+}$-C_{2h}			z	+1.0000	0.0000	0.0000	-0.2943	+0.2943	-0.2943	+0.2943

[a] *x*, *y*, and *z* axes for (*P,P*)-$\mathbf{1}^{2.2+}$-D_2 are shown in red, green, and blue, respectively. Note that the largest components of *D*- and *A*-tensors, i.e., D_{ZZ} and A_{ZZ}, are oriented along *y*-axis of the molecules, which coincides with the $2p_\pi$ orbital axis. Computed components of *g*-matrix for (*P,P*)-$\mathbf{1}^{2.2+}$-D_2: $g_{iso} = (g_{ZZ} + g_{YY} + g_{XX})/3 = (2.00238 + 2.00334 + 2.00366)/3 = 2.0031$ and for (*P,M*)-$\mathbf{1}^{2.2+}$-C_{2h}: $g_{iso} = (g_{ZZ} + g_{YY} + g_{XX})/3 = (2.00238 + 2.00332 + 2.00368)/3 = 2.0031$. Smallest *g*-tensor component, g_{ZZ}, is oriented along the *y*-axis of the molecules, which coincides with the $2p_\pi$ orbital axis, as expected.

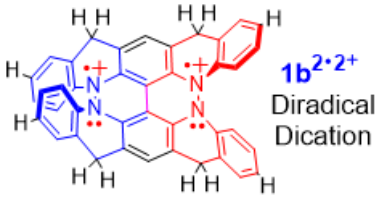
Table S14. Internal reaction coordinate (IRC) from C_1-symmetric TS to D_2- and C_{2h}-symmetric neutral conjoined helicene in DCM at the M06-2X/6-31G(d) level. Following IRC starting from the TS, re-optimization with no symmetry constraints of one of the structures (IRC#6 with IRC Reaction Coordinate of +0.1019) gave C_{2h}-symmetric minimum with total energy of -2701.31593888 a.u. (RMS gradient norm of 1.8×10^{-7} a.u.).

```
Reaction path calculation complete.
Energies reported relative to the TS energy of      -2701.243052
 ----------------------------------------------------------------------------
   Summary of reaction path following
 ----------------------------------------------------------------------------
                     Energy   Rx Coord
  1                 -0.00003  -0.11248
  2                 -0.00003  -0.11240
  3                 -0.00003  -0.10850
  4                 -0.00002  -0.10337
  5                  0.00000   0.00000
  6                 -0.00003   0.10190
 ----------------------------------------------------------------------------
 Total number of points: 5
```

Table S15. Internal reaction coordinate (IRC) from C_1-symmetric TS to D_2- and C_{2h}-symmetric triplet diradical dication of conjoined helicene in the gas phase at the UB3LYP/6-31G(d) level. Following IRC starting from the TS, optimization of one of the structures (IRC#1 with IRC Reaction Coordinate of -0.10748) gave C_{2h}-symmetric minimum with total energy of -2702.34706058 a.u. (RMS gradient norm of 2.2×10^{-7} a.u.).

```
Reaction path calculation complete.
Energies reported relative to the TS energy of      -2701.879557
 ----------------------------------------------------------------------------
   Summary of reaction path following
 ----------------------------------------------------------------------------
                     Energy   Rx Coord
  1                 -0.00002  -0.10748
  2                 -0.00002  -0.10350
  3                 -0.00002  -0.09707
  4                 -0.00002  -0.09654
  5                  0.00000   0.00000
  6                 -0.00002   0.09888
  7                 -0.00002   0.10011
  8                 -0.00002   0.10223
 ----------------------------------------------------------------------------
 Total number of points: 7
```

Table S16. Structure drawing of simplified diradical dication of conjoined [5]helicene $\mathbf{1b}^{2.2+}$, in which *tert*-butyl and *gem*-dimethyl groups were replaced with hydrogens. Triplet states of diradical dications of conjoined [5]helicenes: D_2-symmetric (*P,P*)-$\mathbf{1b}^{2.2+}$-D_2, C_{2h}-symmetric (*meso*) (*P,M*)-$\mathbf{1b}^{2.2+}$-C_{2h}, and C_1-symmetric transition state TS-(*P*)-$\mathbf{1b}^{2.2+}$-C_1: UB3LYP/6-31G(d)+ZPVE, ROMP2/6-31G(d)//UB3LYP/6-31G(d), UMP2/6-31G(d)//UB3LYP/6-31G(d), and UMP3/6-31G(d)//UB3LYP/6-31G(d) energies (hartree), lowest vibrational frequencies (cm^{-1}), RMS gradient norms (a.u.) in Cartesian coordinates, relative energies for triplet states prior to ZPVE correction (ΔE, kcal mol^{-1}).[a]



Level of theory	Point group	Point on PES	El. State	$<S^2>$	$E°$	ZPVE	$E°$ + ZPVE	RMS gradient norm[b] ($\times 10^{-6}$)	Lowest vibrational frequencies	μ	ΔE[c]
UB3LYP/6-31G(d) +ZPVE	D_2	Min	$^3B_3$	2.0219	-1758.40018832	0.557669	-1757.842519	1.99	26.6, 33.2, 55.2	0.00	0.00
	C_{2h}	Min	^3A_u	2.0215	-1758.39891208	0.557788	-1757.841124	3.41	26.7, 32.7, 50.9	0.00	0.80
	C_1	TS	^3A	2.0226	-1758.33941396	0.556858	-1757.782556	0.12	***i68.4,*** 30.4, 37.3	0.80	38.14
ROMP2/6-31G(d) //UB3LYP/6-31G(d)	D_2	Min	$^3B_3$	2.00	-1752.91308755	-	-	-	-	0.00	0.00
	C_{2h}	Min	^3A_u	2.00	-1752.91310985	-	-	-	-	0.00	–0.01
	C_1	TS	^3A	2.00	-1752.85222125	-	-	-	-	0.94	38.19
UMP2/6-31G(d) //UB3LYP/6-31G(d)[d]	D_2	Min	$^3B_3$	4.28	-1752.6927878034	-	-	-	-	0.00	0.00
	C_{2h}	Min	^3A_u	4.28	-1752.6922730086	-	-	-	-	4.66	0.32
	C_1	TS	^3A	4.45	-1752.6183910797	-	-	-	-	0.00	46.68
UMP3/6-31G(d) //UB3LYP/6-31G(d)[d]	C_2	Min	$^3B_3$	-	-1752.84698830	-	-	-	-	0.00	0.00
	D_2	Min	^3A_u	-	-1752.84590140	-	-	-	-	0.00	0.68

[a] 1 Hartree = 627.51 kcal mol^{-1}. [b] In Cartesian coordinates. [c] All relative energies are listed without ZPVE correction; at the UB3LYP/6-31G(d) + ZPVE level, ΔE = 0.00, 0.88, 37.62 kcal mol^{-1} for $\mathbf{1b}^{2\cdot 2+}$. [d] Computations at UMPn (n = 2 and 3) suffer from inadequate starting UHF wf, for which $<S^2>$ = 4.96 (after 12.9), 4.95 (after 12.9), 5.16 (after 14.1) for D_2-, C_{2h}-, C_1-symmetric $\mathbf{1b}^{2\cdot 2+}$. Consequently, the barrier for racemization of 46.7 kcal mol^{-1} at the UMP2/6-31G(d)//UB3LYP/6-31G(d) level is overestimated compared to 38.1 kcal mol^{-1} at the UB3LYP/6-31G(d) level or 37.6 kcal mol^{-1} at the UB3LYP/6-31G(d)+ZPVE level.

2. ^{1}H NMR Spectra of crude mixtures and purified 1-D_2.

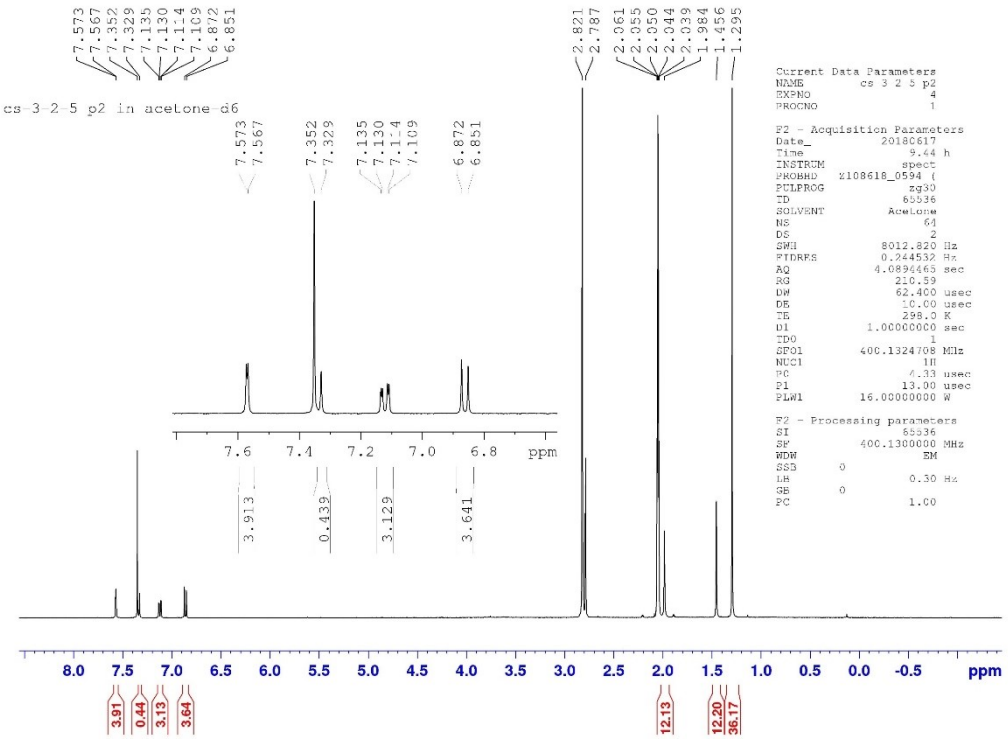


Fig. S37. ^{1}H NMR spectrum (400 MHz, acetone-d_6, CS-3-2-5 p2) of the sample obtained after purification.

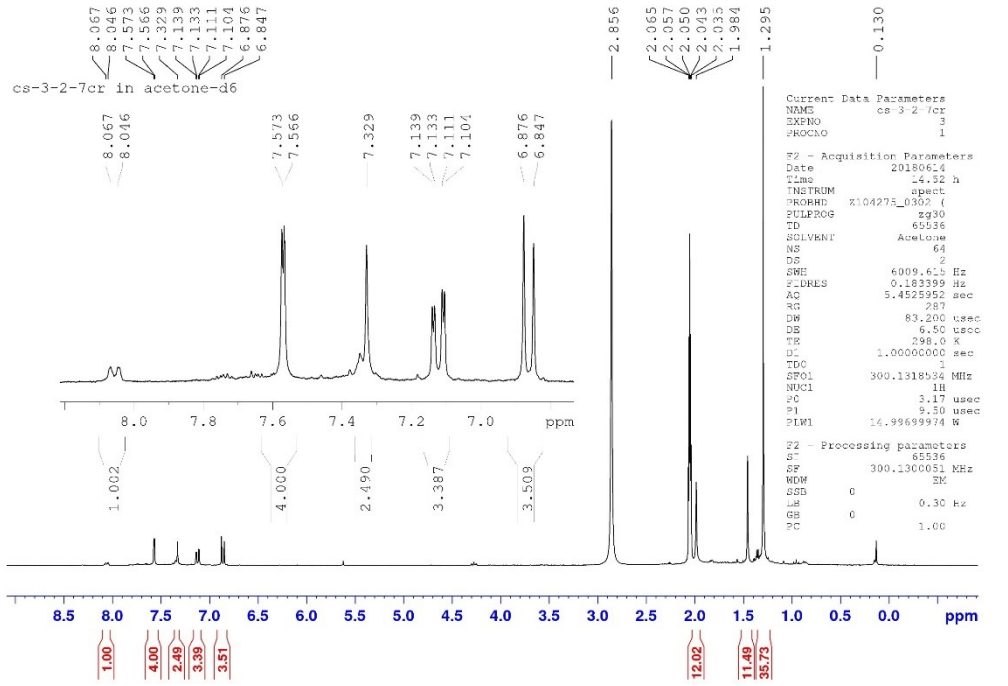


Fig. S38. ^{1}H NMR spectrum (300 MHz, acetone-d_6, CS-3-2-7cr) of the crude mixture obtained after quench.

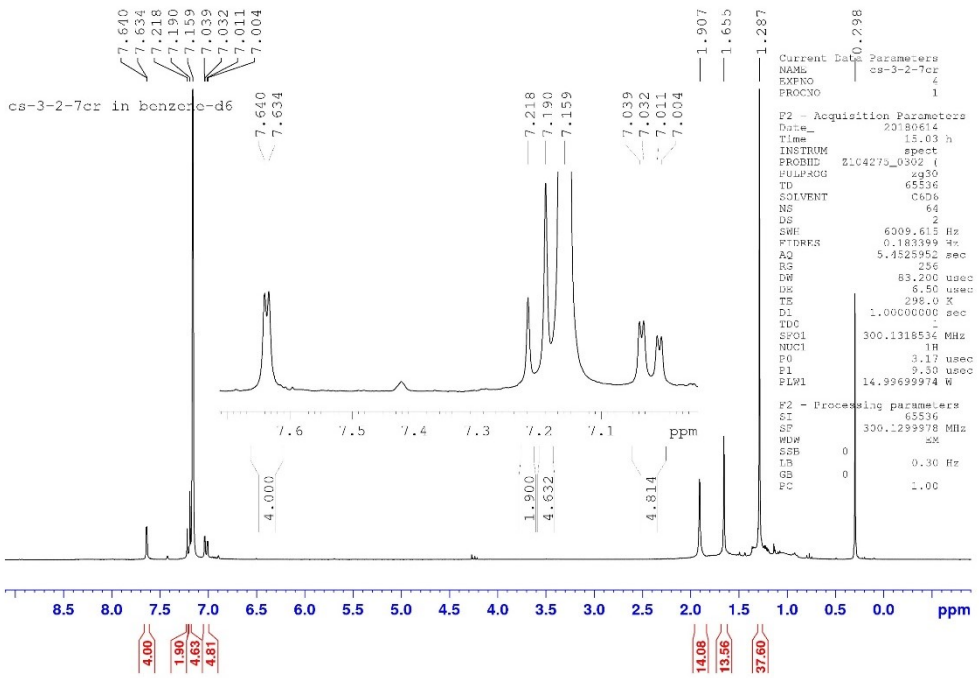


Fig. S39. ^{1}H NMR spectrum (300 MHz, benzene-d_6, CS-3-2-7cr) of the crude mixture obtained after quench.

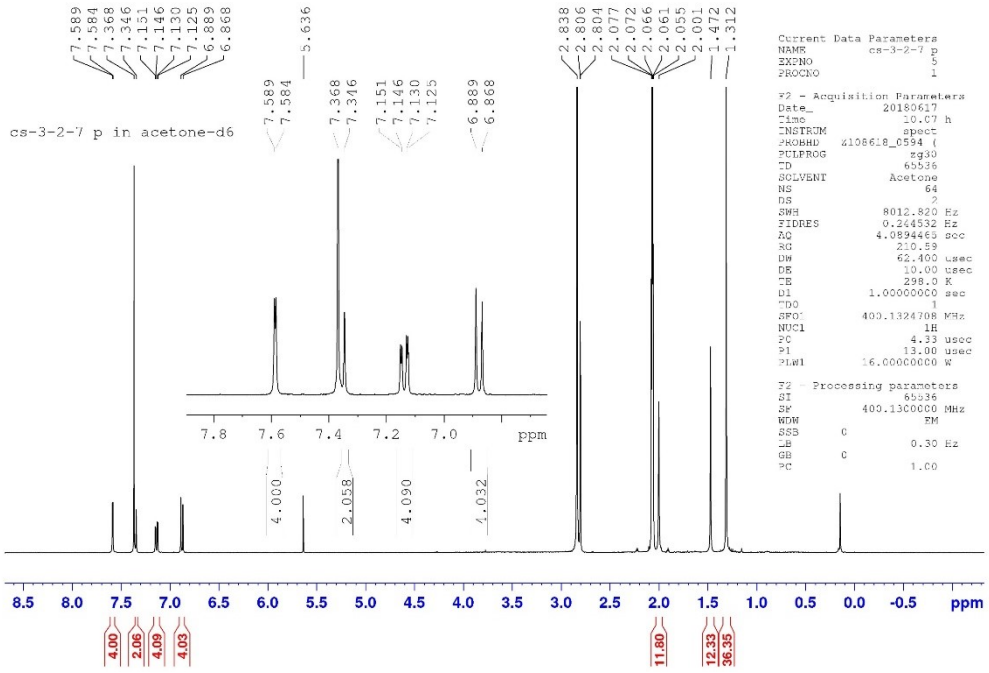


Fig. S40. ^{1}H NMR spectrum (400 MHz, acetone-d_6, CS-3-2-7p) of the sample obtained after purification

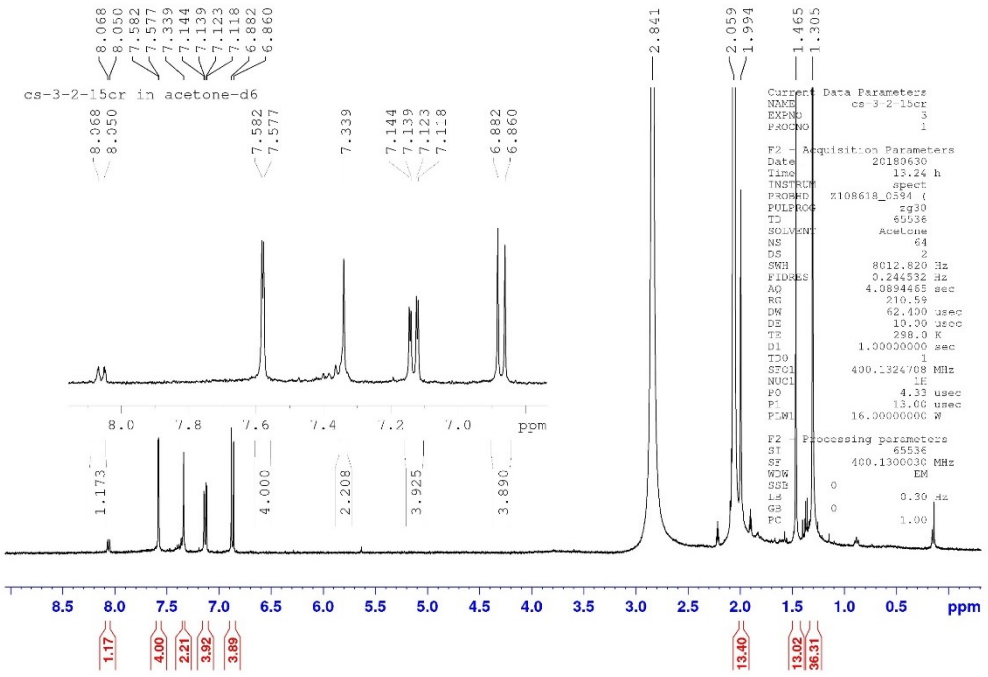


Fig. S41. [1]H NMR spectrum (400 MHz, acetone-d_6, CS-3-2-15cr) of the crude mixture obtained after quench.

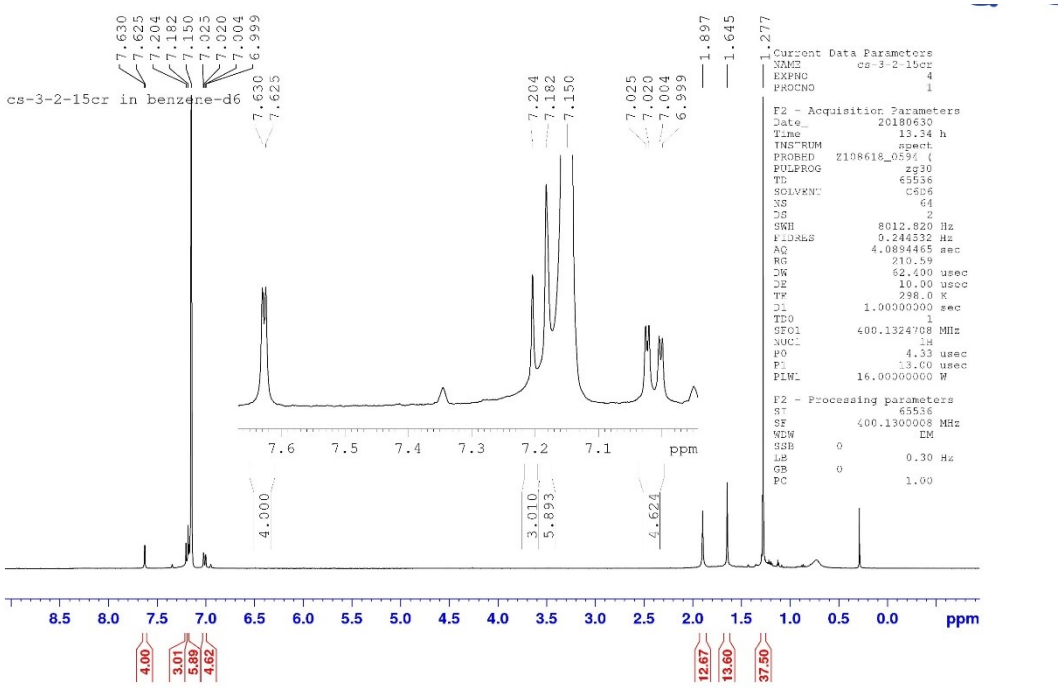


Fig. S42. [1]H NMR spectrum (400 MHz, benzene-d_6, CS-3-2-15bcr) of the crude mixture obtained after quench.

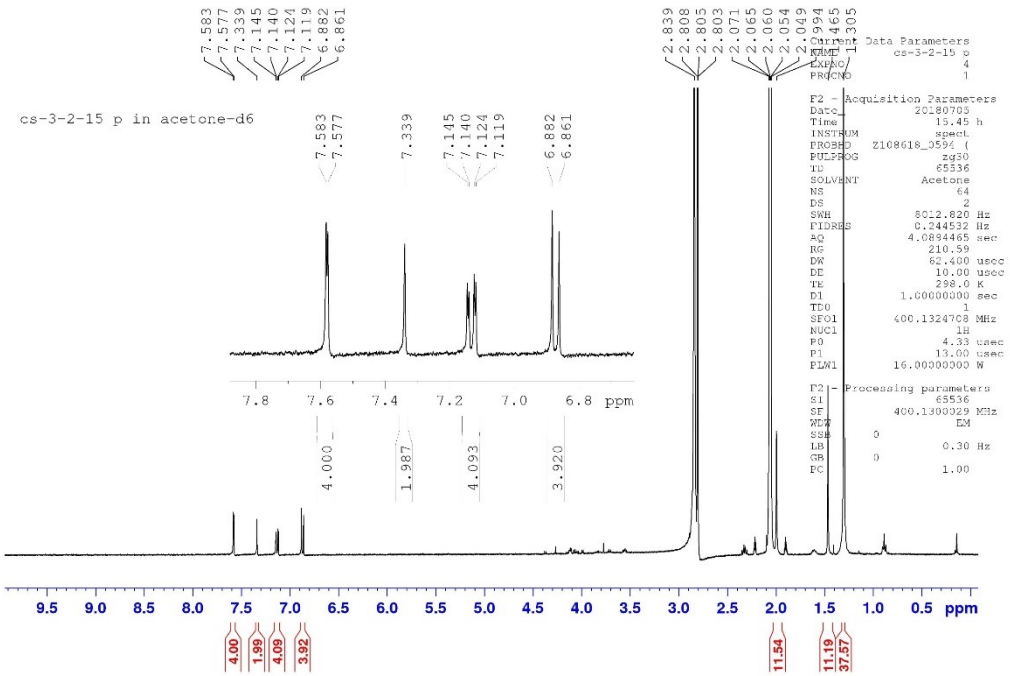


Fig. S43. ^{1}H NMR spectrum (400 MHz, acetone-d_6, CS-3-2-15p) of the sample obtained after purification.

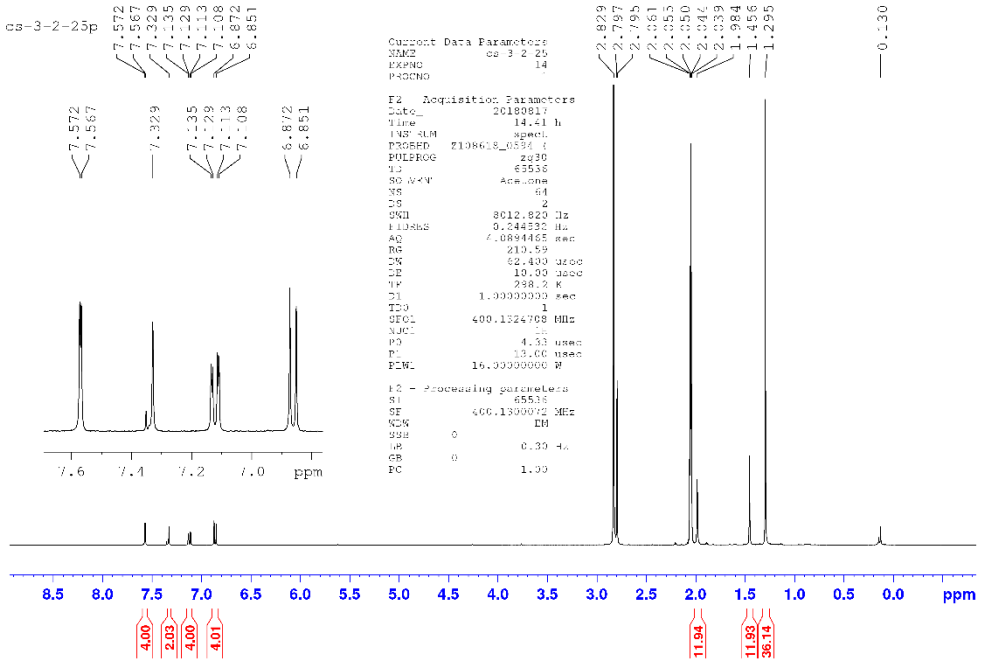


Fig. S44. ^{1}H NMR spectrum (400 MHz, acetone-d_6, CS-3-2-25p) of the sample obtained after purification.

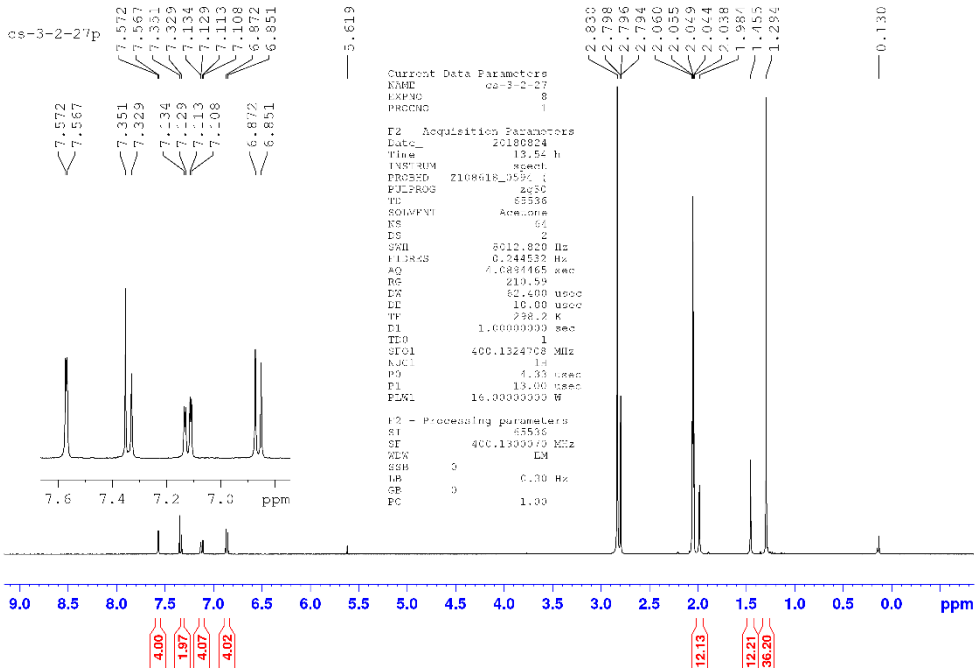


Fig. S45. ^{1}H NMR spectrum (400 MHz, acetone-d_6, CS-3-2-27p) of the sample obtained after purification.

3. Outputs of DFT Calculations for Conjoined [5]Helicenes: Neutrals, Radical Cations, and Diradical Dications.

Conjoined [5]helicene, chiral, D_2 at B3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4
Framework group D2[C2(HCC.CCH),X(C60H72N4)]
Deg. of freedom 105
Full point group D2
Largest Abelian subgroup D2 NOp 4
Largest concise Abelian subgroup D2 NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.429067	0.086661	0.704861
2	7	0	-2.429067	-0.086661	0.704861
3	6	0	5.348004	2.637065	2.446818
4	6	0	4.457145	1.868688	3.216583
5	1	0	4.519465	1.936987	4.296433
6	6	0	3.505185	1.012098	2.664137
7	6	0	2.596300	0.102181	3.512338
8	6	0	1.231797	0.050191	2.817599
9	6	0	0.000000	0.000000	3.481829
10	1	0	0.000000	0.000000	4.563780
11	6	0	-1.231797	-0.050191	2.817599
12	6	0	-2.596300	-0.102181	3.512338
13	6	0	-3.505185	-1.012098	2.664137
14	6	0	-4.457145	-1.868688	3.216583
15	1	0	-4.519465	-1.936987	4.296433
16	6	0	-5.348004	-2.637065	2.446818
17	6	0	-5.251601	-2.511136	1.058603
18	1	0	-5.913605	-3.069518	0.406098
19	6	0	-4.302720	-1.678427	0.465269
20	1	0	-4.249182	-1.606300	-0.613160
21	6	0	-3.417981	-0.944596	1.254998
22	6	0	-1.209343	-0.018176	1.416442
23	6	0	0.000000	0.000000	0.722781
24	6	0	1.209343	0.018176	1.416442
25	6	0	3.417981	0.944596	1.254998
26	6	0	4.302720	1.678427	0.465269
27	6	0	5.251601	2.511136	1.058603
28	1	0	5.913605	3.069518	0.406098
29	6	0	3.199135	-1.332446	3.539025
30	1	0	3.254174	-1.763102	2.535936
31	1	0	2.573891	-1.992077	4.152118
32	1	0	4.209355	-1.314519	3.964207
33	6	0	2.482288	0.591425	4.966725
34	1	0	2.074738	1.606213	5.026016
35	1	0	3.459772	0.581163	5.458262
36	1	0	1.838266	-0.074839	5.548613
37	6	0	-2.482288	-0.591425	4.966725
38	1	0	-2.074738	-1.606213	5.026016
39	1	0	-3.459772	-0.581163	5.458262
40	1	0	-1.838266	0.074839	5.548613
41	6	0	-3.199135	1.332446	3.539025
42	1	0	-3.254174	1.763102	2.535936
43	1	0	-2.573891	1.992077	4.152118
44	1	0	-4.209355	1.314519	3.964207
45	1	0	4.249182	1.606300	-0.613160
46	6	0	0.000000	0.000000	-0.722781
47	6	0	-1.209343	0.018176	-1.416442
48	7	0	-2.429067	0.086661	-0.704861
49	7	0	2.429067	-0.086661	-0.704861
50	6	0	1.209343	-0.018176	-1.416442
51	6	0	-1.231797	0.050191	-2.817599
52	6	0	1.231797	-0.050191	-2.817599
53	6	0	0.000000	0.000000	-3.481829
54	1	0	0.000000	0.000000	-4.563780
55	6	0	2.596300	-0.102181	-3.512338
56	6	0	-2.596300	0.102181	-3.512338
57	6	0	3.505185	-1.012098	-2.664137
58	6	0	-3.505185	1.012098	-2.664137
59	6	0	-3.417981	0.944596	-1.254998
60	6	0	3.417981	-0.944596	-1.254998
61	6	0	-4.457145	1.868688	-3.216583
62	1	0	-4.519465	1.936987	-4.296433
63	6	0	4.457145	-1.868688	-3.216583
64	1	0	4.519465	-1.936987	-4.296433
65	6	0	5.348004	-2.637065	-2.446818
66	6	0	5.251601	-2.511136	-1.058603
67	1	0	5.913605	-3.069518	-0.406098
68	6	0	4.302720	-1.678427	-0.465269
69	1	0	4.249182	-1.606300	0.613160
70	6	0	-5.348004	2.637065	-2.446818
71	6	0	-5.251601	2.511136	-1.058603
72	6	0	-4.302720	1.678427	-0.465269
73	1	0	-4.249182	1.606300	0.613160
74	1	0	-5.913605	3.069518	-0.406098
75	6	0	-3.199135	-1.332446	-3.539025
76	1	0	-3.254174	-1.763102	-2.535936

77	1	0	-4.209355	-1.314519	-3.964207
78	1	0	-2.573891	-1.992077	-4.152118
79	6	0	-2.482288	0.591425	-4.966725
80	1	0	-2.074738	1.606213	-5.026016
81	1	0	-1.838266	-0.074839	-5.548613
82	1	0	-3.459772	0.581163	-5.458262
83	6	0	2.482288	-0.591425	-4.966725
84	1	0	2.074738	-1.606213	-5.026016
85	1	0	1.838266	0.074839	-5.548613
86	1	0	3.459772	-0.581163	-5.458262
87	6	0	3.199135	1.332446	-3.539025
88	1	0	2.573891	1.992077	-4.152118
89	1	0	3.254174	1.763102	-2.535936
90	1	0	4.209355	1.314519	-3.964207
91	6	0	6.373718	-3.550847	-3.142267
92	6	0	-6.373718	3.550847	-3.142267
93	6	0	-6.373718	-3.550847	3.142267
94	6	0	6.373718	3.550847	3.142267
95	6	0	5.634695	-4.586277	-4.023118
96	1	0	5.028376	-4.104645	-4.797648
97	1	0	6.353988	-5.244886	-4.525746
98	1	0	4.967460	-5.210329	-3.417767
99	6	0	7.309650	-2.699524	-4.033046
100	1	0	8.044666	-3.338571	-4.538224
101	1	0	6.754235	-2.156691	-4.805357
102	1	0	7.855070	-1.961565	-3.433717
103	6	0	7.245550	-4.320428	-2.131895
104	1	0	7.827633	-3.643655	-1.496207
105	1	0	6.642342	-4.965175	-1.482564
106	1	0	7.954676	-4.961414	-2.668176
107	6	0	-7.245550	4.320428	-2.131895
108	1	0	-7.827633	3.643655	-1.496207
109	1	0	-6.642342	4.965175	-1.482564
110	1	0	-7.954676	4.961414	-2.668176
111	6	0	-5.634695	4.586277	-4.023118
112	1	0	-4.967460	5.210329	-3.417767
113	1	0	-5.028376	4.104645	-4.797648
114	1	0	-6.353988	5.244886	-4.525746
115	6	0	-7.309650	2.699524	-4.033046
116	1	0	-6.754235	2.156691	-4.805357
117	1	0	-7.855070	1.961565	-3.433717
118	1	0	-8.044666	3.338571	-4.538224
119	6	0	-5.634695	-4.586277	4.023118
120	1	0	-5.028376	-4.104645	4.797648
121	1	0	-6.353988	-5.244886	4.525746
122	1	0	-4.967460	-5.210329	3.417767
123	6	0	-7.245550	-4.320428	2.131895
124	1	0	-7.827633	-3.643655	1.496207
125	1	0	-6.642342	-4.965175	1.482564
126	1	0	-7.954676	-4.961414	2.668176
127	6	0	-7.309650	-2.699524	4.033046
128	1	0	-6.754235	-2.156691	4.805357
129	1	0	-7.855070	-1.961565	3.433717
130	1	0	-8.044666	-3.338571	4.538224
131	6	0	7.309650	2.699524	4.033046
132	1	0	8.044666	3.338571	4.538224
133	1	0	6.754235	2.156691	4.805357
134	1	0	7.855070	1.961565	3.433717
135	6	0	7.245550	4.320428	2.131895
136	1	0	7.827633	3.643655	1.496207
137	1	0	6.642342	4.965175	1.482564
138	1	0	7.954676	4.961414	2.668176
139	6	0	5.634695	4.586277	4.023118
140	1	0	4.967460	5.210329	3.417767
141	1	0	5.028376	4.104645	4.797648
142	1	0	6.353988	5.244886	4.525746

Rotational constants (GHZ): 0.0402957 0.0221548 0.0195110
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(RB+HF-LYP) = -2702.42652661 A.U. after 8 cycles
Convg = 0.7568D-09 -V/T = 2.0098
S**2 = 0.0000

Item	Value	Threshold	Converged?
Maximum Force	0.000053	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.001301	0.001800	YES
RMS Displacement	0.000338	0.001200	YES

Predicted change in Energy=-2.899413D-08
Optimization completed.
-- Stationary point found.

Conjoined [5]helicene, meso, C_{2h} at B3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4
Framework group C2H[SGH(C4H2),X(C60H72N4)]
Deg. of freedom 107
Full point group C2H
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.627544	0.330576	2.426181
2	7	0	-0.627544	0.330576	-2.426181
3	6	0	-3.513233	-0.822110	5.326717
4	6	0	-3.716350	0.252180	4.443711
5	1	0	-4.649452	0.799934	4.506675
6	6	0	-2.774104	0.659400	3.499200
7	6	0	-2.962568	1.891524	2.595905
8	6	0	-2.363328	1.537134	1.232022
9	6	0	-2.937172	1.871303	0.000000
10	1	0	-3.878227	2.404951	0.000000
11	6	0	-2.363328	1.537134	-1.232022
12	6	0	-2.962568	1.891524	-2.595905
13	6	0	-2.774104	0.659400	-3.499200
14	6	0	-3.716350	0.252180	-4.443711
15	1	0	-4.649452	0.799934	-4.506675
16	6	0	-3.513233	-0.822110	-5.326717
17	6	0	-2.293005	-1.496217	-5.229113
18	1	0	-2.068974	-2.329456	-5.885812
19	6	0	-1.331768	-1.132322	-4.286350
20	1	0	-0.398707	-1.677466	-4.231472
21	6	0	-1.570304	-0.074809	-3.408471
22	6	0	-1.160427	0.815463	-1.209899
23	6	0	-0.575465	0.439276	0.000000
24	6	0	-1.160427	0.815463	1.209899
25	6	0	-1.570304	-0.074809	3.408471
26	6	0	-1.331768	-1.132322	4.286350
27	6	0	-2.293005	-1.496217	5.229113
28	1	0	-2.068974	-2.329456	5.885812
29	6	0	-4.438026	2.312243	2.487428
30	1	0	-5.064309	1.510694	2.081533
31	1	0	-4.540719	3.191559	1.843958
32	1	0	-4.833176	2.597248	3.467101
33	6	0	-2.171874	3.089548	3.196624
34	1	0	-1.101404	2.876461	3.253611
35	1	0	-2.533240	3.317987	4.206021
36	1	0	-2.302484	3.979225	2.569427
37	6	0	-4.438026	2.312243	-2.487428
38	1	0	-5.064309	1.510694	-2.081533
39	1	0	-4.833176	2.597248	-3.467101
40	1	0	-4.540719	3.191559	-1.843958
41	6	0	-2.171874	3.089548	-3.196624
42	1	0	-1.101404	2.876461	-3.253611
43	1	0	-2.302484	3.979225	-2.569427
44	1	0	-2.533240	3.317987	-4.206021
45	1	0	-0.398707	-1.677466	4.231472
46	6	0	0.575465	-0.439276	0.000000
47	6	0	1.160427	-0.815463	-1.209899
48	7	0	0.627544	-0.330576	-2.426181
49	7	0	0.627544	-0.330576	2.426181
50	6	0	1.160427	-0.815463	1.209899
51	6	0	2.363328	-1.537134	-1.232022
52	6	0	2.363328	-1.537134	1.232022
53	6	0	2.937172	-1.871303	0.000000
54	1	0	3.878227	-2.404951	0.000000
55	6	0	2.962568	-1.891524	-2.595905
56	6	0	2.962568	-1.891524	2.595905
57	6	0	2.774104	-0.659400	3.499200
58	6	0	2.774104	-0.659400	-3.499200
59	6	0	1.570304	0.074809	-3.408471
60	6	0	3.716350	-0.252180	-4.443711
61	1	0	4.649452	-0.799934	-4.506675
62	6	0	3.513233	0.822110	-5.326717
63	6	0	2.293005	1.496217	-5.229113
64	1	0	2.068974	2.329456	-5.885812
65	6	0	1.331768	1.132322	-4.286350
66	1	0	0.398707	1.677466	-4.231472
67	6	0	1.570304	0.074809	3.408471
68	6	0	3.716350	-0.252180	4.443711
69	1	0	4.649452	-0.799934	4.506675
70	6	0	3.513233	0.822110	5.326717
71	6	0	2.293005	1.496217	5.229113
72	1	0	2.068974	2.329456	5.885812
73	6	0	1.331768	1.132322	4.286350
74	1	0	0.398707	1.677466	4.231472
75	6	0	2.171874	-3.089548	-3.196624
76	1	0	1.101404	-2.876461	-3.253611
77	1	0	2.533240	-3.317987	-4.206021
78	1	0	2.302484	-3.979225	-2.569427
79	6	0	4.438026	-2.312243	-2.487428
80	1	0	5.064309	-1.510694	-2.081533
81	1	0	4.540719	-3.191559	-1.843958

82	1	0	4.833176	-2.597248	-3.467101
83	6	0	4.438026	-2.312243	2.487428
84	1	0	4.540719	-3.191559	1.843958
85	1	0	5.064309	-1.510694	2.081533
86	1	0	4.833176	-2.597248	3.467101
87	6	0	2.171874	-3.089548	3.196624
88	1	0	2.533240	-3.317987	4.206021
89	1	0	1.101404	-2.876461	3.253611
90	1	0	2.302484	-3.979225	2.569427
91	6	0	-4.606213	-1.195842	-6.344740
92	6	0	4.606213	1.195842	-6.344740
93	6	0	-4.606213	-1.195842	6.344740
94	6	0	4.606213	1.195842	6.344740
95	6	0	-4.204677	-2.403330	-7.212961
96	1	0	-3.300369	-2.201925	-7.798516
97	1	0	-4.027792	-3.299371	-6.607151
98	1	0	-5.009914	-2.635420	-7.919343
99	6	0	-4.204677	-2.403330	7.212961
100	1	0	-4.027792	-3.299371	6.607151
101	1	0	-3.300369	-2.201925	7.798516
102	1	0	-5.009914	-2.635420	7.919343
103	6	0	4.204677	2.403330	7.212961
104	1	0	4.027792	3.299371	6.607151
105	1	0	3.300369	2.201925	7.798516
106	1	0	5.009914	2.635420	7.919343
107	6	0	4.204677	2.403330	-7.212961
108	1	0	3.300369	2.201925	-7.798516
109	1	0	4.027792	3.299371	-6.607151
110	1	0	5.009914	2.635420	-7.919343
111	6	0	-4.873961	0.002859	7.285988
112	1	0	-5.202810	0.889584	6.733617
113	1	0	-5.658321	-0.247229	8.011207
114	1	0	-3.969376	0.273207	7.842725
115	6	0	-5.911114	-1.556969	5.595666
116	1	0	-6.277269	-0.722529	4.988056
117	1	0	-5.754942	-2.412035	4.928174
118	1	0	-6.701748	-1.821012	6.309065
119	6	0	-4.873961	0.002859	-7.285988
120	1	0	-5.658321	-0.247229	-8.011207
121	1	0	-5.202810	0.889584	-6.733617
122	1	0	-3.969376	0.273207	-7.842725
123	6	0	-5.911114	-1.556969	-5.595666
124	1	0	-5.754942	-2.412035	-4.928174
125	1	0	-6.277269	-0.722529	-4.988056
126	1	0	-6.701748	-1.821012	-6.309065
127	6	0	4.873961	-0.002859	-7.285988
128	1	0	5.658321	0.247229	-8.011207
129	1	0	5.202810	-0.889584	-6.733617
130	1	0	3.969376	-0.273207	-7.842725
131	6	0	5.911114	1.556969	-5.595666
132	1	0	5.754942	2.412035	-4.928174
133	1	0	6.277269	0.722529	-4.988056
134	1	0	6.701748	1.821012	-6.309065
135	6	0	4.873961	-0.002859	7.285988
136	1	0	5.202810	-0.889584	6.733617
137	1	0	5.658321	0.247229	8.011207
138	1	0	3.969376	-0.273207	7.842725
139	6	0	5.911114	1.556969	5.595666
140	1	0	6.277269	0.722529	4.988056
141	1	0	5.754942	2.412035	4.928174
142	1	0	6.701748	1.821012	6.309065

Rotational constants (GHZ): 0.0401191 0.0250620 0.0178378
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(RB+HF-LYP) = -2702.42829142 A.U. after 8 cycles
Convg = 0.9758D-09 -V/T = 2.0098
S**2 = 0.0000

Item	Value	Threshold	Converged?
Maximum Force	0.000002	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.010363	0.001800	NO
RMS Displacement	0.002186	0.001200	NO

Predicted change in Energy=-1.114960D-06
Optimization completed on the basis of negligible forces.
-- Stationary point found.

Conjoined [5]helicene, chiral, D_2 at B3LYP/6-31G(d) in DCM

Stoichiometry C64H74N4
Framework group D2[C2(HCC.CCH),X(C60H72N4)]
Deg. of freedom 105
Full point group D2 NOp 4
Largest Abelian subgroup D2 NOp 4
Largest concise Abelian subgroup D2 NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.429080	0.087433	0.704789
2	7	0	-2.429080	-0.087433	0.704789
3	6	0	5.346189	2.643735	2.444412
4	6	0	4.456099	1.874201	3.215320
5	1	0	4.519234	1.942068	4.295009
6	6	0	3.504365	1.015806	2.663703
7	6	0	2.596338	0.106660	3.514576
8	6	0	1.232180	0.051498	2.818406
9	6	0	0.000000	0.000000	3.483041
10	1	0	0.000000	0.000000	4.564868
11	6	0	-1.232180	-0.051498	2.818406
12	6	0	-2.596338	-0.106660	3.514576
13	6	0	-3.504365	-1.015806	2.663703
14	6	0	-4.456099	-1.874201	3.215320
15	1	0	-4.519234	-1.942068	4.295009
16	6	0	-5.346189	-2.643735	2.444412
17	6	0	-5.248138	-2.518693	1.055567
18	1	0	-5.907951	-3.078601	0.402142
19	6	0	-4.298948	-1.684166	0.463113
20	1	0	-4.242949	-1.615008	-0.615594
21	6	0	-3.416726	-0.947531	1.254104
22	6	0	-1.209531	-0.018320	1.416977
23	6	0	0.000000	0.000000	0.722940
24	6	0	1.209531	0.018320	1.416977
25	6	0	3.416726	0.947531	1.254104
26	6	0	4.298948	1.684166	0.463113
27	6	0	5.248138	2.518693	1.055567
28	1	0	5.907951	3.078601	0.402142
29	6	0	3.200937	-1.327194	3.545674
30	1	0	3.260508	-1.761374	2.544173
31	1	0	2.574844	-1.984710	4.159921
32	1	0	4.209228	-1.306506	3.974914
33	6	0	2.480869	0.599584	4.967827
34	1	0	2.071855	1.613931	5.024975
35	1	0	3.458191	0.591829	5.459223
36	1	0	1.837381	-0.066122	5.550412
37	6	0	-2.480869	-0.599584	4.967827
38	1	0	-2.071855	-1.613931	5.024975
39	1	0	-3.458191	-0.591829	5.459223
40	1	0	-1.837381	0.066122	5.550412
41	6	0	-3.200937	1.327194	3.545674
42	1	0	-3.260508	1.761374	2.544173
43	1	0	-2.574844	1.984710	4.159921
44	1	0	-4.209228	1.306506	3.974914
45	1	0	4.242949	1.615008	-0.615594
46	6	0	0.000000	0.000000	-0.722940
47	6	0	-1.209531	0.018320	-1.416977
48	7	0	-2.429080	0.087433	-0.704789
49	7	0	2.429080	-0.087433	-0.704789
50	6	0	1.209531	-0.018320	-1.416977
51	6	0	-1.232180	0.051498	-2.818406
52	6	0	1.232180	-0.051498	-2.818406
53	6	0	0.000000	0.000000	-3.483041
54	1	0	0.000000	0.000000	-4.564868
55	6	0	2.596338	-0.106660	-3.514576
56	6	0	-2.596338	0.106660	-3.514576
57	6	0	3.504365	-1.015806	-2.663703
58	6	0	-3.504365	1.015806	-2.663703
59	6	0	-3.416726	0.947531	-1.254104
60	6	0	3.416726	-0.947531	-1.254104
61	6	0	-4.456099	1.874201	-3.215320
62	1	0	-4.519234	1.942068	-4.295009
63	6	0	4.456099	-1.874201	-3.215320
64	1	0	4.519234	-1.942068	-4.295009
65	6	0	5.346189	-2.643735	-2.444412
66	6	0	5.248138	-2.518693	-1.055567
67	1	0	5.907951	-3.078601	-0.402142
68	6	0	4.298948	-1.684166	-0.463113
69	1	0	4.242949	-1.615008	0.615594
70	6	0	-5.346189	2.643735	-2.444412
71	6	0	-5.248138	2.518693	-1.055567
72	6	0	-4.298948	1.684166	-0.463113
73	1	0	-4.242949	1.615008	0.615594
74	1	0	-5.907951	3.078601	-0.402142
75	6	0	-3.200937	-1.327194	-3.545674
76	1	0	-3.260508	-1.761374	-2.544173
77	1	0	-4.209228	-1.306506	-3.974914
78	1	0	-2.574844	-1.984710	-4.159921
79	6	0	-2.480869	0.599584	-4.967827
80	1	0	-2.071855	1.613931	-5.024975
81	1	0	-1.837381	-0.066122	-5.550412

82	1	0	-3.458191	0.591829	-5.459223
83	6	0	2.480869	-0.599584	-4.967827
84	1	0	2.071855	-1.613931	-5.024975
85	1	0	1.837381	0.066122	-5.550412
86	1	0	3.458191	-0.591829	-5.459223
87	6	0	3.200937	1.327194	-3.545674
88	1	0	2.574844	1.984710	-4.159921
89	1	0	3.260508	1.761374	-2.544173
90	1	0	4.209228	1.306506	-3.974914
91	6	0	6.372572	-3.557894	-3.139016
92	6	0	-6.372572	3.557894	-3.139016
93	6	0	-6.372572	-3.557894	3.139016
94	6	0	6.372572	3.557894	3.139016
95	6	0	5.633925	-4.592401	-4.021510
96	1	0	5.028807	-4.109963	-4.796527
97	1	0	6.355044	-5.249400	-4.523232
98	1	0	4.967615	-5.218621	-3.416925
99	6	0	7.308815	-2.706199	-4.029384
100	1	0	8.042508	-3.346955	-4.533931
101	1	0	6.753631	-2.163068	-4.801676
102	1	0	7.856287	-1.970097	-3.429223
103	6	0	7.243071	-4.327629	-2.127576
104	1	0	7.824499	-3.651052	-1.491031
105	1	0	6.639212	-4.972632	-1.479018
106	1	0	7.952124	-4.967919	-2.664559
107	6	0	-7.243071	4.327629	-2.127576
108	1	0	-7.824499	3.651052	-1.491031
109	1	0	-6.639212	4.972632	-1.479018
110	1	0	-7.952124	4.967919	-2.664559
111	6	0	-5.633925	4.592401	-4.021510
112	1	0	-4.967615	5.218621	-3.416925
113	1	0	-5.028807	4.109963	-4.796527
114	1	0	-6.355044	5.249400	-4.523232
115	6	0	-7.308815	2.706199	-4.029384
116	1	0	-6.753631	2.163068	-4.801676
117	1	0	-7.856287	1.970097	-3.429223
118	1	0	-8.042508	3.346955	-4.533931
119	6	0	-5.633925	-4.592401	4.021510
120	1	0	-5.028807	-4.109963	4.796527
121	1	0	-6.355044	-5.249400	4.523232
122	1	0	-4.967615	-5.218621	3.416925
123	6	0	-7.243071	-4.327629	2.127576
124	1	0	-7.824499	-3.651052	1.491031
125	1	0	-6.639212	-4.972632	1.479018
126	1	0	-7.952124	-4.967919	2.664559
127	6	0	-7.308815	-2.706199	4.029384
128	1	0	-6.753631	-2.163068	4.801676
129	1	0	-7.856287	-1.970097	3.429223
130	1	0	-8.042508	-3.346955	4.533931
131	6	0	7.308815	2.706199	4.029384
132	1	0	8.042508	3.346955	4.533931
133	1	0	6.753631	2.163068	4.801676
134	1	0	7.856287	1.970097	3.429223
135	6	0	7.243071	4.327629	2.127576
136	1	0	7.824499	3.651052	1.491031
137	1	0	6.639212	4.972632	1.479018
138	1	0	7.952124	4.967919	2.664559
139	6	0	5.633925	4.592401	4.021510
140	1	0	4.967615	5.218621	3.416925
141	1	0	5.028807	4.109963	4.796527
142	1	0	6.355044	5.249400	4.523232

Rotational constants (GHZ): 0.0402422 0.0221465 0.0195192
Standard basis: 6-31G(d) (6D, 7F)
Error on total polarization charges = 0.01829
SCF Done: E(RB3LYP) = -2702.43460513 A.U. after 3 cycles
Convg = 0.8242D-08 -V/T = 2.0098

Item	Value	Threshold	Converged?
Maximum Force	0.000000	0.000015	YES
RMS Force	0.000000	0.000010	YES
Maximum Displacement	0.000032	0.000060	YES
RMS Displacement	0.000005	0.000040	YES

Predicted change in Energy=-1.883371D-11
Optimization completed.
-- Stationary point found.

Radical cation of conjoined [5]helicene, chiral, D_2 at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(1+,2)
Framework group D2[C2(HCC.CCH),X(C60H72N4)]
Deg. of freedom 105
Full point group D2
Largest Abelian subgroup D2 NOp 4
Largest concise Abelian subgroup D2 NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.412257	0.113444	0.690084
2	7	0	-2.412257	-0.113444	0.690084
3	6	0	5.458360	2.450879	2.500887
4	6	0	4.543318	1.693731	3.253047
5	1	0	4.616407	1.726951	4.332955
6	6	0	3.553209	0.894158	2.681542
7	6	0	2.601976	0.011658	3.511592
8	6	0	1.239288	0.032189	2.810749
9	6	0	0.000000	0.000000	3.466390
10	1	0	0.000000	0.000000	4.548192
11	6	0	-1.239288	-0.032189	2.810749
12	6	0	-2.601976	-0.011658	3.511592
13	6	0	-3.553209	-0.894158	2.681542
14	6	0	-4.543318	-1.693731	3.253047
15	1	0	-4.616407	-1.726951	4.332955
16	6	0	-5.458360	-2.450879	2.500887
17	6	0	-5.342230	-2.387328	1.107312
18	1	0	-6.014136	-2.952475	0.472449
19	6	0	-4.358078	-1.616421	0.494647
20	1	0	-4.282730	-1.602653	-0.585187
21	6	0	-3.465826	-0.878690	1.272970
22	6	0	-1.217616	-0.017168	1.412016
23	6	0	0.000000	0.000000	0.710650
24	6	0	1.217616	0.017168	1.412016
25	6	0	3.465826	0.878690	1.272970
26	6	0	4.358078	1.616421	0.494647
27	6	0	5.342230	2.387328	1.107312
28	1	0	6.014136	2.952475	0.472449
29	6	0	3.136477	-1.450280	3.512862
30	1	0	3.179882	-1.869454	2.503334
31	1	0	2.480820	-2.091480	4.112501
32	1	0	4.143530	-1.485055	3.942201
33	6	0	2.502016	0.482027	4.973277
34	1	0	2.140991	1.512936	5.049355
35	1	0	3.474664	0.418395	5.468470
36	1	0	1.829133	-0.166057	5.542372
37	6	0	-2.502016	-0.482027	4.973277
38	1	0	-2.140991	-1.512936	5.049355
39	1	0	-3.474664	-0.418395	5.468470
40	1	0	-1.829133	0.166057	5.542372
41	6	0	-3.136477	1.450280	3.512862
42	1	0	-3.179882	1.869454	2.503334
43	1	0	-2.480820	2.091480	4.112501
44	1	0	-4.143530	1.485055	3.942201
45	1	0	4.282730	1.602653	-0.585187
46	6	0	0.000000	0.000000	-0.710650
47	6	0	-1.217616	0.017168	-1.412016
48	7	0	-2.412257	0.113444	-0.690084
49	7	0	2.412257	-0.113444	-0.690084
50	6	0	1.217616	-0.017168	-1.412016
51	6	0	-1.239288	0.032189	-2.810749
52	6	0	1.239288	-0.032189	-2.810749
53	6	0	0.000000	0.000000	-3.466390
54	1	0	0.000000	0.000000	-4.548192
55	6	0	2.601976	-0.011658	-3.511592
56	6	0	-2.601976	0.011658	-3.511592
57	6	0	3.553209	-0.894158	-2.681542
58	6	0	-3.553209	0.894158	-2.681542
59	6	0	-3.465826	0.878690	-1.272970
60	6	0	3.465826	-0.878690	-1.272970
61	6	0	-4.543318	1.693731	-3.253047
62	1	0	-4.616407	1.726951	-4.332955
63	6	0	4.543318	-1.693731	-3.253047
64	1	0	4.616407	-1.726951	-4.332955
65	6	0	5.458360	-2.450879	-2.500887
66	6	0	5.342230	-2.387328	-1.107312
67	1	0	6.014136	-2.952475	-0.472449
68	6	0	4.358078	-1.616421	-0.494647
69	1	0	4.282730	-1.602653	0.585187
70	6	0	-5.458360	2.450879	-2.500887
71	6	0	-5.342230	2.387328	-1.107312
72	6	0	-4.358078	1.616421	-0.494647
73	1	0	-4.282730	1.602653	0.585187
74	1	0	-6.014136	2.952475	-0.472449
75	6	0	-3.136477	-1.450280	-3.512862
76	1	0	-3.179882	-1.869454	-2.503334
77	1	0	-4.143530	-1.485055	-3.942201
78	1	0	-2.480820	-2.091480	-4.112501
79	6	0	-2.502016	0.482027	-4.973277

80	1	0	-2.140991	1.512936	-5.049355
81	1	0	-1.829133	-0.166057	-5.542372
82	1	0	-3.474664	0.418395	-5.468470
83	6	0	2.502016	-0.482027	-4.973277
84	1	0	2.140991	-1.512936	-5.049355
85	1	0	1.829133	0.166057	-5.542372
86	1	0	3.474664	-0.418395	-5.468470
87	6	0	3.136477	1.450280	-3.512862
88	1	0	2.480820	2.091480	-4.112501
89	1	0	3.179882	1.869454	-2.503334
90	1	0	4.143530	1.485055	-3.942201
91	6	0	6.526656	-3.296227	-3.215900
92	6	0	-6.526656	3.296227	-3.215900
93	6	0	-6.526656	-3.296227	3.215900
94	6	0	6.526656	3.296227	3.215900
95	6	0	5.834489	-4.328700	-4.138146
96	1	0	5.218388	-3.847551	-4.905332
97	1	0	6.586453	-4.937693	-4.652950
98	1	0	5.189427	-5.002034	-3.562522
99	6	0	7.429807	-2.371196	-4.067042
100	1	0	8.195515	-2.961809	-4.582948
101	1	0	6.860465	-1.829589	-4.830089
102	1	0	7.938436	-1.631297	-3.438812
103	6	0	7.421458	-4.061903	-2.222685
104	1	0	7.970844	-3.384375	-1.559229
105	1	0	6.843771	-4.757823	-1.603512
106	1	0	8.161379	-4.651504	-2.774082
107	6	0	-7.421458	4.061903	-2.222685
108	1	0	-7.970844	3.384375	-1.559229
109	1	0	-6.843771	4.757823	-1.603512
110	1	0	-8.161379	4.651504	-2.774082
111	6	0	-5.834489	4.328700	-4.138146
112	1	0	-5.189427	5.002034	-3.562522
113	1	0	-5.218388	3.847551	-4.905332
114	1	0	-6.586453	4.937693	-4.652950
115	6	0	-7.429807	2.371196	-4.067042
116	1	0	-6.860465	1.829589	-4.830089
117	1	0	-7.938436	1.631297	-3.438812
118	1	0	-8.195515	2.961809	-4.582948
119	6	0	-5.834489	-4.328700	4.138146
120	1	0	-5.218388	-3.847551	4.905332
121	1	0	-6.586453	-4.937693	4.652950
122	1	0	-5.189427	-5.002034	3.562522
123	6	0	-7.421458	-4.061903	2.222685
124	1	0	-7.970844	-3.384375	1.559229
125	1	0	-6.843771	-4.757823	1.603512
126	1	0	-8.161379	-4.651504	2.774082
127	6	0	-7.429807	-2.371196	4.067042
128	1	0	-6.860465	-1.829589	4.830089
129	1	0	-7.938436	-1.631297	3.438812
130	1	0	-8.195515	-2.961809	4.582948
131	6	0	7.429807	2.371196	4.067042
132	1	0	8.195515	2.961809	4.582948
133	1	0	6.860465	1.829589	4.830089
134	1	0	7.938436	1.631297	3.438812
135	6	0	7.421458	4.061903	2.222685
136	1	0	7.970844	3.384375	1.559229
137	1	0	6.843771	4.757823	1.603512
138	1	0	8.161379	4.651504	2.774082
139	6	0	5.834489	4.328700	4.138146
140	1	0	5.189427	5.002034	3.562522
141	1	0	5.218388	3.847551	4.905332
142	1	0	6.586453	4.937693	4.652950

Rotational constants (GHZ): 0.0417392 0.0220542 0.0189078
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB+HF-LYP) = -2702.23141674 A.U. after 6 cycles
Convg = 0.4719D-08 -V/T = 2.0098
S**2 = 0.7601
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7601, after 0.7501

Item	Value	Threshold	Converged?
Maximum Force	0.000020	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001233	0.001800	YES
RMS Displacement	0.000252	0.001200	YES

Predicted change in Energy=-1.634408D-08
Optimization completed.
-- Stationary point found.

Radical cation of conjoined [5]helicene, meso, C_{2h} at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(1+,2)
Framework group C2H[SGH(C4H2),X(C60H72N4)]
Deg. of freedom 107
Full point group C2H
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.645615	0.266344	2.412275
2	7	0	-0.645615	0.266344	-2.412275
3	6	0	-3.399872	-0.831291	5.454566
4	6	0	-3.663673	0.201684	4.538920
5	1	0	-4.610925	0.721434	4.611263
6	6	0	-2.764590	0.600842	3.549788
7	6	0	-3.031473	1.780922	2.598320
8	6	0	-2.439619	1.397839	1.239187
9	6	0	-3.019367	1.701796	0.000000
10	1	0	-3.973218	2.212057	0.000000
11	6	0	-2.439619	1.397839	-1.239187
12	6	0	-3.031473	1.780922	-2.598320
13	6	0	-2.764590	0.600842	-3.549788
14	6	0	-3.663673	0.201684	-4.538920
15	1	0	-4.610925	0.721434	-4.611263
16	6	0	-3.399872	-0.831291	-5.454566
17	6	0	-2.167956	-1.485611	-5.336283
18	1	0	-1.908012	-2.295211	-6.007799
19	6	0	-1.248849	-1.132006	-4.352163
20	1	0	-0.312131	-1.669119	-4.277132
21	6	0	-1.543183	-0.099466	-3.460896
22	6	0	-1.206293	0.734917	-1.218609
23	6	0	-0.590591	0.396623	0.000000
24	6	0	-1.206293	0.734917	1.218609
25	6	0	-1.543183	-0.099466	3.460896
26	6	0	-1.248849	-1.132006	4.352163
27	6	0	-2.167956	-1.485611	5.336283
28	1	0	-1.908012	-2.295211	6.007799
29	6	0	-4.528703	2.120696	2.498609
30	1	0	-5.119954	1.272827	2.137395
31	1	0	-4.687458	2.968563	1.825638
32	1	0	-4.921877	2.426713	3.471671
33	6	0	-2.288383	3.041298	3.128824
34	1	0	-1.206063	2.888463	3.173856
35	1	0	-2.640814	3.292966	4.134924
36	1	0	-2.477354	3.896702	2.470597
37	6	0	-4.528703	2.120696	-2.498609
38	1	0	-5.119954	1.272827	-2.137395
39	1	0	-4.921877	2.426713	-3.471671
40	1	0	-4.687458	2.968563	-1.825638
41	6	0	-2.288383	3.041298	-3.128824
42	1	0	-1.206063	2.888463	-3.173856
43	1	0	-2.477354	3.896702	-2.470597
44	1	0	-2.640814	3.292966	-4.134924
45	1	0	-0.312131	-1.669119	4.277132
46	6	0	0.590591	-0.396623	0.000000
47	6	0	1.206293	-0.734917	-1.218609
48	7	0	0.645615	-0.266344	-2.412275
49	7	0	0.645615	-0.266344	2.412275
50	6	0	1.206293	-0.734917	1.218609
51	6	0	2.439619	-1.397839	-1.239187
52	6	0	2.439619	-1.397839	1.239187
53	6	0	3.019367	-1.701796	0.000000
54	1	0	3.973218	-2.212057	0.000000
55	6	0	3.031473	-1.780922	-2.598320
56	6	0	3.031473	-1.780922	2.598320
57	6	0	2.764590	-0.600842	3.549788
58	6	0	2.764590	-0.600842	-3.549788
59	6	0	1.543183	0.099466	-3.460896
60	6	0	3.663673	-0.201684	-4.538920
61	1	0	4.610925	-0.721434	-4.611263
62	6	0	3.399872	0.831291	-5.454566
63	6	0	2.167956	1.485611	-5.336283
64	1	0	1.908012	2.295211	-6.007799
65	6	0	1.248849	1.132006	-4.352163
66	1	0	0.312131	1.669119	-4.277132
67	6	0	1.543183	0.099466	3.460896
68	6	0	3.663673	-0.201684	4.538920
69	1	0	4.610925	-0.721434	4.611263
70	6	0	3.399872	0.831291	5.454566
71	6	0	2.167956	1.485611	5.336283
72	1	0	1.908012	2.295211	6.007799
73	6	0	1.248849	1.132006	4.352163
74	1	0	0.312131	1.669119	4.277132
75	6	0	2.288383	-3.041298	-3.128824
76	1	0	1.206063	-2.888463	-3.173856
77	1	0	2.640814	-3.292966	-4.134924
78	1	0	2.477354	-3.896702	-2.470597
79	6	0	4.528703	-2.120696	-2.498609

80	1	0	5.119954	-1.272827	-2.137395
81	1	0	4.687458	-2.968563	-1.825638
82	1	0	4.921877	-2.426713	-3.471671
83	6	0	4.528703	-2.120696	2.498609
84	1	0	4.687458	-2.968563	1.825638
85	1	0	5.119954	-1.272827	2.137395
86	1	0	4.921877	-2.426713	3.471671
87	6	0	2.288383	-3.041298	3.128824
88	1	0	2.640814	-3.292966	4.134924
89	1	0	1.206063	-2.888463	3.173856
90	1	0	2.477354	-3.896702	2.470597
91	6	0	-4.445232	-1.194369	-6.523683
92	6	0	4.445232	1.194369	-6.523683
93	6	0	-4.445232	-1.194369	6.523683
94	6	0	4.445232	1.194369	6.523683
95	6	0	-3.965283	-2.333309	-7.443041
96	1	0	-3.051492	-2.064266	-7.985080
97	1	0	-3.776911	-3.258218	-6.886117
98	1	0	-4.736634	-2.551796	-8.188913
99	6	0	-3.965283	-2.333309	7.443041
100	1	0	-3.776911	-3.258218	6.886117
101	1	0	-3.051492	-2.064266	7.985080
102	1	0	-4.736634	-2.551796	8.188913
103	6	0	3.965283	2.333309	7.443041
104	1	0	3.776911	3.258218	6.886117
105	1	0	3.051492	2.064266	7.985080
106	1	0	4.736634	2.551796	8.188913
107	6	0	3.965283	2.333309	-7.443041
108	1	0	3.051492	2.064266	-7.985080
109	1	0	3.776911	3.258218	-6.886117
110	1	0	4.736634	2.551796	-8.188913
111	6	0	-4.736044	0.045606	7.403594
112	1	0	-5.129062	0.883425	6.817687
113	1	0	-5.482240	-0.201357	8.167362
114	1	0	-3.829195	0.388410	7.914447
115	6	0	-5.751810	-1.648818	5.829750
116	1	0	-6.174000	-0.862941	5.194227
117	1	0	-5.579015	-2.531151	5.203301
118	1	0	-6.507079	-1.908595	6.580450
119	6	0	-4.736044	0.045606	-7.403594
120	1	0	-5.482240	-0.201357	-8.167362
121	1	0	-5.129062	0.883425	-6.817687
122	1	0	-3.829195	0.388410	-7.914447
123	6	0	-5.751810	-1.648818	-5.829750
124	1	0	-5.579015	-2.531151	-5.203301
125	1	0	-6.174000	-0.862941	-5.194227
126	1	0	-6.507079	-1.908595	-6.580450
127	6	0	4.736044	-0.045606	-7.403594
128	1	0	5.482240	0.201357	-8.167362
129	1	0	5.129062	-0.883425	-6.817687
130	1	0	3.829195	-0.388410	-7.914447
131	6	0	5.751810	1.648818	-5.829750
132	1	0	5.579015	2.531151	-5.203301
133	1	0	6.174000	0.862941	-5.194227
134	1	0	6.507079	1.908595	-6.580450
135	6	0	4.736044	-0.045606	7.403594
136	1	0	5.129062	-0.883425	6.817687
137	1	0	5.482240	0.201357	8.167362
138	1	0	3.829195	-0.388410	7.914447
139	6	0	5.751810	1.648818	5.829750
140	1	0	6.174000	0.862941	5.194227
141	1	0	5.579015	2.531151	5.203301
142	1	0	6.507079	1.908595	6.580450

Rotational constants (GHZ): 0.0417368 0.0242815 0.0175616
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB+HF-LYP) = -2702.23154745 A.U. after 7 cycles
Convg = 0.2730D-08 -V/T = 2.0098
S**2 = 0.7601
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7601, after 0.7501

Item	Value	Threshold	Converged?
Maximum Force	0.000002	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.005718	0.001800	NO
RMS Displacement	0.001070	0.001200	YES

Predicted change in Energy=-1.210376D-06
Optimization completed on the basis of negligible forces.
-- Stationary point found.

Radical cation of conjoined [5]helicene, meso, C_{2h}, stationary point with two imaginary frequencies at UB3LYP/6-31G(d) in the gas phase.

Stoichiometry C64H74N4(1+,2)
Framework group C2H[C2(HCC.CCH),X(C60H72N4)]
Deg. of freedom 104
Full point group C2H NOp 4
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	3.421924
2	6	0	-0.465191	1.146025	2.753066
3	6	0	-0.171386	1.210712	1.381890
4	6	0	0.000000	0.000000	0.699274
5	6	0	0.171386	-1.210712	1.381890
6	6	0	0.465191	-1.146025	2.753066
7	6	0	0.000000	0.000000	-0.699274
8	6	0	-0.171386	1.210712	-1.381890
9	6	0	-0.465191	1.146025	-2.753066
10	6	0	0.000000	0.000000	-3.421924
11	6	0	0.465191	-1.146025	-2.753066
12	6	0	0.171386	-1.210712	-1.381890
13	1	0	0.000000	0.000000	4.506696
14	1	0	0.000000	0.000000	-4.506696
15	7	0	-0.044687	2.441958	0.728315
16	7	0	-0.044687	2.441958	-0.728315
17	7	0	0.044687	-2.441958	0.728315
18	7	0	0.044687	-2.441958	-0.728315
19	6	0	0.080446	3.580220	1.618778
20	6	0	1.056841	4.573079	1.494737
21	6	0	-0.647384	3.563982	2.840257
22	6	0	1.114852	5.669604	2.350065
23	1	0	1.849053	4.467265	0.781930
24	6	0	-0.582024	4.681973	3.672474
25	1	0	1.883638	6.411995	2.169175
26	1	0	-1.178012	4.669146	4.576910
27	6	0	-0.080446	-3.580220	1.618778
28	6	0	0.647384	-3.563982	2.840257
29	6	0	-1.056841	-4.573079	1.494737
30	6	0	0.582024	-4.681973	3.672474
31	6	0	-1.114852	-5.669604	2.350065
32	1	0	-1.849053	-4.467265	0.781930
33	1	0	1.178012	-4.669146	4.576910
34	1	0	-1.883638	-6.411995	2.169175
35	6	0	-0.080446	-3.580220	-1.618778
36	6	0	0.647384	-3.563982	-2.840257
37	6	0	-1.056841	-4.573079	-1.494737
38	6	0	0.582024	-4.681973	-3.672474
39	6	0	-1.114852	-5.669604	-2.350065
40	1	0	-1.849053	-4.467265	-0.781930
41	1	0	1.178012	-4.669146	-4.576910
42	1	0	-1.883638	-6.411995	-2.169175
43	6	0	0.080446	3.580220	-1.618778
44	6	0	-0.647384	3.563982	-2.840257
45	6	0	1.056841	4.573079	-1.494737
46	6	0	-0.582024	4.681973	-3.672474
47	6	0	1.114852	5.669604	-2.350065
48	1	0	1.849053	4.467265	-0.781930
49	1	0	-1.178012	4.669146	-4.576910
50	1	0	1.883638	6.411995	-2.169175
51	6	0	-1.327697	2.274491	-3.310377
52	6	0	-1.327697	2.274491	3.310377
53	6	0	1.327697	-2.274491	-3.310377
54	6	0	1.327697	-2.274491	3.310377
55	6	0	-0.237900	-5.792971	3.428930
56	6	0	-0.237900	-5.792971	-3.428930
57	6	0	0.237900	5.792971	-3.428930
58	6	0	0.237900	5.792971	3.428930
59	6	0	0.205676	7.009694	-4.365537
60	6	0	0.205676	7.009694	4.365537
61	6	0	-0.205676	-7.009694	4.365537
62	6	0	-0.205676	-7.009694	-4.365537
63	6	0	2.754058	-2.159296	2.700506
64	1	0	3.217966	-1.208082	2.983915
65	1	0	3.383914	-2.975987	3.070331
66	1	0	2.734984	-2.219448	1.607831
67	6	0	2.754058	-2.159296	-2.700506
68	1	0	3.383914	-2.975987	-3.070331
69	1	0	3.217966	-1.208082	-2.983915
70	1	0	2.734984	-2.219448	-1.607831
71	6	0	-2.754058	2.159296	2.700506
72	1	0	-3.217966	1.208082	2.983915
73	1	0	-3.383914	2.975987	3.070331
74	1	0	-2.734984	2.219448	1.607831
75	6	0	-2.754058	2.159296	-2.700506
76	1	0	-3.383914	2.975987	-3.070331

77	1	0	-3.217966	1.208082	-2.983915
78	1	0	-2.734984	2.219448	-1.607831
79	6	0	-1.452130	2.185139	4.840955
80	1	0	-0.488293	2.322884	5.341759
81	1	0	-2.150456	2.932317	5.227901
82	1	0	-1.853922	1.206321	5.122442
83	6	0	-1.452130	2.185139	-4.840955
84	1	0	-2.150456	2.932317	-5.227901
85	1	0	-0.488293	2.322884	-5.341759
86	1	0	-1.853922	1.206321	-5.122442
87	6	0	1.452130	-2.185139	-4.840955
88	1	0	0.488293	-2.322884	-5.341759
89	1	0	1.853922	-1.206321	-5.122442
90	1	0	2.150456	-2.932317	-5.227901
91	6	0	1.452130	-2.185139	4.840955
92	1	0	1.853922	-1.206321	5.122442
93	1	0	0.488293	-2.322884	5.341759
94	1	0	2.150456	-2.932317	5.227901
95	6	0	0.592233	6.574753	-5.799673
96	1	0	-0.099527	5.828005	-6.203565
97	1	0	0.574581	7.439213	-6.473173
98	1	0	1.601130	6.147603	-5.823638
99	6	0	0.592233	6.574753	5.799673
100	1	0	0.574581	7.439213	6.473173
101	1	0	-0.099527	5.828005	6.203565
102	1	0	1.601130	6.147603	5.823638
103	6	0	-0.592233	-6.574753	-5.799673
104	1	0	0.099527	-5.828005	-6.203565
105	1	0	-0.574581	-7.439213	-6.473173
106	1	0	-1.601130	-6.147603	-5.823638
107	6	0	-0.592233	-6.574753	5.799673
108	1	0	-0.574581	-7.439213	6.473173
109	1	0	0.099527	-5.828005	6.203565
110	1	0	-1.601130	-6.147603	5.823638
111	6	0	-1.182279	-8.111506	-3.912621
112	1	0	-0.958240	-8.462699	-2.898876
113	1	0	-2.224263	-7.772460	-3.937702
114	1	0	-1.103236	-8.972302	-4.584836
115	6	0	-1.182279	-8.111506	3.912621
116	1	0	-2.224263	-7.772460	3.937702
117	1	0	-0.958240	-8.462699	2.898876
118	1	0	-1.103236	-8.972302	4.584836
119	6	0	1.182279	8.111506	3.912621
120	1	0	2.224263	7.772460	3.937702
121	1	0	0.958240	8.462699	2.898876
122	1	0	1.103236	8.972302	4.584836
123	6	0	1.182279	8.111506	-3.912621
124	1	0	0.958240	8.462699	-2.898876
125	1	0	2.224263	7.772460	-3.937702
126	1	0	1.103236	8.972302	-4.584836
127	6	0	-1.224993	7.599708	4.374831
128	1	0	-1.965502	6.870890	4.721327
129	1	0	-1.271815	8.465800	5.044909
130	1	0	-1.522140	7.929907	3.373110
131	6	0	-1.224993	7.599708	-4.374831
132	1	0	-1.271815	8.465800	-5.044909
133	1	0	-1.965502	6.870890	-4.721327
134	1	0	-1.522140	7.929907	-3.373110
135	6	0	1.224993	-7.599708	-4.374831
136	1	0	1.965502	-6.870890	-4.721327
137	1	0	1.522140	-7.929907	-3.373110
138	1	0	1.271815	-8.465800	-5.044909
139	6	0	1.224993	-7.599708	4.374831
140	1	0	1.965502	-6.870890	4.721327
141	1	0	1.271815	-8.465800	5.044909
142	1	0	1.522140	-7.929907	3.373110

Rotational constants (GHZ): 0.0434529 0.0233362 0.0162877
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -2702.07993638 A.U. after 2 cycles
Convg = 0.7944D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S**2>= 0.7667 S= 0.5083
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7667, after 0.7502

Item	Value	Threshold	Converged?
Maximum Force	0.000000	0.000015	YES
RMS Force	0.000000	0.000010	YES
Maximum Displacement	0.000043	0.000060	YES
RMS Displacement	0.000008	0.000040	YES

Predicted change in Energy=-1.300174D-11
Optimization completed.
-- Stationary point found.

Radical cation of conjoined [5]helicene, chiral, D_2 at UB3LYP/6-31G(d) in DCM

Stoichiometry C64H74N4(1+,2)
Framework group D2[C2(HCC.CCH),X(C60H72N4)]
Deg. of freedom 105
Full point group D2 NOp 4
Largest Abelian subgroup D2 NOp 4
Largest concise Abelian subgroup D2 NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.412000	0.111999	0.690051
2	7	0	-2.412000	-0.111999	0.690051
3	6	0	5.455466	2.452612	2.498157
4	6	0	4.541564	1.695309	3.251869
5	1	0	4.613913	1.727903	4.331880
6	6	0	3.551858	0.894354	2.680611
7	6	0	2.600950	0.012626	3.511744
8	6	0	1.238851	0.032807	2.810115
9	6	0	0.000000	0.000000	3.466627
10	1	0	0.000000	0.000000	4.548165
11	6	0	-1.238851	-0.032807	2.810115
12	6	0	-2.600950	-0.012626	3.511744
13	6	0	-3.551858	-0.894354	2.680611
14	6	0	-4.541564	-1.695309	3.251869
15	1	0	-4.613913	-1.727903	4.331880
16	6	0	-5.455466	-2.452612	2.498157
17	6	0	-5.339164	-2.389608	1.104537
18	1	0	-6.008892	-2.954898	0.467426
19	6	0	-4.354454	-1.617805	0.492685
20	1	0	-4.276666	-1.608025	-0.586848
21	6	0	-3.463703	-0.878743	1.271862
22	6	0	-1.217473	-0.016945	1.411964
23	6	0	0.000000	0.000000	0.709932
24	6	0	1.217473	0.016945	1.411964
25	6	0	3.463703	0.878743	1.271862
26	6	0	4.354454	1.617805	0.492685
27	6	0	5.339164	2.389608	1.104537
28	1	0	6.008892	2.954898	0.467426
29	6	0	3.134754	-1.449496	3.514001
30	1	0	3.178175	-1.870231	2.505247
31	1	0	2.476474	-2.086724	4.114831
32	1	0	4.141279	-1.483750	3.944689
33	6	0	2.501139	0.483935	4.973116
34	1	0	2.140359	1.514976	5.047957
35	1	0	3.474103	0.419126	5.467626
36	1	0	1.826313	-0.163165	5.540404
37	6	0	-2.501139	-0.483935	4.973116
38	1	0	-2.140359	-1.514976	5.047957
39	1	0	-3.474103	-0.419126	5.467626
40	1	0	-1.826313	0.163165	5.540404
41	6	0	-3.134754	1.449496	3.514001
42	1	0	-3.178175	1.870231	2.505247
43	1	0	-2.476474	2.086724	4.114831
44	1	0	-4.141279	1.483750	3.944689
45	1	0	4.276666	1.608025	-0.586848
46	6	0	0.000000	0.000000	-0.709932
47	6	0	-1.217473	0.016945	-1.411964
48	7	0	-2.412000	0.111999	-0.690051
49	7	0	2.412000	-0.111999	-0.690051
50	6	0	1.217473	-0.016945	-1.411964
51	6	0	-1.238851	0.032807	-2.810115
52	6	0	1.238851	-0.032807	-2.810115
53	6	0	0.000000	0.000000	-3.466627
54	1	0	0.000000	0.000000	-4.548165
55	6	0	2.600950	-0.012626	-3.511744
56	6	0	-2.600950	0.012626	-3.511744
57	6	0	3.551858	-0.894354	-2.680611
58	6	0	-3.551858	0.894354	-2.680611
59	6	0	-3.463703	0.878743	-1.271862
60	6	0	3.463703	-0.878743	-1.271862
61	6	0	-4.541564	1.695309	-3.251869
62	1	0	-4.613913	1.727903	-4.331880
63	6	0	4.541564	-1.695309	-3.251869
64	1	0	4.613913	-1.727903	-4.331880
65	6	0	5.455466	-2.452612	-2.498157
66	6	0	5.339164	-2.389608	-1.104537
67	1	0	6.008892	-2.954898	-0.467426
68	6	0	4.354454	-1.617805	-0.492685
69	1	0	4.276666	-1.608025	0.586848
70	6	0	-5.455466	2.452612	-2.498157
71	6	0	-5.339164	2.389608	-1.104537
72	6	0	-4.354454	1.617805	-0.492685
73	1	0	-4.276666	1.608025	0.586848
74	1	0	-6.008892	2.954898	-0.467426
75	6	0	-3.134754	-1.449496	-3.514001
76	1	0	-3.178175	-1.870231	-2.505247
77	1	0	-4.141279	-1.483750	-3.944689
78	1	0	-2.476474	-2.086724	-4.114831
79	6	0	-2.501139	0.483935	-4.973116

80	1	0	-2.140359	1.514976	-5.047957
81	1	0	-1.826313	-0.163165	-5.540404
82	1	0	-3.474103	0.419126	-5.467626
83	6	0	2.501139	-0.483935	-4.973116
84	1	0	2.140359	-1.514976	-5.047957
85	1	0	1.826313	0.163165	-5.540404
86	1	0	3.474103	-0.419126	-5.467626
87	6	0	3.134754	1.449496	-3.514001
88	1	0	2.476474	2.086724	-4.114831
89	1	0	3.178175	1.870231	-2.505247
90	1	0	4.141279	1.483750	-3.944689
91	6	0	6.522882	-3.299854	-3.212730
92	6	0	-6.522882	3.299854	-3.212730
93	6	0	-6.522882	-3.299854	3.212730
94	6	0	6.522882	3.299854	3.212730
95	6	0	5.829832	-4.335221	-4.130925
96	1	0	5.209881	-3.854925	-4.895356
97	1	0	6.581807	-4.943836	-4.647044
98	1	0	5.188363	-5.008022	-3.550250
99	6	0	7.424183	-2.378481	-4.069504
100	1	0	8.186870	-2.972348	-4.587070
101	1	0	6.850997	-1.837488	-4.829892
102	1	0	7.936006	-1.638747	-3.443330
103	6	0	7.419889	-4.062297	-2.219036
104	1	0	7.966717	-3.381782	-1.556572
105	1	0	6.842624	-4.756399	-1.597511
106	1	0	8.160099	-4.651550	-2.771179
107	6	0	-7.419889	4.062297	-2.219036
108	1	0	-7.966717	3.381782	-1.556572
109	1	0	-6.842624	4.756399	-1.597511
110	1	0	-8.160099	4.651550	-2.771179
111	6	0	-5.829832	4.335221	-4.130925
112	1	0	-5.188363	5.008022	-3.550250
113	1	0	-5.209881	3.854925	-4.895356
114	1	0	-6.581807	4.943836	-4.647044
115	6	0	-7.424183	2.378481	-4.069504
116	1	0	-6.850997	1.837488	-4.829892
117	1	0	-7.936006	1.638747	-3.443330
118	1	0	-8.186870	2.972348	-4.587070
119	6	0	-5.829832	-4.335221	4.130925
120	1	0	-5.209881	-3.854925	4.895356
121	1	0	-6.581807	-4.943836	4.647044
122	1	0	-5.188363	-5.008022	3.550250
123	6	0	-7.419889	-4.062297	2.219036
124	1	0	-7.966717	-3.381782	1.556572
125	1	0	-6.842624	-4.756399	1.597511
126	1	0	-8.160099	-4.651550	2.771179
127	6	0	-7.424183	-2.378481	4.069504
128	1	0	-6.850997	-1.837488	4.829892
129	1	0	-7.936006	-1.638747	3.443330
130	1	0	-8.186870	-2.972348	4.587070
131	6	0	7.424183	2.378481	4.069504
132	1	0	8.186870	2.972348	4.587070
133	1	0	6.850997	1.837488	4.829892
134	1	0	7.936006	1.638747	3.443330
135	6	0	7.419889	4.062297	2.219036
136	1	0	7.966717	3.381782	1.556572
137	1	0	6.842624	4.756399	1.597511
138	1	0	8.160099	4.651550	2.771179
139	6	0	5.829832	4.335221	4.130925
140	1	0	5.188363	5.008022	3.550250
141	1	0	5.209881	3.854925	4.895356
142	1	0	6.581807	4.943836	4.647044

Rotational constants (GHZ): 0.0417322 0.0220665 0.0189270
Standard basis: 6-31G(d) (6D, 7F)
Error on total polarization charges = 0.01738
SCF Done: E(UB3LYP) = -2702.27048330 A.U. after 6 cycles
Convg = 0.4782D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S**2>= 0.7599 S= 0.5049
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7599, after 0.7501

Item	Value	Threshold	Converged?
Maximum Force	0.000001	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.001023	0.001800	YES
RMS Displacement	0.000233	0.001200	YES

Predicted change in Energy=-2.092662D-09
Optimization completed.
-- Stationary point found.

Radical cation of conjoined [5]helicene, meso, C_{2h} at UB3LYP/6-31G(d) in DCM

Stoichiometry C64H74N4(1+,2)
Framework group C2H[SGH(C4H2),X(C60H72N4)]
Deg. of freedom 107
Full point group C2H NOp 4
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.645303	0.266450	2.411916
2	7	0	-0.645303	0.266450	-2.411916
3	6	0	-3.393311	-0.832964	5.457034
4	6	0	-3.660776	0.199234	4.541300
5	1	0	-4.607645	0.719669	4.614259
6	6	0	-2.763428	0.598239	3.549979
7	6	0	-3.033883	1.776611	2.597470
8	6	0	-2.441540	1.393035	1.238818
9	6	0	-3.022532	1.696455	0.000000
10	1	0	-3.976319	2.206345	0.000000
11	6	0	-2.441540	1.393035	-1.238818
12	6	0	-3.033883	1.776611	-2.597470
13	6	0	-2.763428	0.598239	-3.549979
14	6	0	-3.660776	0.199234	-4.541300
15	1	0	-4.607645	0.719669	-4.614259
16	6	0	-3.393311	-0.832964	-5.457034
17	6	0	-2.162385	-1.488766	-5.336012
18	1	0	-1.899586	-2.299092	-6.005569
19	6	0	-1.245727	-1.135404	-4.348782
20	1	0	-0.311759	-1.676298	-4.268846
21	6	0	-1.541643	-0.101559	-3.459249
22	6	0	-1.207431	0.732901	-1.218427
23	6	0	-0.590588	0.395291	0.000000
24	6	0	-1.207431	0.732901	1.218427
25	6	0	-1.541643	-0.101559	3.459249
26	6	0	-1.245727	-1.135404	4.348782
27	6	0	-2.162385	-1.488766	5.336012
28	1	0	-1.899586	-2.299092	6.005569
29	6	0	-4.531976	2.112808	2.498724
30	1	0	-5.120875	1.262762	2.138848
31	1	0	-4.692106	2.958300	1.823561
32	1	0	-4.923763	2.419022	3.472309
33	6	0	-2.292581	3.039011	3.125455
34	1	0	-1.210227	2.887928	3.172267
35	1	0	-2.647889	3.293018	4.129959
36	1	0	-2.483475	3.890239	2.462528
37	6	0	-4.531976	2.112808	-2.498724
38	1	0	-5.120875	1.262762	-2.138848
39	1	0	-4.923763	2.419022	-3.472309
40	1	0	-4.692106	2.958300	-1.823561
41	6	0	-2.292581	3.039011	-3.125455
42	1	0	-1.210227	2.887928	-3.172267
43	1	0	-2.483475	3.890239	-2.462528
44	1	0	-2.647889	3.293018	-4.129959
45	1	0	-0.311759	-1.676298	4.268846
46	6	0	0.590588	-0.395291	0.000000
47	6	0	1.207431	-0.732901	-1.218427
48	7	0	0.645303	-0.266450	-2.411916
49	7	0	0.645303	-0.266450	2.411916
50	6	0	1.207431	-0.732901	1.218427
51	6	0	2.441540	-1.393035	-1.238818
52	6	0	2.441540	-1.393035	1.238818
53	6	0	3.022532	-1.696455	0.000000
54	1	0	3.976319	-2.206345	0.000000
55	6	0	3.033883	-1.776611	-2.597470
56	6	0	3.033883	-1.776611	2.597470
57	6	0	2.763428	-0.598239	3.549979
58	6	0	2.763428	-0.598239	-3.549979
59	6	0	1.541643	0.101559	-3.459249
60	6	0	3.660776	-0.199234	-4.541300
61	1	0	4.607645	-0.719669	-4.614259
62	6	0	3.393311	0.832964	-5.457034
63	6	0	2.162385	1.488766	-5.336012
64	1	0	1.899586	2.299092	-6.005569
65	6	0	1.245727	1.135404	-4.348782
66	1	0	0.311759	1.676298	-4.268846
67	6	0	1.541643	0.101559	3.459249
68	6	0	3.660776	-0.199234	4.541300
69	1	0	4.607645	-0.719669	4.614259
70	6	0	3.393311	0.832964	5.457034
71	6	0	2.162385	1.488766	5.336012
72	1	0	1.899586	2.299092	6.005569
73	6	0	1.245727	1.135404	4.348782
74	1	0	0.311759	1.676298	4.268846
75	6	0	2.292581	-3.039011	-3.125455
76	1	0	1.210227	-2.887928	-3.172267
77	1	0	2.647889	-3.293018	-4.129959
78	1	0	2.483475	-3.890239	-2.462528
79	6	0	4.531976	-2.112808	-2.498724
80	1	0	5.120875	-1.262762	-2.138848

81	1	0	4.692106	-2.958300	-1.823561
82	1	0	4.923763	-2.419022	-3.472309
83	6	0	4.531976	-2.112808	2.498724
84	1	0	4.692106	-2.958300	1.823561
85	1	0	5.120875	-1.262762	2.138848
86	1	0	4.923763	-2.419022	3.472309
87	6	0	2.292581	-3.039011	3.125455
88	1	0	2.647889	-3.293018	4.129959
89	1	0	1.210227	-2.887928	3.172267
90	1	0	2.483475	-3.890239	2.462528
91	6	0	-4.435557	-1.194505	-6.530035
92	6	0	4.435557	1.194505	-6.530035
93	6	0	-4.435557	-1.194505	6.530035
94	6	0	4.435557	1.194505	6.530035
95	6	0	-3.952343	-2.331138	-7.450535
96	1	0	-3.035605	-2.060117	-7.986478
97	1	0	-3.764553	-3.256338	-6.893993
98	1	0	-4.721911	-2.546991	-8.199567
99	6	0	-3.952343	-2.331138	7.450535
100	1	0	-3.764553	-3.256338	6.893993
101	1	0	-3.035605	-2.060117	7.986478
102	1	0	-4.721911	-2.546991	8.199567
103	6	0	3.952343	2.331138	7.450535
104	1	0	3.764553	3.256338	6.893993
105	1	0	3.035605	2.060117	7.986478
106	1	0	4.721911	2.546991	8.199567
107	6	0	3.952343	2.331138	-7.450535
108	1	0	3.035605	2.060117	-7.986478
109	1	0	3.764553	3.256338	-6.893993
110	1	0	4.721911	2.546991	-8.199567
111	6	0	-4.725700	0.046622	7.408416
112	1	0	-5.117361	0.883165	6.820055
113	1	0	-5.471851	-0.199863	8.173006
114	1	0	-3.817376	0.388411	7.917780
115	6	0	-5.744341	-1.650739	5.841751
116	1	0	-6.165566	-0.866464	5.203845
117	1	0	-5.572114	-2.535913	5.218768
118	1	0	-6.497728	-1.907198	6.596092
119	6	0	-4.725700	0.046622	-7.408416
120	1	0	-5.471851	-0.199863	-8.173006
121	1	0	-5.117361	0.883165	-6.820055
122	1	0	-3.817376	0.388411	-7.917780
123	6	0	-5.744341	-1.650739	-5.841751
124	1	0	-5.572114	-2.535913	-5.218768
125	1	0	-6.165566	-0.866464	-5.203845
126	1	0	-6.497728	-1.907198	-6.596092
127	6	0	4.725700	-0.046622	-7.408416
128	1	0	5.471851	0.199863	-8.173006
129	1	0	5.117361	-0.883165	-6.820055
130	1	0	3.817376	-0.388411	-7.917780
131	6	0	5.744341	1.650739	-5.841751
132	1	0	5.572114	2.535913	-5.218768
133	1	0	6.165566	0.866464	-5.203845
134	1	0	6.497728	1.907198	-6.596092
135	6	0	4.725700	-0.046622	7.408416
136	1	0	5.117361	-0.883165	6.820055
137	1	0	5.471851	0.199863	8.173006
138	1	0	3.817376	-0.388411	7.917780
139	6	0	5.744341	1.650739	5.841751
140	1	0	6.165566	0.866464	5.203845
141	1	0	5.572114	2.535913	5.218768
142	1	0	6.497728	1.907198	6.596092

Rotational constants (GHZ): 0.0418295 0.0242614 0.0175621
Standard basis: 6-31G(d) (6D, 7F)
Error on total polarization charges = 0.01737
SCF Done: E(UB3LYP) = -2702.27058593 A.U. after 5 cycles
Convg = 0.8387D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S**2>= 0.7599 S= 0.5049
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7599, after 0.7501

Item	Value	Threshold	Converged?
Maximum Force	0.000001	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000906	0.001800	YES
RMS Displacement	0.000185	0.001200	YES

Predicted change in Energy=-2.030615D-09
Optimization completed.
-- Stationary point found.

C_1-symmetric transition state for radical cation of conjoined [5]helicene, from chiral D_2 structure to meso C_{2h} structure at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(1+,2)
Framework group C1[X(C64H74N4)]
Deg. of freedom 420
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.346953	-0.706833	0.282495
2	7	0	-2.507866	-0.734023	0.370666
3	6	0	1.141253	-2.809056	0.023586
4	6	0	-0.068903	-3.476885	0.252259
5	1	0	-0.083591	-4.555547	0.163922
6	6	0	-1.277144	-2.826673	0.554778
7	6	0	-2.594950	-3.525817	0.878632
8	6	0	-3.661114	-2.853037	-0.000573
9	6	0	-4.711307	-3.559528	-0.588307
10	1	0	-4.748566	-4.632958	-0.446461
11	6	0	-5.727733	-2.949324	-1.341326
12	6	0	-5.648330	-1.562231	-1.497277
13	1	0	-6.401060	-1.027555	-2.064572
14	6	0	-4.606042	-0.822245	-0.941439
15	1	0	-4.582602	0.248196	-1.088202
16	6	0	-3.606550	-1.458156	-0.205127
17	6	0	-1.291879	-1.423748	0.470766
18	6	0	-0.081458	-0.731180	0.322397
19	6	0	1.136817	-1.425607	0.229618
20	6	0	-2.517861	-5.045527	0.663283
21	1	0	-2.325530	-5.307334	-0.382701
22	1	0	-3.451384	-5.525663	0.968773
23	1	0	-1.727337	-5.479668	1.283798
24	6	0	-2.934768	-3.270082	2.376028
25	1	0	-2.978785	-2.201488	2.605921
26	1	0	-2.176490	-3.726075	3.022644
27	1	0	-3.907994	-3.710449	2.617361
28	6	0	-0.086569	0.609736	-0.147464
29	6	0	-1.307920	1.261383	-0.353869
30	7	0	-2.471513	0.661726	0.138878
31	7	0	2.339166	0.631573	-0.198305
32	6	0	1.107433	1.174003	-0.604026
33	6	0	-1.342848	2.530955	-0.926421
34	6	0	1.069197	2.301198	-1.445072
35	6	0	-0.145648	2.986355	-1.521502
36	1	0	-0.180376	3.902472	-2.098359
37	6	0	-2.688552	3.264709	-0.964130
38	6	0	-3.485097	2.846281	0.296214
39	6	0	-3.396568	1.523188	0.785116
40	6	0	-4.356152	3.712253	0.958934
41	1	0	-4.430196	4.734684	0.608467
42	6	0	-5.156386	3.325001	2.048487
43	6	0	-5.050300	1.997260	2.475940
44	6	0	-4.178825	1.101942	1.857968
45	1	0	-4.099717	0.081958	2.216963
46	1	0	-5.641391	1.638703	3.310530
47	6	0	-3.466396	2.817844	-2.234834
48	1	0	-3.579217	1.731150	-2.280801
49	1	0	-4.464714	3.268438	-2.244952
50	1	0	-2.933898	3.136940	-3.138279
51	6	0	-2.485612	4.790263	-1.033188
52	1	0	-1.962096	5.171533	-0.150525
53	1	0	-1.911720	5.066550	-1.922657
54	1	0	-3.444826	5.308141	-1.117776
55	6	0	-6.095288	4.348885	2.711856
56	6	0	-6.861445	-3.800842	-1.939990
57	6	0	-6.904382	3.730623	3.867863
58	1	0	-7.540962	2.906337	3.526425
59	1	0	-6.255893	3.355896	4.667993
60	1	0	-7.559238	4.491248	4.306236
61	6	0	-5.257809	5.519516	3.280176
62	1	0	-4.547186	5.164224	4.035106
63	1	0	-4.687129	6.032395	2.498431
64	1	0	-5.912380	6.261082	3.753107
65	6	0	-7.094601	4.894579	1.663746
66	1	0	-6.586368	5.395761	0.832929
67	1	0	-7.706173	4.087214	1.245370
68	1	0	-7.767994	5.624698	2.127427
69	6	0	-6.262217	-4.859226	-2.896869
70	1	0	-5.567899	-5.531657	-2.381739
71	1	0	-7.060208	-5.474869	-3.327899
72	1	0	-5.718928	-4.383089	-3.721078
73	6	0	-7.868481	-2.948721	-2.735313
74	1	0	-8.358373	-2.199162	-2.103594
75	1	0	-7.392487	-2.432013	-3.576552
76	1	0	-8.651921	-3.593991	-3.146833
77	6	0	-7.626445	-4.515245	-0.800033
78	1	0	-6.974032	-5.178703	-0.222214

79	1	0	-8.066368	-3.789713	-0.106578
80	1	0	-8.438345	-5.125684	-1.212323
81	6	0	2.317689	2.566555	-2.290218
82	6	0	2.395349	-3.412849	-0.619655
83	6	0	3.449257	1.556299	-0.235407
84	6	0	3.505317	-1.500489	0.646202
85	6	0	4.329451	1.758233	0.829287
86	6	0	4.390217	-1.141345	1.666409
87	6	0	3.496981	2.474046	-1.316315
88	6	0	3.584555	-2.822699	0.142608
89	6	0	4.697727	-3.592042	0.480274
90	6	0	4.573966	3.356985	-1.382598
91	6	0	5.484062	-1.937228	1.994838
92	6	0	5.385538	2.660453	0.739810
93	6	0	5.572738	3.445870	-0.399511
94	6	0	5.702614	-3.163042	1.361700
95	1	0	4.770782	-4.588471	0.063010
96	1	0	6.146801	-1.590972	2.779100
97	1	0	4.198027	-0.279575	2.279088
98	1	0	4.158893	1.278540	1.773400
99	1	0	6.044415	2.756066	1.594584
100	1	0	4.623279	4.032011	-2.227692
101	6	0	2.433751	1.458463	-3.376813
102	1	0	2.496624	0.458391	-2.937475
103	1	0	1.565101	1.484579	-4.043445
104	1	0	3.336515	1.618584	-3.976063
105	6	0	2.242471	3.925203	-3.006282
106	1	0	1.356427	3.961011	-3.647385
107	1	0	2.196019	4.761040	-2.300801
108	1	0	3.104404	4.073378	-3.662509
109	6	0	6.918803	-4.057724	1.645618
110	6	0	6.751202	4.416543	-0.573117
111	6	0	7.720258	4.369652	0.623281
112	1	0	7.236449	4.681413	1.555989
113	1	0	8.141109	3.368325	0.769536
114	1	0	8.555727	5.054534	0.445328
115	6	0	7.535166	4.031689	-1.851142
116	1	0	6.908435	4.085099	-2.747693
117	1	0	8.378830	4.716177	-1.994318
118	1	0	7.933440	3.013405	-1.778833
119	6	0	6.219922	5.863809	-0.711164
120	1	0	5.565363	5.983041	-1.581063
121	1	0	5.656362	6.163985	0.179320
122	1	0	7.057745	6.559742	-0.831968
123	6	0	7.672705	-4.317507	0.319010
124	1	0	8.543667	-4.957182	0.501320
125	1	0	7.040700	-4.821001	-0.420320
126	1	0	8.027494	-3.380142	-0.123923
127	6	0	6.445386	-5.405568	2.241653
128	1	0	5.785110	-5.949553	1.557849
129	1	0	7.308783	-6.048217	2.447030
130	1	0	5.904993	-5.253272	3.182633
131	6	0	7.897772	-3.404714	2.639660
132	1	0	8.275758	-2.444747	2.269791
133	1	0	7.438634	-3.240422	3.621187
134	1	0	8.760375	-4.062047	2.789758
135	6	0	2.371865	-4.950416	-0.584441
136	1	0	3.233688	-5.368982	-1.111182
137	1	0	2.367600	-5.339450	0.438811
138	1	0	1.483920	-5.324335	-1.102864
139	6	0	2.444936	-2.968908	-2.111178
140	1	0	1.569027	-3.343620	-2.651430
141	1	0	2.467424	-1.879709	-2.213070
142	1	0	3.345359	-3.369405	-2.589541

Rotational constants (GHZ): 0.0420272 0.0234389 0.0175146
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -2702.16975043 A.U. after 12 cycles
Convg = 0.4903D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S**2>= 0.7598 S= 0.5049
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7598, after 0.7501

Item	Value	Threshold	Converged?
Maximum Force	0.000005	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001613	0.001800	YES
RMS Displacement	0.000290	0.001200	YES

Predicted change in Energy=-7.708971D-09
Optimization completed.
-- Stationary point found.

C_1-symmetric transition state for radical cation of conjoined [5]helicene, from chiral D_2 structure to meso C_{2h} structure at UB3LYP/6-31G(d) in dichloromethane (DCM).

Stoichiometry C64H74N4(1+,2)
Framework group C1[X(C64H74N4)]
Deg. of freedom 420
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.334006	-0.703765	0.275762
2	7	0	-2.524576	-0.732548	0.384356
3	6	0	1.131354	-2.809721	0.047339
4	6	0	-0.075972	-3.477136	0.278133
5	1	0	-0.089911	-4.555844	0.195106
6	6	0	-1.285877	-2.822734	0.572629
7	6	0	-2.604901	-3.524360	0.886652
8	6	0	-3.664473	-2.854806	-0.002985
9	6	0	-4.707862	-3.564755	-0.599426
10	1	0	-4.742016	-4.638286	-0.456430
11	6	0	-5.719508	-2.957011	-1.361785
12	6	0	-5.643207	-1.569745	-1.516888
13	1	0	-6.391859	-1.035189	-2.090114
14	6	0	-4.606456	-0.827007	-0.951693
15	1	0	-4.583427	0.243197	-1.100369
16	6	0	-3.609572	-1.459185	-0.207641
17	6	0	-1.302325	-1.421664	0.483495
18	6	0	-0.094517	-0.729902	0.331120
19	6	0	1.122515	-1.423046	0.240476
20	6	0	-2.524246	-5.044617	0.676145
21	1	0	-2.319917	-5.308661	-0.366863
22	1	0	-3.460886	-5.523823	0.973923
23	1	0	-1.738169	-5.474468	1.304805
24	6	0	-2.958126	-3.265230	2.380486
25	1	0	-3.008101	-2.196310	2.606974
26	1	0	-2.201801	-3.717336	3.031954
27	1	0	-3.930856	-3.710815	2.614972
28	6	0	-0.100657	0.611560	-0.142698
29	6	0	-1.319368	1.259965	-0.358847
30	7	0	-2.490178	0.663267	0.129502
31	7	0	2.322038	0.632445	-0.183299
32	6	0	1.092286	1.174085	-0.597733
33	6	0	-1.350064	2.526888	-0.935754
34	6	0	1.059756	2.295102	-1.448315
35	6	0	-0.152282	2.981516	-1.533233
36	1	0	-0.185879	3.893354	-2.116408
37	6	0	-2.692433	3.266633	-0.965937
38	6	0	-3.481927	2.853737	0.301208
39	6	0	-3.396705	1.529012	0.789886
40	6	0	-4.342714	3.726043	0.969435
41	1	0	-4.411453	4.748376	0.617141
42	6	0	-5.138683	3.343843	2.064638
43	6	0	-5.038887	2.015499	2.491598
44	6	0	-4.176590	1.113767	1.867459
45	1	0	-4.101642	0.093461	2.226338
46	1	0	-5.626744	1.659212	3.329769
47	6	0	-3.481046	2.820363	-2.230357
48	1	0	-3.599778	1.734317	-2.272082
49	1	0	-4.476465	3.277625	-2.235179
50	1	0	-2.950343	3.134736	-3.136285
51	6	0	-2.484247	4.791211	-1.040101
52	1	0	-1.951481	5.171575	-0.162477
53	1	0	-1.915402	5.061212	-1.934185
54	1	0	-3.442748	5.311830	-1.117295
55	6	0	-6.067001	4.374620	2.733141
56	6	0	-6.844888	-3.812831	-1.970878
57	6	0	-6.874725	3.762472	3.893424
58	1	0	-7.517340	2.941788	3.554568
59	1	0	-6.223981	3.381786	4.688895
60	1	0	-7.521760	4.528707	4.334714
61	6	0	-5.219784	5.540169	3.297368
62	1	0	-4.510994	5.179479	4.051857
63	1	0	-4.646320	6.044992	2.512580
64	1	0	-5.867956	6.288084	3.770152
65	6	0	-7.068236	4.928700	1.691277
66	1	0	-6.559534	5.421440	0.855881
67	1	0	-7.690192	4.125353	1.279820
68	1	0	-7.731253	5.666557	2.158719
69	6	0	-6.234100	-4.870039	-2.921632
70	1	0	-5.539278	-5.536227	-2.399404
71	1	0	-7.026210	-5.490568	-3.357634
72	1	0	-5.687732	-4.390877	-3.742371
73	6	0	-7.847585	-2.964883	-2.776042
74	1	0	-8.343460	-2.215420	-2.148913
75	1	0	-7.364503	-2.446569	-3.612214
76	1	0	-8.625175	-3.614077	-3.193540
77	6	0	-7.618562	-4.530508	-0.838925
78	1	0	-6.967001	-5.187227	-0.252673

79	1	0	-8.070673	-3.805153	-0.152693
80	1	0	-8.422287	-5.146800	-1.259644
81	6	0	2.307264	2.545879	-2.299558
82	6	0	2.386697	-3.418851	-0.586792
83	6	0	3.437242	1.551692	-0.234841
84	6	0	3.492148	-1.488965	0.657957
85	6	0	4.311613	1.768818	0.831607
86	6	0	4.375764	-1.113029	1.672560
87	6	0	3.491483	2.448315	-1.332336
88	6	0	3.574255	-2.815406	0.166659
89	6	0	4.693269	-3.575211	0.506548
90	6	0	4.580760	3.314903	-1.417536
91	6	0	5.475455	-1.900382	2.004208
92	6	0	5.376921	2.658794	0.726183
93	6	0	5.576836	3.412943	-0.432194
94	6	0	5.698430	-3.129965	1.380132
95	1	0	4.769548	-4.574529	0.096929
96	1	0	6.137440	-1.540762	2.782923
97	1	0	4.180726	-0.247857	2.278226
98	1	0	4.129219	1.315788	1.786641
99	1	0	6.030765	2.767443	1.583010
100	1	0	4.639940	3.969125	-2.278186
101	6	0	2.404452	1.430762	-3.381410
102	1	0	2.455885	0.431559	-2.938900
103	1	0	1.532330	1.467367	-4.042728
104	1	0	3.306066	1.579901	-3.984980
105	6	0	2.240558	3.902254	-3.021056
106	1	0	1.350022	3.942841	-3.655204
107	1	0	2.206047	4.740733	-2.318205
108	1	0	3.099985	4.038134	-3.682819
109	6	0	6.921537	-4.014223	1.667386
110	6	0	6.766584	4.366458	-0.623352
111	6	0	7.734093	4.332064	0.574676
112	1	0	7.251992	4.667480	1.499905
113	1	0	8.140164	3.328044	0.741933
114	1	0	8.577853	5.003292	0.382110
115	6	0	7.547357	3.948410	-1.892645
116	1	0	6.919900	3.989180	-2.789149
117	1	0	8.397519	4.622600	-2.048255
118	1	0	7.935466	2.927890	-1.797352
119	6	0	6.252359	5.816660	-0.790957
120	1	0	5.598484	5.924184	-1.662694
121	1	0	5.692712	6.139584	0.094233
122	1	0	7.099310	6.499542	-0.925256
123	6	0	7.662235	-4.298259	0.338548
124	1	0	8.536675	-4.932427	0.525482
125	1	0	7.023061	-4.816447	-0.384014
126	1	0	8.009792	-3.367508	-0.124089
127	6	0	6.460184	-5.351499	2.295458
128	1	0	5.789222	-5.906913	1.631824
129	1	0	7.328678	-5.988462	2.499159
130	1	0	5.934674	-5.180323	3.241809
131	6	0	7.909589	-3.337824	2.636429
132	1	0	8.275460	-2.382520	2.243201
133	1	0	7.460594	-3.156353	3.619443
134	1	0	8.777162	-3.989158	2.786897
135	6	0	2.366884	-4.955761	-0.529227
136	1	0	3.233423	-5.378020	-1.044701
137	1	0	2.357162	-5.328667	0.499903
138	1	0	1.482161	-5.337995	-1.046747
139	6	0	2.435071	-2.995176	-2.084811
140	1	0	1.555923	-3.375110	-2.615738
141	1	0	2.462969	-1.907932	-2.203709
142	1	0	3.332616	-3.409337	-2.556612

Rotational constants (GHZ): 0.0420570 0.0234398 0.0175615
Standard basis: 6-31G(d) (6D, 7F)
Error on total polarization charges = 0.01741
SCF Done: E(UB3LYP) = -2702.21029074 A.U. after 10 cycles
Convg = 0.8060D-08 -V/T = 2.0099
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S**2>= 0.7586 S= 0.5043
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7586, after 0.7501

Item	Value	Threshold	Converged?
Maximum Force	0.000011	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001045	0.001800	YES
RMS Displacement	0.000183	0.001200	YES

Predicted change in Energy=-1.982579D-08
Optimization completed.
-- Stationary point found.

Diradical dication of conjoined [5]helicene, chiral, D_2 triplet state at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(2+,3)
Framework group D2[C2(HCC.CCH),X(C60H72N4)]
Deg. of freedom 105
Full point group D2 NOp 4
Largest Abelian subgroup D2 NOp 4
Largest concise Abelian subgroup D2 NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.403168	0.161752	0.671197
2	7	0	-2.403168	-0.161752	0.671197
3	6	0	5.572915	2.315796	2.485587
4	6	0	4.627163	1.596036	3.239826
5	1	0	4.713997	1.618742	4.318204
6	6	0	3.588310	0.859445	2.673222
7	6	0	2.594850	0.042027	3.517745
8	6	0	1.238960	0.064112	2.808297
9	6	0	0.000000	0.000000	3.464442
10	1	0	0.000000	0.000000	4.545282
11	6	0	-1.238960	-0.064112	2.808297
12	6	0	-2.594850	-0.042027	3.517745
13	6	0	-3.588310	-0.859445	2.673222
14	6	0	-4.627163	-1.596036	3.239826
15	1	0	-4.713997	-1.618742	4.318204
16	6	0	-5.572915	-2.315796	2.485587
17	6	0	-5.433444	-2.285875	1.088983
18	1	0	-6.119098	-2.837403	0.457647
19	6	0	-4.411819	-1.569892	0.479754
20	1	0	-4.321297	-1.582165	-0.599238
21	6	0	-3.499420	-0.855731	1.262786
22	6	0	-1.210919	-0.057569	1.406448
23	6	0	0.000000	0.000000	0.711127
24	6	0	1.210919	0.057569	1.406448
25	6	0	3.499420	0.855731	1.262786
26	6	0	4.411819	1.569892	0.479754
27	6	0	5.433444	2.285875	1.088983
28	1	0	6.119098	2.837403	0.457647
29	6	0	3.080821	-1.440209	3.573786
30	1	0	3.139249	-1.891219	2.578173
31	1	0	2.393044	-2.042877	4.176084
32	1	0	4.073898	-1.487747	4.031237
33	6	0	2.492353	0.566571	4.962882
34	1	0	2.164122	1.610089	4.999496
35	1	0	3.455890	0.488391	5.471382
36	1	0	1.797142	-0.041471	5.547944
37	6	0	-2.492353	-0.566571	4.962882
38	1	0	-2.164122	-1.610089	4.999496
39	1	0	-3.455890	-0.488391	5.471382
40	1	0	-1.797142	0.041471	5.547944
41	6	0	-3.080821	1.440209	3.573786
42	1	0	-3.139249	1.891219	2.578173
43	1	0	-2.393044	2.042877	4.176084
44	1	0	-4.073898	1.487747	4.031237
45	1	0	4.321297	1.582165	-0.599238
46	6	0	0.000000	0.000000	-0.711127
47	6	0	-1.210919	0.057569	-1.406448
48	7	0	-2.403168	0.161752	-0.671197
49	7	0	2.403168	-0.161752	-0.671197
50	6	0	1.210919	-0.057569	-1.406448
51	6	0	-1.238960	0.064112	-2.808297
52	6	0	1.238960	-0.064112	-2.808297
53	6	0	0.000000	0.000000	-3.464442
54	1	0	0.000000	0.000000	-4.545282
55	6	0	2.594850	-0.042027	-3.517745
56	6	0	-2.594850	0.042027	-3.517745
57	6	0	3.588310	-0.859445	-2.673222
58	6	0	-3.588310	0.859445	-2.673222
59	6	0	-3.499420	0.855731	-1.262786
60	6	0	3.499420	-0.855731	-1.262786
61	6	0	-4.627163	1.596036	-3.239826
62	1	0	-4.713997	1.618742	-4.318204
63	6	0	4.627163	-1.596036	-3.239826
64	1	0	4.713997	-1.618742	-4.318204
65	6	0	5.572915	-2.315796	-2.485587
66	6	0	5.433444	-2.285875	-1.088983
67	1	0	6.119098	-2.837403	-0.457647
68	6	0	4.411819	-1.569892	-0.479754
69	1	0	4.321297	-1.582165	0.599238
70	6	0	-5.572915	2.315796	-2.485587
71	6	0	-5.433444	2.285875	-1.088983
72	6	0	-4.411819	1.569892	-0.479754
73	1	0	-4.321297	1.582165	0.599238
74	1	0	-6.119098	2.837403	-0.457647
75	6	0	-3.080821	-1.440209	-3.573786
76	1	0	-3.139249	-1.891219	-2.578173
77	1	0	-4.073898	-1.487747	-4.031237
78	1	0	-2.393044	-2.042877	-4.176084

79	6	0	-2.492353	0.566571	-4.962882
80	1	0	-2.164122	1.610089	-4.999496
81	1	0	-1.797142	-0.041471	-5.547944
82	1	0	-3.455890	0.488391	-5.471382
83	6	0	2.492353	-0.566571	-4.962882
84	1	0	2.164122	-1.610089	-4.999496
85	1	0	1.797142	0.041471	-5.547944
86	1	0	3.455890	-0.488391	-5.471382
87	6	0	3.080821	1.440209	-3.573786
88	1	0	2.393044	2.042877	-4.176084
89	1	0	3.139249	1.891219	-2.578173
90	1	0	4.073898	1.487747	-4.031237
91	6	0	6.688820	-3.095084	-3.197238
92	6	0	-6.688820	3.095084	-3.197238
93	6	0	-6.688820	-3.095084	3.197238
94	6	0	6.688820	3.095084	3.197238
95	6	0	6.054732	-4.154845	-4.132469
96	1	0	5.419978	-3.702456	-4.901848
97	1	0	6.843796	-4.714870	-4.645398
98	1	0	5.446373	-4.869587	-3.567300
99	6	0	7.541254	-2.110220	-4.036055
100	1	0	8.339465	-2.656430	-4.549710
101	1	0	6.949132	-1.597242	-4.801460
102	1	0	8.008027	-1.349018	-3.401117
103	6	0	7.618342	-3.817890	-2.203908
104	1	0	8.123287	-3.118053	-1.528285
105	1	0	7.080713	-4.558434	-1.600820
106	1	0	8.396007	-4.353202	-2.757141
107	6	0	-7.618342	3.817890	-2.203908
108	1	0	-8.123287	3.118053	-1.528285
109	1	0	-7.080713	4.558434	-1.600820
110	1	0	-8.396007	4.353202	-2.757141
111	6	0	-6.054732	4.154845	-4.132469
112	1	0	-5.446373	4.869587	-3.567300
113	1	0	-5.419978	3.702456	-4.901848
114	1	0	-6.843796	4.714870	-4.645398
115	6	0	-7.541254	2.110220	-4.036055
116	1	0	-6.949132	1.597242	-4.801460
117	1	0	-8.008027	1.349018	-3.401117
118	1	0	-8.339465	2.656430	-4.549710
119	6	0	-6.054732	-4.154845	4.132469
120	1	0	-5.419978	-3.702456	4.901848
121	1	0	-6.843796	-4.714870	4.645398
122	1	0	-5.446373	-4.869587	3.567300
123	6	0	-7.618342	-3.817890	2.203908
124	1	0	-8.123287	-3.118053	1.528285
125	1	0	-7.080713	-4.558434	1.600820
126	1	0	-8.396007	-4.353202	2.757141
127	6	0	-7.541254	-2.110220	4.036055
128	1	0	-6.949132	-1.597242	4.801460
129	1	0	-8.008027	-1.349018	3.401117
130	1	0	-8.339465	-2.656430	4.549710
131	6	0	7.541254	2.110220	4.036055
132	1	0	8.339465	2.656430	4.549710
133	1	0	6.949132	1.597242	4.801460
134	1	0	8.008027	1.349018	3.401117
135	6	0	7.618342	3.817890	2.203908
136	1	0	8.123287	3.118053	1.528285
137	1	0	7.080713	4.558434	1.600820
138	1	0	8.396007	4.353202	2.757141
139	6	0	6.054732	4.154845	4.132469
140	1	0	5.446373	4.869587	3.567300
141	1	0	5.419978	3.702456	4.901848
142	1	0	6.843796	4.714870	4.645398

Rotational constants (GHZ): 0.0433204 0.0217742 0.0184319
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -2701.93771786 A.U. after 1 cycles
Convg = 0.6988D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S**2>= 2.0205 S= 1.0068
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 2.0205, after 2.0003

Item	Value	Threshold	Converged?
Maximum Force	0.000000	0.000015	YES
RMS Force	0.000000	0.000010	YES
Maximum Displacement	0.000059	0.000060	YES
RMS Displacement	0.000013	0.000040	YES

Predicted change in Energy=-8.650167D-12
Optimization completed.
-- Stationary point found.

Diradical dication of conjoined [5]helicene, chiral, D_2 broken symmetry singlet state at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(2+)
Framework group D2[C2(HCC.CCH),X(C60H72N4)]
Deg. of freedom 105
Full point group D2 NOp 4
Largest Abelian subgroup D2 NOp 4
Largest concise Abelian subgroup D2 NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.404170	0.159613	0.671763
2	7	0	-2.404170	-0.159613	0.671763
3	6	0	5.564863	2.317419	2.494291
4	6	0	4.621852	1.591319	3.245932
5	1	0	4.709186	1.609872	4.324305
6	6	0	3.586939	0.851360	2.676507
7	6	0	2.597024	0.024336	3.516280
8	6	0	1.239912	0.054560	2.807235
9	6	0	0.000000	0.000000	3.462935
10	1	0	0.000000	0.000000	4.543845
11	6	0	-1.239912	-0.054560	2.807235
12	6	0	-2.597024	-0.024336	3.516280
13	6	0	-3.586939	-0.851360	2.676507
14	6	0	-4.621852	-1.591319	3.245932
15	1	0	-4.709186	-1.609872	4.324305
16	6	0	-5.564863	-2.317419	2.494291
17	6	0	-5.426454	-2.291166	1.097079
18	1	0	-6.109918	-2.848061	0.468111
19	6	0	-4.408645	-1.572718	0.485130
20	1	0	-4.317655	-1.588325	-0.593790
21	6	0	-3.498284	-0.852864	1.265756
22	6	0	-1.212596	-0.049470	1.407595
23	6	0	0.000000	0.000000	0.709003
24	6	0	1.212596	0.049470	1.407595
25	6	0	3.498284	0.852864	1.265756
26	6	0	4.408645	1.572718	0.485130
27	6	0	5.426454	2.291166	1.097079
28	1	0	6.109918	2.848061	0.468111
29	6	0	3.084042	-1.457062	3.558728
30	1	0	3.137116	-1.900901	2.559645
31	1	0	2.399252	-2.064347	4.159892
32	1	0	4.079517	-1.508879	4.010621
33	6	0	2.496491	0.536874	4.965392
34	1	0	2.169544	1.580452	5.011226
35	1	0	3.460406	0.453004	5.472495
36	1	0	1.800933	-0.075080	5.546036
37	6	0	-2.496491	-0.536874	4.965392
38	1	0	-2.169544	-1.580452	5.011226
39	1	0	-3.460406	-0.453004	5.472495
40	1	0	-1.800933	0.075080	5.546036
41	6	0	-3.084042	1.457062	3.558728
42	1	0	-3.137116	1.900901	2.559645
43	1	0	-2.399252	2.064347	4.159892
44	1	0	-4.079517	1.508879	4.010621
45	1	0	4.317655	1.588325	-0.593790
46	6	0	0.000000	0.000000	-0.709003
47	6	0	-1.212596	0.049470	-1.407595
48	7	0	-2.404170	0.159613	-0.671763
49	7	0	2.404170	-0.159613	-0.671763
50	6	0	1.212596	-0.049470	-1.407595
51	6	0	-1.239912	0.054560	-2.807235
52	6	0	1.239912	-0.054560	-2.807235
53	6	0	0.000000	0.000000	-3.462935
54	1	0	0.000000	0.000000	-4.543845
55	6	0	2.597024	-0.024336	-3.516280
56	6	0	-2.597024	0.024336	-3.516280
57	6	0	3.586939	-0.851360	-2.676507
58	6	0	-3.586939	0.851360	-2.676507
59	6	0	-3.498284	0.852864	-1.265756
60	6	0	3.498284	-0.852864	-1.265756
61	6	0	-4.621852	1.591319	-3.245932
62	1	0	-4.709186	1.609872	-4.324305
63	6	0	4.621852	-1.591319	-3.245932
64	1	0	4.709186	-1.609872	-4.324305
65	6	0	5.564863	-2.317419	-2.494291
66	6	0	5.426454	-2.291166	-1.097079
67	1	0	6.109918	-2.848061	-0.468111
68	6	0	4.408645	-1.572718	-0.485130
69	1	0	4.317655	-1.588325	0.593790
70	6	0	-5.564863	2.317419	-2.494291
71	6	0	-5.426454	2.291166	-1.097079
72	6	0	-4.408645	1.572718	-0.485130
73	1	0	-4.317655	1.588325	0.593790
74	1	0	-6.109918	2.848061	-0.468111
75	6	0	-3.084042	-1.457062	-3.558728
76	1	0	-3.137116	-1.900901	-2.559645
77	1	0	-4.079517	-1.508879	-4.010621

78	1	0	-2.399252	-2.064347	-4.159892
79	6	0	-2.496491	0.536874	-4.965392
80	1	0	-2.169544	1.580452	-5.011226
81	1	0	-1.800933	-0.075080	-5.546036
82	1	0	-3.460406	0.453004	-5.472495
83	6	0	2.496491	-0.536874	-4.965392
84	1	0	2.169544	-1.580452	-5.011226
85	1	0	1.800933	0.075080	-5.546036
86	1	0	3.460406	-0.453004	-5.472495
87	6	0	3.084042	1.457062	-3.558728
88	1	0	2.399252	2.064347	-4.159892
89	1	0	3.137116	1.900901	-2.559645
90	1	0	4.079517	1.508879	-4.010621
91	6	0	6.680393	-3.094664	-3.208017
92	6	0	-6.680393	3.094664	-3.208017
93	6	0	-6.680393	-3.094664	3.208017
94	6	0	6.680393	3.094664	3.208017
95	6	0	6.049434	-4.133659	-4.168064
96	1	0	5.428116	-3.664443	-4.938448
97	1	0	6.841003	-4.690809	-4.680241
98	1	0	5.428694	-4.852984	-3.622574
99	6	0	7.548521	-2.101281	-4.020705
100	1	0	8.348938	-2.643683	-4.534940
101	1	0	6.967693	-1.571354	-4.783251
102	1	0	8.012897	-1.354203	-3.367503
103	6	0	7.594521	-3.841012	-2.217435
104	1	0	8.100021	-3.156414	-1.526812
105	1	0	7.044762	-4.585402	-1.629987
106	1	0	8.372562	-4.375308	-2.771095
107	6	0	-7.594521	3.841012	-2.217435
108	1	0	-8.100021	3.156414	-1.526812
109	1	0	-7.044762	4.585402	-1.629987
110	1	0	-8.372562	4.375308	-2.771095
111	6	0	-6.049434	4.133659	-4.168064
112	1	0	-5.428694	4.852984	-3.622574
113	1	0	-5.428116	3.664443	-4.938448
114	1	0	-6.841003	4.690809	-4.680241
115	6	0	-7.548521	2.101281	-4.020705
116	1	0	-6.967693	1.571354	-4.783251
117	1	0	-8.012897	1.354203	-3.367503
118	1	0	-8.348938	2.643683	-4.534940
119	6	0	-6.049434	-4.133659	4.168064
120	1	0	-5.428116	-3.664443	4.938448
121	1	0	-6.841003	-4.690809	4.680241
122	1	0	-5.428694	-4.852984	3.622574
123	6	0	-7.594521	-3.841012	2.217435
124	1	0	-8.100021	-3.156414	1.526812
125	1	0	-7.044762	-4.585402	1.629987
126	1	0	-8.372562	-4.375308	2.771095
127	6	0	-7.548521	-2.101281	4.020705
128	1	0	-6.967693	-1.571354	4.783251
129	1	0	-8.012897	-1.354203	3.367503
130	1	0	-8.348938	-2.643683	4.534940
131	6	0	7.548521	2.101281	4.020705
132	1	0	8.348938	2.643683	4.534940
133	1	0	6.967693	1.571354	4.783251
134	1	0	8.012897	1.354203	3.367503
135	6	0	7.594521	3.841012	2.217435
136	1	0	8.100021	3.156414	1.526812
137	1	0	7.044762	4.585402	1.629987
138	1	0	8.372562	4.375308	2.771095
139	6	0	6.049434	4.133659	4.168064
140	1	0	5.428694	4.852984	3.622574
141	1	0	5.428116	3.664443	4.938448
142	1	0	6.841003	4.690809	4.680241

Rotational constants (GHZ): 0.0432582 0.0218071 0.0184429
Standard basis: 6-31G(d) (6D, 7F)
Density matrix has no symmetry -- integrals replicated.
SCF Done: E(UB3LYP) = -2701.93715620 A.U. after 7 cycles
Convg = 0.3439D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.0000 <S**2>= 0.9753 S= 0.6069
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 0.9753, after 0.1255

Item	Value	Threshold	Converged?
Maximum Force	0.000028	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.001076	0.001800	YES
RMS Displacement	0.000303	0.001200	YES

Predicted change in Energy=-2.361160D-08
Optimization completed.
-- Stationary point found.

Diradical dication of conjoined [5]helicene, *meso*, C_{2h} triplet state at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(2+,3)
Framework group C2H[SGH(C4H2),X(C60H72N4)]
Deg. of freedom 107
Full point group C2H NOp 4
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.661445	0.197658	2.405851
2	7	0	-0.661445	0.197658	-2.405851
3	6	0	-3.295656	-0.836819	5.566995
4	6	0	-3.610478	0.160467	4.624968
5	1	0	-4.567632	0.657868	4.711464
6	6	0	-2.757846	0.538204	3.589166
7	6	0	-3.104250	1.658565	2.594269
8	6	0	-2.503382	1.278479	1.239559
9	6	0	-3.083873	1.585235	0.000000
10	1	0	-4.043962	2.081562	0.000000
11	6	0	-2.503382	1.278479	-1.239559
12	6	0	-3.104250	1.658565	-2.594269
13	6	0	-2.757846	0.538204	-3.589166
14	6	0	-3.610478	0.160467	-4.624968
15	1	0	-4.567632	0.657868	-4.711464
16	6	0	-3.295656	-0.836819	-5.566995
17	6	0	-2.057046	-1.482195	-5.424242
18	1	0	-1.769210	-2.272917	-6.106014
19	6	0	-1.177914	-1.143164	-4.404634
20	1	0	-0.238466	-1.673534	-4.312843
21	6	0	-1.519125	-0.135004	-3.497269
22	6	0	-1.251141	0.646371	-1.212431
23	6	0	-0.619394	0.350588	0.000000
24	6	0	-1.251141	0.646371	1.212431
25	6	0	-1.519125	-0.135004	3.497269
26	6	0	-1.177914	-1.143164	4.404634
27	6	0	-2.057046	-1.482195	5.424242
28	1	0	-1.769210	-2.272917	6.106014
29	6	0	-4.621244	1.906971	2.501077
30	1	0	-5.166735	1.013192	2.182239
31	1	0	-4.838375	2.719407	1.802194
32	1	0	-5.019009	2.229722	3.465863
33	6	0	-2.426193	2.983008	3.065971
34	1	0	-1.336769	2.891682	3.118052
35	1	0	-2.795817	3.254778	4.059587
36	1	0	-2.662649	3.798185	2.374157
37	6	0	-4.621244	1.906971	-2.501077
38	1	0	-5.166735	1.013192	-2.182239
39	1	0	-5.019009	2.229722	-3.465863
40	1	0	-4.838375	2.719407	-1.802194
41	6	0	-2.426193	2.983008	-3.065971
42	1	0	-1.336769	2.891682	-3.118052
43	1	0	-2.662649	3.798185	-2.374157
44	1	0	-2.795817	3.254778	-4.059587
45	1	0	-0.238466	-1.673534	4.312843
46	6	0	0.619394	-0.350588	0.000000
47	6	0	1.251141	-0.646371	-1.212431
48	7	0	0.661445	-0.197658	-2.405851
49	7	0	0.661445	-0.197658	2.405851
50	6	0	1.251141	-0.646371	1.212431
51	6	0	2.503382	-1.278479	-1.239559
52	6	0	2.503382	-1.278479	1.239559
53	6	0	3.083873	-1.585235	0.000000
54	1	0	4.043962	-2.081562	0.000000
55	6	0	3.104250	-1.658565	-2.594269
56	6	0	3.104250	-1.658565	2.594269
57	6	0	2.757846	-0.538204	3.589166
58	6	0	2.757846	-0.538204	-3.589166
59	6	0	1.519125	0.135004	-3.497269
60	6	0	3.610478	-0.160467	-4.624968
61	1	0	4.567632	-0.657868	-4.711464
62	6	0	3.295656	0.836819	-5.566995
63	6	0	2.057046	1.482195	-5.424242
64	1	0	1.769210	2.272917	-6.106014
65	6	0	1.177914	1.143164	-4.404634
66	1	0	0.238466	1.673534	-4.312843
67	6	0	1.519125	0.135004	3.497269
68	6	0	3.610478	-0.160467	4.624968
69	1	0	4.567632	-0.657868	4.711464
70	6	0	3.295656	0.836819	5.566995
71	6	0	2.057046	1.482195	5.424242
72	1	0	1.769210	2.272917	6.106014
73	6	0	1.177914	1.143164	4.404634
74	1	0	0.238466	1.673534	4.312843
75	6	0	2.426193	-2.983008	-3.065971
76	1	0	1.336769	-2.891682	-3.118052
77	1	0	2.795817	-3.254778	-4.059587
78	1	0	2.662649	-3.798185	-2.374157

79	6	0	4.621244	-1.906971	-2.501077
80	1	0	5.166735	-1.013192	-2.182239
81	1	0	4.838375	-2.719407	-1.802194
82	1	0	5.019009	-2.229722	-3.465863
83	6	0	4.621244	-1.906971	2.501077
84	1	0	4.838375	-2.719407	1.802194
85	1	0	5.166735	-1.013192	2.182239
86	1	0	5.019009	-2.229722	3.465863
87	6	0	2.426193	-2.983008	3.065971
88	1	0	2.795817	-3.254778	4.059587
89	1	0	1.336769	-2.891682	3.118052
90	1	0	2.662649	-3.798185	2.374157
91	6	0	-4.294626	-1.182724	-6.681025
92	6	0	4.294626	1.182724	-6.681025
93	6	0	-4.294626	-1.182724	6.681025
94	6	0	4.294626	1.182724	6.681025
95	6	0	-3.768195	-2.292861	-7.610325
96	1	0	-2.840199	-2.001344	-8.115344
97	1	0	-3.592625	-3.231528	-7.072525
98	1	0	-4.510166	-2.498673	-8.387818
99	6	0	-3.768195	-2.292861	7.610325
100	1	0	-3.592625	-3.231528	7.072525
101	1	0	-2.840199	-2.001344	8.115344
102	1	0	-4.510166	-2.498673	8.387818
103	6	0	3.768195	2.292861	7.610325
104	1	0	3.592625	3.231528	7.072525
105	1	0	2.840199	2.001344	8.115344
106	1	0	4.510166	2.498673	8.387818
107	6	0	3.768195	2.292861	-7.610325
108	1	0	2.840199	2.001344	-8.115344
109	1	0	3.592625	3.231528	-7.072525
110	1	0	4.510166	2.498673	-8.387818
111	6	0	-4.563045	0.082189	7.534309
112	1	0	-4.989866	0.898945	6.942444
113	1	0	-5.276470	-0.153497	8.331040
114	1	0	-3.642577	0.447555	8.003014
115	6	0	-5.621227	-1.666687	6.043965
116	1	0	-6.079771	-0.901003	5.409120
117	1	0	-5.464743	-2.563866	5.434898
118	1	0	-6.340806	-1.914734	6.831396
119	6	0	-4.563045	0.082189	-7.534309
120	1	0	-5.276470	-0.153497	-8.331040
121	1	0	-4.989866	0.898945	-6.942444
122	1	0	-3.642577	0.447555	-8.003014
123	6	0	-5.621227	-1.666687	-6.043965
124	1	0	-5.464743	-2.563866	-5.434898
125	1	0	-6.079771	-0.901003	-5.409120
126	1	0	-6.340806	-1.914734	-6.831396
127	6	0	4.563045	-0.082189	-7.534309
128	1	0	5.276470	0.153497	-8.331040
129	1	0	4.989866	-0.898945	-6.942444
130	1	0	3.642577	-0.447555	-8.003014
131	6	0	5.621227	1.666687	-6.043965
132	1	0	5.464743	2.563866	-5.434898
133	1	0	6.079771	0.901003	-5.409120
134	1	0	6.340806	1.914734	-6.831396
135	6	0	4.563045	-0.082189	7.534309
136	1	0	4.989866	-0.898945	6.942444
137	1	0	5.276470	0.153497	8.331040
138	1	0	3.642577	-0.447555	8.003014
139	6	0	5.621227	1.666687	6.043965
140	1	0	6.079771	0.901003	5.409120
141	1	0	5.464743	2.563866	5.434898
142	1	0	6.340806	1.914734	6.831396

Rotational constants (GHZ): 0.0432669 0.0236479 0.0173148
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -2701.93695236 A.U. after 6 cycles
Convg = 0.9611D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S**2>= 2.0201 S= 1.0067
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 2.0201, after 2.0003

Item	Value	Threshold	Converged?
Maximum Force	0.000022	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.001062	0.001800	YES
RMS Displacement	0.000248	0.001200	YES

Predicted change in Energy=-3.874733D-08
Optimization completed.
-- Stationary point found.

Diradical dication of conjoined [5]helicene, *meso*, C_{2h} broken symmetry singlet state at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(2+)
Framework group C2H[SGH(C4H2),X(C60H72N4)]
Deg. of freedom 107
Full point group C2H NOp 4
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.661050	0.198367	2.406876
2	7	0	-0.661050	0.198367	-2.406876
3	6	0	-3.305786	-0.836379	5.557625
4	6	0	-3.615833	0.163619	4.616773
5	1	0	-4.572287	0.662728	4.701251
6	6	0	-2.758419	0.543531	3.585891
7	6	0	-3.096505	1.670386	2.595119
8	6	0	-2.497282	1.287470	1.239989
9	6	0	-3.077641	1.593323	0.000000
10	1	0	-4.036237	2.092754	0.000000
11	6	0	-2.497282	1.287470	-1.239989
12	6	0	-3.096505	1.670386	-2.595119
13	6	0	-2.758419	0.543531	-3.585891
14	6	0	-3.615833	0.163619	-4.616773
15	1	0	-4.572287	0.662728	-4.701251
16	6	0	-3.305786	-0.836379	-5.557625
17	6	0	-2.066591	-1.482219	-5.418875
18	1	0	-1.782223	-2.274411	-6.100393
19	6	0	-1.183266	-1.142079	-4.403611
20	1	0	-0.244043	-1.673254	-4.314176
21	6	0	-1.520659	-0.132462	-3.495907
22	6	0	-1.248369	0.653105	-1.213506
23	6	0	-0.616215	0.352615	0.000000
24	6	0	-1.248369	0.653105	1.213506
25	6	0	-1.520659	-0.132462	3.495907
26	6	0	-1.183266	-1.142079	4.403611
27	6	0	-2.066591	-1.482219	5.418875
28	1	0	-1.782223	-2.274411	6.100393
29	6	0	-4.611632	1.928717	2.501401
30	1	0	-5.162786	1.039489	2.179470
31	1	0	-4.822622	2.744423	1.804383
32	1	0	-5.008306	2.251486	3.466695
33	6	0	-2.410494	2.987960	3.071890
34	1	0	-1.321532	2.890104	3.122621
35	1	0	-2.777293	3.258764	4.066880
36	1	0	-2.642246	3.807279	2.383318
37	6	0	-4.611632	1.928717	-2.501401
38	1	0	-5.162786	1.039489	-2.179470
39	1	0	-5.008306	2.251486	-3.466695
40	1	0	-4.822622	2.744423	-1.804383
41	6	0	-2.410494	2.987960	-3.071890
42	1	0	-1.321532	2.890104	-3.122621
43	1	0	-2.642246	3.807279	-2.383318
44	1	0	-2.777293	3.258764	-4.066880
45	1	0	-0.244043	-1.673254	4.314176
46	6	0	0.616215	-0.352615	0.000000
47	6	0	1.248369	-0.653105	-1.213506
48	7	0	0.661050	-0.198367	-2.406876
49	7	0	0.661050	-0.198367	2.406876
50	6	0	1.248369	-0.653105	1.213506
51	6	0	2.497282	-1.287470	-1.239989
52	6	0	2.497282	-1.287470	1.239989
53	6	0	3.077641	-1.593323	0.000000
54	1	0	4.036237	-2.092754	0.000000
55	6	0	3.096505	-1.670386	-2.595119
56	6	0	3.096505	-1.670386	2.595119
57	6	0	2.758419	-0.543531	3.585891
58	6	0	2.758419	-0.543531	-3.585891
59	6	0	1.520659	0.132462	-3.495907
60	6	0	3.615833	-0.163619	-4.616773
61	1	0	4.572287	-0.662728	-4.701251
62	6	0	3.305786	0.836379	-5.557625
63	6	0	2.066591	1.482219	-5.418875
64	1	0	1.782223	2.274411	-6.100393
65	6	0	1.183266	1.142079	-4.403611
66	1	0	0.244043	1.673254	-4.314176
67	6	0	1.520659	0.132462	3.495907
68	6	0	3.615833	-0.163619	4.616773
69	1	0	4.572287	-0.662728	4.701251
70	6	0	3.305786	0.836379	5.557625
71	6	0	2.066591	1.482219	5.418875
72	1	0	1.782223	2.274411	6.100393
73	6	0	1.183266	1.142079	4.403611
74	1	0	0.244043	1.673254	4.314176
75	6	0	2.410494	-2.987960	-3.071890
76	1	0	1.321532	-2.890104	-3.122621
77	1	0	2.777293	-3.258764	-4.066880
78	1	0	2.642246	-3.807279	-2.383318

79	6	0	4.611632	-1.928717	-2.501401
80	1	0	5.162786	-1.039489	-2.179470
81	1	0	4.822622	-2.744423	-1.804383
82	1	0	5.008306	-2.251486	-3.466695
83	6	0	4.611632	-1.928717	2.501401
84	1	0	4.822622	-2.744423	1.804383
85	1	0	5.162786	-1.039489	2.179470
86	1	0	5.008306	-2.251486	3.466695
87	6	0	2.410494	-2.987960	3.071890
88	1	0	2.777293	-3.258764	4.066880
89	1	0	1.321532	-2.890104	3.122621
90	1	0	2.642246	-3.807279	2.383318
91	6	0	-4.309004	-1.183380	-6.667273
92	6	0	4.309004	1.183380	-6.667273
93	6	0	-4.309004	-1.183380	6.667273
94	6	0	4.309004	1.183380	6.667273
95	6	0	-3.787359	-2.295964	-7.596365
96	1	0	-2.861035	-2.006491	-8.105603
97	1	0	-3.610757	-3.233759	-7.057382
98	1	0	-4.532566	-2.502486	-8.370562
99	6	0	-3.787359	-2.295964	7.596365
100	1	0	-3.610757	-3.233759	7.057382
101	1	0	-2.861035	-2.006491	8.105603
102	1	0	-4.532566	-2.502486	8.370562
103	6	0	3.787359	2.295964	7.596365
104	1	0	3.610757	3.233759	7.057382
105	1	0	2.861035	2.006491	8.105603
106	1	0	4.532566	2.502486	8.370562
107	6	0	3.787359	2.295964	-7.596365
108	1	0	2.861035	2.006491	-8.105603
109	1	0	3.610757	3.233759	-7.057382
110	1	0	4.532566	2.502486	-8.370562
111	6	0	-4.579099	0.080274	7.522029
112	1	0	-5.002911	0.898597	6.930187
113	1	0	-5.295629	-0.156285	8.315705
114	1	0	-3.659934	0.443708	7.994758
115	6	0	-5.633894	-1.664429	6.024332
116	1	0	-6.089253	-0.896920	5.389431
117	1	0	-5.476292	-2.560580	5.414049
118	1	0	-6.356529	-1.913187	6.808730
119	6	0	-4.579099	0.080274	-7.522029
120	1	0	-5.295629	-0.156285	-8.315705
121	1	0	-5.002911	0.898597	-6.930187
122	1	0	-3.659934	0.443708	-7.994758
123	6	0	-5.633894	-1.664429	-6.024332
124	1	0	-5.476292	-2.560580	-5.414049
125	1	0	-6.089253	-0.896920	-5.389431
126	1	0	-6.356529	-1.913187	-6.808730
127	6	0	4.579099	-0.080274	-7.522029
128	1	0	5.295629	0.156285	-8.315705
129	1	0	5.002911	-0.898597	-6.930187
130	1	0	3.659934	-0.443708	-7.994758
131	6	0	5.633894	1.664429	-6.024332
132	1	0	5.476292	2.560580	-5.414049
133	1	0	6.089253	0.896920	-5.389431
134	1	0	6.356529	1.913187	-6.808730
135	6	0	4.579099	-0.080274	7.522029
136	1	0	5.002911	-0.898597	6.930187
137	1	0	5.295629	0.156285	8.315705
138	1	0	3.659934	-0.443708	7.994758
139	6	0	5.633894	1.664429	6.024332
140	1	0	6.089253	0.896920	5.389431
141	1	0	5.476292	2.560580	5.414049
142	1	0	6.356529	1.913187	6.808730

Rotational constants (GHZ): 0.0431306 0.0236994 0.0173345
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -2701.93612640 A.U. after 7 cycles
Convg = 0.6445D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.0000 <S**2>= 0.9899 S= 0.6135
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 0.9899, after 0.1296

Item	Value	Threshold	Converged?
Maximum Force	0.000039	0.000450	YES
RMS Force	0.000005	0.000300	YES
Maximum Displacement	0.001655	0.001800	YES
RMS Displacement	0.000426	0.001200	YES

Predicted change in Energy=-1.407464D-07
Optimization completed.
-- Stationary point found.

Diradical dication of conjoined [5]helicene, triplet state, C_1-symmetric transition state from chiral D_2 structure to meso C_{2h} structure at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(2+,3)
Framework group C1[X(C64H74N4)]
Deg. of freedom 420
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.419230	-0.678557	0.316039
2	7	0	-2.434562	-0.725755	0.300407
3	6	0	1.209830	-2.774091	-0.020015
4	6	0	-0.000510	-3.462490	0.177382
5	1	0	0.003194	-4.539034	0.072696
6	6	0	-1.218121	-2.831519	0.460126
7	6	0	-2.527957	-3.543825	0.783582
8	6	0	-3.631541	-2.831716	-0.012555
9	6	0	-4.717467	-3.515186	-0.557171
10	1	0	-4.771908	-4.586695	-0.414595
11	6	0	-5.743721	-2.889664	-1.287377
12	6	0	-5.628914	-1.505442	-1.482343
13	1	0	-6.373495	-0.968955	-2.057514
14	6	0	-4.562613	-0.784211	-0.959849
15	1	0	-4.510945	0.279802	-1.145609
16	6	0	-3.573061	-1.434358	-0.215459
17	6	0	-1.221335	-1.423963	0.421377
18	6	0	-0.014308	-0.719937	0.362835
19	6	0	1.206682	-1.399841	0.250245
20	6	0	-2.456230	-5.051153	0.485674
21	1	0	-2.296023	-5.257099	-0.577624
22	1	0	-3.376393	-5.550857	0.797215
23	1	0	-1.648889	-5.514993	1.060096
24	6	0	-2.806524	-3.366366	2.309202
25	1	0	-2.852265	-2.311818	2.598880
26	1	0	-2.019407	-3.847317	2.899176
27	1	0	-3.763600	-3.831764	2.564132
28	6	0	-0.025772	0.653028	-0.003268
29	6	0	-1.243269	1.310440	-0.171186
30	7	0	-2.403881	0.656844	0.270897
31	7	0	2.398389	0.677562	-0.072808
32	6	0	1.160455	1.238708	-0.443147
33	6	0	-1.308215	2.588010	-0.738402
34	6	0	1.104008	2.372359	-1.270783
35	6	0	-0.123672	3.048297	-1.342974
36	1	0	-0.164939	3.964861	-1.917209
37	6	0	-2.653285	3.315469	-0.803207
38	6	0	-3.569099	2.780644	0.318381
39	6	0	-3.458400	1.451252	0.789098
40	6	0	-4.581843	3.558592	0.878174
41	1	0	-4.695284	4.579289	0.536321
42	6	0	-5.470845	3.091269	1.865103
43	6	0	-5.305064	1.767333	2.304528
44	6	0	-4.312392	0.952892	1.778270
45	1	0	-4.189569	-0.059515	2.146074
46	1	0	-5.946185	1.361933	3.077449
47	6	0	-3.311647	3.010543	-2.183175
48	1	0	-3.437879	1.935436	-2.346494
49	1	0	-4.296117	3.485061	-2.240262
50	1	0	-2.692781	3.403919	-2.996573
51	6	0	-2.446275	4.841835	-0.682080
52	1	0	-2.032887	5.118007	0.292563
53	1	0	-1.771955	5.207326	-1.460804
54	1	0	-3.388442	5.376128	-0.824275
55	6	0	-6.557194	4.024508	2.420391
56	6	0	-6.911720	-3.719807	-1.840191
57	6	0	-7.429670	3.333157	3.485342
58	1	0	-7.957339	2.460992	3.082718
59	1	0	-6.843772	3.015407	4.355290
60	1	0	-8.188807	4.034591	3.844570
61	6	0	-5.884649	5.261185	3.067225
62	1	0	-5.229644	4.968657	3.895291
63	1	0	-5.288048	5.832534	2.348065
64	1	0	-6.652022	5.933509	3.465341
65	6	0	-7.475577	4.483840	1.260273
66	1	0	-6.925846	5.031816	0.487555
67	1	0	-7.970900	3.630284	0.784232
68	1	0	-8.252646	5.152028	1.646218
69	6	0	-6.360392	-4.793062	-2.811558
70	1	0	-5.665761	-5.480915	-2.317665
71	1	0	-7.186690	-5.390953	-3.210502
72	1	0	-5.838311	-4.332072	-3.657400
73	6	0	-7.931467	-2.852362	-2.602259
74	1	0	-8.379429	-2.084827	-1.960815
75	1	0	-7.484382	-2.360842	-3.473915
76	1	0	-8.745601	-3.484939	-2.968960
77	6	0	-7.642980	-4.414611	-0.664640
78	1	0	-6.984363	-5.089886	-0.108056

79	1	0	-8.049272	-3.680248	0.039677
80	1	0	-8.477264	-5.011566	-1.048038
81	6	0	2.342353	2.668423	-2.120023
82	6	0	2.462562	-3.361504	-0.674398
83	6	0	3.511210	1.602928	-0.106836
84	6	0	3.586730	-1.478440	0.639808
85	6	0	4.403218	1.783173	0.954153
86	6	0	4.501135	-1.138286	1.641523
87	6	0	3.539942	2.541141	-1.171592
88	6	0	3.657389	-2.783129	0.088406
89	6	0	4.787299	-3.549684	0.364248
90	6	0	4.624366	3.411740	-1.243851
91	6	0	5.607364	-1.937350	1.910734
92	6	0	5.462115	2.680137	0.861165
93	6	0	5.641837	3.475507	-0.274390
94	6	0	5.817114	-3.139869	1.229710
95	1	0	4.860275	-4.530363	-0.087672
96	1	0	6.291138	-1.614668	2.686435
97	1	0	4.323498	-0.296944	2.284561
98	1	0	4.234056	1.298936	1.897362
99	1	0	6.131214	2.767214	1.708585
100	1	0	4.668409	4.102197	-2.076140
101	6	0	2.426338	1.589676	-3.242991
102	1	0	2.497648	0.576159	-2.836691
103	1	0	1.546238	1.639926	-3.892454
104	1	0	3.316533	1.769332	-3.853730
105	6	0	2.260297	4.049161	-2.793954
106	1	0	1.371993	4.107374	-3.430107
107	1	0	2.225713	4.864880	-2.064993
108	1	0	3.116066	4.211837	-3.453319
109	6	0	7.047939	-4.030462	1.447585
110	6	0	6.823704	4.438140	-0.452733
111	6	0	7.816293	4.358488	0.722438
112	1	0	7.358150	4.661858	1.670717
113	1	0	8.230117	3.350684	0.841956
114	1	0	8.655338	5.036180	0.537537
115	6	0	7.574690	4.068915	-1.756146
116	1	0	6.931378	4.146208	-2.639272
117	1	0	8.419484	4.750204	-1.902829
118	1	0	7.968545	3.047467	-1.712007
119	6	0	6.298268	5.891632	-0.553184
120	1	0	5.631346	6.034047	-1.410256
121	1	0	5.754603	6.180759	0.353046
122	1	0	7.140148	6.581204	-0.675664
123	6	0	7.761954	-4.235448	0.088487
124	1	0	8.641125	-4.874182	0.224241
125	1	0	7.113449	-4.719425	-0.649732
126	1	0	8.099651	-3.281192	-0.330822
127	6	0	6.601690	-5.403089	2.009157
128	1	0	5.932590	-5.934515	1.323964
129	1	0	7.478380	-6.039417	2.169713
130	1	0	6.086212	-5.290626	2.969382
131	6	0	8.048717	-3.401450	2.435272
132	1	0	8.407795	-2.425460	2.089251
133	1	0	7.619330	-3.279964	3.436271
134	1	0	8.921518	-4.053925	2.535021
135	6	0	2.444025	-4.900652	-0.672942
136	1	0	3.306327	-5.300337	-1.211534
137	1	0	2.447700	-5.313910	0.340570
138	1	0	1.560053	-5.270201	-1.200912
139	6	0	2.491310	-2.883195	-2.158761
140	1	0	1.612309	-3.249360	-2.699288
141	1	0	2.515520	-1.792035	-2.238788
142	1	0	3.387152	-3.275465	-2.650121

Rotational constants (GHZ): 0.0439113 0.0229142 0.0171732
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -2701.87955672 A.U. after 1 cycles
Convg = 0.4359D-08 -V/T = 2.0098
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S**2>= 2.0214 S= 1.0071
<L.S>= 0.000000000000E+00
Annihilation of the first spin contaminant:
S**2 before annihilation 2.0214, after 2.0003

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000567	0.001800	YES
RMS Displacement	0.000082	0.001200	YES

Predicted change in Energy=-6.308443D-10
Optimization completed.
-- Stationary point found.

Diradical dication of conjoined [5]helicene, broken-symmetry singlet state, C_1-symmetric transition state from chiral D_2 structure to meso C_{2h} structure at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C64H74N4(2+)
Framework group C1[X(C64H74N4)]
Deg. of freedom 420
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.386476	-0.698884	0.244304
2	7	0	-2.454650	-0.717408	0.275045
3	6	0	1.175247	-2.790651	-0.072361
4	6	0	-0.041484	-3.457367	0.166168
5	1	0	-0.050817	-4.536559	0.078657
6	6	0	-1.250113	-2.818583	0.485054
7	6	0	-2.558664	-3.512277	0.855483
8	6	0	-3.650349	-2.828432	0.016136
9	6	0	-4.722975	-3.528853	-0.533706
10	1	0	-4.771535	-4.598326	-0.373979
11	6	0	-5.750993	-2.919362	-1.274216
12	6	0	-5.652243	-1.533219	-1.475974
13	1	0	-6.402874	-1.009368	-2.054889
14	6	0	-4.594889	-0.796749	-0.958941
15	1	0	-4.551366	0.266198	-1.152517
16	6	0	-3.596625	-1.433451	-0.213222
17	6	0	-1.259510	-1.417483	0.409015
18	6	0	-0.041882	-0.716708	0.253346
19	6	0	1.183684	-1.416151	0.150230
20	6	0	-2.493876	-5.030861	0.624911
21	1	0	-2.337324	-5.285869	-0.428446
22	1	0	-3.415642	-5.512361	0.960395
23	1	0	-1.685548	-5.471035	1.216874
24	6	0	-2.842907	-3.263106	2.365623
25	1	0	-2.872325	-2.196226	2.609501
26	1	0	-2.066276	-3.729487	2.981151
27	1	0	-3.808849	-3.699419	2.639081
28	6	0	-0.047783	0.618622	-0.143207
29	6	0	-1.271442	1.303520	-0.290352
30	7	0	-2.416295	0.669621	0.194168
31	7	0	2.373593	0.658912	-0.139871
32	6	0	1.160185	1.213787	-0.551560
33	6	0	-1.309366	2.589784	-0.815863
34	6	0	1.118303	2.369976	-1.344611
35	6	0	-0.104811	3.049543	-1.396910
36	1	0	-0.142601	3.971436	-1.964420
37	6	0	-2.657476	3.314591	-0.897951
38	6	0	-3.528088	2.822816	0.281269
39	6	0	-3.437278	1.489481	0.745503
40	6	0	-4.476114	3.637772	0.898461
41	1	0	-4.566153	4.663915	0.566110
42	6	0	-5.335705	3.197393	1.922950
43	6	0	-5.203909	1.863447	2.341412
44	6	0	-4.266613	1.015614	1.766359
45	1	0	-4.165780	-0.002462	2.125066
46	1	0	-5.826284	1.474753	3.137994
47	6	0	-3.349876	2.932463	-2.237371
48	1	0	-3.460698	1.848820	-2.347059
49	1	0	-4.345217	3.385261	-2.290898
50	1	0	-2.762059	3.295664	-3.087666
51	6	0	-2.462842	4.843751	-0.863534
52	1	0	-2.015120	5.176841	0.077925
53	1	0	-1.823642	5.173318	-1.687387
54	1	0	-3.415223	5.362285	-0.998391
55	6	0	-6.360721	4.165912	2.531741
56	6	0	-6.910827	-3.763753	-1.821361
57	6	0	-7.205693	3.501335	3.635208
58	1	0	-7.784574	2.651836	3.255201
59	1	0	-6.590131	3.156411	4.473812
60	1	0	-7.919701	4.228246	4.034270
61	6	0	-5.615198	5.375394	3.149071
62	1	0	-4.933273	5.056337	3.945042
63	1	0	-5.032364	5.927524	2.404066
64	1	0	-6.338371	6.073566	3.583902
65	6	0	-7.316616	4.662637	1.418179
66	1	0	-6.784707	5.194151	0.621857
67	1	0	-7.863043	3.828838	0.963554
68	1	0	-8.050935	5.355728	1.842223
69	6	0	-6.347190	-4.846451	-2.775310
70	1	0	-5.649898	-5.522305	-2.268853
71	1	0	-7.167614	-5.455608	-3.169349
72	1	0	-5.824784	-4.393396	-3.625214
73	6	0	-7.932853	-2.913838	-2.600008
74	1	0	-8.392133	-2.143334	-1.970312
75	1	0	-7.484048	-2.428030	-3.473985
76	1	0	-8.738835	-3.557709	-2.965053

77	6	0	-7.643602	-4.448177	-0.640234
78	1	0	-6.983495	-5.112397	-0.072328
79	1	0	-8.057400	-3.707337	0.052776
80	1	0	-8.472557	-5.054616	-1.020328
81	6	0	2.363526	2.661636	-2.186658
82	6	0	2.429982	-3.397984	-0.707839
83	6	0	3.490820	1.577886	-0.158374
84	6	0	3.538389	-1.500851	0.605595
85	6	0	4.366681	1.750964	0.920338
86	6	0	4.437113	-1.154181	1.622858
87	6	0	3.540560	2.528577	-1.214539
88	6	0	3.608501	-2.820587	0.081225
89	6	0	4.723525	-3.591974	0.397641
90	6	0	4.629128	3.395084	-1.260025
91	6	0	5.527112	-1.958439	1.930998
92	6	0	5.427624	2.645342	0.853764
93	6	0	5.630830	3.448589	-0.273584
94	6	0	5.739820	-3.176615	1.276597
95	1	0	4.796546	-4.579812	-0.038559
96	1	0	6.193863	-1.631323	2.719543
97	1	0	4.248661	-0.307726	2.255234
98	1	0	4.171593	1.272589	1.861050
99	1	0	6.077837	2.728882	1.716123
100	1	0	4.690214	4.088049	-2.089220
101	6	0	2.468281	1.591466	-3.312030
102	1	0	2.526123	0.573950	-2.912165
103	1	0	1.601346	1.649101	-3.978560
104	1	0	3.371246	1.767156	-3.905349
105	6	0	2.292935	4.047697	-2.849699
106	1	0	1.410612	4.112263	-3.493785
107	1	0	2.250698	4.857285	-2.114125
108	1	0	3.155381	4.215457	-3.499386
109	6	0	6.957821	-4.072031	1.534674
110	6	0	6.819555	4.405538	-0.424994
111	6	0	7.790382	4.315529	0.767430
112	1	0	7.316782	4.616818	1.708767
113	1	0	8.197494	3.305292	0.889418
114	1	0	8.635659	4.990126	0.600818
115	6	0	7.591881	4.038458	-1.717095
116	1	0	6.964970	4.123507	-2.611122
117	1	0	8.442231	4.716645	-1.844411
118	1	0	7.980192	3.015023	-1.670885
119	6	0	6.302249	5.862049	-0.528831
120	1	0	5.651786	6.011344	-1.397188
121	1	0	5.743981	6.150160	0.368743
122	1	0	7.149929	6.547425	-0.633185
123	6	0	7.699518	-4.300886	0.193688
124	1	0	8.570677	-4.943684	0.358438
125	1	0	7.063734	-4.790907	-0.551442
126	1	0	8.053425	-3.355097	-0.231268
127	6	0	6.488332	-5.433987	2.104125
128	1	0	5.830911	-5.969925	1.411329
129	1	0	7.356979	-6.073741	2.292134
130	1	0	5.952956	-5.305187	3.051268
131	6	0	7.941478	-3.436837	2.535438
132	1	0	8.316569	-2.468961	2.183693
133	1	0	7.491028	-3.297729	3.524834
134	1	0	8.806282	-4.094828	2.663847
135	6	0	2.394848	-4.936044	-0.685725
136	1	0	3.259484	-5.354686	-1.206363
137	1	0	2.377526	-5.335747	0.333232
138	1	0	1.513098	-5.301145	-1.220996
139	6	0	2.500519	-2.937642	-2.193536
140	1	0	1.631683	-3.303396	-2.750775
141	1	0	2.533443	-1.847338	-2.286644
142	1	0	3.404499	-3.339558	-2.662141

Rotational constants (GHZ): 0.0431081 0.0231609 0.0172967

Standard basis: 6-31G(d) (6D, 7F)

SCF Done: E(UB3LYP) = -2701.86866592 A.U. after 11 cycles

Convg = 0.7181D-08 -V/T = 2.0099

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.0000 <S**2>= 0.0000 S= 0.0000

<L.S>= 0.000000000000E+00

Annihilation of the first spin contaminant:

S**2 before annihilation 0.0000, after 0.0000

Item	Value	Threshold	Converged?
Maximum Force	0.000031	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001261	0.001800	YES
RMS Displacement	0.000237	0.001200	YES

Predicted change in Energy=-2.024484D-08

Optimization completed.

-- Stationary point found.

Simplified structure diradical dication $1b^{2\bullet 2+}$, chiral, D_2 triplet state at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C40H26N4(2+,3)
Framework group D2[C2(HCC.CCH),X(C36H24N4)]
Deg. of freedom 51
Full point group D2 NOp 4
Largest Abelian subgroup D2 NOp 4
Largest concise Abelian subgroup D2 NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.406331	-0.168805	-0.668771
2	7	0	-2.406331	0.168805	-0.668771
3	6	0	5.574798	-2.260946	-2.485747
4	6	0	4.636946	-1.576269	-3.258522
5	1	0	4.711791	-1.594577	-4.342090
6	6	0	3.594105	-0.864344	-2.664072
7	6	0	2.568475	-0.121595	-3.496138
8	6	0	1.230142	-0.077304	-2.804036
9	6	0	0.000000	0.000000	-3.471855
10	1	0	0.000000	0.000000	-4.558686
11	6	0	-1.230142	0.077304	-2.804036
12	6	0	-2.568475	0.121595	-3.496138
13	6	0	-3.594105	0.864344	-2.664072
14	6	0	-4.636946	1.576269	-3.258522
15	1	0	-4.711791	1.594577	-4.342090
16	6	0	-5.574798	2.260946	-2.485747
17	6	0	-5.465283	2.261044	-1.090888
18	1	0	-6.176523	2.814215	-0.486249
19	6	0	-4.434383	1.567224	-0.469270
20	1	0	-4.339615	1.588641	0.609417
21	6	0	-3.513282	0.862319	-1.256499
22	6	0	-1.210156	0.066544	-1.403373
23	6	0	0.000000	0.000000	-0.709066
24	6	0	1.210156	-0.066544	-1.403373
25	6	0	3.513282	-0.862319	-1.256499
26	6	0	4.434383	-1.567224	-0.469270
27	6	0	5.465283	-2.261044	-1.090888
28	1	0	6.176523	-2.814215	-0.486249
29	1	0	4.339615	-1.588641	0.609417
30	6	0	0.000000	0.000000	0.709066
31	6	0	-1.210156	-0.066544	1.403373
32	7	0	-2.406331	-0.168805	0.668771
33	7	0	2.406331	0.168805	0.668771
34	6	0	1.210156	0.066544	1.403373
35	6	0	-1.230142	-0.077304	2.804036
36	6	0	1.230142	0.077304	2.804036
37	6	0	0.000000	0.000000	3.471855
38	1	0	0.000000	0.000000	4.558686
39	6	0	2.568475	0.121595	3.496138
40	6	0	-2.568475	-0.121595	3.496138
41	6	0	3.594105	0.864344	2.664072
42	6	0	-3.594105	-0.864344	2.664072
43	6	0	-3.513282	-0.862319	1.256499
44	6	0	3.513282	0.862319	1.256499
45	6	0	-4.636946	-1.576269	3.258522
46	1	0	-4.711791	-1.594577	4.342090
47	6	0	4.636946	1.576269	3.258522
48	1	0	4.711791	1.594577	4.342090
49	6	0	5.574798	2.260946	2.485747
50	6	0	5.465283	2.261044	1.090888
51	1	0	6.176523	2.814215	0.486249
52	6	0	4.434383	1.567224	0.469270
53	1	0	4.339615	1.588641	-0.609417
54	6	0	-5.574798	-2.260946	2.485747
55	6	0	-5.465283	-2.261044	1.090888
56	6	0	-4.434383	-1.567224	0.469270
57	1	0	-4.339615	-1.588641	-0.609417
58	1	0	-6.176523	-2.814215	0.486249
59	1	0	-6.379955	2.804787	-2.969018
60	1	0	6.379955	-2.804787	-2.969018
61	1	0	6.379955	2.804787	2.969018
62	1	0	-6.379955	-2.804787	2.969018
63	1	0	-2.909793	-0.911355	-3.675657
64	1	0	-2.477641	0.582262	-4.484683
65	1	0	-2.909793	0.911355	3.675657
66	1	0	-2.477641	-0.582262	4.484683
67	1	0	2.477641	-0.582262	-4.484683
68	1	0	2.909793	0.911355	-3.675657
69	1	0	2.477641	0.582262	4.484683
70	1	0	2.909793	-0.911355	3.675657

Rotational constants (GHZ): 0.1309975 0.0606618 0.0485619
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -1758.40018832 A.U. after 5 cycles
NFock= 5 Conv=0.80D-08 -V/T= 2.0097
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S**2>= 2.0219 S= 1.0073
<L.S>= 0.00000000000
Annihilation of the first spin contaminant:
S**2 before annihilation 2.0219, after 2.0003

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000015	YES
RMS Force	0.000001	0.000010	YES
Maximum Displacement	0.000051	0.000060	YES
RMS Displacement	0.000010	0.000040	YES

Predicted change in Energy=-8.632029D-10
Optimization completed.
-- Stationary point found.

Simplified structure diradical dication $1b^{2\bullet 2+}$, *meso*, C_{2h} triplet state at UB3LYP/6-31G(d) in the gas phase

Stoichiometry C40H26N4(2+,3)
Framework group C2H[SGH(C4H2),X(C36H24N4)]
Deg. of freedom 53
Full point group C2H NOp 4
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.682762	0.096690	2.410269
2	7	0	-0.682762	0.096690	-2.410269
3	6	0	-3.123677	-1.236976	5.573279
4	6	0	-3.605312	-0.319453	4.639747
5	1	0	-4.625446	0.045917	4.716168
6	6	0	-2.798160	0.139954	3.598141
7	6	0	-3.313613	1.125162	2.569906
8	6	0	-2.659753	0.896749	1.231636
9	6	0	-3.289001	1.120932	0.000000
10	1	0	-4.316849	1.473828	0.000000
11	6	0	-2.659753	0.896749	-1.231636
12	6	0	-3.313613	1.125162	-2.569906
13	6	0	-2.798160	0.139954	-3.598141
14	6	0	-3.605312	-0.319453	-4.639747
15	1	0	-4.625446	0.045917	-4.716168
16	6	0	-3.123677	-1.236976	-5.573279
17	6	0	-1.819659	-1.730962	-5.458688
18	1	0	-1.449038	-2.466220	-6.165433
19	6	0	-0.993949	-1.297404	-4.428733
20	1	0	0.006632	-1.699978	-4.331302
21	6	0	-1.480948	-0.353992	-3.513268
22	6	0	-1.331054	0.451298	-1.212222
23	6	0	-0.662718	0.253784	0.000000
24	6	0	-1.331054	0.451298	1.212222
25	6	0	-1.480948	-0.353992	3.513268
26	6	0	-0.993949	-1.297404	4.428733
27	6	0	-1.819659	-1.730962	5.458688
28	1	0	-1.449038	-2.466220	6.165433
29	1	0	0.006632	-1.699978	4.331302
30	6	0	0.662718	-0.253784	0.000000
31	6	0	1.331054	-0.451298	-1.212222
32	7	0	0.682762	-0.096690	-2.410269
33	7	0	0.682762	-0.096690	2.410269
34	6	0	1.331054	-0.451298	1.212222
35	6	0	2.659753	-0.896749	-1.231636
36	6	0	2.659753	-0.896749	1.231636
37	6	0	3.289001	-1.120932	0.000000
38	1	0	4.316849	-1.473828	0.000000
39	6	0	3.313613	-1.125162	-2.569906
40	6	0	3.313613	-1.125162	2.569906
41	6	0	2.798160	-0.139954	3.598141
42	6	0	2.798160	-0.139954	-3.598141
43	6	0	1.480948	0.353992	-3.513268
44	6	0	3.605312	0.319453	-4.639747
45	1	0	4.625446	-0.045917	-4.716168
46	6	0	3.123677	1.236976	-5.573279
47	6	0	1.819659	1.730962	-5.458688
48	1	0	1.449038	2.466220	-6.165433
49	6	0	0.993949	1.297404	-4.428733
50	1	0	-0.006632	1.699978	-4.331302
51	6	0	1.480948	0.353992	3.513268
52	6	0	3.605312	0.319453	4.639747
53	1	0	4.625446	-0.045917	4.716168
54	6	0	3.123677	1.236976	5.573279
55	6	0	1.819659	1.730962	5.458688
56	1	0	1.449038	2.466220	6.165433
57	6	0	0.993949	1.297404	4.428733
58	1	0	-0.006632	1.699978	4.331302
59	1	0	3.766845	1.577974	6.378035
60	1	0	-3.766845	-1.577974	6.378035
61	1	0	3.766845	1.577974	-6.378035
62	1	0	-3.766845	-1.577974	-6.378035
63	1	0	-4.402227	1.053347	2.487317
64	1	0	-4.402227	1.053347	-2.487317
65	1	0	-3.102110	2.156349	-2.898145
66	1	0	3.102110	-2.156349	-2.898145
67	1	0	4.402227	-1.053347	-2.487317
68	1	0	3.102110	-2.156349	2.898145
69	1	0	4.402227	-1.053347	2.487317
70	1	0	-3.102110	2.156349	2.898145

Rotational constants (GHZ): 0.1309565 0.0634746 0.0469196
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -1758.39891208 A.U. after 5 cycles
NFock= 5 Conv=0.10D-07 -V/T= 2.0097
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S**2>= 2.0215 S= 1.0072
<L.S>= 0.00000000000
Annihilation of the first spin contaminant:
S**2 before annihilation 2.0215, after 2.0003
-- Stationary point found

Item	Value	Threshold	Converged?
Maximum Force	0.000007	0.000015	YES
RMS Force	0.000001	0.000010	YES
Maximum Displacement	0.000021	0.000060	YES
RMS Displacement	0.000006	0.000040	YES

Predicted change in Energy=-1.448165D-09
Optimization completed.
-- Stationary point found.

Simplified structure of diradical dication $1b^{2\bullet 2+}$, triplet state, C_1-symmetric transition state from chiral D_2 structure to meso C_{2h} structure at UB3LYP/6-31G(d) in the gas phase.

Stoichiometry C40H26N4(2+,3)
Framework group C1[X(C40H26N4)]
Deg. of freedom 204
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.437072	0.690443	0.190766
2	7	0	2.432895	0.732960	0.196812
3	6	0	-1.208433	2.756267	-0.267459
4	6	0	-0.002581	3.462221	-0.141176
5	1	0	-0.003189	4.530498	-0.340646
6	6	0	1.209050	2.842879	0.177495
7	6	0	2.510120	3.570565	0.370247
8	6	0	3.645673	2.797777	-0.263403
9	6	0	4.745517	3.456807	-0.815194
10	1	0	4.792667	4.540292	-0.753031
11	6	0	5.767022	2.751412	-1.448177
12	6	0	5.677889	1.361219	-1.565676
13	1	0	6.450372	0.804828	-2.086433
14	6	0	4.593363	0.678120	-1.028370
15	1	0	4.533400	-0.395099	-1.146272
16	6	0	3.590054	1.392793	-0.357476
17	6	0	1.215757	1.438434	0.261310
18	6	0	0.004360	0.733216	0.263688
19	6	0	-1.216602	1.404197	0.097178
20	6	0	0.014330	-0.660166	-0.007009
21	6	0	1.232766	-1.321566	-0.138976
22	7	0	2.397107	-0.645660	0.267014
23	7	0	-2.415034	-0.687170	-0.110519
24	6	0	-1.168360	-1.273377	-0.422931
25	6	0	1.304668	-2.618262	-0.658141
26	6	0	-1.095018	-2.452941	-1.180979
27	6	0	0.130866	-3.131830	-1.231152
28	1	0	0.177929	-4.079644	-1.761074
29	6	0	2.648691	-3.304510	-0.666617
30	6	0	3.564994	-2.754240	0.412441
31	6	0	3.454432	-1.413351	0.837854
32	6	0	4.553712	-3.541574	1.003997
33	1	0	4.656863	-4.578843	0.697989
34	6	0	5.408301	-3.016351	1.974789
35	6	0	5.274220	-1.684938	2.384537
36	6	0	4.294031	-0.876122	1.822174
37	1	0	4.168610	0.148929	2.152155
38	1	0	5.924075	-1.281501	3.154203
39	6	0	-2.323221	-2.814629	-1.974984
40	6	0	-2.451077	3.301127	-0.919978
41	6	0	-3.540556	-1.609704	-0.105185
42	6	0	-3.619357	1.510327	0.437200
43	6	0	-4.462938	-1.719421	0.943724
44	6	0	-4.567184	1.236362	1.432713
45	6	0	-3.546836	-2.599563	-1.116347
46	6	0	-3.669987	2.765268	-0.211823
47	6	0	-4.792303	3.574822	-0.035869
48	6	0	-4.619688	-3.487926	-1.184185
49	6	0	-5.675754	2.060622	1.603383
50	6	0	-5.520717	-2.620640	0.865573
51	6	0	-5.638200	-3.470153	-0.232603
52	6	0	-5.823938	3.206870	0.825472
53	1	0	-4.833009	4.528238	-0.554984
54	1	0	-6.402322	1.817020	2.371643
55	1	0	-4.414880	0.441215	2.137568
56	1	0	-4.318312	-1.181287	1.861265
57	1	0	-6.229615	-2.676631	1.685221
58	1	0	-4.630259	-4.231998	-1.975579
59	1	0	6.171218	-3.647313	2.419185
60	1	0	-6.466772	-4.166995	-0.306406
61	1	0	-6.691004	3.848345	0.945141
62	1	0	6.616615	3.282607	-1.864774
63	1	0	2.689210	3.692279	1.451273
64	1	0	2.459142	4.581212	-0.044989
65	1	0	-2.461485	4.394669	-0.909969
66	1	0	-2.431499	3.002616	-1.980830
67	1	0	-2.286607	-3.850059	-2.324223
68	1	0	-2.341641	-2.182295	-2.877374
69	1	0	3.115761	-3.169812	-1.656073
70	1	0	2.527065	-4.385541	-0.541883

Rotational constants (GHZ): 0.1298603 0.0621358 0.0463891
Standard basis: 6-31G(d) (6D, 7F)
SCF Done: E(UB3LYP) = -1758.33941396 A.U. after 4 cycles
NFock= 4 Conv=0.34D-08 -V/T= 2.0097
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S**2>= 2.0226 S= 1.0075
<L.S>= 0.00000000000
Annihilation of the first spin contaminant:
S**2 before annihilation 2.0226, after 2.0004
SCF Done: E(UB3LYP) = -1758.33941396 A.U. after 4 cycles
NFock= 4 Conv=0.34D-08 -V/T= 2.0097
<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S**2>= 2.0226 S= 1.0075
<L.S>= 0.00000000000
Annihilation of the first spin contaminant:
S**2 before annihilation 2.0226, after 2.0004

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