Supplementary Information

Nitrogen-Coupled Blatter Diradicals: The Fused *versus* Unfused Bridges

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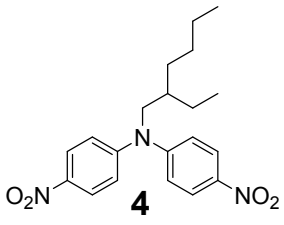
1. Methods and Materials

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 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/Vis/NIR absorption spectra were recorded on a Shimadzu UV-2600 UV-VIS spectrophotometer in spectroscopy grade dichloromethane (DCM). 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. 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. Cyclic voltammograms were measured on a Shanghai Chenhua CHI 660E electrochemical workstation. Melting points were measured on a Shanghai YiCe Apparatus & Equipment co., LTD WRX-4 Melting-point Apparatus.

2. Preparation of diradicals NDR and CDR

Synthesis of *N*-(2-ethylhexyl)-4,4′-dinitrodiphenylamine (4).

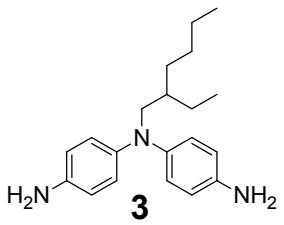


4

Compound 4,4′-dinitrophenylamine (**6**) (5.0 g, 19.3 mmol) and KO^{t}Bu (4.3 g, 38.6 mmol) were charged to a 250 mL two neck flask with dry DMSO (30 mL), and stirred at room temperature for 30 min. Then 2-ethylhexyl bromide (**5**) (7.5 g, 38.6 mmol) was added under nitrogen and the resulting mixture was stirred at 100 ^{o}C overnight. After cooling to room temperature, the mixture was quenched with water (50 mL) followed by extraction with ethyl acetate (3 x 50 mL). The combined organic fractions were washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography (silica gel, hexane/ethyl acetate, V/V = 9 :1 as eluent) to give compound **4** as yellow oil (3.2 g, 45%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.84-0.89 (m, 6H), 1.22-1.45 (m, 8H), 1.74-1.81 (m, 1H), 3.79 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 12.0 Hz, 4H), 8.18 (d, J = 12.0 Hz, 4H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 10.6, 13.9, 22.9, 24.0, 28.5, 30.6, 37.7, 56.8, 120.8, 125.6, 142.2, 152.4. HRMS (ESI$^+$): $[M+Na]^+$ calcd. for $C_{20}H_{25}N_3NaO_4$ 394.1743, found 394.1715.

Synthesis of *N*-(2-ethylhexyl)-4,4′-diaminodiphenylamine (3).



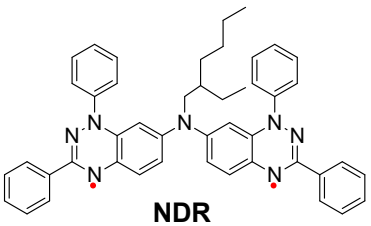
3

Compound **3** (3.1 g, 8.4 mmol) and $SnCl_2$•$2H_2O$ (13.2 g, 58.6 mmol) were charged to a 100 mL two neck flask with 30 mL of ethanol, and refluxed overnight. After cooling to room temperature the solution was alkalinized with aqueous NaOH (50%), and then extracted with DCM. The combined organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced

pressure. The residue was purified by column chromatography (silica gel, hexane/ethyl acetate, V/V = 1:1 as eluent) to give compound **3** as a brown oil (2.6 g, 98%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.83-0.89 (m, 6H), 1.23-1.46 (m, 8H), 1.64-1.71 (m, 1H), 3.739 (s, 6H), 6.69 (d, *J* = 56.0 Hz, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 10.7, 14.1, 23.1, 24.0, 28.7, 30.7, 115.2, 122.4, 140.0. HRMS (ESI$^+$): $[M+H]^+$ calcd. for $C_{20}H_{30}N_3$ 312.2440, found 312.2414.

Synthesis of *N*-(2-ethylhexyl)-4,4′-bis(1,3-Diphenyl-1,4-dihydro-1,2,4-benzotriazin-4-yl)amine (NDR).

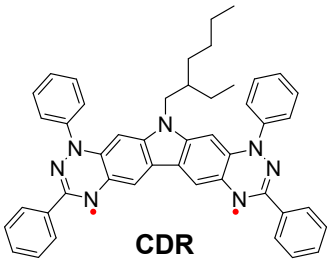


To an anhydrous THF solution (20 mL) of **3** (1.0 g, 3.2 mmol) and (*E*/*Z*)-1-[chloro(phenyl)-methylene]-2-phenyl- hydrazine **1**[1] (1.6 g, 6.9 mmol) was added triethylamine (TEA) (1 mL) at room temperature. Then the mixture was heated to reflux for 24 h, monitored by TLC. The resulting mixture was cooled to room temperature and Et_3NHCl was removed by suction filtration, followed by evaporation of THF under a reduced pressure. The residue was dissolved in dry DCM (20 ml) and treated with 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (1 ml) and 10 wt% Pd/C powder (0.2 g). Then this solution was stirred exposed to air, after 24 h the solution was filtered and evaporated to yield a crude dark green solid. This solid was purified by TEA pretreated column chromatography (SiO_2, hexane/ethyl acetate, V/V = 8: 1) followed by recrystallization from DCM/hexane to give the radical **NDR** as dark green powder (82.0 mg, 4%).

HRMS (ESI$^+$): $[M+H]^+$ calcd. for $C_{46}H_{44}N_7$ 694.3658, found 694.3640. UV/vis/NIR (DCM) λ_{max} nm (ε): 256 (28728), 322 (28150), 570 (3715), 695 (5201). Elemental

analysis (%) calcd. for $C_{46}H_{43}N_7$ C 79.62, H 6.25, N 14.13; found C 79.58, H 6.26, N 14.15. Melting range: 79.2-79.9 °C.

Synthesis of CDR.



To an anhydrous THF solution (20 mL) of 3,6-diamino-9-(2-ethylhexyl)carbazole **2**[2, 3] (619.0 mg, 2.0 mmol) and **1**[1] (1.0 g, 4.0 mmol) was added triethylamine (1 mL) at room temperature. Then the mixture was heated to reflux for 24 h, monitored by TLC. The resulting mixture was cooled to room temperature and Et_3NHCl was removed by suction filtration, followed by evaporation of THF under a reduced pressure. The residue was dissolved in dry DCM (20 ml) and treated with DBU (0.5 ml) and 10 wt% Pd/C powder (20 mg). 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 (SiO_2, hexane/ethyl acetate, V/V = 5: 1) to give the radical **CDR** as wine red powder (235 mg, 17%).

HRMS (ESI$^+$): $[M+H]^+$ calcd. for $C_{46}H_{42}N_7$ 692.3502, found 692.3475. UV/vis/NIR (DCM) λ_{max} nm (ε): 281 (22234), 334 (25050), 399 (7962), 541 (4563), 934 (4175). Elemental analysis (%) calcd. for $C_{46}H_{41}N_7$ C 79.86, H 5.97, N 14.17; found C 79.89, H 5.96, N 14.16. Melting range: 115.5-116.4 °C.

Methods to grow single crystals of diradicals NDR and CDR

Three major methods have been used to grow single crystals for x-ray diffraction. Method a: slow evaporation of **NDR** and **CDR** in pure or mixed solutions (DCM, toluene, THF, DCM/toluene, DCM/hexane, DCM/EA, DCM/acetone, DCM/acetonitrile) in 4 mL glass vials (with cap). Method b: slow diffusion of poor solvents e.g. hexane, toluene and acetonitrile to saturated DCM solution of **NDR** and **CDR** 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 **NDR** and **CDR** in pure or mixed solvents (e.g. toluene, THF, EA, acetone, DCM/toluene, DCM/hexane, DCM/EA, DCM/acetone, DCM/acetonitrile). Both diradicals are not stable in alcohol such as MeOH and EtOH, thus alcohol is not used for growing single crystal.

3. NMR and Mass spectra

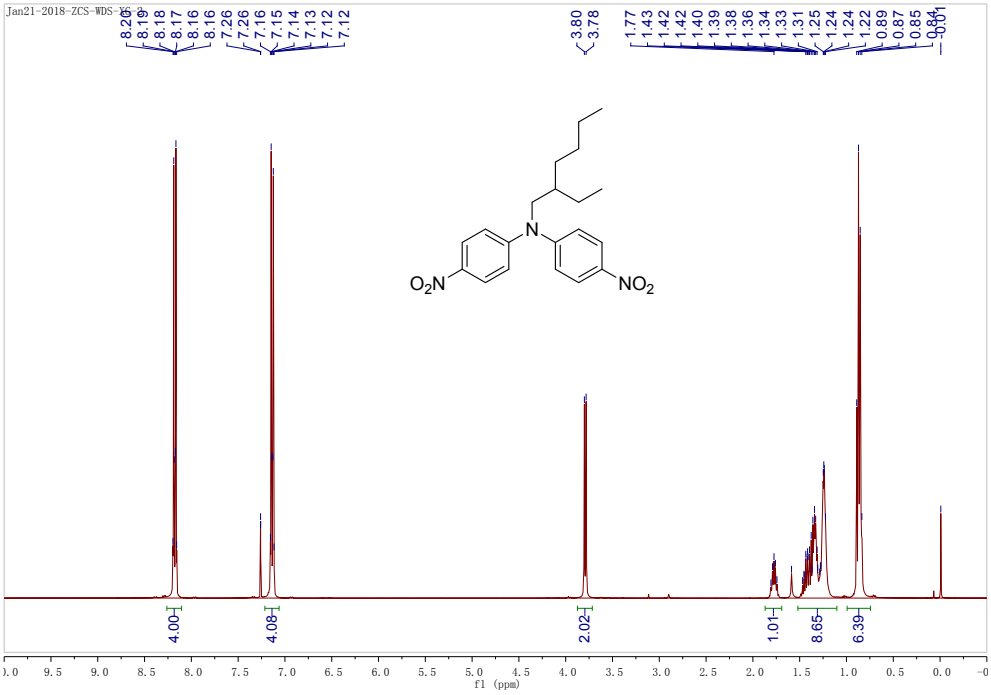


Figure S1. ^{1}H NMR spectrum of **4**.

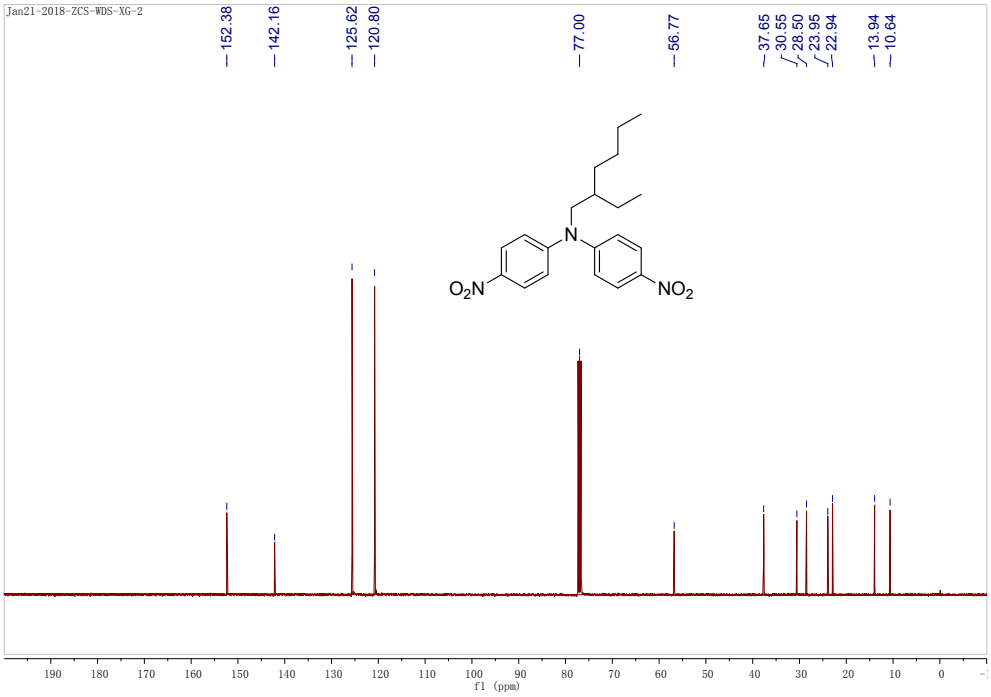


Figure S2. ^{13}C NMR spectrum of **4**.

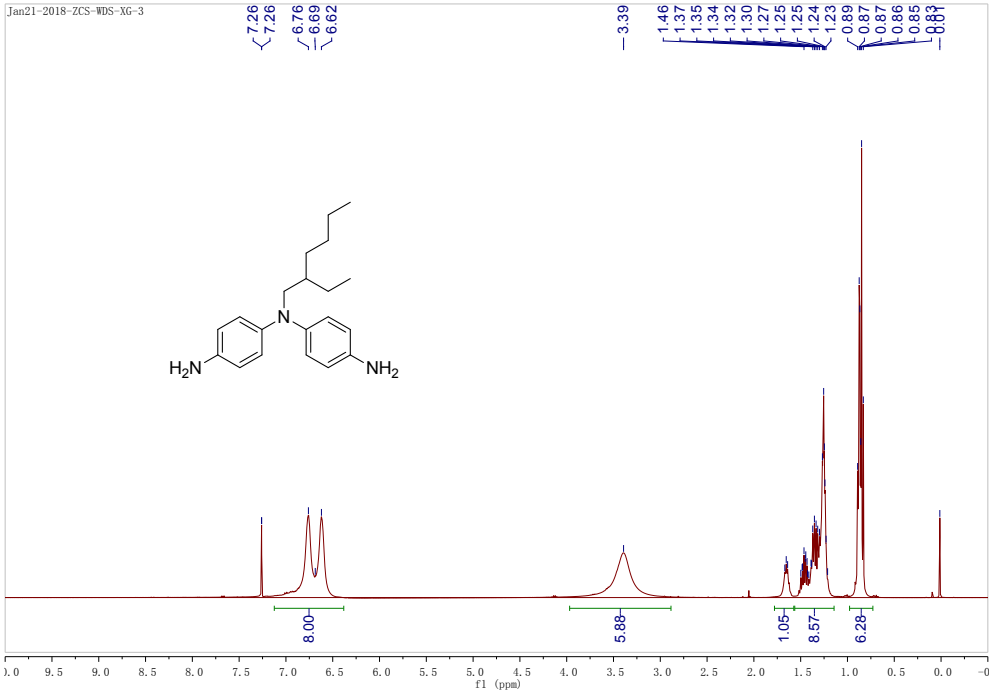


Figure S3. ^{1}H NMR spectrum of **3**.

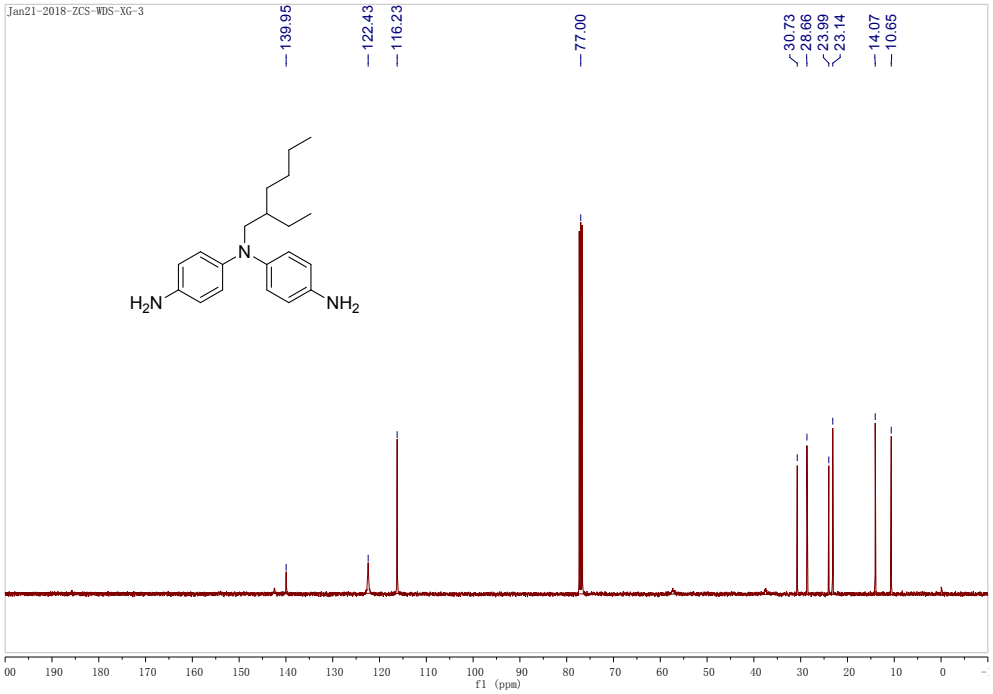


Figure S4. ^{13}C NMR spectrum of **3**.

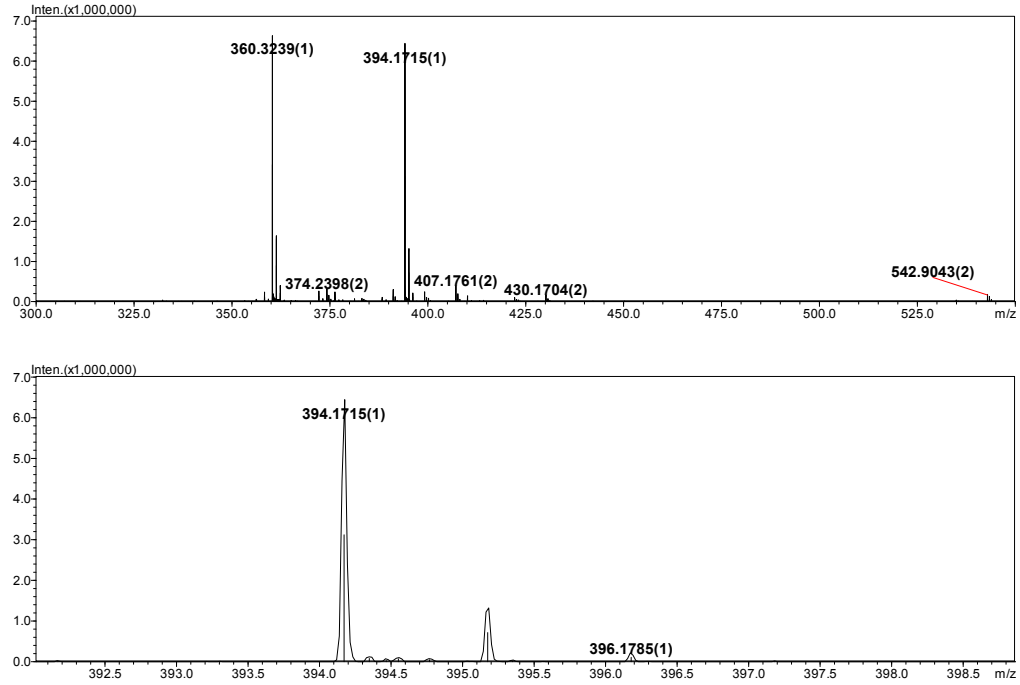


Figure S5. Mass spectra of **4** (ESI+)

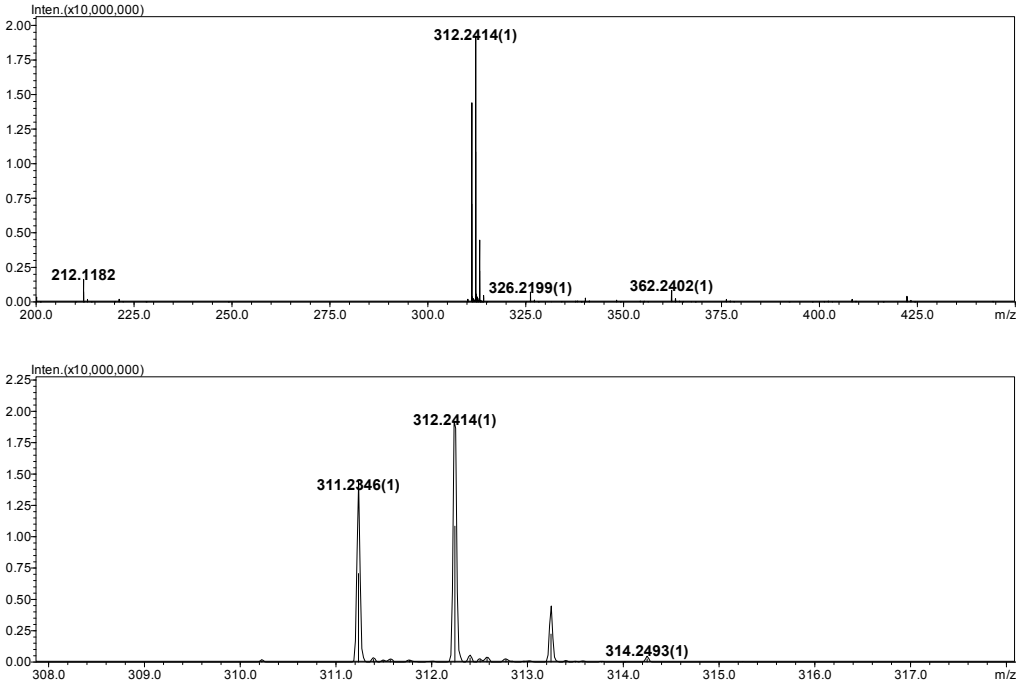


Figure S6. Mass spectra of **3** (ESI+)

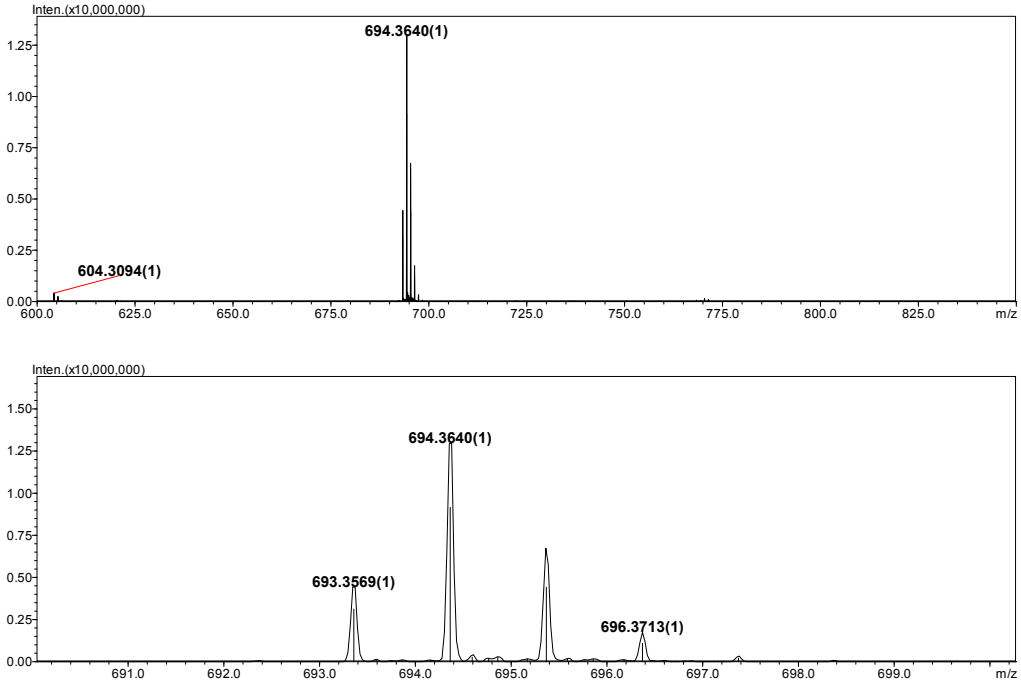


Figure S7. Mass spectra of **NDR** (ESI+)

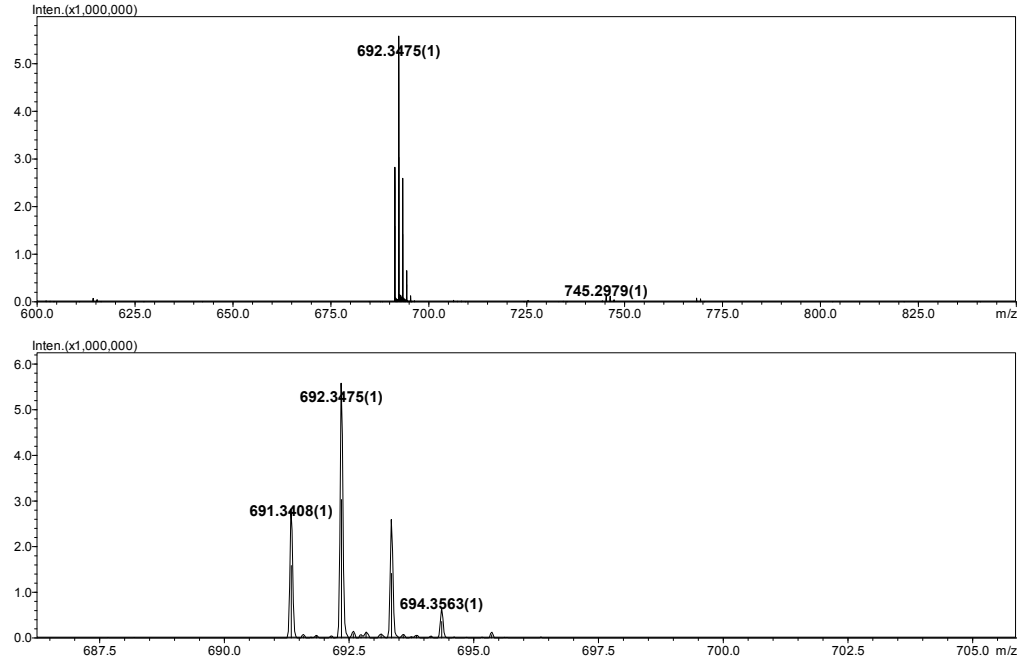


Figure S8. Mass spectra of **CDR** (ESI+).

4. ESR spectra and simulation

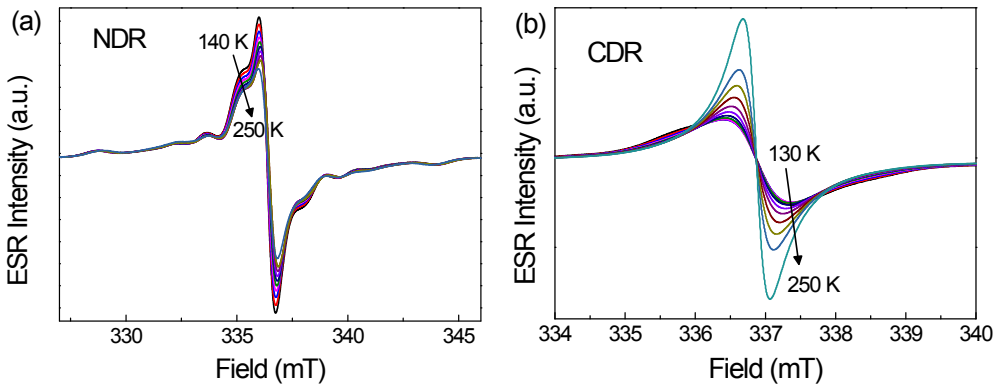


Figure S9. Variable temperature ESR spectra of **NDR** (a) and **CDR** (b) in benzothiophene solid solution from 130 to 250 K.

ESR simulation

All the ESR spectra were simulated by *easyspin* program in Matlab.[4] The detail parameters for **NDR** at 150 K are D= 0.0057 cm^{-1}, E= 0.00067 cm^{-1}, A_N= [33 59 45] MHz with 10% monoradical impurity at g= 2.0031. For **CDR** at 140 K, the fitting parameters are D= 0.0027 cm^{-1}, E= 0.00083 cm^{-1}, A_N= [55 9 30] MHz with 3% monoradical impurity at g= 2.0031.

Estimate of the population of diradical character

A standard curve method was used to estimate the population of **NDR** and **CDR** molecules possess diradical character, and 2,2-diphenyl-1-picrylhydrazyl (DPPH) was used as standard. First, the ESR spectra (**Figure S10a**) of 0.01, 0.03, 0.1, 0.3 and 1.0 mM DPPH solutions in degassed toluene were measured. Then the intensity of the doubly integrated ESR signal (DI) of 18.14, 41.18, 117.50, 354.24 and 1172.16 was

plotted as a function of concentration to get a standard curve (**Figure S10b**). It was estimated that 47% and 9% of the molecules possess diradical character in solution for **NDR** and **CDR**, respectively, by measuring the DI values of 0.3 and 1.0 mM solutions.

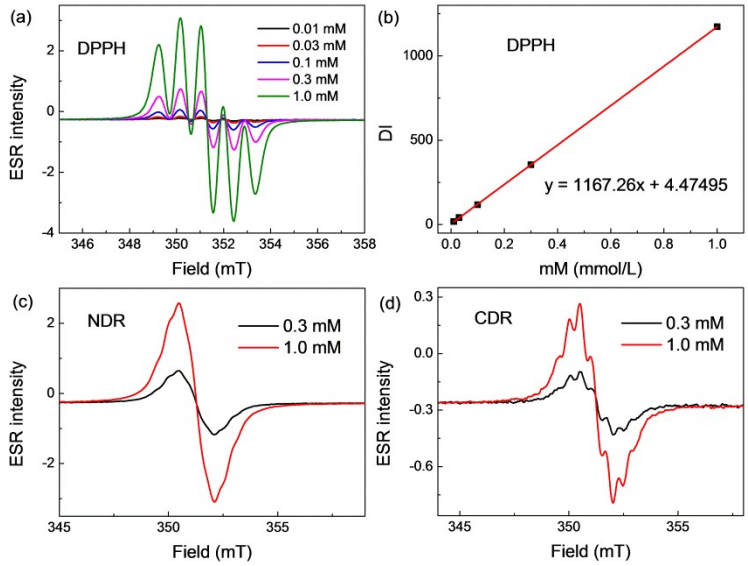


Figure S10. ESR spectra of 0.01, 0.03, 0.1, 0.3 and 1.0 mM DPPH solutions in degassed toluene (a). DPPH Standard curve plot of 0.01, 0.03, 0.1, 0.3 and 1.0 mM DPPH solutions against the intensity of the double integrated ESR signal (DI) (b). ESR spectra of 0.3 and 1.0 mM **NDR** (c) and **CDR** (d) solutions in degassed toluene.

5. Cyclic voltammetry

Cyclic voltammograms were measured 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. They display two reversible oxidation waves and two quasi-reversible reduction waves. The HOMO and LUMO energy levels of these two compounds were estimated from the half-wave potential $E_{1/2}$ in **Figure S11**

using ferrocene as reference. The equations used to calculate the energy level are: HOMO = - (E^{ox}_{sample} - $E^{ox}_{Fc/Fc+}$ + 4.8), LUMO = - (E^{red}_{sample} – $E^{red}_{Fc/Fc+}$ + 4.8). The values for HOMO and LUMO energy levels are summarized in **Table 1**. **NDR** and **CDR** possess similar HOMO and LUMO energy levels with small HOMO-LUMO energy gap of 1.01 and 1.02 eV, respectively.

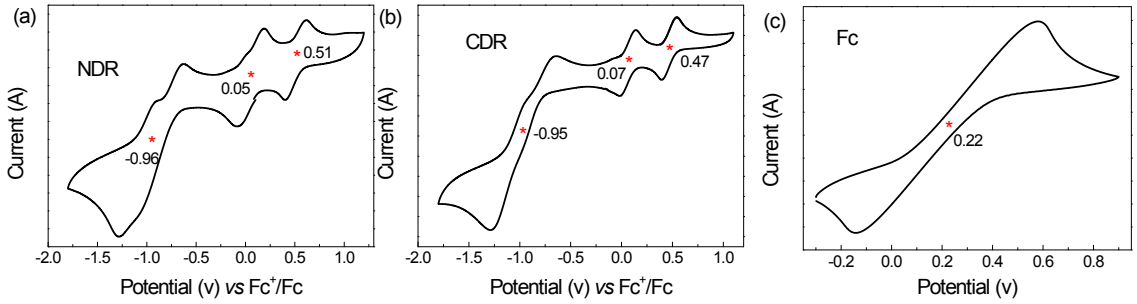


Figure S11. Cyclic voltammograms of **NDR** (a), **CDR** (b) and ferrocene (c) in dry DCM with 0.1 M Bu_4NPF_6 as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 100 mV/s. The red stars indicate the half-wave potential $E_{1/2}$.

6. Fourier transform infrared (FT-IR) spectra

Before FT-IR measurements, the two diradicals were dried in vacuum at 30 °C for 48 hours, and the potassium bromide (KBr) was grinded to fine powders using an agate mortar then dried in oven at 150 °C for 4 hours. Then the mixture of each diradical (~3 mg) and KBr (~150 mg) was grinded for 3-5 minutes under an infrared lamp. Finally, thin pellets were obtained by pressing the mixture under 10 MPa for 1 minute. The absence of typical N-H stretching vibration absorption above 3100 cm^{-1} indicates that

both starting materials **3** and **2** are fully converted into diradicals **NDR** and **CDR**, respectively

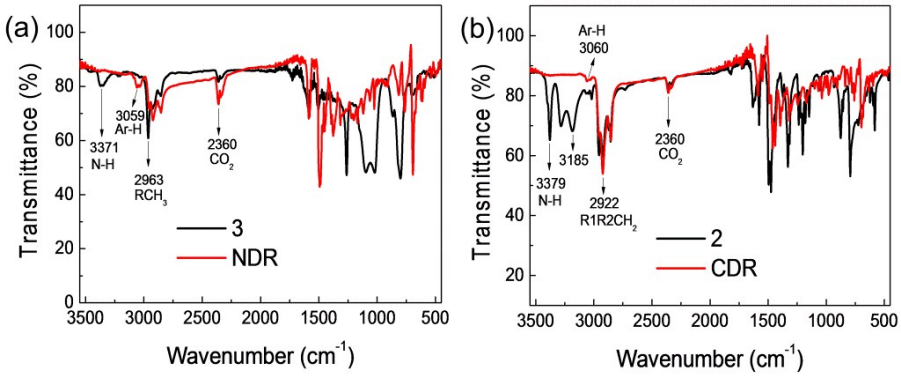


Figure S12. FT-IR spectra of compounds **3** & **NDR** (a), and **2** & **CDR** (b).

7. Optical energy gaps

UV/vis/NIR absorption spectra (**Figure S13**) reveal that the absorption onsets are 1092, and 1125 nm for **NDR** and **CDR**, respectively. The corresponding optical energy gaps Eg^{Opt} are 1.14 and 1.10 eV for **NDR** and **CDR**, respectively.

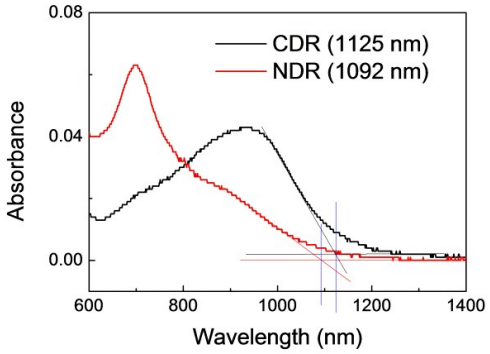


Figure S13. The partial UV/vis/NIR absorption spectra of **NDR** and **CDR** in DCM. The cross indicates the onset of each compound.

8. Stability test

Chemical stability

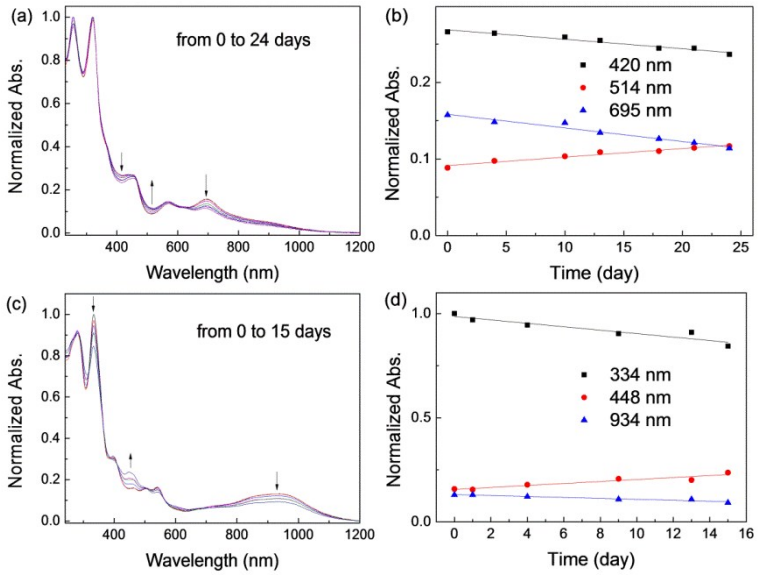


Figure S14. Normalized UV/vis/NIR absorption spectra (a) and the changes of the optical density at 420, 514 and 695 nm (b) of **NDR** in DCM for different time. Normalized UV/vis/NIR absorption spectra (c) and the changes of the optical density at 334, 448 and 934 (d) of **CDR** in DCM for different time. The half-life was estimated to be 45 and 29 days for **NDR** (695 nm) and **CDR** (934 nm), respectively.

9. Computational details

All calculations were performed with the Gaussian 16 program suite.[5] Full geometry optimizations were carried out at the (U)B3LYP/6–31G(d) level,[6-9] and the obtained stationary points were characterized by frequency calculations. The diradical character *y* was calculated by a broken-symmetry 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 diradical structures.[10, 11] Both **NDR** and **CDR** were calculated to be an open-shell singlet diradical with a typical disjoint HOMO and LUMO orbitals profile, leading to large diradical character of 0.89 and 0.68, respectively. The spin densities were illustrated using Multiwfn and VMD.[12, 13]

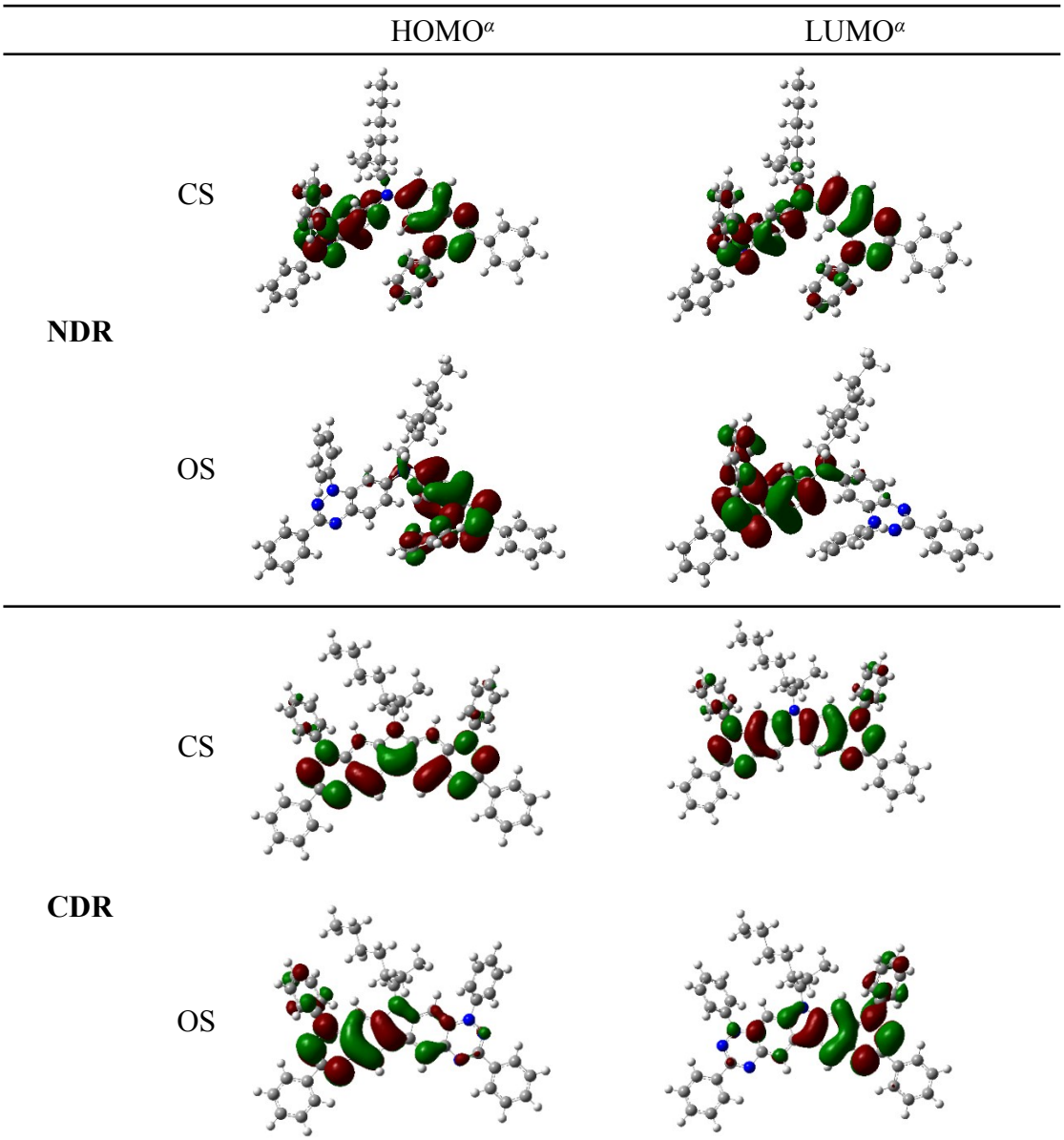


Figure S15. Frontier orbitals of **NDR** and **CDR** calculated at the UB3LYP/6-31G(d) level ($^{\alpha}$HOMO(α) and LUMO(α)) for the OS states.

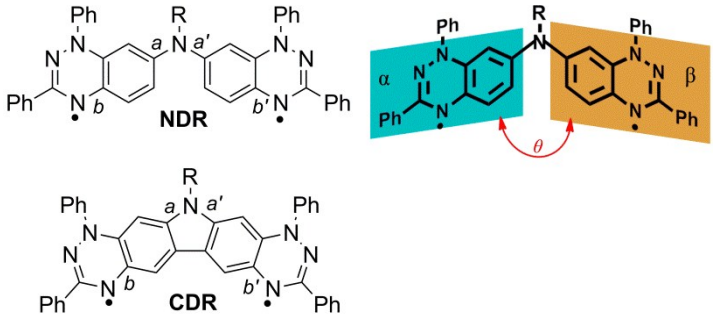


Table S1. Selected calculated relative energy ΔE (kcal/mol), bond lengths (Å), dihedral θ (°), and diradical characters (y) of **NDR** and **CDR**.

Compounds	States	ΔE	avg. a& a'	avg. b&b'	θ	y[a]
NDR	CS[b]	10.97	1.402	1.341	60.4	
	OS[c]	0	1.425	1.367	85.6	0.89
	T	0.05	1.425	1.367	85.8	
CDR	CS[b]	10.00	1.393	1.372	-	
	OS[c]	0	1.393	1.371	-	0.68
	T	0.01	1.392	1.367	-	

[a] Calculated at the level of UB3LYP/6-31G(d). [b] CS = closed-shell singlet, calculated at the level of B3LYP/6-31G. [c] OS = open-shell singlet, calculated at the level of UB3LYP/6-31G.

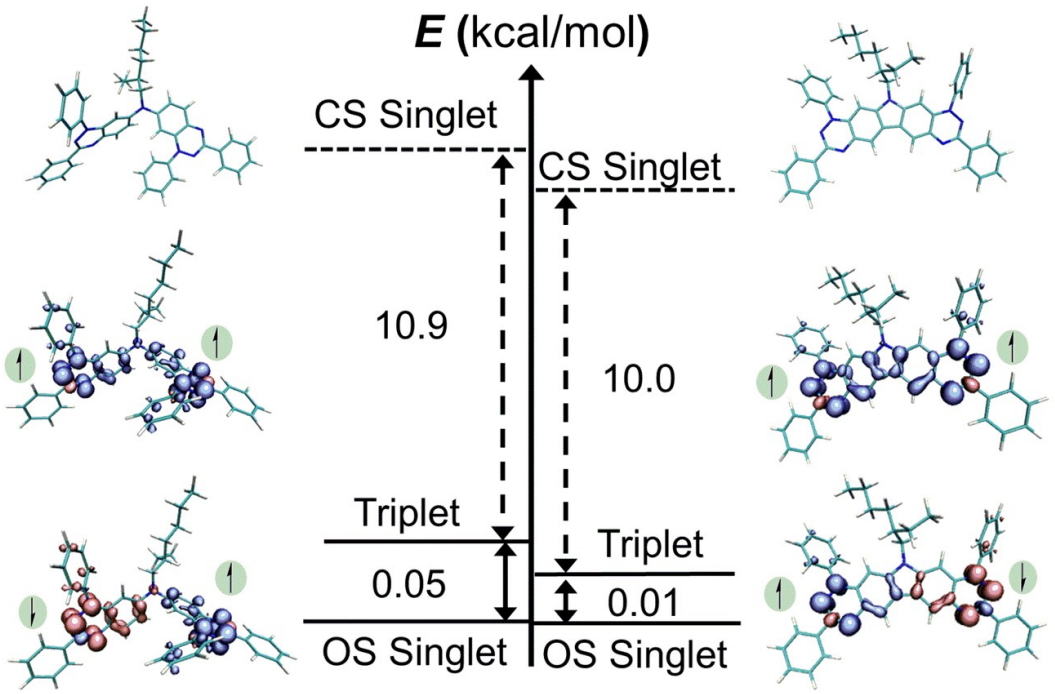


Figure S16. Calculated spin density distribution plot and relative energy of each spin state of **NDR** and **CDR**.

10. Supporting References

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Coordinates for calculated geometries:

NDR-OS

N	-5.45443400	-0.65219700	0.07093100
C	-5.31243900	-1.66614200	-0.78673800
N	-4.28626900	-1.87313700	-1.62327500
C	-3.24301700	-0.99680000	-1.51811400
C	-3.26642600	0.11133600	-0.62638600
N	-4.45279900	0.28227700	0.09007300
C	-2.07447800	-1.19043400	-2.28513200
C	-0.98069000	-0.35843200	-2.15873000
C	-0.98529600	0.71299000	-1.22837600
C	-2.13816200	0.92681600	-0.45762900
C	-6.42864800	-2.65118900	-0.80516300
C	-7.56779800	-2.47640500	-0.00374500
C	-8.59978400	-3.41180100	-0.03288300
C	-8.51131800	-4.53311100	-0.86156800
C	-7.38166600	-4.71164500	-1.66278600
C	-6.34684200	-3.77850600	-1.63599100
C	1.72694300	-0.10910800	-0.20859800
C	1.42590200	0.85274900	-1.17765100
N	0.15755900	1.53325500	-1.13455300
C	2.94956400	-0.78931100	-0.24911500
C	3.92862200	-0.45355200	-1.23069000
C	3.59324000	0.51172400	-2.20117900
C	2.36002100	1.14586300	-2.18572500

N	3.31610300	-1.78996800	0.65468400
N	4.58839600	-2.27821000	0.71400600
C	5.43810700	-1.86727900	-0.23426300
N	5.17078500	-1.02259900	-1.23859600
C	-4.71374600	1.38991900	0.95228000
C	0.10364000	2.73764900	-0.28942500
C	2.42870700	-2.35169000	1.62520200
C	6.81097300	-2.43419700	-0.15292300
C	2.87134800	-2.50147900	2.94444700
C	2.02851200	-3.07831400	3.89171600
C	0.74851700	-3.50734900	3.53238200
C	0.31717900	-3.36604900	2.21225900
C	1.15401400	-2.79600600	1.25328500
C	7.78879300	-2.01941800	-1.06948000
C	9.08024100	-2.53870100	-1.00492100
C	9.41280600	-3.47764600	-0.02621500
C	8.44329300	-3.89595600	0.88861200
C	7.15093700	-3.37981700	0.82742800
C	1.08555700	3.86300200	-0.68197600
C	0.72162600	4.43542500	-2.07437700
C	1.89828100	4.97445800	-2.89952200
C	2.01599200	6.10022900	0.32359400
C	1.05891400	4.90793300	0.45690400
C	2.97246700	8.19108300	1.45024400
C	2.03510900	6.98599800	1.57737600
C	-4.51887000	2.70314500	0.50618100
C	-4.80803500	3.77125400	1.35480200
C	-5.30309900	3.53952400	2.63950900
C	-5.51448300	2.22793000	3.07132900
C	-5.22327500	1.15294200	2.23436200
H	-2.06838300	-2.02152000	-2.98339000
H	-0.10415000	-0.51746600	-2.77715900
H	-2.16082500	1.69870500	0.29738100
H	-7.63472900	-1.60199100	0.63383000
H	-9.47729800	-3.26396100	0.59139700
H	-9.31806200	-5.26131900	-0.88342300

H	-7.30552800	-5.58075200	-2.31119000
H	-5.46512200	-3.90498000	-2.25398100
H	0.99893100	-0.32715800	0.56305700
H	4.33810600	0.73867900	-2.95693100
H	2.10026100	1.86869300	-2.95135800
H	-0.90847200	3.14448500	-0.37538900
H	0.25688200	2.46830700	0.76909600
H	3.86979800	-2.17133500	3.20745300
H	2.37354100	-3.18952300	4.91589400
H	0.09406000	-3.95491500	4.27481700
H	-0.66963300	-3.71219100	1.91861300
H	0.82585600	-2.71228000	0.22255200
H	7.51794800	-1.29071600	-1.82503000
H	9.82896300	-2.20910300	-1.72050900
H	10.42041100	-3.88229100	0.02297500
H	8.69406700	-4.62888300	1.65098900
H	6.39405200	-3.70586300	1.53186600
H	2.09934200	3.44227100	-0.72589000
H	0.23396800	3.64235200	-2.65514600
H	-0.03398000	5.22493700	-1.94882600
H	1.55479800	5.32380100	-3.88027300
H	2.40650400	5.81037400	-2.41048800
H	2.64909500	4.19367100	-3.07125300
H	3.03429800	5.73620200	0.12299100
H	1.73296800	6.71691700	-0.53930200
H	0.03127700	5.28934900	0.56407500
H	1.28632200	4.39062900	1.40064900
H	2.96559300	8.80092900	2.36077800
H	4.00654400	7.87183100	1.27112900
H	2.67707600	8.83737700	0.61449200
H	1.01459000	7.33638700	1.78867300
H	2.33314900	6.37938100	2.44431500
H	-4.16486700	2.88327900	-0.50349500
H	-4.66122100	4.78814200	1.00124700
H	-5.53061400	4.37457200	3.29594700
H	-5.90613000	2.03847600	4.06695300

H	-5.39216400	0.13076800	2.55334200

NDR CS

N	-4.98372000	-1.37049100	0.50300300
C	-4.75403000	-2.06948500	-0.59018600
N	-3.74173500	-1.88000900	-1.47803100
C	-2.82937300	-0.95316600	-1.14232000
C	-2.94836600	-0.13989300	0.03921100
N	-4.12723400	-0.32404800	0.76465000
C	-1.67989000	-0.75942600	-1.95384500
C	-0.68166600	0.11923100	-1.59056700
C	-0.77632800	0.86825000	-0.39402300
C	-1.91842100	0.71614600	0.41917400
C	-5.70934100	-3.17297300	-0.87671100
C	-6.81519700	-3.41327200	-0.04528900
C	-7.69667200	-4.45310100	-0.32861600
C	-7.49006500	-5.26819200	-1.44531300
C	-6.39430600	-5.03319300	-2.27720700
C	-5.50885900	-3.99315300	-1.99665500
C	1.94851300	0.01962000	-0.00004000
C	1.58537400	1.38537300	-0.08150100
N	0.24969200	1.77516200	-0.05589900
C	3.27939500	-0.36957000	-0.02796100
C	4.33500200	0.60936500	-0.06766100
C	3.94796100	1.97483100	-0.14693500
C	2.62653500	2.35363200	-0.15826000
N	3.71530000	-1.69741600	0.03458100
N	5.03491600	-2.01933600	0.20232000
C	5.91159900	-1.03444900	0.17445400
N	5.63184700	0.28667500	0.01435500
C	-4.50353900	0.46329700	1.88772100
C	-0.10429300	3.13354000	0.40141900
C	2.84131600	-2.82512500	0.05089500
C	7.33933400	-1.41556700	0.33272000
C	3.05682300	-3.84132500	0.99114700
C	2.22920100	-4.96128900	1.00030000

C	1.18468100	-5.07911500	0.08006000
C	0.98200500	-4.07095300	-0.86408700
C	1.80947400	-2.94953300	-0.88890900
C	8.32566000	-0.41895700	0.37096700
C	9.66873100	-0.76153400	0.52219600
C	10.04503000	-2.10072900	0.63600600
C	9.06708200	-3.09869900	0.59637200
C	7.72475700	-2.76125300	0.44572900
C	-0.21952200	4.20677800	-0.71285200
C	-1.46135600	3.98409200	-1.61532500
C	-1.23886000	4.31042400	-3.09825600
C	-0.23162300	6.81258600	-0.95548300
C	-0.19997400	5.59153800	-0.02653800
C	-0.14170900	9.36574500	-1.11350800
C	-0.10280600	8.14009900	-0.19523300
C	-4.43384200	1.86349000	1.83823500
C	-4.83772500	2.61780800	2.93840100
C	-5.32264400	1.99098400	4.08825100
C	-5.40887300	0.59721200	4.12592300
C	-5.00449600	-0.16793200	3.03471200
H	-1.62135100	-1.33217300	-2.87363900
H	0.17703700	0.26748600	-2.23771000
H	-1.98617600	1.24975600	1.35801600
H	-6.97460800	-2.77508300	0.81676500
H	-8.54959700	-4.62756300	0.32228700
H	-8.18013000	-6.07882800	-1.66498800
H	-6.22721500	-5.66129500	-3.14853700
H	-4.65513100	-3.79951500	-2.63587000
H	1.17072200	-0.72278600	0.10300900
H	4.74349800	2.71144000	-0.18729400
H	2.38724800	3.40682300	-0.23770600
H	-1.05708600	3.07510200	0.93370000
H	0.64381800	3.43623000	1.13972900
H	3.87191100	-3.74077700	1.69849200
H	2.39806800	-5.74268400	1.73617300
H	0.53677900	-5.95067900	0.09574500

H	0.18114700	-4.15688100	-1.59293900
H	1.66557400	-2.18391600	-1.64310200
H	8.02235800	0.61777100	0.28055200
H	10.42290600	0.02069900	0.55102900
H	11.09238800	-2.36679300	0.75308200
H	9.35231300	-4.14412300	0.68113500
H	6.96358800	-3.53276800	0.40978600
H	0.67517600	4.12639600	-1.34608600
H	-1.78010200	2.93907000	-1.54956500
H	-2.29963400	4.57861400	-1.22384200
H	-2.15481400	4.14043400	-3.67544500
H	-0.93352500	5.34946900	-3.25664200
H	-0.45742200	3.66818900	-3.52239300
H	0.58302800	6.73676000	-1.69065900
H	-1.16608300	6.82325600	-1.53165500
H	-1.05212900	5.65157800	0.66853000
H	0.70217800	5.65887400	0.60012200
H	-0.04637500	10.29589900	-0.54212300
H	0.67508000	9.33922400	-1.84521500
H	-1.08442000	9.41332000	-1.67233000
H	-0.91094200	8.21207300	0.54662700
H	0.83565400	8.14041600	0.37722500
H	-4.09253500	2.35517400	0.93323200
H	-4.78905600	3.70225100	2.88745500
H	-5.63808300	2.58291800	4.94260100
H	-5.79043100	0.09914800	5.01310900
H	-5.07529700	-1.24917800	3.05082400

NDR T

N	-5.49392300	-0.65194100	0.05993300
C	-5.34569100	-1.68694500	-0.77147500
N	-4.31176600	-1.91678000	-1.59185400
C	-3.26690400	-1.04067300	-1.49691100
C	-3.29657300	0.08878900	-0.63273700
N	-4.49000700	0.28033700	0.06648800
C	-2.09018200	-1.25643200	-2.24460300

C	-0.99481800	-0.42510700	-2.12597000
C	-1.00682300	0.67023500	-1.22365500
C	-2.16807100	0.90534800	-0.47144300
C	-6.46453700	-2.66926000	-0.77748200
C	-7.61201600	-2.47132700	0.00645600
C	-8.64635400	-3.40445000	-0.01063500
C	-8.55195100	-4.54654400	-0.80973100
C	-7.41396200	-4.74819800	-1.59349300
C	-6.37679500	-3.81740300	-1.57864400
C	1.73549400	-0.10934000	-0.19717700
C	1.40540200	0.81659900	-1.19083300
N	0.13453400	1.49274700	-1.13786700
C	2.96161100	-0.78370000	-0.24456800
C	3.91257500	-0.47833400	-1.26297600
C	3.54691700	0.44969600	-2.25797800
C	2.31063200	1.07849600	-2.23256000
N	3.35703900	-1.74923700	0.68424700
N	4.63218400	-2.23136900	0.72660000
C	5.45504900	-1.85000000	-0.25780100
N	5.15765800	-1.04216400	-1.28293700
C	-4.75704900	1.40939900	0.89846900
C	0.08505500	2.69829700	-0.29455600
C	2.49809700	-2.27933800	1.69755100
C	6.83214200	-2.40874400	-0.19270800
C	2.97455200	-2.37559400	3.00989900
C	2.15964100	-2.92098100	3.99930900
C	0.87432200	-3.37159800	3.68863100
C	0.40937100	-3.28387600	2.37529900
C	1.21804200	-2.74567300	1.37463800
C	7.78395700	-2.02227300	-1.14819100
C	9.07900500	-2.53417900	-1.09935200
C	9.44107200	-3.43743800	-0.09776500
C	8.49754300	-3.82743600	0.85588400
C	7.20165100	-3.31852700	0.81056900
C	1.08054200	3.81275000	-0.68319600
C	0.72910200	4.38947000	-2.07717900

C	1.91746300	4.90603600	-2.89983400
C	2.03157800	6.04052600	0.32240100
C	1.06140000	4.85879500	0.45471900
C	3.00549700	8.12414900	1.44756400
C	2.05444500	6.92972800	1.57366600
C	-4.55372400	2.71085800	0.42260200
C	-4.84891800	3.80012800	1.24174100
C	-5.35835800	3.60117100	2.52632500
C	-5.57809200	2.30106100	2.98769900
C	-5.28101400	1.20519900	2.18039300
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H	-0.11192800	-0.60399200	-2.72954900
H	-2.19803000	1.69535200	0.26411900
H	-7.68347100	-1.58090600	0.62097100
H	-9.53033800	-3.23856900	0.59984200
H	-9.36052100	-5.27295300	-0.82226000
H	-7.33313300	-5.63360600	-2.21887600
H	-5.48860100	-3.96171000	-2.18332200
H	1.02830800	-0.30386100	0.59977500
H	4.27095600	0.65368400	-3.04004500
H	2.02740700	1.77483400	-3.01432000
H	-0.92240900	3.11488500	-0.38796100
H	0.22821700	2.42974800	0.76567700
H	3.97682100	-2.02932800	3.23498400
H	2.53065600	-2.99069900	5.01804000
H	0.24175000	-3.79454000	4.46374500
H	-0.58178700	-3.64747900	2.11991500
H	0.86425600	-2.70360300	0.34984100
H	7.49026800	-1.32118400	-1.92113600
H	9.80744900	-2.22679600	-1.84510700
H	10.45147200	-3.83637300	-0.06086700
H	8.77137000	-4.53255600	1.63633200
H	6.46479100	-3.62271700	1.54535200
H	2.08971200	3.38068800	-0.72337300
H	0.22848900	3.60463800	-2.65809800
H	-0.01245000	5.19259400	-1.95424600

H	1.58312400	5.26135300	-3.88162000
H	2.43977300	5.73263500	-2.40970400
H	2.65368000	4.11097200	-3.06877900
H	3.04683700	5.66507300	0.12746400
H	1.75905200	6.65755100	-0.54366600
H	0.03757900	5.25130100	0.55826100
H	1.28044600	4.34027000	1.39977100
H	3.00086400	8.73676000	2.35625700
H	4.03689000	7.79313300	1.27441900
H	2.72122300	8.77112200	0.60849000
H	1.03682400	7.29183200	1.77908800
H	2.34172900	6.32246300	2.44378300
H	-4.18832700	2.86536400	-0.58725600
H	-4.69547700	4.80768500	0.86502900
H	-5.59055400	4.45259900	3.15968400
H	-5.98097500	2.13700100	3.98335400
H	-5.45632400	0.19155800	2.52231100

CDR OS

C	1.26480200	0.39318200	-0.05940600
C	0.96066900	-0.99987800	0.00504800
C	-0.47708200	-1.11305800	-0.02491800
C	-0.98730500	0.21481200	-0.11854000
N	0.07418500	1.11565200	-0.11944100
C	2.57671800	0.85974300	-0.08017800
C	3.60908800	-0.08931900	-0.02794000
C	3.32992900	-1.49866800	0.01188900
C	1.99557300	-1.92919400	0.04109100
N	4.95840600	0.25149300	-0.04602800
N	5.95594000	-0.67475700	-0.16276800
C	5.58136900	-1.96129700	-0.13354700
N	4.33763100	-2.42790400	-0.01315600
C	-1.36209100	-2.18599700	0.01656200
C	-2.74535200	-1.95999300	-0.05214000
C	-3.22875900	-0.61475700	-0.20143100
C	-2.35112500	0.47989800	-0.21105100

N	-3.60779500	-3.02065100	0.04928300
C	-4.91109700	-2.73590400	0.05538900
N	-5.46920900	-1.52811500	-0.10572200
N	-4.61085100	-0.48304100	-0.29993000
C	6.68893000	-2.95057700	-0.23681900
C	-5.86789500	-3.86060400	0.24433200
C	-0.07198600	2.56364800	-0.21615200
C	5.43654300	1.60040000	-0.02540500
C	-5.27370600	0.76114700	-0.54316400
C	6.33737100	2.01772900	-1.01068900
C	6.83785600	3.31783300	-0.98032600
C	6.44677900	4.20247100	0.02771300
C	5.55788200	3.77583500	1.01610100
C	5.05536500	2.47442800	0.99794800
C	-6.32414600	1.14764600	0.29640100
C	-7.00235000	2.33908100	0.04815200
C	-6.64147800	3.14618400	-1.03376500
C	-5.60095000	2.74879000	-1.87597800
C	-4.91859800	1.55542000	-1.63925600
C	-0.60518900	3.23827300	1.07071700
C	0.37332100	3.11269200	2.26075500
C	1.62949100	3.99168000	2.19556800
C	-2.28240500	4.88731100	-0.04459900
C	-1.01108000	4.70342700	0.79850900
C	-3.94725600	6.54944300	-1.05487900
C	-2.69313400	6.35859300	-0.19607000
C	6.39520700	-4.32198100	-0.26632700
C	7.42035000	-5.26061800	-0.36510200
C	8.75153500	-4.84427800	-0.43604400
C	9.05091600	-3.48014500	-0.40623600
C	8.02886900	-2.53842900	-0.30687400
C	-7.25517400	-3.65134100	0.20104300
C	-8.13408700	-4.71692000	0.38354000
C	-7.64252900	-6.00465500	0.61041600
C	-6.26324100	-6.21953000	0.65291800
C	-5.38087000	-5.15640000	0.47155200

H	2.80438400	1.91455300	-0.15316900
H	1.81003800	-2.99801300	0.06571000
H	-1.02249200	-3.21182800	0.11527500
H	-2.72905100	1.49077000	-0.28146500
H	0.90055900	2.98065500	-0.49232800
H	-0.74705000	2.77324200	-1.05399200
H	6.64035400	1.31627400	-1.77998700
H	7.53493500	3.64049000	-1.74864400
H	6.83941000	5.21513400	0.04771200
H	5.26437800	4.45016000	1.81572700
H	4.38786500	2.13025300	1.78097100
H	-6.60084200	0.50500500	1.12456100
H	-7.81584400	2.63756600	0.70351700
H	-7.17507800	4.07263200	-1.22622100
H	-5.32833700	3.35924500	-2.73224200
H	-4.13019500	1.22917200	-2.30965400
H	-1.51464500	2.69437800	1.36089800
H	-0.17908300	3.36304600	3.17631400
H	0.66811500	2.06105200	2.36653300
H	2.27043200	3.80016800	3.06384000
H	2.23128800	3.79895500	1.30003900
H	1.38076200	5.05844100	2.20243100
H	-2.14521100	4.45626700	-1.04655000
H	-3.11023600	4.32842800	0.41581400
H	-1.16466100	5.19947900	1.76750600
H	-0.17883900	5.23840300	0.31808600
H	-4.22664400	7.60677000	-1.12469500
H	-3.78794800	6.17966300	-2.07555000
H	-4.80092600	6.00310800	-0.63576800
H	-2.86197400	6.78933700	0.80097500
H	-1.85926400	6.92520100	-0.63440900
H	5.35789600	-4.63220400	-0.21033700
H	7.17904400	-6.32023100	-0.38732700
H	9.55043200	-5.57737600	-0.51301200
H	10.08468400	-3.14819000	-0.45847700
H	8.25707200	-1.47885600	-0.27903000

H	-7.63253700	-2.65117500	0.01993600
H	-9.20628200	-4.54197900	0.34633200
H	-8.32990900	-6.83475600	0.75191400
H	-5.87270300	-7.21860700	0.82845300
H	-4.30810100	-5.31009900	0.50180100

CDR CS

C	1.25827000	0.37308600	-0.05897700
C	0.94401900	-1.02762600	0.00797900
C	-0.46502900	-1.13704600	-0.01172100
C	-0.98445900	0.19712400	-0.10341900
N	0.07269400	1.10367800	-0.10775500
C	2.55850400	0.84404200	-0.09158300
C	3.60118700	-0.11052000	-0.04967500
C	3.31612600	-1.53749900	-0.00147300
C	1.99575300	-1.96327800	0.03974300
N	4.92061600	0.22963700	-0.08140000
N	5.94795800	-0.67052200	-0.15543100
C	5.58135700	-1.96353800	-0.11941200
N	4.34771100	-2.44219100	-0.01984500
C	-1.36768500	-2.21694200	0.03706500
C	-2.73650500	-1.99102400	-0.02479700
C	-3.22649100	-0.62866300	-0.17627900
C	-2.33747400	0.47090800	-0.19059800
N	-3.62700900	-3.03108900	0.06776400
C	-4.92046900	-2.73446500	0.03985300
N	-5.47030300	-1.51958200	-0.12749800
N	-4.57925900	-0.49045200	-0.27240900
C	6.70454800	-2.93901300	-0.18908100
C	-5.89455800	-3.85075900	0.19326300
C	-0.07220300	2.55157000	-0.20716100
C	5.38314300	1.59103700	-0.09445600
C	-5.22836600	0.77249300	-0.49160400
C	6.20748800	2.01159200	-1.14116200
C	6.69180100	3.31819400	-1.14870300
C	6.36406700	4.19807900	-0.11393400

C	5.55412000	3.76387500	0.93685800
C	5.06431600	2.45719100	0.95404900
C	-6.22462400	1.18115800	0.39937600
C	-6.88855400	2.38616700	0.17942100
C	-6.56939100	3.17610800	-0.92828200
C	-5.58484300	2.75188500	-1.82293500
C	-4.91387100	1.54695400	-1.61178500
C	-0.59272000	3.23182500	1.08201200
C	0.39088300	3.10037700	2.26718700
C	1.65346600	3.96949800	2.19464700
C	-2.26423400	4.89396300	-0.02341300
C	-0.98770500	4.69990900	0.80945700
C	-3.91849400	6.57133100	-1.02665900
C	-2.65731900	6.36945300	-0.18086600
C	6.42987500	-4.31443300	-0.19752000
C	7.46909000	-5.24010100	-0.26485700
C	8.79543000	-4.80609500	-0.32474700
C	9.07566900	-3.43778700	-0.31591000
C	8.03904100	-2.50881200	-0.24826100
C	-7.27779200	-3.62403900	0.12480500
C	-8.17277000	-4.68180900	0.27409300
C	-7.70063400	-5.97803400	0.49271300
C	-6.32486900	-6.20989000	0.56050100
C	-5.42691200	-5.15486600	0.41202500
H	2.78407000	1.89855600	-0.16843400
H	1.80554000	-3.03059600	0.06943300
H	-1.02509100	-3.24114100	0.13652000
H	-2.71197100	1.48281100	-0.25830100
H	0.89883200	2.96575100	-0.49266600
H	-0.75313300	2.76096400	-1.04024700
H	6.46507600	1.30973200	-1.92657900
H	7.32855700	3.64848800	-1.96446600
H	6.74645800	5.21480800	-0.12202500
H	5.31190500	4.43620300	1.75493600
H	4.45508200	2.10478700	1.77987000
H	-6.47159900	0.54636000	1.24292600

H	-7.65983900	2.70687600	0.87393100
H	-7.09427000	4.11152000	-1.10027800
H	-5.34718100	3.35043800	-2.69766200
H	-4.16685400	1.19819200	-2.31746200
H	-1.50488400	2.69547800	1.37779500
H	-0.15506000	3.35637300	3.18500800
H	0.67803700	2.04671200	2.37349800
H	2.29679000	3.77439400	3.06033200
H	2.24960600	3.77049500	1.29672800
H	1.41313700	5.03818400	2.20079500
H	-2.14182800	4.45457600	-1.02365800
H	-3.09463800	4.34862300	0.44850700
H	-1.12854200	5.20001800	1.77825800
H	-0.15450700	5.22583600	0.32072100
H	-4.18316700	7.63198900	-1.10255500
H	-3.77689900	6.19029400	-2.04578300
H	-4.77509800	6.04160600	-0.59241700
H	-2.80889800	6.80955200	0.81485800
H	-1.82107400	6.92166800	-0.63278900
H	5.39569900	-4.63646400	-0.15029800
H	7.24309700	-6.30331700	-0.27097700
H	9.60539900	-5.52921900	-0.37714300
H	10.10545600	-3.09245700	-0.36020800
H	8.25155500	-1.44570400	-0.23756400
H	-7.63922300	-2.61675000	-0.04900200
H	-9.24198100	-4.49388400	0.21782400
H	-8.40025300	-6.80195500	0.60846900
H	-5.94977100	-7.21596300	0.72983400
H	-4.35648500	-5.31968600	0.46162100

CDR T

C	1.26613200	0.39838800	-0.05957300
C	0.96293100	-0.99473800	0.00455200
C	-0.47780200	-1.10848100	-0.02715800
C	-0.98752100	0.21938400	-0.12143600
N	0.07478900	1.11798600	-0.12183300

C	2.57982700	0.86453000	-0.07783400
C	3.61101600	-0.08309600	-0.02341400
C	3.33276500	-1.49241700	0.01352600
C	1.99516900	-1.92350900	0.04156900
N	4.96451100	0.25617300	-0.03652200
N	5.95711500	-0.67487000	-0.16342200
C	5.58216100	-1.95756300	-0.13868100
N	4.33414500	-2.42292400	-0.01476200
C	-1.35988000	-2.18087900	0.01370400
C	-2.74644300	-1.95529800	-0.05552700
C	-3.22924900	-0.61036100	-0.20728700
C	-2.35302000	0.48315300	-0.21576000
N	-3.60240900	-3.01601700	0.04979200
C	-4.91000600	-2.73298200	0.06054600
N	-5.46803100	-1.52959400	-0.10377900
N	-4.61494700	-0.48175900	-0.30950900
C	6.68500300	-2.95082500	-0.25136300
C	-5.86175700	-3.85988800	0.26010500
C	-0.07167700	2.56647100	-0.21695900
C	5.44656200	1.60213900	-0.00667400
C	-5.28100400	0.75750800	-0.56149200
C	6.36530500	2.01853600	-0.97621600
C	6.86962300	3.31683100	-0.93575000
C	6.46454600	4.20205700	0.06618800
C	5.55758600	3.77699100	1.03877400
C	5.05136100	2.47731800	1.01091000
C	-6.34581300	1.13879300	0.26284800
C	-7.02705900	2.32640000	0.00503800
C	-6.65520300	3.13637900	-1.07096100
C	-5.60029600	2.74482800	-1.89794900
C	-4.91495800	1.55515900	-1.65202700
C	-0.60797800	3.23833600	1.06998000
C	0.36967200	3.11408200	2.26087700
C	1.62352100	3.99652900	2.19786500
C	-2.28756300	4.88377000	-0.04688900
C	-1.01749300	4.70266800	0.79872400

C	-3.95606000	6.54171500	-1.05780600
C	-2.70374200	6.35378800	-0.19571400
C	6.38564500	-4.32082700	-0.28690000
C	7.40670300	-5.26313800	-0.39461100
C	8.73915800	-4.85191400	-0.46851300
C	9.04416000	-3.48903700	-0.43261000
C	8.02645200	-2.54384200	-0.32434700
C	-7.25003400	-3.65585800	0.22128500
C	-8.12433400	-4.72327600	0.41372700
C	-7.62733300	-6.00804800	0.64627400
C	-6.24727400	-6.21777800	0.68429400
C	-5.36928900	-5.15259100	0.49292000
H	2.80757300	1.91947800	-0.14947800
H	1.81041100	-2.99251100	0.06501400
H	-1.02070100	-3.20679400	0.11322200
H	-2.73126300	1.49384100	-0.28784600
H	0.90122100	2.98413000	-0.49064300
H	-0.74544000	2.77613300	-1.05569300
H	6.67874200	1.31741100	-1.74156100
H	7.58054500	3.63782700	-1.69202600
H	6.85993300	5.21346100	0.09379800
H	5.25275100	4.45129400	1.83421200
H	4.37025900	2.13494500	1.78288700
H	-6.63084100	0.49489700	1.08715000
H	-7.85149200	2.61994700	0.64891100
H	-7.19092300	4.06007100	-1.27060200
H	-5.31857800	3.35702200	-2.75005100
H	-4.11564600	1.23392600	-2.31179500
H	-1.51633900	2.69185700	1.35856800
H	-0.18440000	3.36198600	3.17609000
H	0.66720400	2.06312400	2.36587500
H	2.26423700	3.80564600	3.06643600
H	2.22661600	3.80657700	1.30261600
H	1.37189100	5.06259400	2.20589100
H	-2.14633900	4.45580400	-1.04960400
H	-3.11433000	4.32055000	0.41011600

H	-1.17465200	5.19678700	1.76812900
H	-0.18582700	5.24081600	0.32089000
H	-4.23987700	7.59801900	-1.12525200
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H	-4.80859500	5.99027800	-0.64311300
H	-2.87733400	6.78116800	0.80196100
H	-1.87087000	6.92494300	-0.63003800
H	5.34744200	-4.62749400	-0.22846800
H	7.16092500	-6.32161300	-0.42145700
H	9.53479900	-5.58777500	-0.55240000
H	10.07905600	-3.16097700	-0.48698800
H	8.25913600	-1.48534900	-0.29161600
H	-7.63173000	-2.65813400	0.03565300
H	-9.19727300	-4.55230200	0.37982600
H	-8.31123600	-6.83965300	0.79551100
H	-5.85242300	-7.21439400	0.86410600
H	-4.29595100	-5.30274700	0.51957900