Supplementary Information

Air Stable High-Spin Blatter Diradicals: Non-Kekulé versus Kekulé Structures

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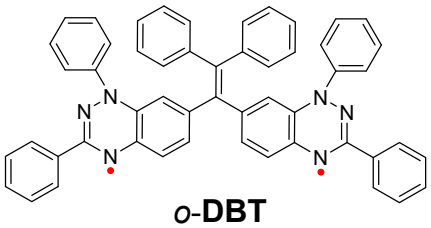
1. Methods and Materials

All reagents were purchased from Sigma-Aldrich, Alfa, Acros and Adamas and used as received. Flash column chromatography was performed with Haiyang silica gel (200-300 mesh), and Greagent neutral Aluminum Oxide (200-300 mesh). Solvent toluene was freshly distilled from CaH_2 under N_2, tetrahydrofuran (THF) was freshly distilled from Na under N_2. Anhydrous Na_2SO_4 was used for drying organic extracts, and all volatiles were removed under reduced pressure. All reaction mixtures and column eluents were monitored by TLC using commercial Huanghai glass plates (HSGF 254, 2.5 x 8 cm). The plates were visualized under UV radiation at 254 and 365 nm. UV absorption spectra were recorded on a Shimadzu UV-2600 UV-VIS spectrophotometer in spectroscopy grade dichloromethane (DCM). Fluorescence spectra were recorded on a Hitachi F-4600 FL Spectrophotometer. NMR spectra were obtained on a Bruker AV II-400 MHz. MALDI-TOF mass spectra (MS) were recorded on a SHIMADZU iD plus Performance using anthracene-1, 8, 9-triol as matrix. High resolution mass spectra (HRMS) were measured on a Waters-Q-TOF-Premier (ESI). ESR measurements were carried out on a Bruker EMX plus X-band spectrometer with 9.8 GHz microwave frequency. SQUID measurements were carried out on a Quantum Design (MPMS-SQUID VSM-094). Thermogravimetric analysis (TGA) measurements were performed on NETZSCH TG 209F1 Iris thermal gravimetric analyzer. Differential scanning calorimetry (DSC) measurements were performed on a Mettler-Toledo differential scanning calorimeter (DSC1). Fourier transform infrared (FT-IR) spectra were measured on a Thermo Fisher Scientific Nicolet 6700 spectrometer. Elemental analysis measurements were performed on a Leeman Labs Euro EA 3000 elemental analyzer.

2. Synthetic details

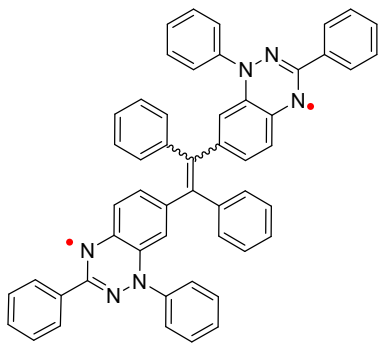
Synthesis of diradical 4,4'-(2,2-Diphenylethenylidene)bis[1,3-Diphenyl-1,4-dihydro-1,2,4-benzotriazin-4-yl] (*o*-DBT)



o-DBT

Compounds 1,1-Bis(4-aminophenyl)-2,2-diphenylethene (**1**) (1.0 g, 2.76 mmol) and (*Z*)-N-phenylbenzohydrazonoyl chloride (**3**) (1.5 g, 6.50 mmol) were charged to a 25 mL two neck flask with dry toluene (10 mL) and refluxed overnight under N_2 flow. After cooling to room temperature, the mixture was concentrated under reduced pressure. Then the residue was dissolved in dry DCM (20 ml) and treated with 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (1.5 ml) and 10 wt% Pd/C powder (0.20 g). Then this solution was stirred exposed to air, after 24 h the solution was filtered and evaporated to yield a crude black solid. This solid was purified by column chromatography (neutral Al_2O_3, EA: Hexane = 1: 30 then 1: 10) and recrystallized from DCM/EtOH to give the diradical *o*-**DBT** as a black solid (0.48 g, 23%). HRMS (ESI+): calcd. for $C_{52}H_{36}N_6^{2\bullet}$ 744.3001, found $[M+H]^+$ 745.3063. UV/vis/NIR (DCM) λ_{max}nm (ε): 304 (74650), 387 (18800), 528 (6450). Melting range from DSC: 239-247 °C. Element analysis (%) calcd. C 83.85, H 4.87, N 11.28; found C 83.77, H 4.90, N 11.31.

Synthesis of diradical 4,4'-(1,2-Diphenyl-1,2-ethenediyl)bis[1,3-Diphenyl-1,4-dihydro-1,2,4-benzotriazin-4-yl] (*p*-DBT)



p-DBT

Compound 1,2-Bis(4-aminophenyl)-1,2-diphenylethene (**2**) (1.0 g, 2.76 mmol) and compound **3** (1.5 g, 6.50 mmol) were charged to a 25 mL two neck flask with dry toluene (10 mL) and refluxed overnight under N_2 flow. After cooling to room temperature, the mixture was concentrated under reduced pressure. Then the residue was dissolved in dry DCM (20 ml) and treated with DBU (1.5 ml) and 10 wt% Pd/C powder (0.20 g). Then this solution was stirred exposed to air, after 24 h the solution was filtered and evaporated to yield a crude black solid. This solid was purified by column chromatography (neutral Al_2O_3, EA: Hexane = 1: 30 then 1: 10) and recrystallized from DCM/EtOH to give the diradical *p*-**DBT** as a black solid (0.39 g, 19%). HRMS (ESI^+): calcd. for $C_{52}H_{36}N_6^{2\bullet}$ 744.3001, found $[M+H]^+$ 745.3077. UV/vis/NIR (DCM) λ_{max}nm (ε): 277 (65950), 324 (38050), 387 (17850), 524 (5450), 659 (2900). Melting range from DSC: 245-258 °C. Element analysis (%) calcd. C 83.85, H 4.87, N 11.28; found C 83.94, H 4.84, N 11.26.

Methods to grow single crystals of diradicals *o*-DBT and *p*-DBT

Three major methods have been used to grow single crystals for x-ray diffraction. Method a: slow evaporation of *o*-**DBT** and *p*-**DBT** in pure or mixed solutions (DCM, toluene, THF, DCM/toluene, DCM/hexane, DCM/MeOH, DCM/EtOH, DCM/EA, DCM/acetone, DCM/acetonitrile) in 4 mL glass vials (with cap). Method b: slow diffusion of poor solvents e.g. hexane, toluene, MeOH, EtOH and acetonitrile to saturated DCM solution of *o*-**DBT** and *p*-**DBT** in NMR tubes (with cap) and 4 mL glass vials (with cap) at room temperature and -20 ^{o}C (in refrigerator). Method c: slow cooling the hot solutions of *o*-**DBT** and *p*-**DBT** in pure or mixed solvents (e.g. toluene, THF, EA, acetone, DCM/toluene, DCM/hexane, DCM/MeOH, DCM/EtOH, DCM/EA, DCM/acetone, DCM/acetonitrile).

Possible resonance structures of diradical *p*-DBT

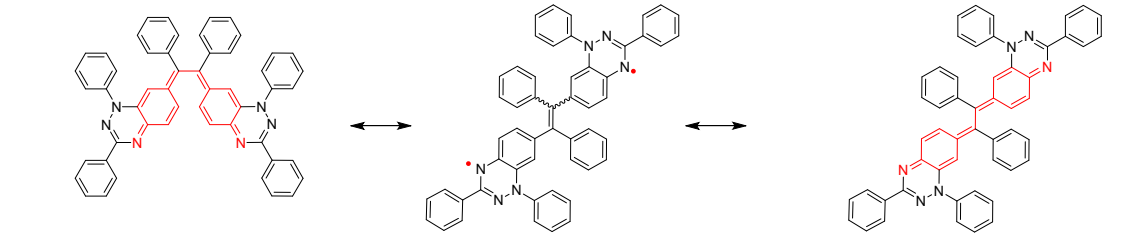


Figure S1. Possible resonance structures of *p*-**DBT**.

Analys of the possible structure of *p*-DBT (trans- or cis-):

The isometric trans- and cis- mixtures of the intermediate compound **2** is inseparable. Moreover, the ratio of trans- and cis- isomers of **2** is almost same after recrystallization.[1-3] As for diradical *p*-**DBT**, we purified it by column chromatography, prep TLC plate, and recrystallization, and finally only one spot was observed in TLC plate. But it is hard to say it is a mixture or pure compound (either trans- or cis-isomer) since the purity cannot be checked by NMR spectroscopy. The DFT calculation indicates that the ground state (open-shell singlet) of the *trans*-isomer of p-DBT is 0.49 kcal/mol lower than that of *cis*-isomer, suggesting that the *trans*-isomer is the thermodynamically favourable isomer. Thus, we used the *trans*-isomer in this manuscript that can explain the experimental data (SQUID and ESR) well.

3. NMR and Mass spectra

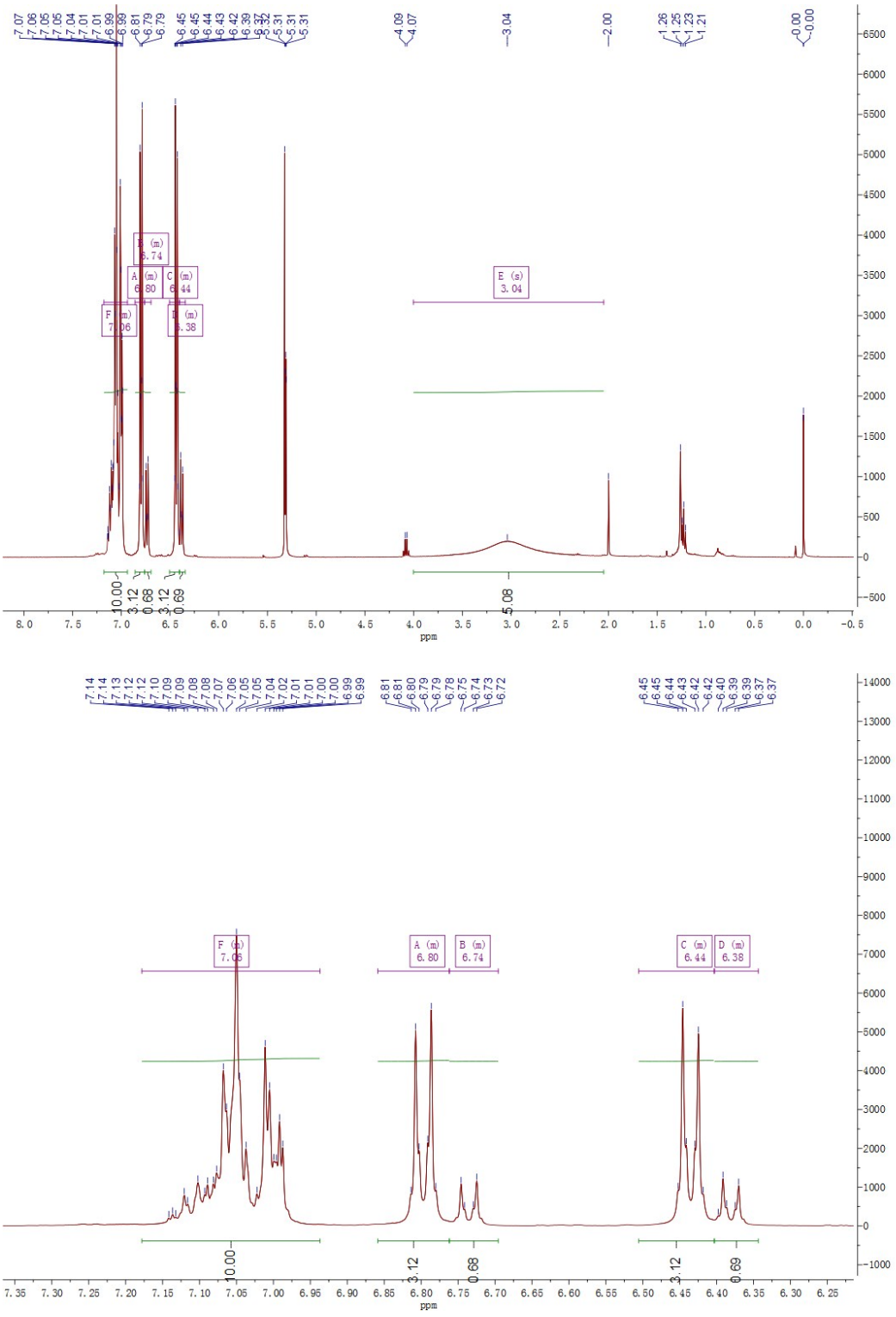


Figure S2. [1]HNMR spectrum of **2** in CD_2Cl_2.

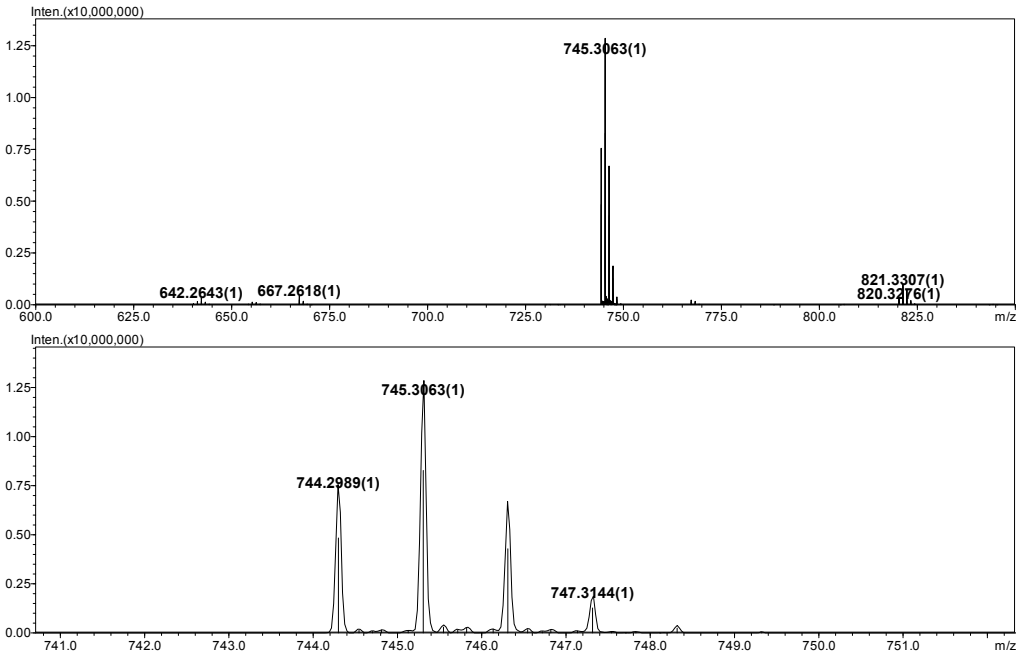


Figure S3. HRMS (ESI) spectrum of *o*-**DBT**.

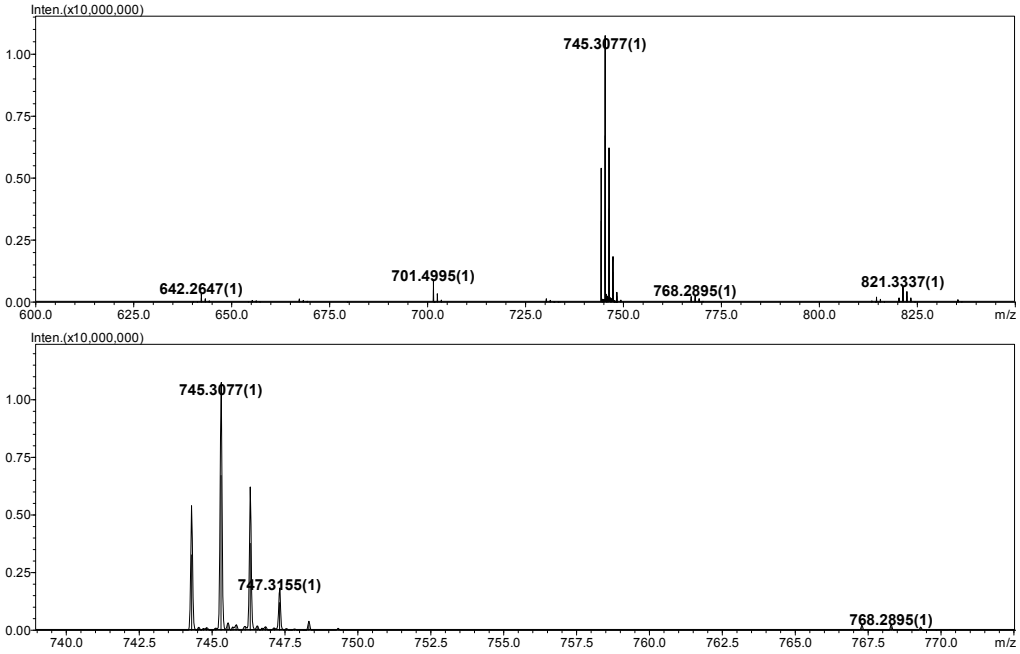


Figure S4. HRMS (ESI) spectrum of *p*-**DBT**.

4. UV-vis-NIR spectroscopy and cyclic voltammetry

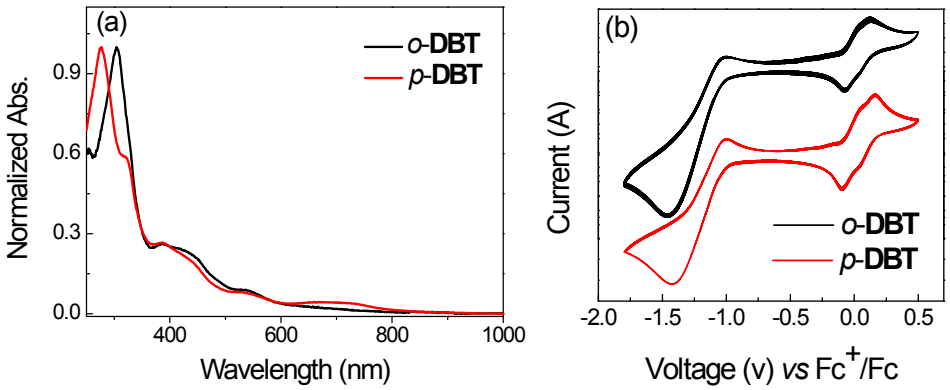


Figure S5. (a) Normalized UV/vis/NIR absorption spectra of diradicals *o*-**DBT** (blackline) and *p*-**DBT** (red line) in DCM. (b) Cyclic voltammograms of *o*-**DBT** and *p*-**DBT** in dry DCM with 0.1 M Bu_4NPF_6 as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 100 mV/s.

Table S1. Photophysical and electrochemical data of diradicals *o*-**DBT**, and *p*-**DBT**.

Compound	HOMO(eV)	LUMO (eV)	E_g^{EC} (eV)	E_g^{opt} (eV)	$\Delta E_{s\text{-}t}$ (kcal/mol)
o-**DBT**	-4.28	-3.49	0.79	1.38	-0.21
p-**DBT**	-4.51	-3.51	1.00	1.24	-0.26

5. Fourier transform infrared (IR) spectra

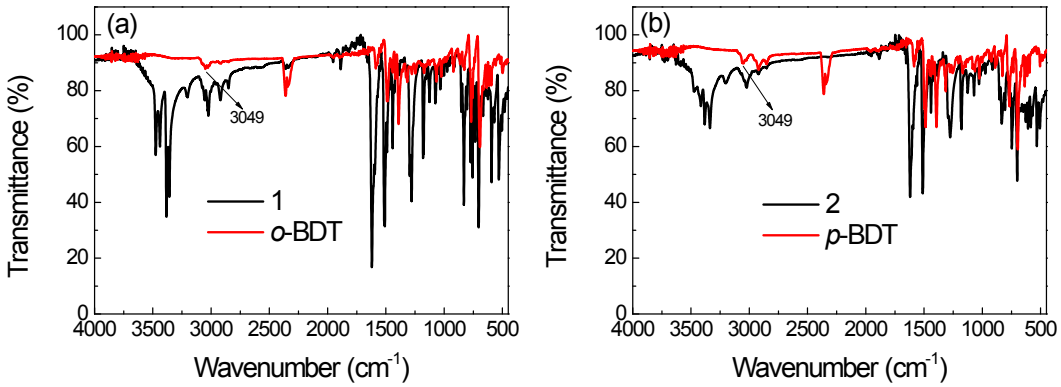


Figure S6. FT-IR spectra of compounds **1** & *o*-**DBT** (a), and **2** & *p*-**DBT** (b). The absence of typical N-H stretching vibration absorption above 3100 cm^{-1} indicates that both **1** and **2** are fully converted into diradicals *o*-**DBT** and *p*-**DBT**.

6. ESR spectra/simulation

Simulations of ESR spectra were performed with the *Easyspin* program in Matlab.[4]

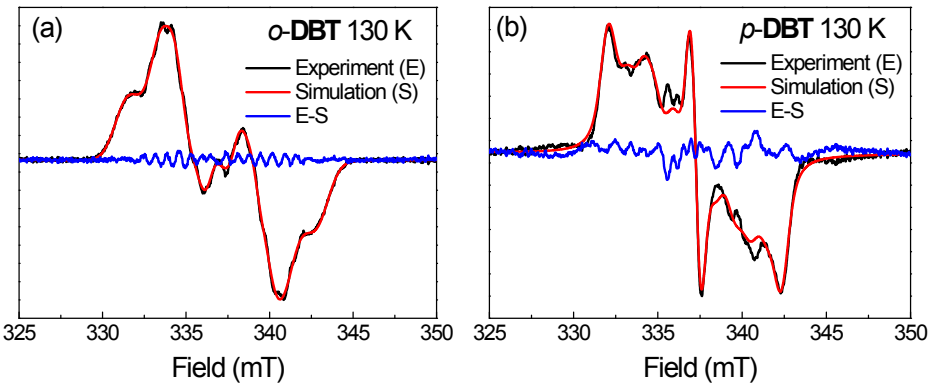


Figure S7. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 130 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

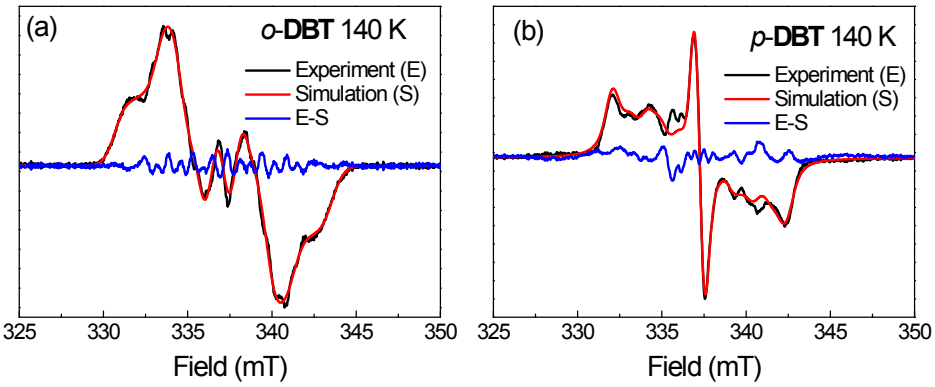


Figure S8. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 140 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

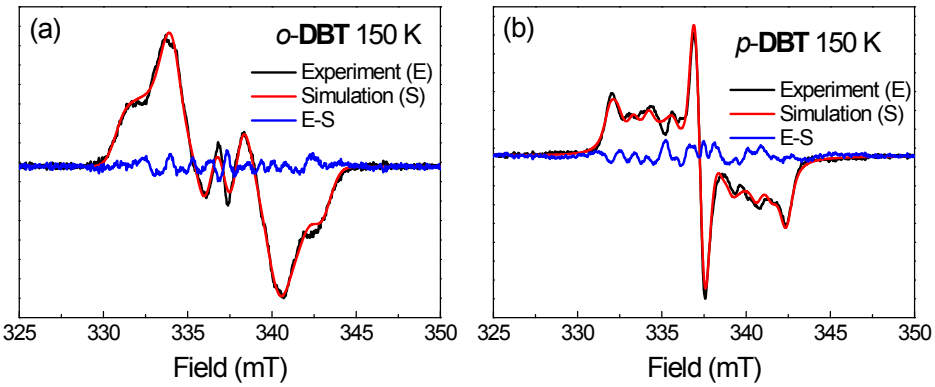


Figure S9. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 150 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

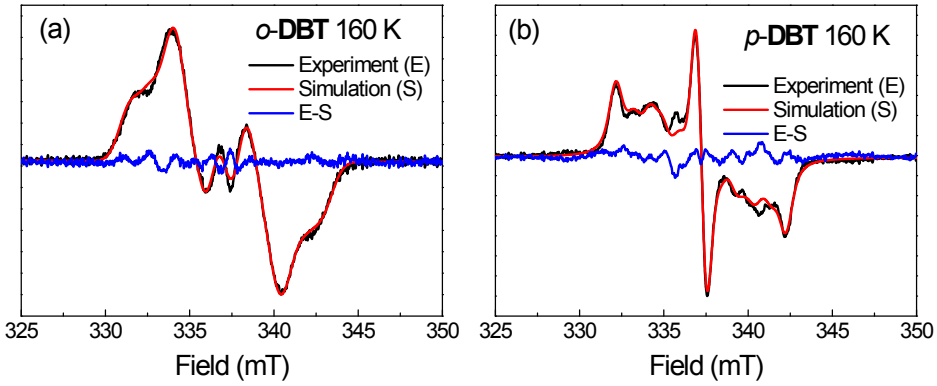


Figure S10. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 160 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively..

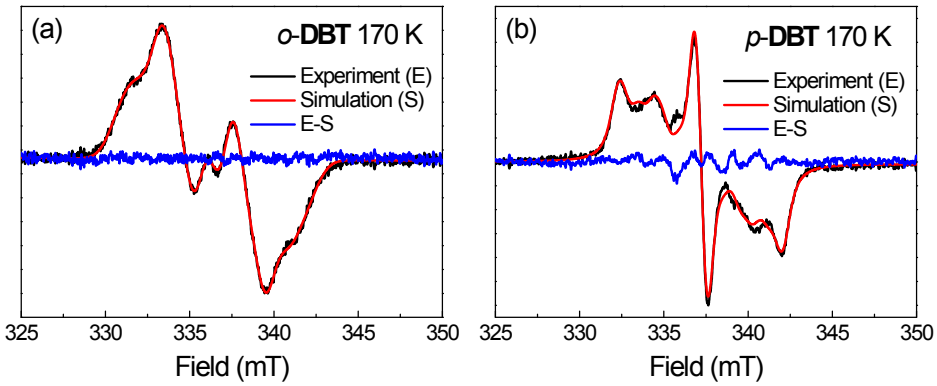


Figure S11. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 170 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

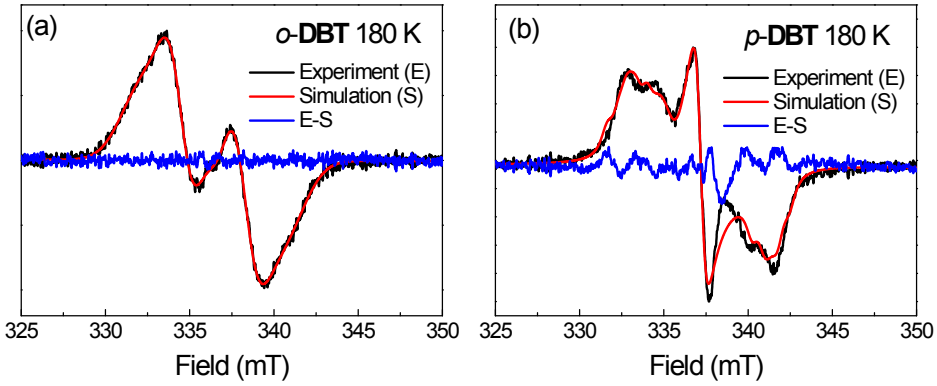


Figure S12. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 180 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

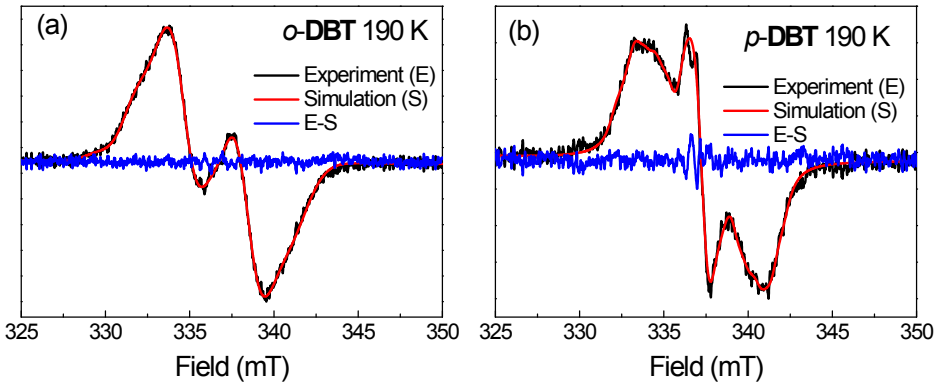


Figure S13. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 190 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

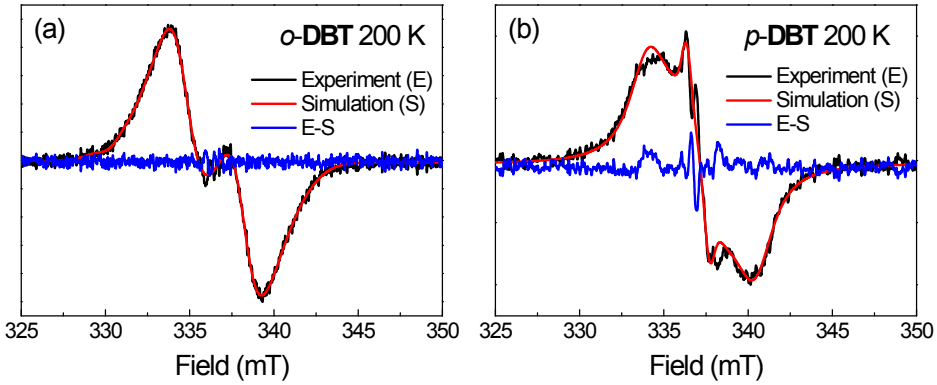


Figure S14. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 200 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

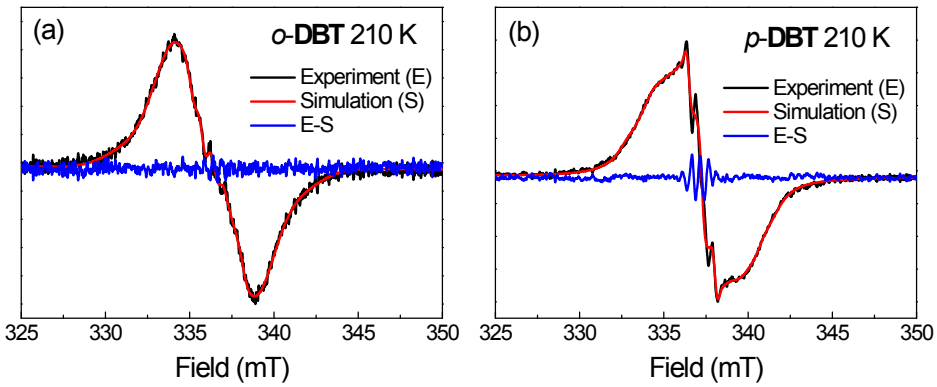


Figure S15. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 210 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

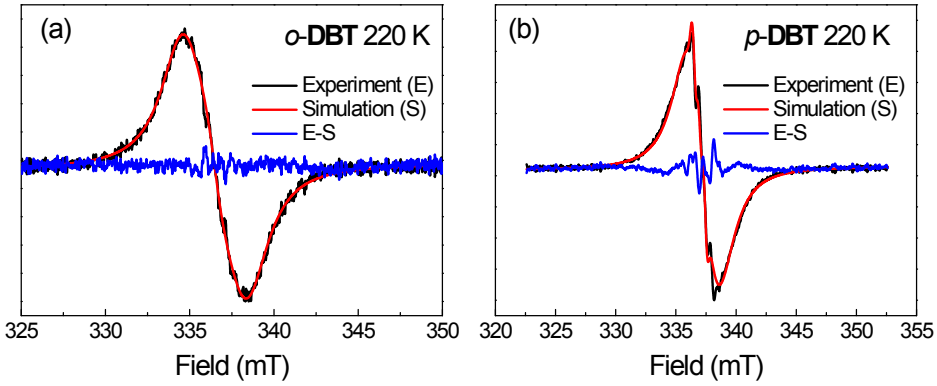


Figure S16. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 220 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

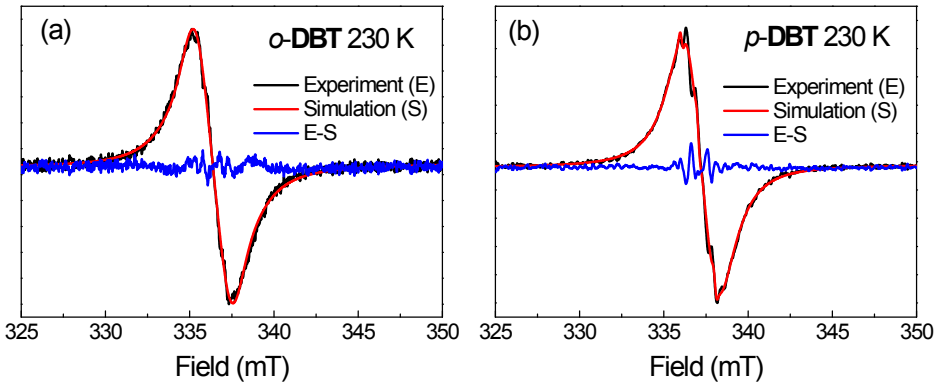


Figure S17. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 230 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

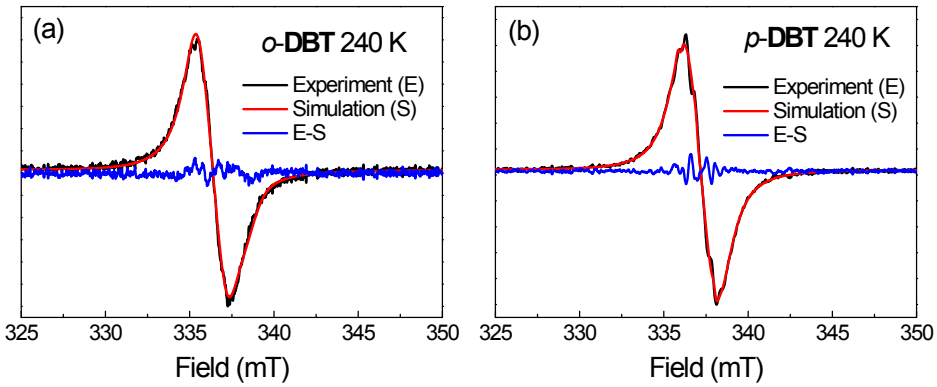


Figure S18. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 240 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

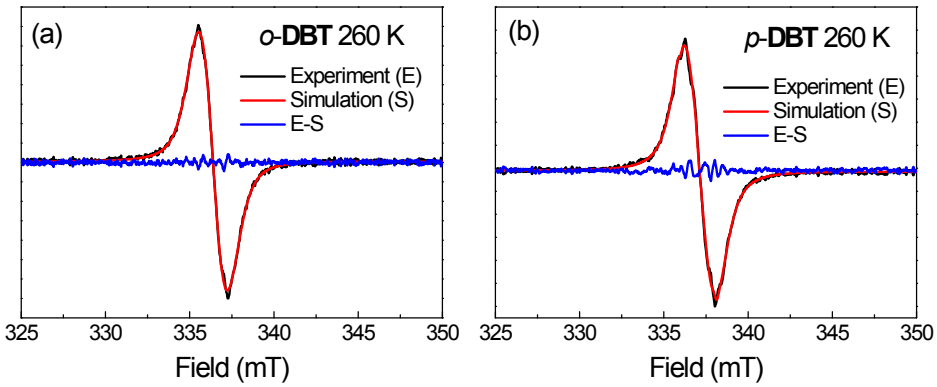


Figure S19. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 260 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

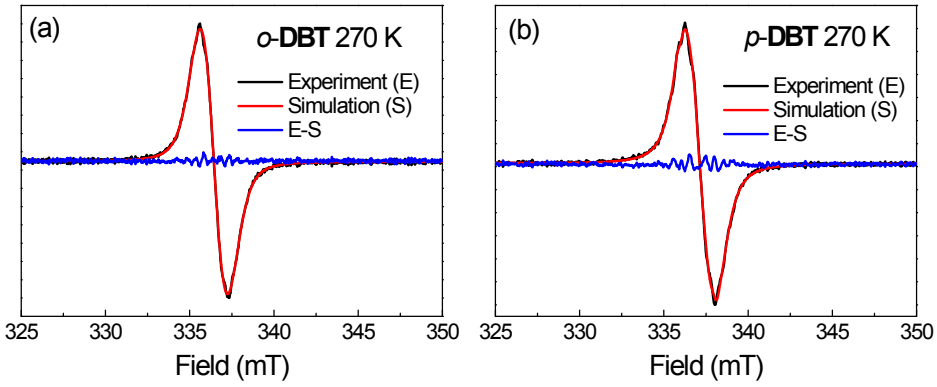


Figure S20. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 270 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

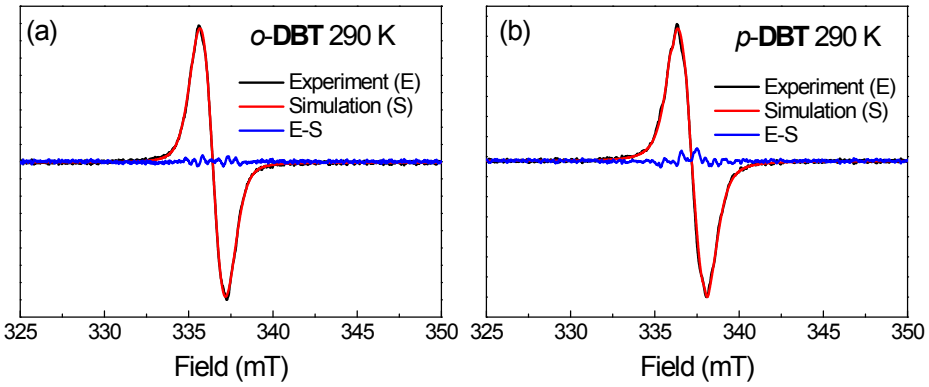


Figure S21. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 290 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

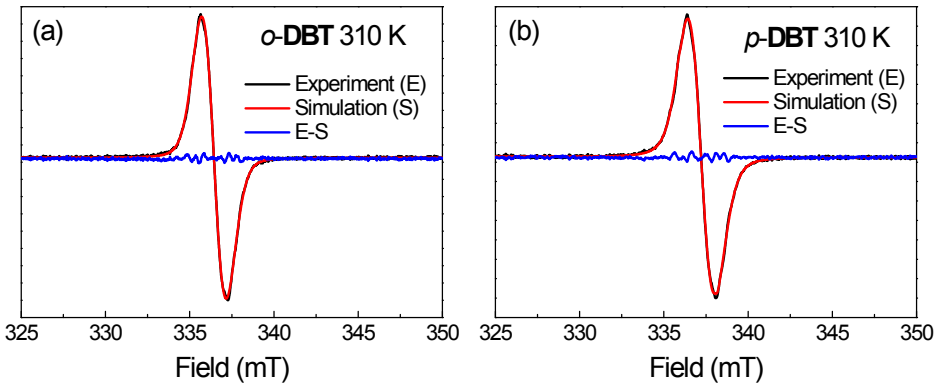


Figure S22. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 310 K. The black, red and blue lines indicate experimental, simulated and difference (experimental - simulated) ESR spectra, respectively.

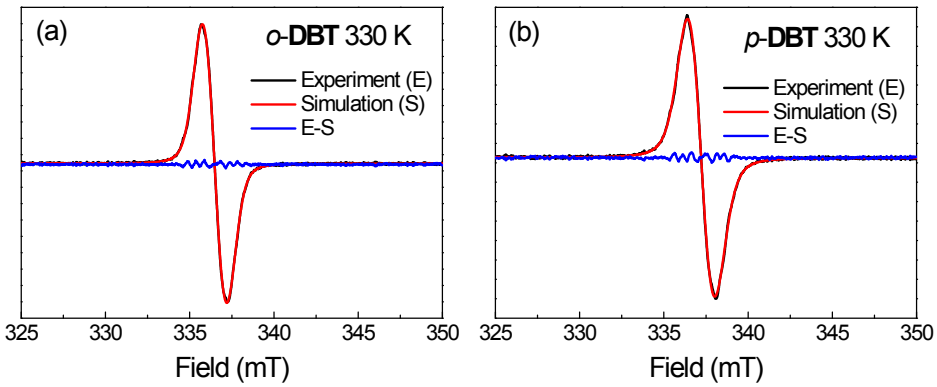


Figure S23. ESR spectra of *o*-**DBT** (a) and *p*-**DBT** (b) (in toluene/$CHCl_3$, v/v= 4:1) at 330 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

7. Magnetization measurements and data analysis

Magnetization measurements

For SUQID measurements, first the two diradicals are dried in vacuum at 50 °C for 48 hours, then confirmed by Mass Spectra, FT-IR and combustion analyses. Magnetic susceptibility of powder samples of *o*-DBT (16.3 mg) and *p*-DBT (14.7 mg) was measured in a polycarbonate capsule fitted in a plastic straw as a function of temperature in heating (3 K→ 300 K) mode with 30 seconds of temperature stability at each temperature (1 K increment in a range 3–10 K, 2 K increment in a range 10–30 K, 5 K increment in a range 30–80 K, and 10 K increment in a range 80-300 K) at 1.0 T using a SQUID magnetometer (Quantum Design MPMS-SQUID VSM-094). The data was corrected for both sample diamagnetism (Pascal′s constants) and the diamagnetism of the sample holder (polycarbonate capsule).

Data analysis

The SQUID data in Fig. 3a were fitted with a modified Bleaney-Bowers equation.[5, 6]

$$\chi = \frac{Ng^2\mu_\beta^2}{kT}\left[\frac{2}{3 + e^{-2J/kT}}\right](1-\rho) + \frac{Ng^2\mu_\beta^2}{2kT}\rho + TIP(1-\rho) \qquad Equation\ S1$$

Where ρ is the fraction of s=1/2 impurity, *TIP* is the temperature independent paramagnetism due to a small energy gap between group singlet state and excited triplet state.

The yield ρ= 5.0%, *TIP*= 1.7 x 10^{-3} emu/mol, and 2*J*= -0.21 kal/mol for *o*-**DBT**, ρ= 20.1%, *TIP*= 1.1 x 10^{-3} emu/mol, and 2*J*= -0.18 kcal/mol for *p*-**DBT**, with the Adj. R-Square >0.995. However, both **1** and **2** are fully converted into diradicals *o*-**DBT** and *p*-**DBT** according to the FT-IR spectra (**Figure S6**). We assume that the large monoradical impurity ρ value of *p*-**DBT** is due to the intermolecular exchange interactions between adjacent molecules in the solid states. The spins between adjacent molecules are paired if the exchange interactions between two overlapping nitrogen containing rings are large enough. Then the left spin of each molecule might pair with the spin of other molecules, or stay as a doublet monoradical. Thus there is a lot of triplet disappear with some or no increase in doublet depending on how complete the spin pairing between molecules.

To confirm this assumption the ESR signals of *p*-**DBT** in solid state and dilute solid matrix were measured and compared. First, the ESR signal of a small amount of solid *p*-**DBT** (~ 1 mg) at room temperature was measured. Then excess benzophenone was added to the tube and melted to dissolve *p*-**DBT**. Followed by rapid cooling to get a solid solution, in which each radical center is surrounded by benzophenone molecule without intermolecular exchange interactions and spin pairing. Finally, the ESR spectra of the solid solution at room temperature were taken. As expected, ESR spectrum with an unresolved single peak was observed for solid *p*-**DBT**, while triplet ESR spectrum and increased double integrals were obtained for the solid solution (**Figure S24**). Hence, the s=1/2 impurity (ρ) in SQUID is from the intermolecular exchange interactions in the solid state.

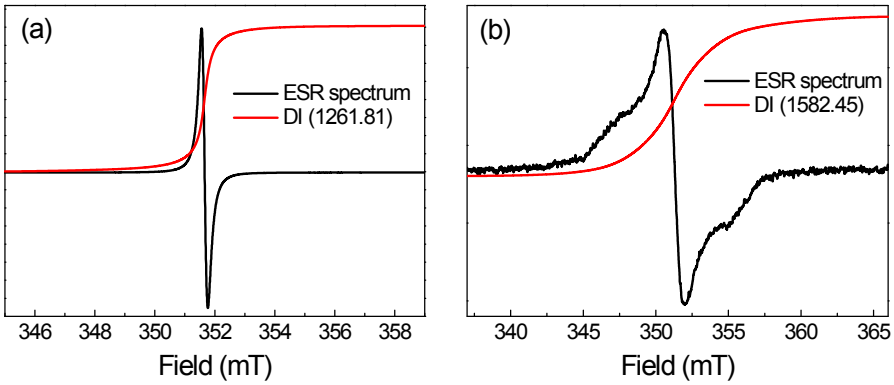


Figure S24. Room temperature ESR spectra and double integrals (DI) of diradical *p*-**DBT** in the absence (a) and presence (b) of benzophenone matrix. Inset shows the magnified ESR spectra in benzophenone matrix.

8. Stability test

8.1 Chemical Stability

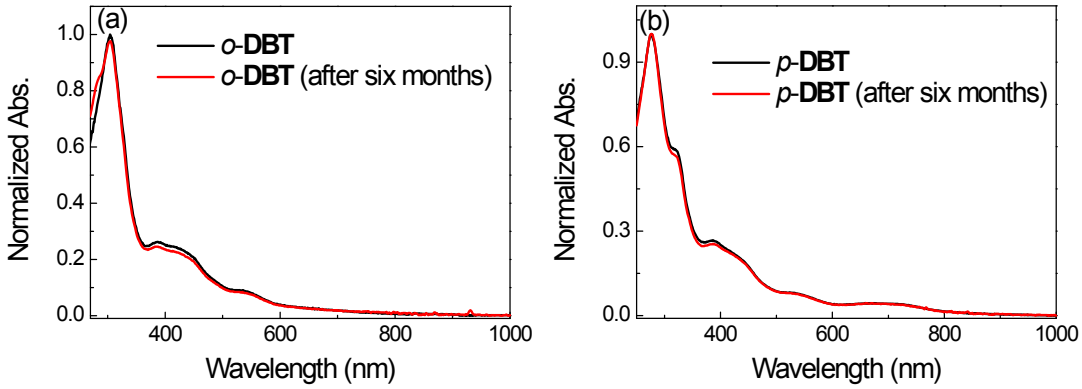


Figure S25. Normalized UV/vis/NIR absorption spectra of (a) ***o*-DBT** and (b) ***p*-DBT** in DCM. Black line: fresh prepared solution samples, red line: solution samples stored for six months under ambient conditions.

8.2 Photo Stability

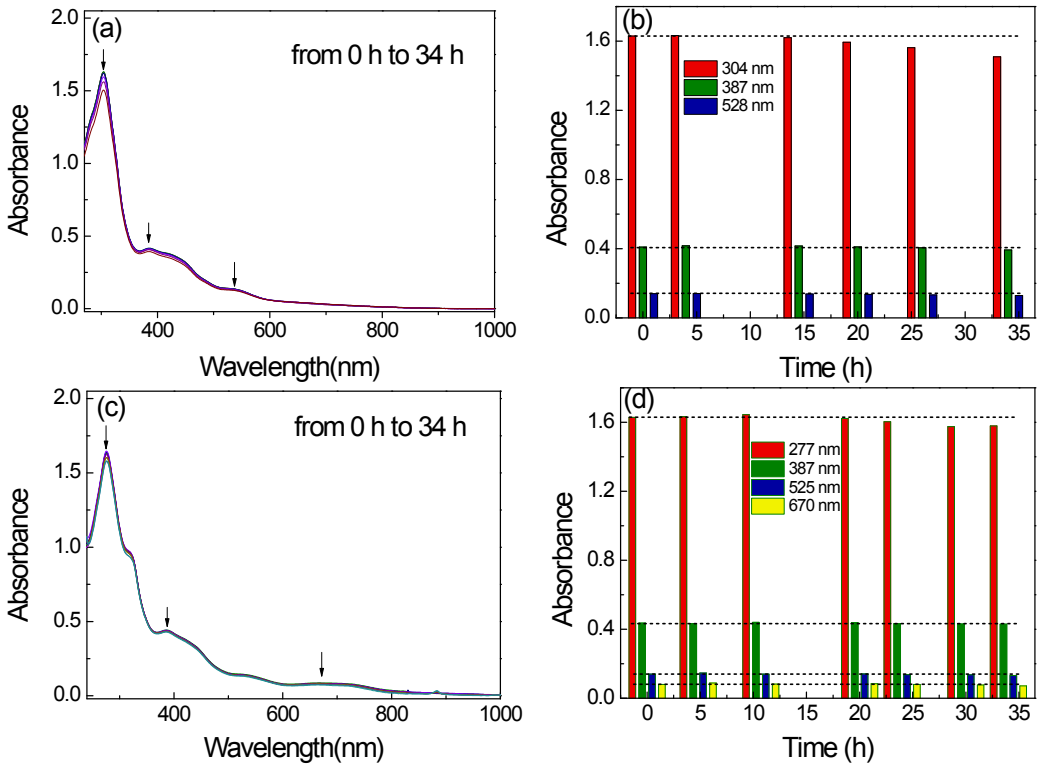


Figure S26. UV-Vis-NIR absorption spectra (a) and the changes of the optical density at 304, 387 and 528 nm of ***o*-DBT** (b) in DCM upon irradiation with white light (400 W) for different time. The distance

between sample and lamp is 20 cm. UV-Vis-NIR absorption spectra (c) and the changes of the optical density at 277, 387, 525 and 670 nm of ***p*-DBT** (d) in DCM upon irradiation with white light (400 W) for different time. The dotted lines are the original optical intensities used as reference.

8.3 Thermal Stability

TGA diagram (Fig. 4a) indicates that ***o*-DBT** and ***p*-DBT** are stable up to ~ 320 °C and ~ 160 °C, respectively. To verify whether both diradicals remain intact at high temperature, we annealed ***o*-DBT** at 220, 270, 300 and 350 °C, ***p*-DBT** at 126 and 200 °C for 15 minutes under N_2 using the TGA apparatus. The UV-Vis-NIR (Figure S24), MS (Figure S25) and ESR (Figure S26) spectra reveal that ***o*-DBT** is stable up to 200 °C without any decomposition, it begins to decompose at 270 °C and completely disappears at 350 °C. While ***p*-DBT** is stable up to 200 °C without obvious decomposition.

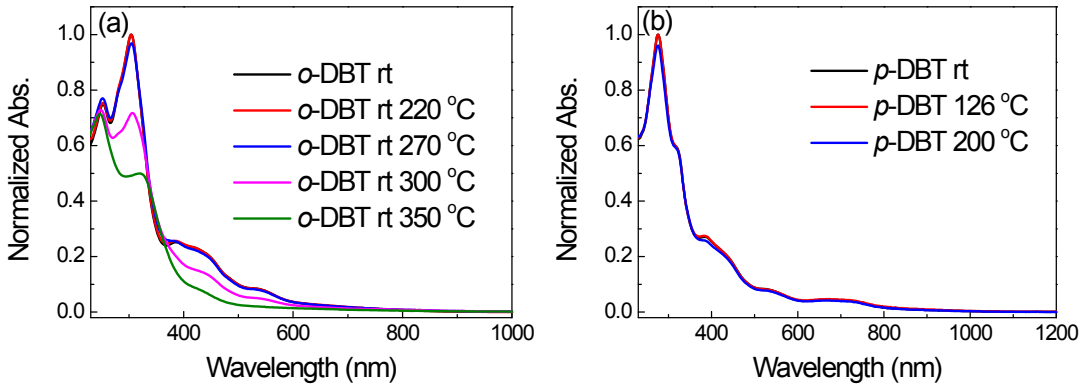


Figure S27. Room temperature UV-Vis-NIR absorption spectra of ***o*-DBT** (a) and ***p*-DBT** (b) in DCM after annealing for different temperatures under N_2 for 15 minutes (using TGA apparatus). Spectra intensities are normalized relative to sample concentration.

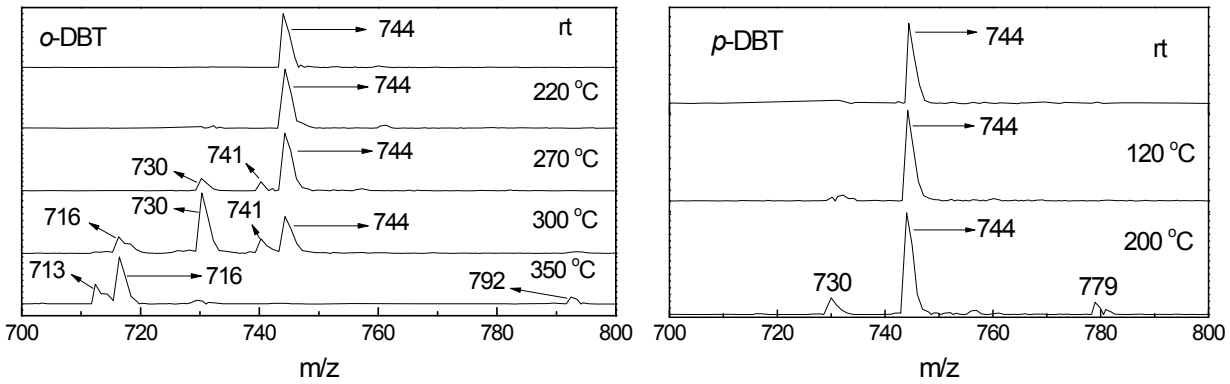


Figure S28. MALDI-TOF mass spectra of ***o*-DBT** (left) and ***p*-DBT** (right) after annealing for different temperatures under N_2 for 15 minutes (using TGA apparatus).

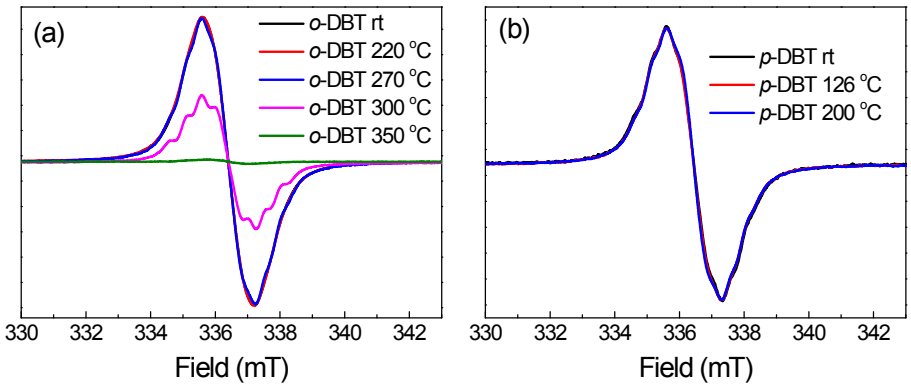


Figure S29. Room temperature ESR spectra of ***o*-DBT** (a) and ***p*-DBT** (b) in toluene after annealing for different temperatures under N_2 for 15 minutes (using TGA apparatus). Spectra intensities are normalized relative to sample concentration.

9. Differential scanning calorimetry (DSC)

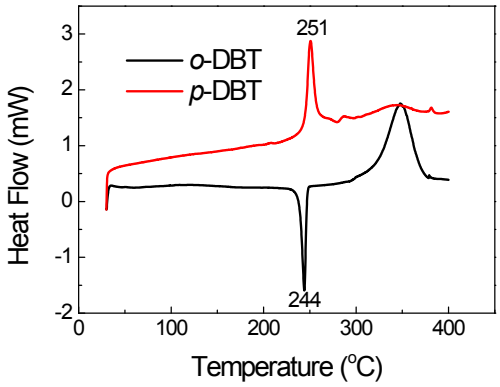


Figure S30. DSC of ***o*-DBT** and ***p*-DBT** under N_2. Heating rate: 10 °C/min.

10. Computational details

All calculations were performed with the Gaussian 16 program suite.[7] Full geometry optimizations were carried out at the (U)B3LYP/6–31G(d) level,[8-11] and the obtained stationary points were characterized by frequency calculations. All energies were obtained from electronic with zero-point energies. Diradical character parameter (y) was calculated by a symmetry-broken UB3LYP/6-31G(d) method,

basing on the LUMO occupation number (nLUMO) in natural orbital analysis for the optimized singlet geometry. The y is formally expressed as $y = 1 - (2T/(1 + T^2))$, where T is represented by calculating the occupation numbers of natural orbitals as: T = (nHOMO – nLUMO)/2. A molecule with y = 0 implies a closed-shell structure, whereas a molecule with y = 1 indicates a pure diradical structure. Any intermediate value of y refers to diradicaloid (i.e. diradical like) structures.[12, 13] The HOMO and LUMO orbitals of *o*-**DBT** and *p*-**DBT** (*trans* isomer) OS state were delocalized mainly at the backbone of benzotriazinyl moiety and double bond**.** The spin densities were illustrated using Multiwfn and VMD.[14, 15]

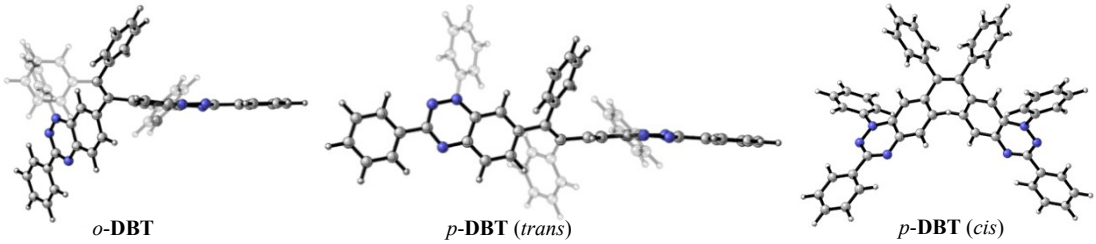
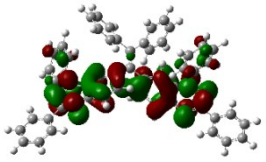
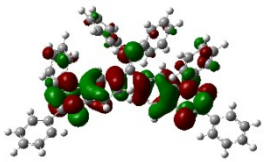
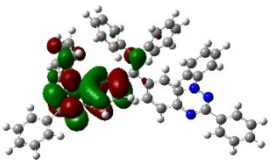
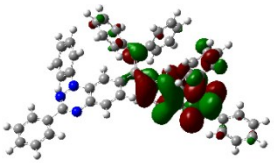
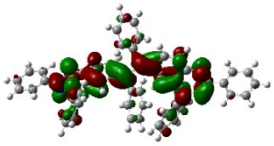
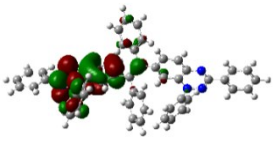
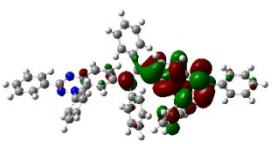


Figure S31. Optimized conformations of diradicals *o*-**DBT** and *p*-**DBT** in open-shell state (UB3LYP/6-31G(d)). Blue for nitrogen; gray for carbon and white for hydrogen.[16]

		HOMO$^{\alpha}$	LUMO$^{\alpha}$
o-**DBT**	CS		
	OS		
p-**DBT (trans)**	CS		
	OS		

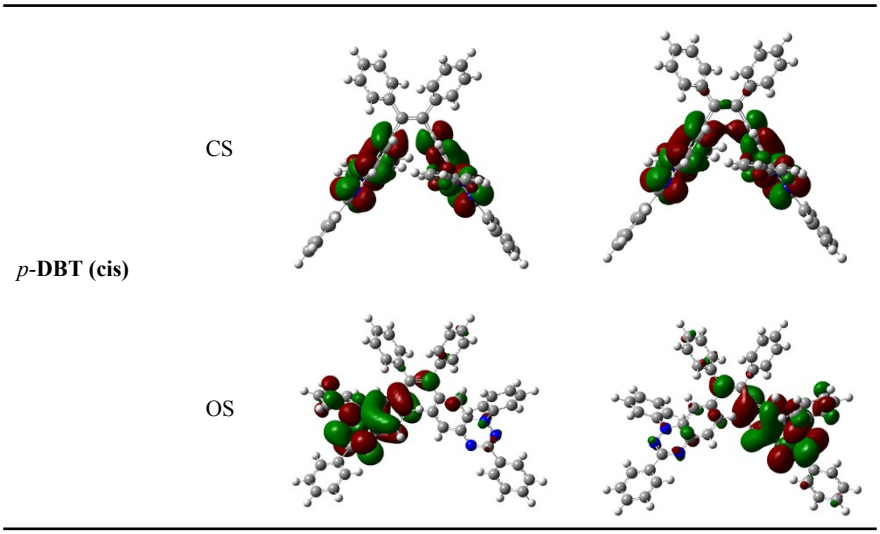
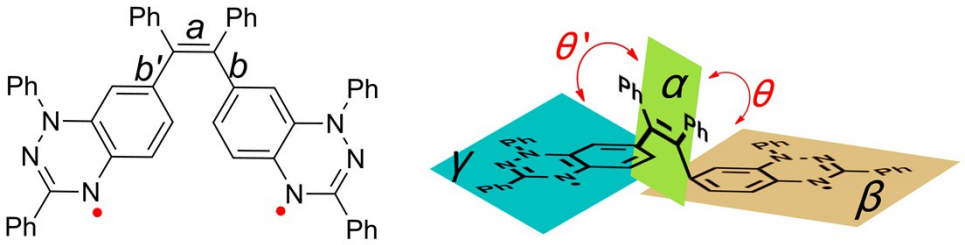


Figure S31. Frontier orbitals of *o*-**DBT** and *p*-**DBT** (*trans* and *cis* isomer) calculated at the UB3LYP/6-31G(d) level (HOMO(α) and LUMO(α) for the OS states).

Table S2. Calculated relative energy (ΔE), bond lengths (Å) and dihedral θ (°) of *cis*-isomer of *p*-**DBT**.



p-**DBT** (*cis*)

States	ΔE (kcal/mol)	α	Avg. b&b'	Avg. θ&θ'
CS	23.58	1.36	1.500	87.72
OS	0	1.37	1.487	41.43
T	0.73	1.37	1.491	43.72

CS=closed-shell singlet, OS= open-shell singlet, T= open-shell triplet. Calculated at the level of (U)B3LYP/6-31G(d).

11. References

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12. Coordinates for calculated geometries:

o-DBT-CS

N	-5.77466100	-1.27676600	-0.29108300
C	-5.52711100	-2.22705700	0.59861400
N	-4.39630400	-2.37842900	1.32208800
C	-3.38881300	-1.52537100	1.04335900
C	-3.52349500	-0.47388000	0.06864900
N	-4.78469100	-0.35594300	-0.50534500
C	-2.14341300	-1.65699100	1.70221400
C	-1.07561000	-0.84227000	1.37972200
C	-1.19842600	0.17080500	0.39739300
C	-2.42772100	0.32721000	-0.26410700
C	-6.62103500	-3.20887000	0.82320600
C	-5.15877000	0.68881400	-1.40295100
C	-0.00672600	0.96237900	0.00055000
C	0.01767800	2.32678600	-0.08308900
C	1.15283800	3.06138300	-0.71437900
C	1.16090400	0.09250700	-0.30335900
C	-1.08291100	3.18295400	0.44748700
C	1.73024000	4.16997900	-0.06952200
C	2.78563200	4.86697300	-0.65442800
C	3.26957900	4.48584900	-1.90796700
C	2.69018700	3.40210400	-2.57064200
C	1.64342000	2.69616400	-1.97992500
C	-1.62844200	2.97000700	1.72613600
C	-2.63862500	3.79419700	2.21985300
C	-3.12440100	4.85252700	1.44785300
C	-2.58347600	5.08496300	0.18093800
C	-1.56843200	4.26467600	-0.30986000

C	1.00498200	-1.01094500	-1.17659700
C	2.06523900	-1.85041600	-1.45938800
C	3.32779600	-1.66524000	-0.84823600
C	3.45776400	-0.59894800	0.11012400
C	2.39472900	0.27848100	0.34131300
N	4.36872600	-2.45521100	-1.18673600
C	5.55631000	-2.15725500	-0.61698800
N	5.78060500	-1.23532300	0.30858400
N	4.69954300	-0.50848700	0.73084500
C	6.74093800	-2.94514000	-1.05013200
C	8.00193600	-2.74558800	-0.46569600
C	9.09942200	-3.49128600	-0.88839100
C	8.95552100	-4.44644400	-1.89845200
C	7.70395400	-4.65100600	-2.48204000
C	6.60268800	-3.90666100	-2.06197900
C	-7.85465300	-3.08814500	0.16349100
C	-8.86490800	-4.02070200	0.38444700
C	-8.66023800	-5.08578000	1.26595500
C	-7.43659000	-5.21026800	1.92625500
C	-6.42252400	-4.27892800	1.70811100
C	4.99399000	0.38691000	1.80128900
C	4.13783400	0.48916500	2.90587900
C	4.46502500	1.34423400	3.95677700
C	5.64422600	2.09110200	3.92075500
C	6.50280400	1.97126700	2.82513400
C	6.18588100	1.12239700	1.76777800
C	-5.86654500	0.36247000	-2.56727700
C	-6.26846000	1.37365800	-3.43606400
C	-5.97412500	2.70989200	-3.15253900
C	-5.28174000	3.02989700	-1.98332000
C	-4.87702000	2.02793300	-1.10257600
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H	-2.51635800	1.07929400	-1.03690200
H	1.35265400	4.47675900	0.90174600
H	3.22857200	5.71077800	-0.13206300
H	4.08740000	5.03400500	-2.36791500
H	3.05085200	3.10654300	-3.55222800
H	1.19402100	1.85745100	-2.50183700
H	-1.24920800	2.15662800	2.33609400
H	-3.04052000	3.61488400	3.21348800
H	-3.90888300	5.49701000	1.83518900
H	-2.94559300	5.91263900	-0.42355700
H	-1.14704500	4.45684300	-1.29212300
H	0.04287900	-1.17428800	-1.65250200
H	1.97171200	-2.66733600	-2.16719800
H	2.51757700	1.11735000	1.01398800
H	8.10786300	-2.00733700	0.32137000
H	10.07006800	-3.32881400	-0.42694700
H	9.81344200	-5.02784900	-2.22628300
H	7.58364300	-5.39281900	-3.26732700
H	5.62526200	-4.05684700	-2.50594400

H	-8.01065700	-2.25749100	-0.51578000
H	-9.81607100	-3.91562600	-0.13102000
H	-9.45037800	-5.81236100	1.43707100
H	-7.26990100	-6.03556900	2.61365300
H	-5.46818700	-4.36393900	2.21510200
H	3.23732900	-0.11380700	2.95055100
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H	-6.28835700	3.49512100	-3.83426400
H	-5.06066000	4.06528600	-1.74088000
H	-4.36827300	2.28716100	-0.18050000

***o*-DBT-OS**

N	-5.89468600	-1.16019000	-0.32206800
C	-5.71289100	-2.12227000	0.58742500
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C	-3.53649800	-1.54492700	1.02995300
C	-3.60355900	-0.49453800	0.06677700
N	-4.85458700	-0.30132100	-0.52779100
C	-2.30243700	-1.77668700	1.67216600
C	-1.18161400	-1.03217600	1.35346200
C	-1.24063500	-0.00443700	0.38459000
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C	-6.87489200	-3.02498300	0.80674500
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C	-1.60750000	2.79907100	1.73812700
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C	-3.04061300	4.73278200	1.47766000
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C	-1.51114600	4.10174500	-0.28909400
C	1.07114500	-1.24480500	-1.06876600
C	2.17028800	-2.04025100	-1.33647000
C	3.42788400	-1.76117300	-0.76194300
C	3.52242700	-0.65487200	0.13347500
C	2.41743300	0.17285900	0.36001500
N	4.50940600	-2.52760900	-1.08572000
C	5.68067800	-2.14777600	-0.55633800

N	5.87878500	-1.15943500	0.32130000
N	4.77708000	-0.46063000	0.72090200
C	6.89865900	-2.90114400	-0.95915400
C	8.15384200	-2.60679500	-0.40346000
C	9.28268600	-3.32191600	-0.79668100
C	9.17574600	-4.33999000	-1.74752200
C	7.92971400	-4.63877300	-2.30260900
C	6.79794100	-3.92545300	-1.91248400
C	-8.09128600	-2.82178600	0.13591200
C	-9.16641200	-3.68049400	0.35284300
C	-9.04419200	-4.75175200	1.24136700
C	-7.83743000	-4.95806100	1.91305800
C	-6.75915700	-4.10177500	1.69854200
C	5.04286700	0.50957200	1.73577600
C	4.23238200	0.59006400	2.87427700
C	4.52941000	1.52240100	3.86772400
C	5.63539900	2.36430000	3.73830200
C	6.45026700	2.26612300	2.60788300
C	6.15997100	1.34248000	1.60641300
C	-5.81353400	0.44843100	-2.63993000
C	-6.13760600	1.47065600	-3.52875900
C	-5.80364800	2.79517300	-3.23510000
C	-5.15113600	3.09366300	-2.03796600
C	-4.82718100	2.08021100	-1.13624000
H	-2.26542300	-2.57365500	2.40791400
H	-0.23844100	-1.23685600	1.85094900
H	-2.50325400	1.00078500	-1.03217900
H	1.41485600	4.24349200	0.91837800
H	3.28592800	5.46583400	-0.13665900
H	4.09785600	4.80185800	-2.39415200
H	3.01857100	2.89614500	-3.57679800
H	1.16843600	1.65681400	-2.50359300
H	-1.25507300	1.96949100	2.34271400
H	-2.99318200	3.47981100	3.23400800
H	-3.80149500	5.40104200	1.87176700
H	-2.82964300	5.79803500	-0.38725900
H	-1.08635800	4.28740000	-1.27113600
H	0.11132900	-1.48176100	-1.51752500
H	2.10489000	-2.89401500	-2.00327100
H	2.51242300	1.04168800	0.99806600
H	8.23128100	-1.81950800	0.33793900
H	10.24872400	-3.08570700	-0.35804000
H	10.05781700	-4.89725000	-2.05235500
H	7.83837800	-5.42992800	-3.04227800
H	5.82484200	-4.14818200	-2.33521200
H	-8.18313400	-1.98619800	-0.54881600
H	-10.10351500	-3.51199500	-0.17143200
H	-9.88460600	-5.42030800	1.40945000
H	-7.73476500	-5.78915600	2.60597000
H	-5.81708000	-4.25101900	2.21376700
H	3.39064200	-0.08481600	2.98825800
H	3.90086400	1.57778700	4.75213800

H	5.86500200	3.08691800	4.51617900
H	7.31589900	2.91409500	2.50191600
H	6.78770500	1.25046700	0.72751200
H	-6.07279400	-0.58276200	-2.85111000
H	-6.64964100	1.22972400	-4.45625100
H	-6.05610200	3.58912100	-3.93231100
H	-4.89808100	4.12035000	-1.79041600
H	-4.34700200	2.32161300	-0.19407200

***o*-DBT-T**

N	5.90810400	1.14592100	-0.32300100
C	5.73232900	2.11252900	0.58284200
N	4.62882100	2.34003800	1.30852500
C	3.55194900	1.55120500	1.02559100
C	3.61282000	0.49578200	0.06762800
N	4.86349400	0.29222800	-0.52536600
C	2.31804700	1.79616400	1.66343100
C	1.19239200	1.05897000	1.34553300
C	1.24526300	0.02520700	0.38244800
C	2.46323300	-0.23165500	-0.26177000
C	6.89994600	3.00852200	0.79942200
C	5.15139500	-0.76738600	-1.44122500
C	0.01077600	-0.72980600	0.02302000
C	-0.02824600	-2.09699700	-0.06938000
C	-1.16885300	-2.81872000	-0.71117400
C	-1.18401400	0.12643400	-0.23029300
C	1.05269500	-2.97947900	0.46225500
C	-1.77468200	-3.91599200	-0.07364900
C	-2.82559600	-4.60435400	-0.67755500
C	-3.27872300	-4.22542700	-1.94295800
C	-2.67234800	-3.15159300	-2.59796200
C	-1.62986400	-2.45551700	-1.98835300
C	1.60216000	-2.77799400	1.74156000
C	2.57769600	-3.63539900	2.24776900
C	3.02521400	-4.72023600	1.48916400
C	2.48073400	-4.94200800	0.22210200
C	1.50230200	-4.08565200	-0.28209400
C	-1.07523400	1.28055400	-1.04005800
C	-2.17747800	2.07259700	-1.30423600
C	-3.43708100	1.77777700	-0.74178100
C	-3.52978400	0.65922400	0.13845200
C	-2.42127300	-0.16423000	0.36107700
N	-4.52092500	2.54198700	-1.06191200
C	-5.69291600	2.14930700	-0.54309200
N	-5.88965300	1.14909500	0.32118100
N	-4.78685300	0.45030900	0.71668300
C	-6.91285600	2.90131000	-0.94223300
C	-8.16910800	2.59337000	-0.39637500
C	-9.29982800	3.30749700	-0.78595900
C	-9.19376200	4.33807600	-1.72333700
C	-7.94671100	4.65037400	-2.26859700

C	-6.81303500	3.93812600	-1.88205600
C	8.11535900	2.79500600	0.12999900
C	9.19589900	3.64752600	0.34439000
C	9.08016600	4.72277200	1.22895700
C	7.87441900	4.93933300	1.89924200
C	6.79072700	4.08929300	1.68723200
C	-5.05256500	-0.53407000	1.71788500
C	-4.24775900	-0.62434800	2.85966000
C	-4.54492700	-1.57071300	3.83971700
C	-5.64549800	-2.41698300	3.69373800
C	-6.45477900	-2.30918500	2.56018400
C	-6.16421100	-1.37150800	1.57192700
C	5.81759100	-0.46887400	-2.63564900
C	6.13576300	-1.49540900	-3.52164100
C	5.79428500	-2.81714700	-3.22419200
C	5.14009900	-3.10851900	-2.02621700
C	4.82198400	-2.09073400	-1.12729800
H	2.28540100	2.59739600	2.39474400
H	0.24981300	1.27369600	1.83986300
H	2.50400600	-0.99668500	-1.02602700
H	-1.42123100	-4.22310600	0.90666600
H	-3.28919400	-5.43997700	-0.15977200
H	-4.09317500	-4.76636200	-2.41728600
H	-3.00868500	-2.85631700	-3.58837400
H	-1.16147200	-1.62264900	-2.50380200
H	1.25301000	-1.94506200	2.34346700
H	2.98164300	-3.46174100	3.24170100
H	3.78171500	-5.39154900	1.88650500
H	2.81136000	-5.78959800	-0.37304100
H	1.07849100	-4.27181200	-1.26444000
H	-0.11452100	1.52947400	-1.48025400
H	-2.11315500	2.93564900	-1.95908400
H	-2.51488800	-1.04133000	0.98779100
H	-8.24593700	1.79634200	0.33461000
H	-10.26667200	3.06069000	-0.35500400
H	-10.07731100	4.89452100	-2.02535900
H	-7.85604800	5.45128700	-2.99777100
H	-5.83915600	4.17135300	-2.29725900
H	8.20218600	1.95634700	-0.55162300
H	10.13216200	3.47105000	-0.17875700
H	9.92481000	5.38646700	1.39507700
H	7.77678300	5.77357600	2.58908800
H	5.84938500	4.24656200	2.20141300
H	-3.41039100	0.05363400	2.98665000
H	-3.92081800	-1.63377100	4.72675200
H	-5.87525000	-3.15055900	4.46124600
H	-7.31615700	-2.96059000	2.44137800
H	-6.78759900	-1.27210900	0.69073000
H	6.08267400	0.56022800	-2.84979000
H	6.64904900	-1.25999800	-4.44985900
H	6.04213700	-3.61450500	-3.91916100
H	4.88107300	-4.13300300	-1.77581500

H	4.34035900	-2.32673800	-0.18451200

***p*-DBT-CS (*trans*)**

C	11.06210900	-0.06702600	-0.71248400
C	10.26955800	-1.06114700	-1.29399100
C	8.88395200	-1.01754100	-1.16898600
C	8.26752800	0.02576800	-0.45833700
C	9.06844200	1.01942000	0.12429300
C	10.45607000	0.97115600	-0.00358600
C	6.79165000	0.09098800	-0.31633100
N	6.09383600	-0.84316600	-0.92415400
N	4.73807200	-0.81778700	-0.78199000
C	4.07026900	0.21644000	-0.11807500
C	4.95259500	1.18627500	0.50411500
N	6.27616000	1.11246000	0.43077400
C	2.69714100	0.38176900	-0.07981900
C	2.10018900	1.49309000	0.58338000
C	2.98507000	2.43175200	1.21342300
C	4.34311800	2.27678100	1.19433400
C	4.07727700	-1.88702800	-1.46385100
C	4.46497400	-2.19562800	-2.77355000
C	3.86270600	-3.26059900	-3.43872500
C	2.87613200	-4.02093800	-2.80606200
C	2.50105300	-3.71285100	-1.49756500
C	3.09932600	-2.65138100	-0.81898100
C	0.67821800	1.69407900	0.63259400
C	-0.26047100	0.61761900	0.62900900
C	0.10527100	-0.68303700	1.26525900
C	0.78913000	-0.71489900	2.49528300
C	-0.26059900	-1.91381900	0.68767700
C	0.03665300	-3.12247800	1.31655000
C	0.71796600	-3.13370000	2.53591500
C	1.09476200	-1.92196200	3.12069600
C	0.19479900	3.09959900	0.74543500
C	-0.80000700	3.45118300	1.67886800
C	-1.88811400	1.69519500	-0.92599400
C	-1.59909100	0.76556700	0.13231100
C	0.73630100	4.12438900	-0.05533100
C	0.29753900	5.44269900	0.06733000
C	-0.68924100	5.77068000	0.99804000
C	-1.23415700	4.76777800	1.80535800
C	-3.12783400	1.79747000	-1.48777900
C	-4.22032200	0.99731700	-1.02802000
C	-3.96229100	0.10981400	0.08857100
C	-2.68948700	-0.02298900	0.60839800
N	-5.39527400	1.06813800	-1.63755500
C	-6.37794500	0.23659400	-1.16958600
N	-6.27978800	-0.55511400	-0.12564600
N	-5.09412600	-0.57457200	0.54858200
C	-5.10728200	-1.40193700	1.71223800
C	-5.70732800	-2.66536800	1.64453200

C	-5.76135600	-3.46645700	2.78279600
C	-5.22138000	-3.01840800	3.99052600
C	-4.63413300	-1.75339300	4.05565100
C	-4.57899700	-0.94069800	2.92450900
C	-7.67530100	0.24323300	-1.89001900
C	-8.75367100	-0.54448200	-1.45376600
C	-9.96186000	-0.52838800	-2.14454700
C	-10.11463000	0.27228400	-3.28047800
C	-9.04785900	1.05816400	-3.71841700
C	-7.83564400	1.04604700	-3.02937700
H	12.14391600	-0.10387600	-0.81104500
H	10.73414500	-1.87458100	-1.84527500
H	8.26618300	-1.78930900	-1.61490000
H	8.58812300	1.82121900	0.67324300
H	11.06476400	1.74774700	0.45228100
H	2.05499400	-0.31375700	-0.60247600
H	2.55556000	3.26959500	1.75132700
H	5.00679900	2.98037400	1.68604300
H	5.23756400	-1.60260600	-3.24975600
H	4.16335700	-3.49397200	-4.45639000
H	2.40691100	-4.85004800	-3.32815400
H	1.74529700	-4.30435600	-0.98958200
H	2.82078000	-2.43306000	0.20592900
H	1.07427700	0.22217400	2.96347900
H	-0.78286800	-1.91767300	-0.26434700
H	-0.26646300	-4.05790900	0.85279600
H	0.94847500	-4.07513600	3.02720700
H	1.61869200	-1.91624800	4.07298200
H	-1.22462700	2.67819600	2.31228900
H	-1.07811500	2.29287000	-1.32603300
H	1.49526400	3.87492900	-0.79136700
H	0.72378300	6.21277700	-0.57039600
H	-1.03217600	6.79726400	1.09430300
H	-1.99599400	5.01490500	2.54014400
H	-3.32206200	2.46015800	-2.32464300
H	-2.51263900	-0.72016500	1.41573100
H	-6.12951600	-2.99946400	0.70366800
H	-6.22459200	-4.44749400	2.72319200
H	-5.26274500	-3.64758700	4.87500900
H	-4.22670000	-1.38793100	4.99413100
H	-4.14597900	0.05197600	2.98363600
H	-8.63314500	-1.16132200	-0.56997200
H	-10.78883300	-1.14130500	-1.79541100
H	-11.05929000	0.28312800	-3.81793300
H	-9.15817400	1.68440000	-4.59992600
H	-7.00189400	1.65440900	-3.36046300

***p*-DBT-OS (*trans*)**

C	11.15111600	0.14333300	0.28262000
C	10.48024600	-0.70444700	-0.60241200
C	9.08846900	-0.70148400	-0.65905700

C	8.34670200	0.15369600	0.17127600
C	9.02639400	1.00157400	1.05856400
C	10.41890500	0.99493200	1.11243300
C	6.85994300	0.17532200	0.12484900
N	6.30009600	-0.62111200	-0.78923900
N	4.93674900	-0.64299900	-0.83782200
C	4.15217700	0.22984000	-0.07613600
C	4.86378400	1.02529200	0.87153100
N	6.22049000	0.97036900	0.99506600
C	2.76973600	0.37963600	-0.23354500
C	2.05061000	1.27628800	0.56977300
C	2.75649600	2.05086000	1.52009600
C	4.12379100	1.92067900	1.67246200
C	4.40775900	-1.57665900	-1.78272100
C	4.97391800	-1.64130300	-3.06138500
C	4.49283200	-2.56971200	-3.98145400
C	3.45138900	-3.43412700	-3.63464500
C	2.89943900	-3.37139500	-2.35430000
C	3.37660200	-2.45082200	-1.42148600
C	0.58401800	1.46218300	0.39590000
C	-0.29917600	0.41514200	0.31811800
C	0.07078500	-0.98253800	0.69919300
C	0.74514000	-1.25774700	1.90199400
C	-0.30837500	-2.06930000	-0.10943900
C	-0.00632500	-3.37977800	0.25989100
C	0.67467100	-3.63538700	1.45244800
C	1.04647100	-2.56747800	2.27296700
C	0.14385000	2.88880000	0.32756100
C	-0.91050900	3.36607000	1.12532500
C	-2.01290800	1.34258200	-1.29443700
C	-1.70674700	0.59305100	-0.13447600
C	0.81884000	3.80545700	-0.49833600
C	0.43132000	5.14349500	-0.54989800
C	-0.62512100	5.59974000	0.24110900
C	-1.29035700	4.70636500	1.08338600
C	-3.31105200	1.44384700	-1.75641700
C	-4.37914700	0.81984400	-1.07709900
C	-4.07972900	0.09979700	0.11803500
C	-2.75701000	-0.03886800	0.55019200
N	-5.64088300	0.88726500	-1.58779000
C	-6.58230500	0.19449600	-0.92938500
N	-6.42524200	-0.48007900	0.21235400
N	-5.18027100	-0.46661800	0.77103300
C	-5.10548100	-1.13022800	2.03441700
C	-5.72439000	-2.37624300	2.18674800
C	-5.68924700	-3.01665000	3.42330300
C	-5.04248100	-2.42294300	4.50984900
C	-4.43790800	-1.17419000	4.35552000
C	-4.47186900	-0.52116700	3.12397700
C	-7.95424500	0.17434300	-1.50412800
C	-9.01036900	-0.47473400	-0.84508500
C	-10.28705200	-0.48497400	-1.40203300

C	-10.52860300	0.15188200	-2.62194500
C	-9.48272300	0.80078100	-3.28144600
C	-8.20381000	0.81307600	-2.72803600
H	12.23723600	0.13891800	0.32554200
H	11.04333600	-1.37214600	-1.24935400
H	8.56350100	-1.36130100	-1.34065700
H	8.44644100	1.65775000	1.69757200
H	10.93362200	1.65708600	1.80383300
H	2.24391800	-0.18956600	-0.98886100
H	2.20972000	2.75687000	2.13750900
H	4.67467500	2.51507600	2.39433500
H	5.78636000	-0.96947600	-3.31394200
H	4.93145300	-2.61444800	-4.97447200
H	3.07737400	-4.15519100	-4.35599900
H	2.09907400	-4.04677400	-2.06683000
H	2.96380400	-2.42669000	-0.41876700
H	1.02869900	-0.43509500	2.55090800
H	-0.84427000	-1.88080300	-1.03515200
H	-0.31131000	-4.20287000	-0.38147700
H	0.90400600	-4.65647900	1.74498400
H	1.56362000	-2.75462100	3.21035500
H	-1.42940800	2.67695000	1.78451900
H	-1.20841600	1.82368300	-1.83989900
H	1.64838800	3.45966900	-1.10868200
H	0.95838200	5.83146800	-1.20571800
H	-0.92316900	6.64413600	0.20667000
H	-2.10500900	5.05456500	1.71292700
H	-3.54810300	1.98567100	-2.66635900
H	-2.53349100	-0.64056400	1.42222300
H	-6.22967800	-2.82180000	1.33746700
H	-6.16687600	-3.98591400	3.53634800
H	-5.01571400	-2.92697200	5.47168500
H	-3.94866900	-0.69584900	5.19936700
H	-4.02809500	0.46237400	3.01150200
H	-8.81958400	-0.96328200	0.10383600
H	-11.09683700	-0.98959200	-0.88142700
H	-11.52580200	0.14313900	-3.05439600
H	-9.66290500	1.29902600	-4.23048300
H	-7.38364200	1.31390900	-3.22973600

***p*-DBT-T (*trans*)**

C	11.15178900	0.16315300	0.31849200
C	10.48767000	-0.68722100	-0.56906400
C	9.09610100	-0.68880000	-0.63190300
C	8.34793500	0.16437700	0.19466600
C	9.02090200	1.01491500	1.08453700
C	10.41312800	1.01282400	1.14463700
C	6.86119700	0.18141400	0.14158800
N	6.30884000	-0.61872400	-0.77564000
N	4.94590000	-0.64410400	-0.83169900
C	4.15535700	0.22771700	-0.07531600

C	4.85761200	1.02437000	0.87675100
N	6.21559700	0.97352600	1.00788000
C	2.77285400	0.37371200	-0.24193200
C	2.04661600	1.26569700	0.55853200
C	2.74259200	2.04082900	1.51447400
C	4.11026800	1.91590500	1.67393900
C	4.42364800	-1.58344100	-1.77464500
C	4.99638600	-1.65331000	-3.05008800
C	4.52144000	-2.58699500	-3.96801700
C	3.47973000	-3.45153400	-3.62226600
C	2.92133400	-3.38372600	-2.34495700
C	3.39234100	-2.45790600	-1.41423800
C	0.57900400	1.44798700	0.37056800
C	-0.30043600	0.39978400	0.30451100
C	0.07016000	-0.99448500	0.69672800
C	0.74669300	-1.26079400	1.90032400
C	-0.31016100	-2.08712600	-0.10342800
C	-0.00559200	-3.39471800	0.27392700
C	0.67797300	-3.64152300	1.46685700
C	1.04979500	-2.56773100	2.27963800
C	0.14016000	2.87331400	0.27042900
C	-0.92024800	3.36716000	1.04961300
C	-2.01054700	1.28043400	-1.33989200
C	-1.70910500	0.57018600	-0.15557800
C	0.82307000	3.77281600	-0.56764500
C	0.43710800	5.10970500	-0.64932400
C	-0.62569400	5.58252600	0.12331700
C	-1.29867100	4.70666800	0.97757600
C	-3.30979300	1.37482100	-1.80308900
C	-4.37971000	0.78156200	-1.10160400
C	-4.08384900	0.10011700	0.11580400
C	-2.76066900	-0.03191800	0.55146300
N	-5.64409000	0.83987600	-1.61256000
C	-6.58641900	0.17374600	-0.93183300
N	-6.43144000	-0.46593500	0.23183800
N	-5.18578700	-0.43952300	0.78819100
C	-5.11208100	-1.06196800	2.07254300
C	-5.73490700	-2.30033400	2.26555600
C	-5.70067700	-2.90045300	3.52217300
C	-5.05114600	-2.27381600	4.58841000
C	-4.44281300	-1.03262400	4.39330900
C	-4.47571000	-0.41978300	3.14122800
C	-7.95987800	0.14146400	-1.50277900
C	-9.01772700	-0.48008700	-0.82048900
C	-10.29569900	-0.50229200	-1.37429400
C	-10.53664800	0.09507600	-2.61407200
C	-9.48894300	0.71654800	-3.29680700
C	-8.20885300	0.74061900	-2.74666000
H	12.23771900	0.16231400	0.36625100
H	11.05580400	-1.35339900	-1.21315700
H	8.57631900	-1.35067400	-1.31545600
H	8.43587200	1.66951700	1.72053800

H	10.92263500	1.67698700	1.83796600
H	2.25337100	-0.19685900	-1.00063500
H	2.18950900	2.74486700	2.12862300
H	4.65475700	2.51209100	2.39920500
H	5.80887600	-0.98123600	-3.30181900
H	4.96507600	-2.63575900	-4.95861400
H	3.11056000	-4.17668000	-4.34201800
H	2.12076700	-4.05918200	-2.05817200
H	2.97476900	-2.42992600	-0.41357700
H	1.03077800	-0.43365600	2.54322100
H	-0.84852200	-1.90557200	-1.02910600
H	-0.31087900	-4.22243300	-0.36131800
H	0.90908700	-4.66035500	1.76579500
H	1.56862700	-2.74798800	3.21744100
H	-1.44532500	2.69189800	1.71816300
H	-1.20345400	1.73855700	-1.90124700
H	1.65806700	3.41463700	-1.16326000
H	0.97050300	5.78405700	-1.31411300
H	-0.92249200	6.62623900	0.06545400
H	-2.11846200	5.06782100	1.59299800
H	-3.54494100	1.88794000	-2.73002500
H	-2.53913000	-0.60609500	1.44245700
H	-6.24231800	-2.77148000	1.43148900
H	-6.18121900	-3.86402900	3.66696500
H	-5.02521500	-2.74644900	5.56607700
H	-3.95150100	-0.52869400	5.22089700
H	-4.02918600	0.55830700	2.99657300
H	-8.82735200	-0.93789700	0.14369800
H	-11.10687600	-0.98530600	-0.83567700
H	-11.53479900	0.07707700	-3.04404000
H	-9.66870700	1.18402200	-4.26144800
H	-7.38716700	1.22034800	-3.26620800

***p*-DBT-CS (*cis*)**

C	0.63055200	-3.00716400	0.25494600
C	-0.63152800	-3.00671300	-0.25554200
C	-1.29848100	-1.71612700	-0.63090300
C	-1.15632900	-1.18874900	-1.92860400
C	1.15679300	-1.19017000	1.92854800
C	1.29824700	-1.71703500	0.63056300
C	-2.06133900	-1.01897000	0.30950800
C	-2.67224600	0.19890000	-0.03288900
C	-2.58529300	0.70274200	-1.37248000
C	-1.79964900	-0.01279200	-2.29586200
C	1.80060000	-0.01454700	2.29603100
C	2.58613100	0.70109000	1.37265100
C	2.67246200	0.19776500	0.03282100
C	2.06092600	-1.01972200	-0.30987200
C	1.46778900	-4.23326500	0.43295000
C	2.26185700	-4.41297100	1.57897700
C	-2.26367400	-4.41137200	-1.57970200

C	-1.46967500	-4.23219100	-0.43354700
C	1.54531600	-5.20252900	-0.58323700
C	2.36395000	-6.32134200	-0.44631400
C	3.12729000	-6.49878100	0.70953300
C	3.07265500	-5.53863900	1.72078900
C	-3.07534400	-5.53640700	-1.72154400
C	-3.13091400	-6.49640200	-0.71019400
C	-2.36762800	-6.31946600	0.44576400
C	-1.54812600	-5.20128900	0.58271900
N	-3.41590200	0.97042700	0.84991200
N	-4.16753300	2.03321800	0.43709100
C	-4.04284200	2.39348700	-0.84150500
N	-3.25317700	1.82366300	-1.76282200
N	3.25451600	1.82165800	1.76320400
C	4.04415200	2.39149300	0.84189000
N	4.16841200	2.03162500	-0.43686200
N	3.41615900	0.96932600	-0.84988100
C	-4.86188600	3.56279800	-1.25965400
C	-3.51939800	0.70387600	2.24912100
C	3.51929900	0.70317600	-2.24921500
C	4.86381400	3.56034100	1.26026300
C	-2.37112400	0.48292700	3.02031000
C	-2.49742900	0.26101100	4.39073500
C	-3.75543500	0.26735700	4.99694900
C	-4.89405200	0.50682400	4.22355100
C	-4.78245600	0.72889500	2.85335400
C	-5.66071200	4.25893800	-0.33883500
C	-6.42346300	5.34867200	-0.75224000
C	-6.39930300	5.75922400	-2.08755900
C	-5.60500300	5.07201300	-3.00768600
C	-4.84060800	3.98095700	-2.59837100
C	2.37076900	0.48313100	-3.02026800
C	2.49671000	0.26158300	-4.39078900
C	3.75461700	0.26741200	-4.99721100
C	4.89350200	0.50598800	-4.22393100
C	4.78226900	0.72768000	-2.85364300
C	4.84308800	3.97797600	2.59914700
C	5.60802100	5.06858600	3.00865600
C	6.40230900	5.75584600	2.08855700
C	6.42592200	5.34579900	0.75307100
C	5.66262900	4.25651900	0.33947100
H	-0.54545700	-1.72018300	-2.65320200
H	0.54600100	-1.72168700	2.65315200
H	-2.18963500	-1.43065900	1.30258600
H	-1.72992000	0.38401000	-3.30364000
H	1.73135600	0.38189400	3.30398300
H	2.18871000	-1.43104700	-1.30316700
H	2.24552000	-3.66464500	2.36533600
H	-2.24657700	-3.66312800	-2.36612800
H	0.96138600	-5.07034400	-1.48827800
H	2.41008200	-7.05327700	-1.24846200
H	3.76617100	-7.37135000	0.81591400

H	3.66924100	-5.65974100	2.62121200
H	-3.67186800	-5.65713400	-2.62205700
H	-3.77047200	-7.36847200	-0.81659800
H	-2.41447400	-7.05129400	1.24796800
H	-0.96421200	-5.06948200	1.48782800
H	-1.39042100	0.50956000	2.55667700
H	-1.60457800	0.10005400	4.98848600
H	-3.84715300	0.09612100	6.06564700
H	-5.87608400	0.51925700	4.68805400
H	-5.65602600	0.92517700	2.24246100
H	-5.67179800	3.94040300	0.69743800
H	-7.03664700	5.88105200	-0.02979100
H	-6.99467800	6.61040400	-2.40776600
H	-5.58035400	5.38633200	-4.04786700
H	-4.21883800	3.43925900	-3.30201300
H	1.39016600	0.51019400	-2.55644800
H	1.60366700	0.10132900	-4.98844200
H	3.84606000	0.09647000	-6.06598000
H	5.87545900	0.51802300	-4.68860300
H	5.65605100	0.92327700	-2.24283500
H	4.22132200	3.43623300	3.30275800
H	5.58380000	5.38251600	4.04896500
H	6.99810100	6.60667800	2.40891200
H	7.03910400	5.87822200	0.03065200
H	5.67328300	3.93837100	-0.69692600

***p*-DBT-OS (*cis*)**

C	-0.67704400	2.26025600	0.11302900
C	0.67703600	2.26026500	-0.11305000
C	1.44179700	1.01884700	-0.40388300
C	0.95496500	0.05665600	-1.32113600
C	-0.95493400	0.05662700	1.32108300
C	-1.44179000	1.01882700	0.40385400
C	2.70548100	0.81162200	0.17325800
C	3.44741800	-0.33668700	-0.11958800
C	2.97085900	-1.28329400	-1.07678300
C	1.70233700	-1.05610100	-1.65357400
C	-1.70229200	-1.05614000	1.65351900
C	-2.97082400	-1.28333100	1.07675000
C	-3.44741000	-0.33671100	0.11958100
C	-2.70548500	0.81160600	-0.17326300
C	-1.48705500	3.51666900	0.08967700
C	-2.39498000	3.80312600	1.12471000
C	2.39492500	3.80318600	-1.12473600
C	1.48702900	3.51669000	-0.08968800
C	-1.40038400	4.41784400	-0.98491800
C	-2.18005500	5.57310400	-1.01530600
C	-3.06266900	5.85375000	0.02935000
C	-3.16659600	4.96352900	1.10043000
C	3.16652100	4.96360400	-1.10045000
C	3.06260100	5.85380000	-0.02934900

C	2.18001400	5.57311700	1.01532000
C	1.40036300	4.41784400	0.98492500
N	4.69184400	-0.63026700	0.44696500
N	5.47237000	-1.65330700	-0.00799900
C	4.94002600	-2.45302900	-0.93420200
N	3.71128500	-2.35695000	-1.46655300
N	-3.71123500	-2.35699900	1.46651700
C	-4.93998400	-2.45308200	0.93418700
N	-5.47235400	-1.65334800	0.00800700
N	-4.69184900	-0.63028700	-0.44694700
C	5.80897500	-3.56718200	-1.39899500
C	5.29087800	0.13111600	1.49791200
C	-5.29092100	0.13112000	-1.49785500
C	-5.80890500	-3.56726400	1.39896000
C	4.57103800	0.43240600	2.65990400
C	5.18582300	1.14996100	3.68528000
C	6.51570500	1.55661400	3.56383100
C	7.23380300	1.23650700	2.40920000
C	6.62817300	0.52504900	1.37598900
C	7.08522200	-3.77224900	-0.85102800
C	7.88488700	-4.81946400	-1.30260600
C	7.42350800	-5.67656900	-2.30496200
C	6.15432500	-5.47902100	-2.85260700
C	5.35109600	-4.43223400	-2.40408800
C	-4.57113100	0.43242000	-2.65987500
C	-5.18595400	1.14999800	-3.68521200
C	-6.51582600	1.55666300	-3.56369600
C	-7.23387600	1.23654500	-2.40903700
C	-6.62820600	0.52506400	-1.37586500
C	-5.35099100	-4.43234400	2.40401300
C	-6.15419500	-5.47915900	2.85251300
C	-7.42338600	-5.67670800	2.30488900
C	-7.88480000	-4.81957400	1.30257300
C	-7.08516100	-3.77233200	0.85101300
H	-0.00994200	0.21679200	-1.78970800
H	0.00998300	0.21676200	1.78963700
H	3.10428400	1.55505900	0.85188200
H	1.35168400	-1.77760600	-2.38447800
H	-1.35162000	-1.77765400	2.38440300
H	-3.10430600	1.55505500	-0.85186400
H	-2.48788400	3.11059800	1.95673200
H	2.48782200	3.11067900	-1.95677500
H	-0.71618000	4.20565200	-1.80062000
H	-2.09986000	6.25334400	-1.85920000
H	-3.66903900	6.75528100	0.00636900
H	-3.85258700	5.17097000	1.91760300
H	3.85249000	5.17107400	-1.91763400
H	3.66895500	6.75534300	-0.00636400
H	2.09982500	6.25333900	1.85922900
H	0.71618100	4.20562400	1.80063800
H	3.54682100	0.09085900	2.76608700
H	4.62475200	1.37795800	4.58718300

H	6.99134400	2.11341900	4.36610700
H	8.27077300	1.54477000	2.30901400
H	7.17585700	0.26295100	0.47793100
H	7.43718800	-3.10791200	-0.06980200
H	8.87049900	-4.96888400	-0.86940300
H	8.04896400	-6.49363900	-2.65525300
H	5.78793500	-6.14220900	-3.63190500
H	4.36354300	-4.26906500	-2.82037300
H	-3.54692200	0.09086200	-2.76611000
H	-4.62492200	1.37800300	-4.58713700
H	-6.99149600	2.11348600	-4.36594100
H	-8.27083800	1.54481700	-2.30880000
H	-7.17585300	0.26295600	-0.47778700
H	-4.36343200	-4.26917400	2.82028200
H	-5.78777700	-6.14236800	3.63178000
H	-8.04882200	-6.49379900	2.65516500
H	-8.87042000	-4.96899500	0.86938700
H	-7.43715400	-3.10797300	0.06981800

***p*-DBT-T (*cis*)**

C	0.67320100	-2.27277700	0.12687200
C	-0.67303500	-2.27283800	-0.12695300
C	-1.43791200	-1.02796200	-0.42265400
C	-0.95901900	-0.07635500	-1.35188500
C	0.95884300	-0.07607600	1.35152400
C	1.43794100	-1.02783400	0.42255400
C	-2.69093800	-0.81257800	0.17089400
C	-3.43248200	0.33787700	-0.12016500
C	-2.96521200	1.27392400	-1.08898200
C	-1.70702000	1.03876300	-1.68108400
C	1.70670300	1.03916400	1.68063100
C	2.96497400	1.27431200	1.08869500
C	3.43247900	0.33808600	0.12016500
C	2.69107000	-0.81246300	-0.17081500
C	1.48576500	-3.52790000	0.13243400
C	2.37538100	-3.79929600	1.18718300
C	-2.37503300	-3.79952400	-1.18734500
C	-1.48553900	-3.52800800	-0.13253200
C	1.42363900	-4.44015800	-0.93450600
C	2.20854000	-5.59224100	-0.93788600
C	3.07185600	-5.85857200	0.12649000
C	3.15167900	-4.95687400	1.18995200
C	-3.15130000	-4.95712400	-1.19007100
C	-3.07156700	-5.85870500	-0.12650300
C	-2.20836900	-5.59224900	0.93793700
C	-1.42349300	-4.44014800	0.93451600
N	-4.67005500	0.63717800	0.45993400
N	-5.45535300	1.65567600	0.00454700
C	-4.92976800	2.45007400	-0.93395800
N	-3.70929100	2.35053900	-1.47721100
N	3.70889800	2.35107300	1.47680800

C	4.92945300	2.45060400	0.93371400
N	5.45524700	1.65603900	-0.00452500
N	4.67013800	0.63736200	-0.45978000
C	-5.80448000	3.56127100	-1.39575600
C	-5.25572900	-0.11411700	1.52531200
C	5.25610000	-0.11424000	-1.52479700
C	5.80397100	3.56202800	1.39535600
C	-4.51978200	-0.40828600	2.67908500
C	-5.12140100	-1.11623400	3.71885900
C	-6.45396300	-1.52018000	3.61998000
C	-7.18803000	-1.20698900	2.47347500
C	-6.59580800	-0.50517200	1.42605400
C	-7.07347700	3.77096900	-0.83309800
C	-7.87849500	4.81525400	-1.28228800
C	-7.42953800	5.66461900	-2.29665900
C	-6.16740600	5.46243400	-2.85897200
C	-5.35908200	4.41861500	-2.41302300
C	4.52051900	-0.40848500	-2.67878200
C	5.12238900	-1.11673700	-3.71820500
C	6.45484400	-1.52090000	-3.61875500
C	7.18854800	-1.20763200	-2.47203900
C	6.59606300	-0.50551600	-1.42496500
C	5.35831700	4.41958000	2.41233800
C	6.16645400	5.46360900	2.85813200
C	7.42864400	5.66579500	2.29594900
C	7.87785300	4.81622000	1.28186600
C	7.07302300	3.77172500	0.83282600
H	0.00149500	-0.24129200	-1.82817900
H	-0.00172000	-0.24099500	1.82772300
H	-3.08447800	-1.55111500	0.85811300
H	-1.36231700	1.75524800	-2.41977800
H	1.36181600	1.75576600	2.41912600
H	3.08477100	-1.55108200	-0.85785300
H	2.45060300	-3.09720800	2.01296000
H	-2.45019100	-3.09751300	-2.01319400
H	0.75463200	-4.23929400	-1.76549500
H	2.14767200	-6.28118600	-1.77631300
H	3.68233400	-6.75761300	0.12436100
H	3.82302300	-5.15266600	2.02202500
H	-3.82255500	-5.15302700	-2.02218900
H	-3.68203000	-6.75775700	-0.12434700
H	-2.14757900	-6.28110800	1.77644100
H	-0.75455100	-4.23917700	1.76553200
H	-3.49347000	-0.06806800	2.76793400
H	-4.54787600	-1.33859900	4.61431400
H	-6.91933100	-2.06938800	4.43343400
H	-8.22714200	-1.51322500	2.39083900
H	-7.15575500	-0.24855300	0.53402400
H	-7.41565700	3.11271800	-0.04247600
H	-8.85844800	4.96838200	-0.83769700
H	-8.05905200	6.47938700	-2.64504700
H	-5.81075200	6.11966700	-3.64777200

H	-4.37698300	4.25163400	-2.84059700
H	3.49429200	-0.06811500	-2.76804300
H	4.54915600	-1.33917000	-4.61383000
H	6.92041200	-2.07034100	-4.43193700
H	8.22757400	-1.51403900	-2.38896700
H	7.15573200	-0.24883000	-0.53277600
H	4.37617600	4.25257900	2.83980600
H	5.80961400	6.12100900	3.64670900
H	8.05801100	6.48072900	2.64421600
H	8.85785700	4.96935000	0.83738800
H	7.41539100	3.11329800	0.04243200