# Supporting Information for

## Correlation Between the Strength of Conjugation and Spin-Spin Interaction in Stable Diradicaloids

Xiaoguang Hu, ǂ[ab] Hanjiao Chen, ǂ[c] Guodong Xue, ǂ[a] Yonghao Zheng [a]*

[a] School of Optoelectronic Science and Engineering, University of Electronic Science and Technology of China (UESTC), Chengdu 610054, People Republic of China.

[b] School of Materials Science and Engineering, Zhengzhou University, Zhengzhou, 450001, Henan, People Republic of China.

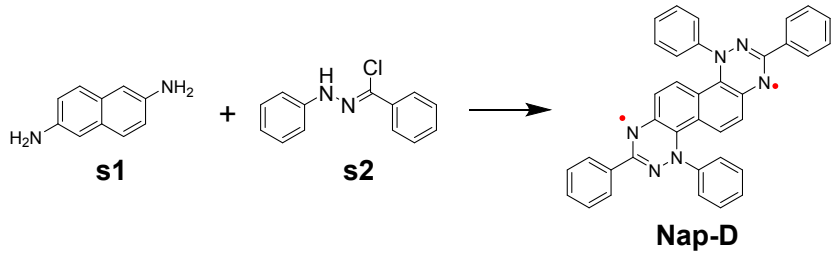
[c] Analytical & Testing Center, Sichuan University, Chengdu 610064, People Republic of China.

Email address: zhengyonghao@uestc.edu.cn (Y.Z.)

## 1. Methods and Materials

All reagents were purchased from Sigma-Aldrich, 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 $N_2$. 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. High resolution mass spectra (HRMS) were measured on a Waters-Q-TOF-Premier (ESI). MALDI-TOF mass spectra (MS) were recorded on a SHIMADZU iD plus Performance using anthracene-1, 8, 9-triol as matrix. 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). Elemental analysis measurements were performed on a Leeman Labs Euro EA 3000 elemental analyzer. Cyclic voltammograms were measured in dry $CH_2Cl_2$ 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. Single Crystal X-Ray Diffraction were measured by a Gemini X-ray Single Crystal Diffractometer.

## 2. Experimental Procedures




**Nap-D**

To an anhydrous THF solution (20 mL) of 2,6-naphthalenediamine **s1** (1.0 g, 6.0 mmol) and **s2** (3.0 g, 12.0 mmol) was added triethylamine (TEA) (3.0 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 the precipitate was removed by suction filtration, followed by evaporation of THF under a reduced pressure. The residue was dissolved in dichloromethane/methanol (30/300 mL), and treated with 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (2.0 mL), while air was bubbled through the reaction mixture for 24 h. The resulting precipitation was filtered, and was washed with methanol (20 mL x 5), followed by hot ethyl acetate to give the diradical **Nap-D** as a black powder (1.4 g, 43%). HRMS ($ESI^+$): $[M+H]^+$ calcd. for $C_{36}H_{25}N_6$ 541.2141, found 541.2101. Elemental analysis (%) calcd. C 79.98 H 4.47, N 15.55; found C 80.02, H 4.46, N 15.52. IR (KBr, $cm^{-1}$) 3054, 1574, 1475, 1436, 1408, 1344, 1302, 1294, 1282, 1231, 1168, 1149, 1058.

## 3. Mass spectra

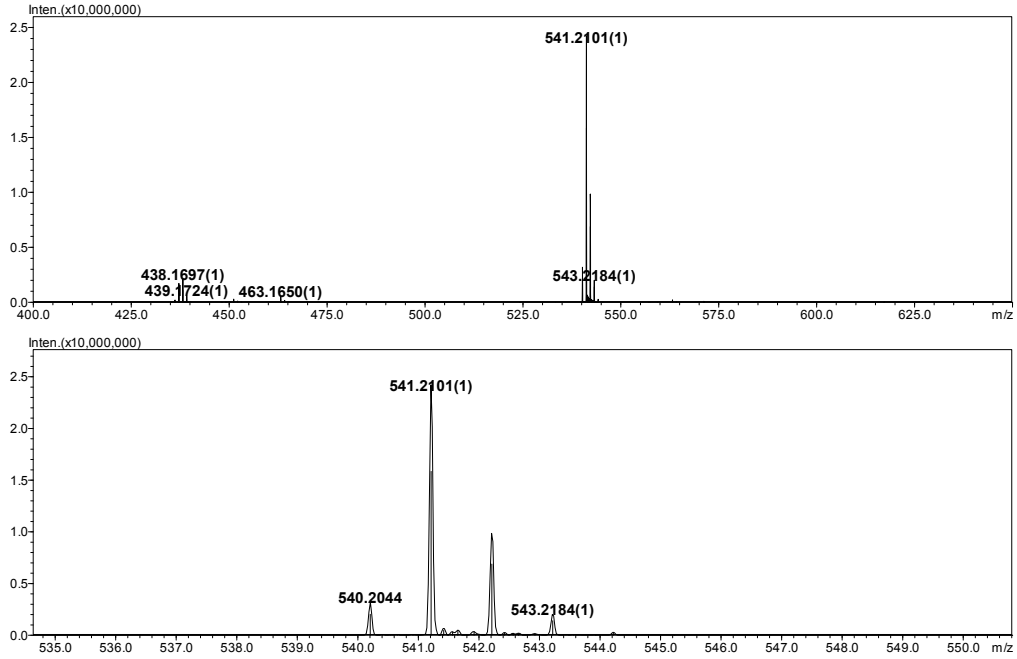



**Figure S1**. Mass spectra of **Nap-D** (ESI+)

## 4. Stability test

## Chemical stability

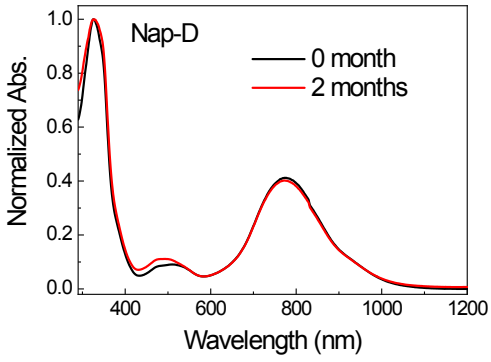



**Figure S2.** UV/vis/NIR absorption spectra of **Nap-D** in $CH_2Cl_2$ for different time.

**Thermal stability**

TGA diagram (**Figure S3**) indicates that **Nap-D** is stable up to ~ 290 °C. To verify whether the diradicaloid remains intact at high temperature, we annealed it at different temperatures for 15 minutes under $N_2$ using the TGA apparatus. The UV-Vis-NIR and MS spectra (**Figure S4**) reveal that **Nap-D** is stable up to 275 °C without any decomposition, it begins to decompose at 300 °C.

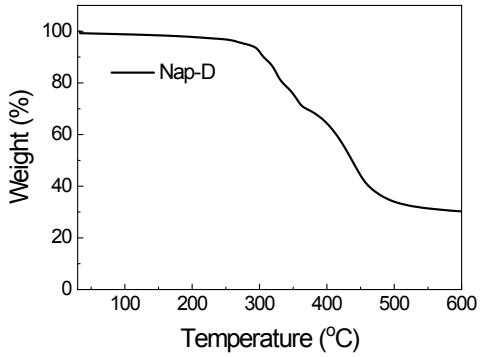



**Figure S3**. TGA of **Nap-D** under $N_2$; heating rate = 10 °C/min.

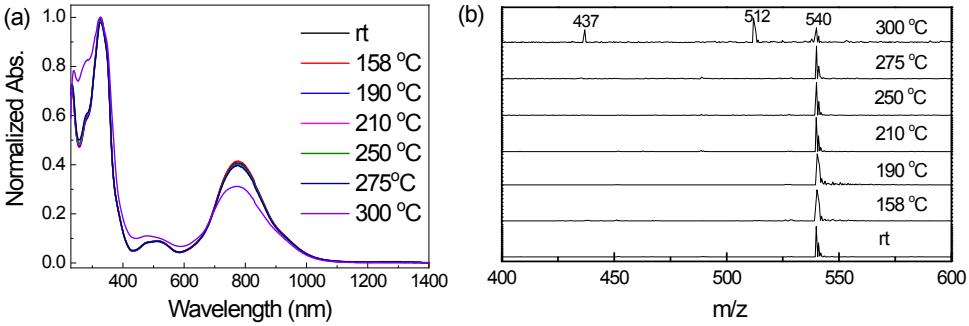



**Figure S4.** Room temperature UV-Vis-NIR absorption spectra (a) and MALDI-TOF mass spectra (b) of **Nap-D** after annealing at different temperatures under $N_2$ for 15 minutes (using TGA apparatus).

**Photo stability**

The Photo stability was studied in $CH_2Cl_2$ upon irradiation with a white light (400 W), and the distance between sample and lamp is 20 cm. The yield half-life ($t_{1/2}$) was 9.6 h (775 nm) for **Nap-D**.

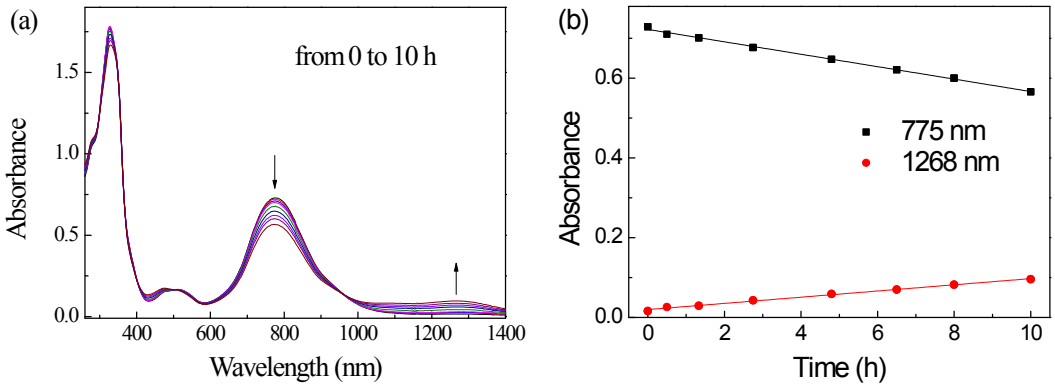



**Figure S5.** UV-Vis-NIR absorption spectra of **Nap-D** (a) in $CH_2Cl_2$ upon irradiation with white light (400 W). The changes of the optical density at 775 and 1268 nm for **Nap-D** (b) as a function of irradiation time.

## 5. Electrochemical energy gaps

Cyclic voltammograms were measured in dry $CH_2Cl_2$ 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. **Nap-D** displays two reversible oxidation waves and one reduction wave. The HOMO and LUMO energy levels were estimated from the half-wave potential $E_{1/2}$ in **Figure S6** 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 of LUMO and HOMO energy levels for **Nap-D** are -3.33 and -4.50 eV, respectively.

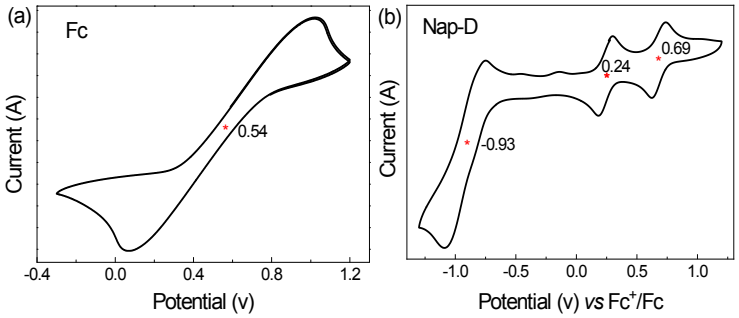



**Figure S6.** Cyclic voltammogram of ferrocene (a), **Nap-D** (b) in dry $CH_2Cl_2$ with 0.1 M $Bu_4NPF_6$ as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 100 mV/s. The red stars indicate the half-wave potential $E_{1/2}$.

## 6. X-ray crystallography

Dark purple single crystals of **Nap-D** was grown by allowing slow evaporation of a nearly saturated solution of **Nap-D** in $CH_2Cl_2$ at room temperature. **Nap-D** has centrosymmetric and planar core backbone (**Figure S7**), and the phenyl at the N3 position is twisted relative to the core plane with a dihedral angle of c.a. 56.5°. The torsion angles between the phenyl at C7(a) position and the triazinyl ring is 4.6° for **Nap-D**.

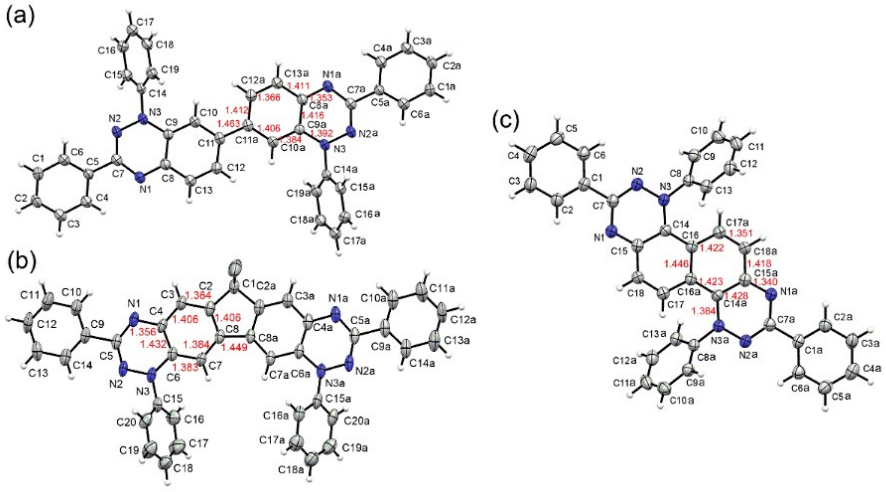



**Figure S7**. Single-crystal X-ray structures of **DPh-D** (a), **FDT** (b) and **Nap-D** (c) with selected bond lengths (Å) with thermal ellipsoids shown at the 50% probability level.

**Table S1**. Sample and crystal data for **Nap-D**

| Identification code | **Nap-D** | |
|---|---|---|
| Chemical formula | $C_{36}H_{24}N_6$ | |
| Formula weight | 540.61 g/mol | |
| Temperature | 150(2) K | |
| Wavelength | 1.54178 Å | |
| Crystal size | 0.050 x 0.100 x 0.200 mm | |
| Crystal system | monoclinic | |
| Space group | P 1 21/c 1 | |
| Unit cell dimensions | a = 9.1579(5) Å | α = 90° |
| | b = 21.3968(10) Å | β = 104.940(3)° |
| | c = 6.9520(3) Å | γ = 90° |
| Volume | 1316.19(11) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.364 $g/cm^3$ | |
| Absorption coefficient | 0.652 $mm^{-1}$ | |
| F(000) | 564 | |

**Table S2.** Data collection and structure refinement for **Nap-D.**

| Theta range for data collection | 4.13 to 68.17° | |
|---|---|---|
| Index ranges | -11<=h<=11, -23<=k<=25, -8<=l<=7 | |
| Reflections collected | 7101 | |
| Independent reflections | 2370 [R(int) = 0.0491] | |
| Absorption correction | none | |
| Max. and min. transmission | 0.9680 and 0.8810 | |
| Structure solution technique | direct methods | |
| Structure solution program | SHELXS-97 (Sheldrick 2008) | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Refinement program | SHELXL-2014 (Sheldrick 2014) | |
| Function minimized | $\Sigma\, w(F_o^2 - F_c^2)^2$ | |
| Data / restraints / parameters | 2370 / 0 / 191 | |
| Goodness-of-fit on $F^2$ | 1.068 | |
| $\Delta/\sigma_{max}$ | 0.002 | |
| Final R indices | 1784 data; I>2σ(I) | R1 = 0.0497, wR2 = 0.1289 |
| | all data | R1 = 0.0673, wR2 = 0.1441 |
| Weighting scheme | $w=1/[\sigma^2(F_o^2)+(0.0661P)^2+0.3119P]$ where $P=(F_o^2+2F_c^2)/3$ | |
| Extinction coefficient | 0.0033(7) | |
| Largest diff. peak and hole | 0.217 and -0.177 $eÅ^{-3}$ | |

R.M.S. deviation from mean 0.045 eÅ$^{-3}$

**Table S3.** Bond lengths (Å) for **Nap-D.**

| | | | |
|---|---|---|---|
| N1-C15 | 1.340(2) | N1-C7 | 1.346(3) |
| C1-C6 | 1.387(3) | C1-C2 | 1.393(3) |
| C1-C7 | 1.495(3) | C2-C3 | 1.388(3) |
| C2-H2 | 0.95 | N2-C7 | 1.315(3) |
| N2-N3 | 1.380(2) | C3-C4 | 1.381(3) |
| C3-H3 | 0.95 | N3-C14 | 1.384(2) |
| N3-C8 | 1.438(2) | C4-C5 | 1.392(3) |
| C4-H4 | 0.95 | C5-C6 | 1.381(3) |
| C5-H5 | 0.95 | C6-H6 | 0.95 |
| C8-C9 | 1.379(3) | C8-C13 | 1.389(3) |
| C9-C10 | 1.390(3) | C9-H9 | 0.95 |
| C10-C11 | 1.377(3) | C10-H10 | 0.95 |
| C11-C12 | 1.382(3) | C11-H11 | 0.95 |
| C12-C13 | 1.387(3) | C12-H12 | 0.95 |
| C13-H13 | 0.95 | C14-C16 | 1.423(3) |
| C14-C15 | 1.428(3) | C15-C18 | 1.418(3) |
| C16-C17 | 1.422(3) | C16-C16 | 1.446(4) |
| C17-C18 | 1.351(3) | C17-H17 | 0.95 |
| C18-H18 | 0.95 | | |

**Table S4.** Bond angles (°) for **Nap-D.**

| | | | |
|---|---|---|---|
| C15-N1-C7 | 116.16(17) | C6-C1-C2 | 118.83(18) |
| C6-C1-C7 | 121.53(18) | C2-C1-C7 | 119.63(19) |
| C3-C2-C1 | 120.1(2) | C3-C2-H2 | 119.9 |
| C1-C2-H2 | 119.9 | C7-N2-N3 | 115.82(16) |
| C4-C3-C2 | 120.7(2) | C4-C3-H3 | 119.7 |
| C2-C3-H3 | 119.7 | N2-N3-C14 | 122.93(16) |
| N2-N3-C8 | 110.91(15) | C14-N3-C8 | 125.74(15) |
| C3-C4-C5 | 119.4(2) | C3-C4-H4 | 120.3 |
| C5-C4-H4 | 120.3 | C6-C5-C4 | 120.0(2) |
| C6-C5-H5 | 120.0 | C4-C5-H5 | 120.0 |
| C5-C6-C1 | 121.0(2) | C5-C6-H6 | 119.5 |
| C1-C6-H6 | 119.5 | N2-C7-N1 | 126.94(18) |
| N2-C7-C1 | 115.49(18) | N1-C7-C1 | 117.42(17) |
| C9-C8-C13 | 121.12(18) | C9-C8-N3 | 119.38(19) |
| C13-C8-N3 | 119.48(18) | C8-C9-C10 | 119.2(2) |
| C8-C9-H9 | 120.4 | C10-C9-H9 | 120.4 |

| | | | |
|---|---|---|---|
| C11-C10-C9 | 119.9(2) | C11-C10-H10 | 120.1 |
| C9-C10-H10 | 120.1 | C10-C11-C12 | 120.9(2) |
| C10-C11-H11 | 119.6 | C12-C11-H11 | 119.6 |
| C11-C12-C13 | 119.7(2) | C11-C12-H12 | 120.2 |
| C13-C12-H12 | 120.2 | C12-C13-C8 | 119.2(2) |
| C12-C13-H13 | 120.4 | C8-C13-H13 | 120.4 |
| N3-C14-C16 | 125.21(17) | N3-C14-C15 | 114.05(17) |
| C16-C14-C15 | 120.74(18) | N1-C15-C18 | 119.28(17) |
| N1-C15-C14 | 123.02(18) | C18-C15-C14 | 117.63(17) |
| C17-C16-C14 | 123.07(18) | C17-C16-C16 | 118.1(2) |
| C14-C16-C16 | 118.9(2) | C18-C17-C16 | 121.88(19) |
| C18-C17-H17 | 119.1 | C16-C17-H17 | 119.1 |
| C17-C18-C15 | 122.10(18) | C17-C18-H18 | 119.0 |
| C15-C18-H18 | 119.0 | | |

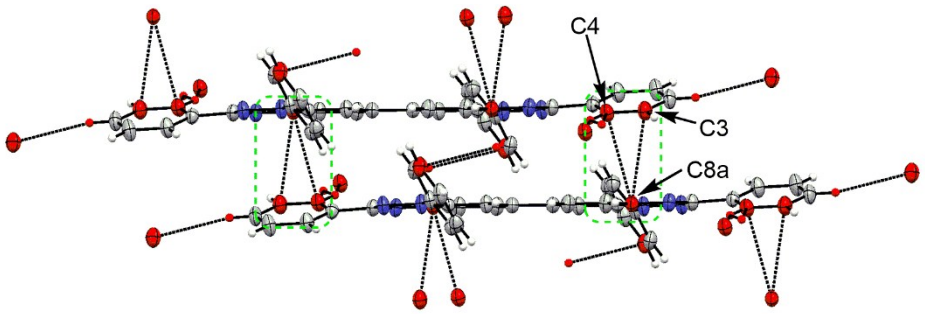



**Figure S8**. Solid-state packing diagrams of **DPh-D** with short contacts (dashed lines). Red colored atoms are short contact atoms.

## 7. Fourier transform infrared (IR) spectra

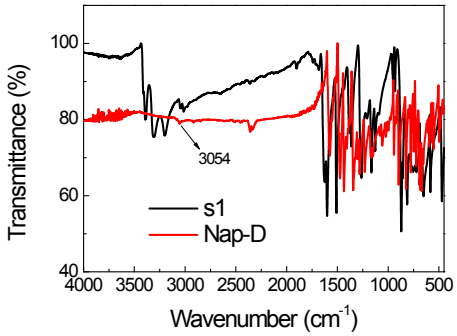



**Figure S9**. FT-IR spectra of compounds **s1** & **Nap-D**.

## 8. Magnetization measurements and data analysis

### SQUID measurements

For SUQID measurement, first the diradicaloid was dried in vacuum at 50 °C for 48 hours, then confirmed by Mass Spectra, FT-IR and combustion analyses. Magnetic susceptibility of powder sample of **Nap-D** (43.3 mg) was measured in a polycarbonate capsule fitted in a plastic straw as a function of temperature in heating (2 K→ 300 K) mode with 30 seconds of temperature stability at each temperature (1 K increment in a range 2–10 K, 3 K increment in a range 10–300 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) (**Figure S10**).

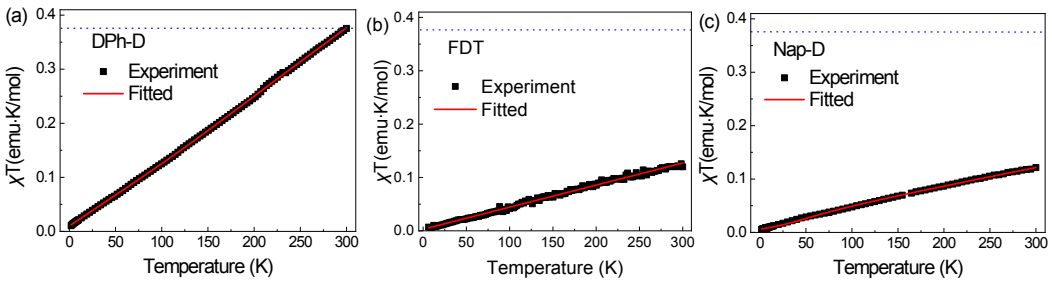



**Figure S10**. Temperature-dependent plots of χT for **DPh-D** (a), **FDT** (b) and **Nap-D** (c) measured at 1.0 T in the stable mode from 2 to 300 K. The solid lines are the fitting curves according to Bleaney−Bowers equation; g-factor was taken to be 2. The

horizontal dot line $\chi T$ = 0.375 emu·K/mol indicates the theoretical value for an ideal paramagnetic monoradical.

## SQUID Data analysis

The SQUID data in **Figure S10** were fitted with a modified Bleaney-Bowers equation.[4, 5] However, singlet-triplet energy gap ($\Delta E_{S\text{-}T}$) cannot be fitted well. The yield monoradical impurity values are too high.

## ESR spectra/simulation

Simulations of ESR spectra were performed with the *Easyspin* program in Matlab.[6]

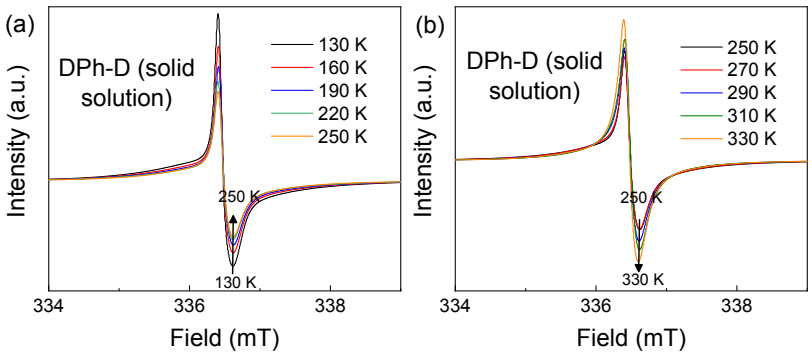



**Figure S11**. Variable temperature ESR spectra of **DPh-D** in benzophenone solid solution.

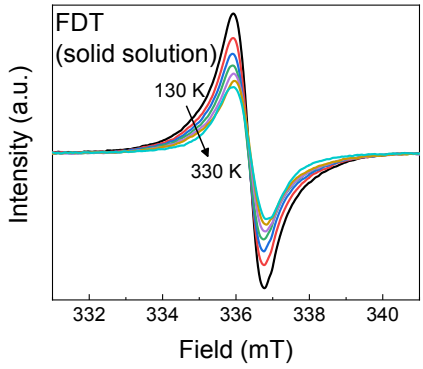



**Figure S12**. Variable temperature ESR spectra of **FDT** in benzophenone solid solution.

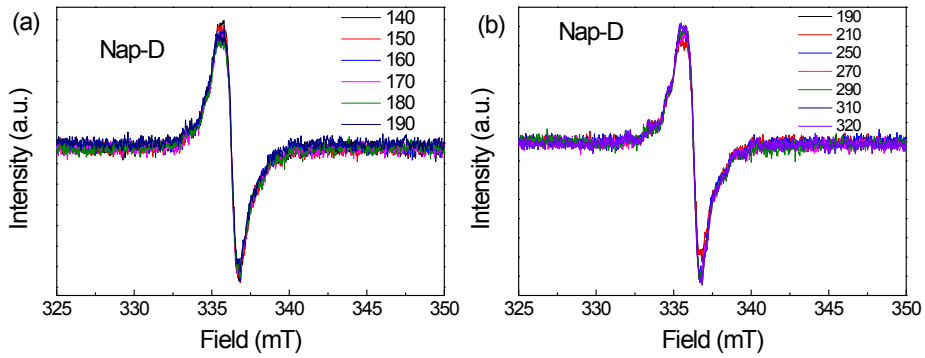



**Figure S13**. Variable temperature ESR spectra of **Nap-D** in benzophenone solid solution.

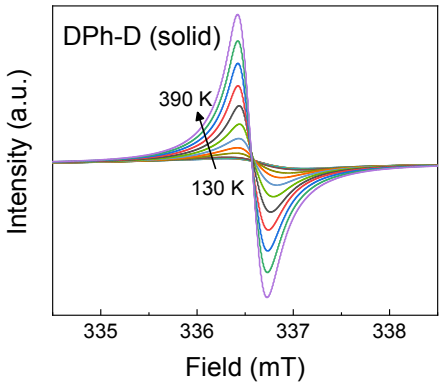



**Figure S14**. Variable temperature ESR spectra of **DPh-D** in solid state.

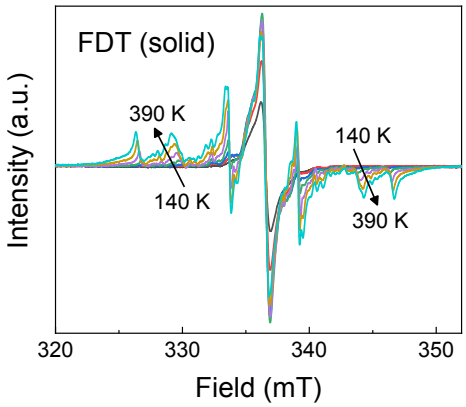



**Figure S15**. Variable temperature ESR spectra of **FDT** in solid state.

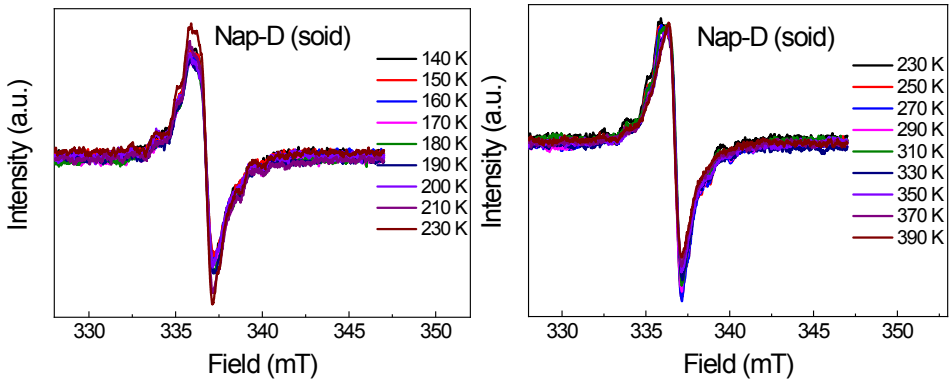



**Figure S16**. Variable temperature ESR spectra of **Nap-D** in solid state.

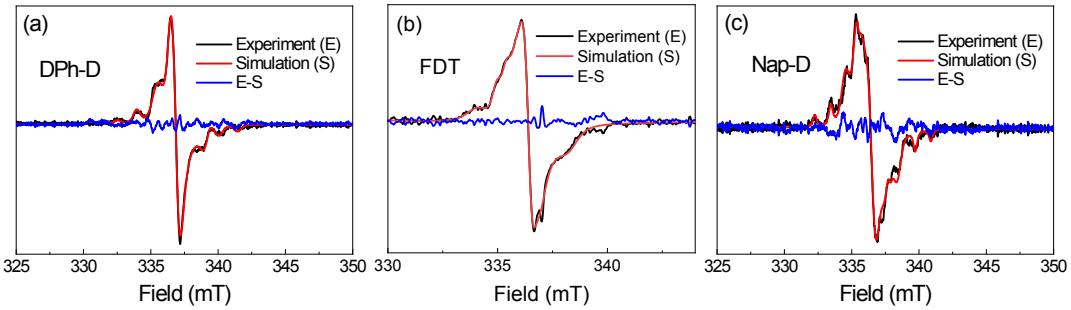



**Figure S17**. ESR spectra of **DPh-D** (a), **FDT** (b) and **Nap-D** (c) (in toluene/$CHCl_3$, v/v= 1:1) at 130 K. The black, red and blue lines indicate experimental, simulated and difference ESR (experimental - simulated) spectra, respectively.

## 9. Electronic devices

### Charge mobility and conductivity

Bottom-gate, bottom-contact OFETs were fabricated on $SiO_2$ (300 nm)/$Si^{++}$ substrates. The source/drain electrodes were defined by photolithography, followed by the evaporation of Cr/Au (2 nm/ 50 nm). The materials were dissolved in chlorobenzene with a concentration of about 1 mg/mL, and films or microcrystals were obtained when the solutions were drop-casted onto the substrates, which were cleaned by water, Acetone and IPA in sequence, and then treated by ozone for 10 minutes.

The electrical performance of the OFETs were measured at ambient conditions using a B2912A. Since there is gate modulation on the drain current, the mobility of

the thin film can be obtained using the conventional method, namely: $\mu_{saturation} = \frac{2L}{WC_i}\left(\frac{\partial\sqrt{I_{DS}}}{\partial V_G}\right)^2$. Here, $L$ and $W$ are the channel length and width of devices, respectively, and $C_i$ is the gate-dielectric capacitance per unit area. For the estimation of conductivity, we measured the $I_d$-$V_d$ cruve at $V_g$=0 V, which is related conductivity. Since the materials do not form continuous films but small aggregates or crystals, we employed optical microscopy and atomic force microscopy (AFM) to determine the actual device geometry. It should also be noted that since the **DPh-D** crystals are pretty thick, which it is hard to determine the real thickness of the crystals that contribute to current conduction. Therefore, we used both the thickness of electrodes and crystals for calculating conductivity, which should correspond to the upper ($5.21\times10^{-3}$ S/cm) and lower limit ($7.44\times10^{-5}$ S/cm) of the conductivity, respectively.

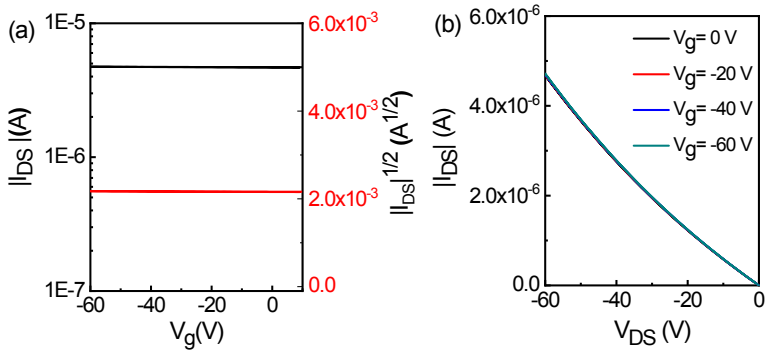



**Figure S18**. The typical transfer (a) and output characteristics (b) of **DPh-D** based devices, respectively.

**Photodiodes**

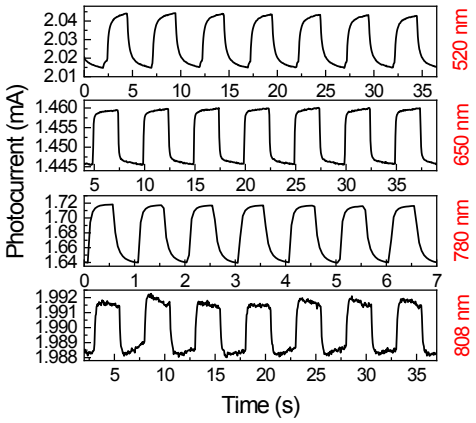



**Figure S19.** Transient photocurrent measurements of the photodiodes were fabricated from **DPh-D** upon alternative illumination with lasers at different illumination wavelength (520 nm at 6.28 mW, 650 nm at 20 mW, 780 nm at 30 mW, 808 nm at 110 mW).

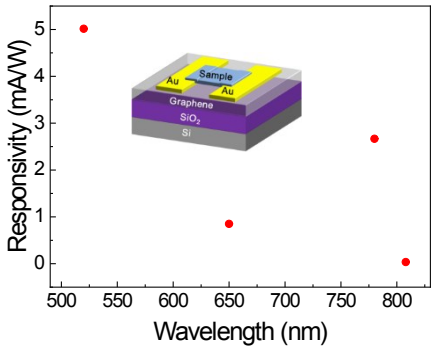



**Figure S20.** Responsivity of the photodiode fabricated from **DPh-D** at different illumination wavelength (520 nm at 6.28 mW, 650 nm at 20 mW, 780 nm at 30 mW, 808 nm at 110 mW). Inset shows the device structure of OPD was used in this study.

## 10. Computational details

All calculations were performed with the Gaussian 16 program suite[1] using the density functional theory (DFT) with the Becke's three-parameter hybrid exchange functionals[2] and the Lee-Yang-Parr correlation functional[3] (B3LYP) employing the 6-31G(d) basis set[4] for all atoms. Closed-shell singlet structures were optimized using restricted B3LYP and open-shell singlet and triplet were optimized using unrestricted UB3LYP

method. Optimized geometries were checked as minima by frequency calculations while finding no negative frequencies. The alkyl chains in **FDT** were replaced by methyl groups to reduce the computation cost. The diradical character $y_0$ is calculated by Yamaguchi's equation[5] based natural orbital analysis for the optimized open-shell singlet geometry:

$$y_0 = 1 - \left(2T/\left(1 + T^2\right)\right)$$

where T is represented by calculating the occupation numbers of natural orbitals:

$$T = (nHONO - nLUNO)/2$$

A molecule with $y_0 = 0$ implies a closed-shell structure, whereas a molecule with $y_0 = 1$ indicates a pure diradical structure. The $\Delta E_{ST}$ were calculated using zero-point vibrational energy correct singlet-triplet energy gaps. The spin densities were illustrated using Multiwfn[6] and VMD[7]. The NICS(1)zz value was calculated by standard gauge independent atomic orbital (GIAO) method[8] based on the optimized geometries at the UB3LYP/6-31(d) level. The AICD plots was calculated by using the method developed by Herges[9].

**Table S5.** Selected calculated relative energy (kcal/mol) of **DPh-D**, **FDT** and **Nap-D**.

| Compounds | States | $\Delta E$[a] |
|---|---|---|
| **DPh-D** | CS[b] | 8.091 |
| | OS[b] | 0 |
| | T | 0.948 |
| **FDT** | CS[b] | 4.220 |
| | OS[b] | 0 |
| | T | 2.566 |
| **Nap-D** | CS[b] | 2.576 |
| | OS[b] | 0 |
| | T | 3.746 |

[a] Energy relative to the OS state. [b] CS=closed-shell singlet, OS=open-shell singlet.

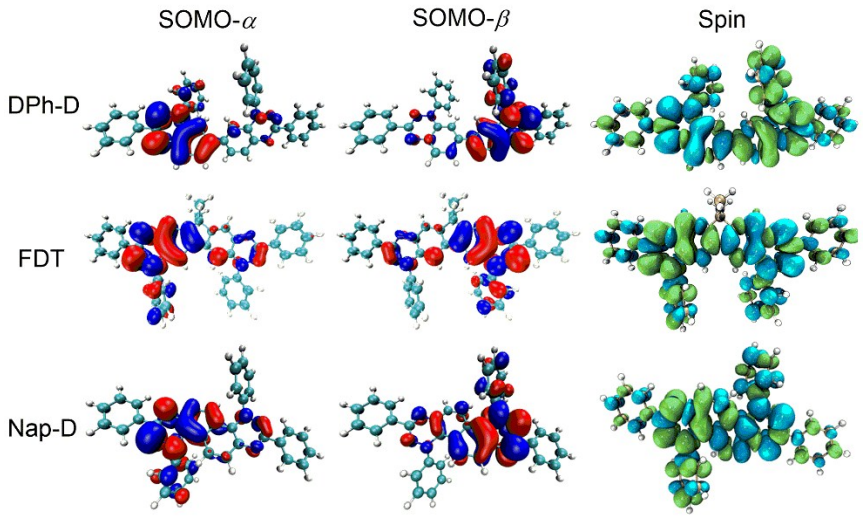



**Figure S21**. Frontier orbitals and spin density distribution of **DPh-D**, **FDT** and **Nap-D** calculated at the UB3LYP/6-31G(d) level.

## References


1. R. A. Gaussian 16, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT., 2016.
2. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
3. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B. Condens. Matter.*, 1988, **37**, 785-789.
4. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.
5. M. Nakano, R. Kishi, T. Nitta, T. Kubo, K. Nakasuji, K. Kamada, K. Ohta, B. Champagne, E. Botek and K. Yamaguchi, *J. Phys. Chem. A*, 2005, **109**, 885-891.
6. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.
7. W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graph.*, 1996, **14**, 33-38.
8. F. B. S. Hossein, C. S. Wannere, C. Clémence, P. Ralph and P. V. R. Schleyer, *Org. Lett.*, 2006, **8**, 863-866.
9. D. Geuenich, K. Hess, F. Kohler and R. Herges, *Chem. Rev.*, 2005, **105**, 3758-3772.


## Coordinates for calculated geometries

**Dph_CS**

| | | | |
|---|---|---|---|
| C | -2.84947300 | -0.72120700 | -0.23244500 |
| C | -3.59321400 | -1.94526700 | -0.01872900 |
| C | -2.83620000 | -3.14683700 | 0.11458000 |
| C | -1.46753300 | -3.13073300 | 0.09874500 |
| C | -0.71925500 | -1.91774500 | -0.03129800 |
| C | -1.46643700 | -0.71774000 | -0.19859900 |
| C | 0.71927900 | -1.91774300 | 0.03111900 |
| C | 1.46645300 | -0.71774300 | 0.19850600 |
| C | 2.84948800 | -0.72120500 | 0.23235900 |
| C | 3.59323900 | -1.94524800 | 0.01858800 |
| C | 2.83623300 | -3.14681200 | -0.11482400 |
| C | 1.46756600 | -3.13071600 | -0.09900600 |
| N | 3.64781400 | 0.40323900 | 0.45448700 |
| N | 5.00237800 | 0.38258900 | 0.27983000 |
| C | 5.56578300 | -0.77762100 | 0.02271200 |
| N | 4.91828400 | -1.97789400 | -0.07166500 |
| C | 3.13469500 | 1.68654200 | 0.81553700 |
| C | 7.03868800 | -0.78173500 | -0.16175700 |
| C | 7.69864100 | -1.98076200 | -0.46976600 |
| C | 9.08119800 | -1.99815900 | -0.64989800 |
| C | 9.82230700 | -0.82235700 | -0.52425300 |
| C | 9.17070700 | 0.37540800 | -0.21552400 |
| C | 7.79069600 | 0.39800200 | -0.03541100 |
| C | 2.22350300 | 1.82039000 | 1.87064500 |
| C | 1.76409000 | 3.08682200 | 2.22898700 |
| C | 2.21451700 | 4.22096800 | 1.55052500 |
| C | 3.13579000 | 4.08227500 | 0.50991600 |
| C | 3.59798400 | 2.82147000 | 0.13927600 |
| N | -3.64781200 | 0.40324300 | -0.45450800 |
| N | -5.00236700 | 0.38258700 | -0.27974700 |
| C | -5.56575700 | -0.77763900 | -0.02267600 |
| N | -4.91825500 | -1.97792100 | 0.07156700 |
| C | -3.13473100 | 1.68655300 | -0.81557200 |
| C | -7.03865100 | -0.78176600 | 0.16188500 |
| C | -7.69856900 | -1.98079800 | 0.46995500 |
| C | -9.08111500 | -1.99821000 | 0.65017500 |
| C | -9.82224600 | -0.82241900 | 0.52455600 |
| C | -9.17068200 | 0.37535000 | 0.21576700 |
| C | -7.79068300 | 0.39795800 | 0.03556500 |
| C | -2.22354800 | 1.82042200 | -1.87068700 |
| C | -1.76418100 | 3.08686400 | -2.22904600 |

| | | | |
|---|---|---|---|
| C | -2.21464100 | 4.22100400 | -1.55059700 |
| C | -3.13590800 | 4.08229200 | -0.50998300 |
| C | -3.59805800 | 2.82147600 | -0.13932700 |
| H | -3.39292200 | -4.06700000 | 0.25711800 |
| H | -0.94729900 | -4.07069800 | 0.24157200 |
| H | -0.94422000 | 0.21777500 | -0.34048600 |
| H | 0.94422900 | 0.21775900 | 0.34044900 |
| H | 3.39296300 | -4.06696200 | -0.25741800 |
| H | 0.94733900 | -4.07067300 | -0.24191100 |
| H | 7.11422600 | -2.88882000 | -0.56331600 |
| H | 9.57997500 | -2.93384400 | -0.88875400 |
| H | 10.90006100 | -0.83726500 | -0.66411600 |
| H | 9.74132600 | 1.29482100 | -0.11325300 |
| H | 7.28248000 | 1.32450600 | 0.20820800 |
| H | 1.89399400 | 0.94290900 | 2.41678400 |
| H | 1.06151900 | 3.18524500 | 3.05173100 |
| H | 1.85482300 | 5.20572100 | 1.83465800 |
| H | 3.49596900 | 4.95966100 | -0.02017300 |
| H | 4.31939700 | 2.70158100 | -0.66093700 |
| H | -7.11413500 | -2.88884500 | 0.56348300 |
| H | -9.57986500 | -2.93389700 | 0.88907700 |
| H | -10.89999100 | -0.83734000 | 0.66448600 |
| H | -9.74132000 | 1.29475200 | 0.11351600 |
| H | -7.28249500 | 1.32446400 | -0.20810300 |
| H | -1.89401300 | 0.94294800 | -2.41682000 |
| H | -1.06161800 | 3.18530100 | -3.05179600 |
| H | -1.85498200 | 5.20576600 | -1.83474400 |
| H | -3.49611500 | 4.95967200 | 0.02009600 |
| H | -4.31946500 | 2.70157300 | 0.66088900 |

**Dph_OS**

| | | | |
|---|---|---|---|
| C | 2.86084700 | -0.74126100 | 0.27630800 |
| C | 3.58110100 | -1.90732100 | -0.12567200 |
| C | 2.83738600 | -3.07181300 | -0.41619000 |
| C | 1.45785200 | -3.07415500 | -0.35015200 |
| C | 0.73758000 | -1.90445800 | -0.00831000 |
| C | 1.46398200 | -0.74236400 | 0.30143700 |
| C | -0.73756400 | -1.90446500 | 0.00818100 |
| C | -1.46397700 | -0.74236000 | -0.30150000 |
| C | -2.86084200 | -0.74127100 | -0.27637200 |
| C | -3.58108500 | -1.90735300 | 0.12556000 |
| C | -2.83736000 | -3.07185700 | 0.41600600 |

| | | | |
|---|---|---|---|
| C | -1.45782700 | -3.07418700 | 0.34996000 |
| N | -3.64971300 | 0.36435800 | -0.60967000 |
| N | -4.99644800 | 0.38642400 | -0.38887800 |
| C | -5.55893800 | -0.74796300 | 0.03079800 |
| N | -4.93485100 | -1.91612700 | 0.25638600 |
| C | -3.13075400 | 1.58363100 | -1.14604900 |
| C | -7.02903700 | -0.69661100 | 0.24945900 |
| C | -7.69849700 | -1.82818400 | 0.73893700 |
| C | -9.07521600 | -1.79479100 | 0.95258300 |
| C | -9.80146500 | -0.63358300 | 0.68081900 |
| C | -9.14093700 | 0.49636100 | 0.19171700 |
| C | -7.76517700 | 0.46736100 | -0.02352800 |
| C | -2.27847400 | 1.56790700 | -2.25642600 |
| C | -1.80800500 | 2.77128700 | -2.78107900 |
| C | -2.19300300 | 3.98749200 | -2.21415600 |
| C | -3.05903800 | 3.99629800 | -1.11811700 |
| C | -3.53023600 | 2.80018100 | -0.58146100 |
| N | 3.64970800 | 0.36435800 | 0.60965800 |
| N | 4.99645400 | 0.38642800 | 0.38893700 |
| C | 5.55895500 | -0.74793800 | -0.03078300 |
| N | 4.93487000 | -1.91608300 | -0.25647300 |
| C | 3.13072000 | 1.58363100 | 1.14601700 |
| C | 7.02906600 | -0.69658600 | -0.24936000 |
| C | 7.69855300 | -1.82815500 | -0.73881300 |
| C | 9.07528400 | -1.79476200 | -0.95237900 |
| C | 9.80151900 | -0.63355700 | -0.68056200 |
| C | 9.14096400 | 0.49638200 | -0.19148600 |
| C | 7.76519200 | 0.46738200 | 0.02368100 |
| C | 2.27847000 | 1.56790600 | 2.25641500 |
| C | 1.80797100 | 2.77128400 | 2.78104700 |
| C | 2.19291400 | 3.98748600 | 2.21407800 |
| C | 3.05892100 | 3.99629300 | 1.11801700 |
| C | 3.53014700 | 2.80017600 | 0.58138300 |
| H | 3.39204700 | -3.95457900 | -0.71736500 |
| H | 0.91649900 | -3.97721100 | -0.61352000 |
| H | 0.93389400 | 0.15574700 | 0.59093200 |
| H | -0.93389600 | 0.15577200 | -0.59094700 |
| H | -3.39201300 | -3.95464300 | 0.71714000 |
| H | -0.91646600 | -3.97725400 | 0.61327400 |
| H | -7.12385500 | -2.72394300 | 0.94528000 |
| H | -9.58204800 | -2.67799300 | 1.33257800 |
| H | -10.87526500 | -0.60881400 | 0.84750100 |
| H | -9.70014000 | 1.40284400 | -0.02495200 |
| H | -7.24944700 | 1.34033600 | -0.40758200 |

| | | | |
|---|---|---|---|
| H | -2.00366300 | 0.62400500 | -2.71538800 |
| H | -1.15014800 | 2.75486500 | -3.64542000 |
| H | -1.82650500 | 4.92247600 | -2.62812900 |
| H | -3.36826500 | 4.93888400 | -0.67507500 |
| H | -4.20940000 | 2.79242900 | 0.26349900 |
| H | 7.12392100 | -2.72391000 | -0.94519900 |
| H | 9.58213700 | -2.67796000 | -1.33235400 |
| H | 10.87532800 | -0.60878800 | -0.84718200 |
| H | 9.70015600 | 1.40286300 | 0.02522300 |
| H | 7.24944100 | 1.34035400 | 0.40771300 |
| H | 2.00370200 | 0.62400400 | 2.71540600 |
| H | 1.15013400 | 2.75486600 | 3.64540400 |
| H | 1.82639300 | 4.92246900 | 2.62803400 |
| H | 3.36810300 | 4.93887800 | 0.67494200 |
| H | 4.20929100 | 2.79242300 | -0.26359300 |

**Dph_T**

| | | | |
|---|---|---|---|
| C | -2.86554700 | -0.74135800 | -0.29160300 |
| C | -3.57699200 | -1.88713100 | 0.16929600 |
| C | -2.83193200 | -3.03419600 | 0.50875100 |
| C | -1.45052700 | -3.03917200 | 0.43139100 |
| C | -0.74048900 | -1.88761100 | 0.02387900 |
| C | -1.46630200 | -0.74247800 | -0.33257000 |
| C | 0.74030900 | -1.88768100 | -0.02266800 |
| C | 1.46620900 | -0.74237200 | 0.33301800 |
| C | 2.86545600 | -0.74139800 | 0.29211300 |
| C | 3.57680700 | -1.88747200 | -0.16817400 |
| C | 2.83166600 | -3.03473000 | -0.50682300 |
| C | 1.45027000 | -3.03957200 | -0.42940200 |
| N | 3.65559600 | 0.35110600 | 0.66189700 |
| N | 4.99851400 | 0.38717000 | 0.42248500 |
| C | 5.55729600 | -0.73354900 | -0.04990100 |
| N | 4.93566600 | -1.88941700 | -0.31276900 |
| C | 3.14072400 | 1.54435100 | 1.25772000 |
| C | 7.02499500 | -0.66723000 | -0.28289400 |
| C | 7.69214900 | -1.77468500 | -0.82766500 |
| C | 9.06608600 | -1.72763800 | -1.05505300 |
| C | 9.79195000 | -0.57632600 | -0.74234100 |
| C | 9.13385200 | 0.52949400 | -0.19838400 |
| C | 7.76055900 | 0.48657500 | 0.03106200 |
| C | 2.30343900 | 1.47742800 | 2.37754900 |
| C | 1.83657800 | 2.65539300 | 2.96000500 |

| | | | |
|---|---|---|---|
| C | 2.21070100 | 3.89625100 | 2.44132000 |
| C | 3.06224000 | 3.95551300 | 1.33546300 |
| C | 3.52981800 | 2.78544600 | 0.74138700 |
| N | -3.65559400 | 0.35097300 | -0.66203400 |
| N | -4.99862200 | 0.38709600 | -0.42326700 |
| C | -5.55750100 | -0.73333900 | 0.04969500 |
| N | -4.93588200 | -1.88895300 | 0.31368000 |
| C | -3.14041000 | 1.54422300 | -1.25765400 |
| C | -7.02529800 | -0.66696900 | 0.28203800 |
| C | -7.69283000 | -1.77458900 | 0.82600400 |
| C | -9.06686300 | -1.72747500 | 1.05280000 |
| C | -9.79244000 | -0.57592000 | 0.74031100 |
| C | -9.13396300 | 0.53007000 | 0.19716500 |
| C | -7.76057200 | 0.48707700 | -0.03170100 |
| C | -2.30353800 | 1.47726100 | -2.37777300 |
| C | -1.83632700 | 2.65520500 | -2.96000000 |
| C | -2.20972700 | 3.89605400 | -2.44077200 |
| C | -3.06086600 | 3.95535600 | -1.33461000 |
| C | -3.52876900 | 2.78529600 | -0.74076100 |
| H | -3.38310800 | -3.90198500 | 0.85649300 |
| H | -0.90103700 | -3.92710900 | 0.72844900 |
| H | -0.93689200 | 0.14107700 | -0.66600100 |
| H | 0.93686300 | 0.14145300 | 0.66583800 |
| H | 3.38277500 | -3.90277200 | -0.85404100 |
| H | 0.90071500 | -3.92768000 | -0.72582700 |
| H | 7.11741600 | -2.66257700 | -1.06550300 |
| H | 9.57125500 | -2.59210000 | -1.47792900 |
| H | 10.86370900 | -0.54085600 | -0.91992700 |
| H | 9.69281400 | 1.42787300 | 0.05028200 |
| H | 7.24668400 | 1.34051200 | 0.45787300 |
| H | 2.03786600 | 0.51359600 | 2.79900600 |
| H | 1.19037700 | 2.59934500 | 3.83143700 |
| H | 1.84721700 | 4.81118900 | 2.90028900 |
| H | 3.36290100 | 4.91746700 | 0.92975900 |
| H | 4.19784900 | 2.81636000 | -0.11184500 |
| H | -7.11831800 | -2.66266200 | 1.06370600 |
| H | -9.57233500 | -2.59207100 | 1.47504100 |
| H | -10.86427200 | -0.54039600 | 0.91744400 |
| H | -9.69270000 | 1.42864200 | -0.05131100 |
| H | -7.24639700 | 1.34115000 | -0.45787900 |
| H | -2.03852800 | 0.51342100 | -2.79957400 |
| H | -1.19042900 | 2.59916700 | -3.83165700 |
| H | -1.84598400 | 4.81098000 | -2.89956200 |
| H | -3.36095200 | 4.91731800 | -0.92849900 |

| | | | |
|---|---|---|---|
| H | -4.19651200 | 2.81622600 | 0.11270300 |

**FDT_CS**

| | | | |
|---|---|---|---|
| C | 3.47086200 | -1.45257600 | 0.11059700 |
| C | 2.98208600 | -0.08010600 | 0.15461300 |
| C | 1.62613800 | 0.19563100 | 0.08350000 |
| C | 0.70905900 | -0.87712800 | 0.03448900 |
| C | 1.17490100 | -2.23104100 | 0.05028300 |
| C | 2.51180000 | -2.51416900 | 0.08694200 |
| C | -0.70908300 | -0.87712600 | -0.03431100 |
| C | -1.17493200 | -2.23103700 | -0.05005900 |
| C | -0.00002100 | -3.20390800 | 0.00019000 |
| C | -1.62615600 | 0.19563800 | -0.08339400 |
| C | -2.98209800 | -0.08010100 | -0.15457900 |
| C | -3.47088600 | -1.45256300 | -0.11054000 |
| C | -2.51183000 | -2.51416100 | -0.08678400 |
| C | -0.05276500 | -4.09041900 | 1.26479300 |
| N | -3.98615700 | 0.88210600 | -0.24992400 |
| N | -5.31332500 | 0.57994700 | -0.12270500 |
| C | -5.63767200 | -0.69052400 | -0.03798000 |
| N | -4.76620200 | -1.74319200 | -0.06979200 |
| N | 4.76617400 | -1.74321600 | 0.06979600 |
| C | 5.63764500 | -0.69055300 | 0.03785000 |
| N | 5.31330700 | 0.57992300 | 0.12253200 |
| N | 3.98615500 | 0.88209500 | 0.24985400 |
| C | -3.72950100 | 2.27927600 | -0.40772800 |
| C | -7.08266400 | -1.00698400 | 0.09037300 |
| C | 3.72954000 | 2.27927100 | 0.40773500 |
| C | 7.08262500 | -1.00702500 | -0.09059000 |
| C | 0.05271300 | -4.09070600 | -1.26419800 |
| C | -7.49534300 | -2.34141400 | 0.22010200 |
| C | -8.84901000 | -2.65176000 | 0.34521800 |
| C | -9.80712400 | -1.63712900 | 0.34156400 |
| C | -9.40237300 | -0.30535300 | 0.21069300 |
| C | -8.05227500 | 0.00941000 | 0.08596600 |
| C | -4.39497400 | 3.19286400 | 0.41783400 |
| C | -4.18175300 | 4.55918700 | 0.24786300 |
| C | -3.30956400 | 5.02192300 | -0.74002400 |
| C | -2.65699000 | 4.10659000 | -1.56835600 |
| C | -2.86658300 | 2.73734000 | -1.41071600 |
| C | 2.86665200 | 2.73732000 | 1.41075700 |
| C | 2.65711700 | 4.10657000 | 1.56846600 |

| | | | |
|---|---|---|---|
| C | 3.30971500 | 5.02191900 | 0.74017200 |
| C | 4.18187600 | 4.55919700 | -0.24774700 |
| C | 4.39504300 | 3.19287400 | -0.41778600 |
| C | 8.05224800 | 0.00935800 | -0.08624700 |
| C | 9.40233400 | -0.30541900 | -0.21105400 |
| C | 9.80706400 | -1.63720100 | -0.34193900 |
| C | 8.84893900 | -2.65182100 | -0.34553200 |
| C | 7.49528200 | -2.34146100 | -0.22033900 |
| H | 1.27054900 | 1.21850000 | 0.06931800 |
| H | 2.90328000 | -3.52657500 | 0.07469800 |
| H | -1.27056600 | 1.21850600 | -0.06922500 |
| H | -2.90331500 | -3.52656400 | -0.07453000 |
| H | 0.83307800 | -4.73277700 | 1.32080400 |
| H | -0.93852900 | -4.73506900 | 1.24599600 |
| H | -0.09203100 | -3.48113500 | 2.17329200 |
| H | 0.09186200 | -3.48163900 | -2.17284900 |
| H | 0.93853200 | -4.73527600 | -1.24530900 |
| H | -0.83307600 | -4.73315800 | -1.31999300 |
| H | -6.74332900 | -3.12201300 | 0.22020400 |
| H | -9.15502300 | -3.68988100 | 0.44556800 |
| H | -10.86206000 | -1.88022600 | 0.43845700 |
| H | -10.14272800 | 0.49042700 | 0.20422100 |
| H | -7.73492300 | 1.04100300 | -0.01978000 |
| H | -5.07602700 | 2.82153000 | 1.17514100 |
| H | -4.69803200 | 5.26432200 | 0.89341500 |
| H | -3.14464300 | 6.08794300 | -0.86790200 |
| H | -1.99105500 | 4.45691600 | -2.35203000 |
| H | -2.37936900 | 2.02785900 | -2.07113000 |
| H | 2.37942200 | 2.02783100 | 2.07114800 |
| H | 1.99120600 | 4.45688300 | 2.35216700 |
| H | 3.14483600 | 6.08794000 | 0.86810400 |
| H | 4.69817500 | 5.26434200 | -0.89327100 |
| H | 5.07607300 | 2.82155300 | -1.17511900 |
| H | 7.73491300 | 1.04095500 | 0.01951300 |
| H | 10.14269700 | 0.49035400 | -0.20463400 |
| H | 10.86199200 | -1.88030900 | -0.43889000 |
| H | 9.15493400 | -3.68994600 | -0.44589200 |
| H | 6.74326000 | -3.12205100 | -0.22039900 |

**FDT_OS**

| | | | |
|---|---|---|---|
| C | -3.47163200 | 1.45555600 | 0.11924300 |
| C | -2.99458400 | 0.09885800 | 0.15359700 |

| | | | |
|---|---|---|---|
| C | -1.62830600 | -0.18165100 | 0.08097300 |
| C | -0.72314400 | 0.88399200 | 0.03490900 |
| C | -1.17737700 | 2.23053800 | 0.05063900 |
| C | -2.52380700 | 2.51106900 | 0.08720500 |
| C | 0.72315400 | 0.88399200 | -0.03490900 |
| C | 1.17738800 | 2.23053800 | -0.05061900 |
| C | 0.00000600 | 3.20232400 | 0.00001800 |
| C | 1.62831500 | -0.18165100 | -0.08098900 |
| C | 2.99459200 | 0.09886000 | -0.15360800 |
| C | 3.47164200 | 1.45555600 | -0.11923700 |
| C | 2.52381800 | 2.51106900 | -0.08718200 |
| C | 0.05321500 | 4.08935400 | 1.26433800 |
| N | 3.99087400 | -0.87735600 | -0.23297600 |
| N | 5.31786000 | -0.58063300 | -0.10477800 |
| C | 5.64296700 | 0.70608900 | -0.04190200 |
| N | 4.79193500 | 1.75081700 | -0.08966100 |
| N | -4.79192400 | 1.75082000 | 0.08966600 |
| C | -5.64295700 | 0.70609500 | 0.04187900 |
| N | -5.31785300 | -0.58062900 | 0.10474700 |
| N | -3.99086900 | -0.87735600 | 0.23294900 |
| C | 3.72394900 | -2.27373700 | -0.38214200 |
| C | 7.09429300 | 1.00570500 | 0.07983400 |
| C | -3.72395400 | -2.27374200 | 0.38210100 |
| C | -7.09428500 | 1.00571600 | -0.07981900 |
| C | -0.05320300 | 4.08937100 | -1.26429000 |
| C | 7.52225900 | 2.33620000 | 0.20078000 |
| C | 8.87915200 | 2.63218900 | 0.31878100 |
| C | 9.82595700 | 1.60615700 | 0.31743000 |
| C | 9.40632700 | 0.27879400 | 0.19578300 |
| C | 8.05163000 | -0.02148500 | 0.07736500 |
| C | 4.37044600 | -3.18497600 | 0.46053100 |
| C | 4.14573100 | -4.55065800 | 0.30092800 |
| C | 3.28130800 | -5.01412300 | -0.69367000 |
| C | 2.64852100 | -4.10110500 | -1.53936600 |
| C | 2.87061100 | -2.73227200 | -1.39272300 |
| C | -2.87064600 | -2.73229900 | 1.39269600 |
| C | -2.64857100 | -4.10113600 | 1.53932600 |
| C | -3.28134600 | -5.01413600 | 0.69360100 |
| C | -4.14574400 | -4.55064900 | -0.30100800 |
| C | -4.37044300 | -3.18496300 | -0.46059600 |
| C | -8.05162400 | -0.02147200 | -0.07734700 |
| C | -9.40632300 | 0.27881200 | -0.19573200 |
| C | -9.82595300 | 1.60617900 | -0.31735000 |
| C | -8.87914500 | 2.63220800 | -0.31870200 |

| | | | |
|---|---|---|---|
| C | -7.52225100 | 2.33621400 | -0.20073300 |
| H | -1.27686600 | -1.20613000 | 0.05731300 |
| H | -2.91460300 | 3.52404600 | 0.07380500 |
| H | 1.27687500 | -1.20613100 | -0.05734800 |
| H | 2.91461400 | 3.52404500 | -0.07376800 |
| H | -0.83221600 | 4.73252400 | 1.32063400 |
| H | 0.93917600 | 4.73401500 | 1.24573000 |
| H | 0.09224800 | 3.48039100 | 2.17309400 |
| H | -0.09224000 | 3.48042100 | -2.17305500 |
| H | -0.93916200 | 4.73403600 | -1.24567300 |
| H | 0.83223000 | 4.73253900 | -1.32057900 |
| H | 6.77790200 | 3.12425900 | 0.19970100 |
| H | 9.19753400 | 3.66721300 | 0.41230000 |
| H | 10.88388700 | 1.83815000 | 0.40917000 |
| H | 10.13773200 | -0.52522000 | 0.19102100 |
| H | 7.72217300 | -1.04972300 | -0.02202400 |
| H | 5.04548600 | -2.81215100 | 1.22248100 |
| H | 4.64688800 | -5.25476900 | 0.95933000 |
| H | 3.10790500 | -6.07972300 | -0.81364800 |
| H | 1.98954400 | -4.45270900 | -2.32828800 |
| H | 2.40175800 | -2.02419300 | -2.06794000 |
| H | -2.40180500 | -2.02423500 | 2.06793800 |
| H | -1.98961700 | -4.45275800 | 2.32825900 |
| H | -3.10795600 | -6.07974000 | 0.81356800 |
| H | -4.64689300 | -5.25474600 | -0.95943200 |
| H | -5.04546400 | -2.81212200 | -1.22255500 |
| H | -7.72216700 | -1.04971200 | 0.02201800 |
| H | -10.13773000 | -0.52520100 | -0.19096900 |
| H | -10.88388300 | 1.83817500 | -0.40906300 |
| H | -9.19752700 | 3.66723500 | -0.41219800 |
| H | -6.77789200 | 3.12427200 | -0.19965700 |

**FDT_T**

| | | | |
|---|---|---|---|
| C | 3.47246000 | -1.45938600 | 0.12614500 |
| C | 3.00041800 | -0.10990500 | 0.15737300 |
| C | 1.62897400 | 0.17269400 | 0.08241200 |
| C | 0.72978900 | -0.89036800 | 0.03610900 |
| C | 1.17943300 | -2.23400800 | 0.05208100 |
| C | 2.53041800 | -2.51261800 | 0.08983500 |
| C | -0.72984900 | -0.89036700 | -0.03600100 |
| C | -1.17949900 | -2.23400600 | -0.05202900 |
| C | -0.00002200 | -3.20418000 | 0.00006000 |

| | | | |
|---|---|---|---|
| C | -1.62902100 | 0.17270500 | -0.08230600 |
| C | -3.00046200 | -0.10988800 | -0.15733500 |
| C | -3.47251200 | -1.45936500 | -0.12617800 |
| C | -2.53048300 | -2.51260500 | -0.08985200 |
| C | -0.05458600 | -4.09102100 | 1.26449100 |
| N | -3.99130600 | 0.87370200 | -0.22968900 |
| N | -5.31794800 | 0.58237400 | -0.09629200 |
| C | -5.64525000 | -0.71390300 | -0.04179400 |
| N | -4.80682800 | -1.75479500 | -0.10005200 |
| N | 4.80676300 | -1.75483000 | 0.09993500 |
| C | 5.64519100 | -0.71394200 | 0.04166600 |
| N | 5.31790700 | 0.58233100 | 0.09625200 |
| N | 3.99129100 | 0.87366400 | 0.22978500 |
| C | -3.71809900 | 2.26817000 | -0.38249100 |
| C | -7.09978800 | -1.00141000 | 0.08114800 |
| C | 3.71815300 | 2.26815600 | 0.38248900 |
| C | 7.09973400 | -1.00147300 | -0.08119200 |
| C | 0.05448900 | -4.09121000 | -1.26421000 |
| C | -7.53789300 | -2.32889800 | 0.19982300 |
| C | -8.89651700 | -2.61464800 | 0.31871400 |
| C | -9.83538200 | -1.58083800 | 0.32099100 |
| C | -9.40588600 | -0.25678000 | 0.20192200 |
| C | -8.04865700 | 0.03323300 | 0.08216000 |
| C | -4.36074100 | 3.18402700 | 0.45838400 |
| C | -4.12913200 | 4.54810700 | 0.29636000 |
| C | -3.26254100 | 5.00564800 | -0.69932300 |
| C | -2.63463800 | 4.08827300 | -1.54378500 |
| C | -2.86349800 | 2.72070700 | -1.39488200 |
| C | 2.86383600 | 2.72084200 | 1.39505900 |
| C | 2.63506800 | 4.08843100 | 1.54386900 |
| C | 3.26279300 | 5.00568600 | 0.69913900 |
| C | 4.12912500 | 4.54800200 | -0.29670100 |
| C | 4.36064200 | 3.18389200 | -0.45862800 |
| C | 8.04865100 | 0.03312600 | -0.08170000 |
| C | 9.40587800 | -0.25691400 | -0.20141600 |
| C | 9.83531900 | -1.58095000 | -0.32093900 |
| C | 8.89640300 | -2.61471300 | -0.31916300 |
| C | 7.53777900 | -2.32893800 | -0.20031400 |
| H | 1.27917800 | 1.19776000 | 0.05409100 |
| H | 2.92136800 | -3.52568700 | 0.07585700 |
| H | -1.27922200 | 1.19777300 | -0.05395200 |
| H | -2.92145700 | -3.52566500 | -0.07594300 |
| H | 0.83072000 | -4.73439800 | 1.32195500 |
| H | -0.94071200 | -4.73558200 | 1.24534000 |

| | | | |
|---|---|---|---|
| H | -0.09438200 | -3.48185300 | 2.17308200 |
| H | 0.09449800 | -3.48221600 | -2.17291100 |
| H | 0.94046500 | -4.73597300 | -1.24489000 |
| H | -0.83094300 | -4.73441600 | -1.32167300 |
| H | -6.79900900 | -3.12217200 | 0.19632600 |
| H | -9.22306700 | -3.64728000 | 0.41040700 |
| H | -10.89495300 | -1.80490600 | 0.41369100 |
| H | -10.13104600 | 0.55287300 | 0.19995100 |
| H | -7.71129000 | 1.05891800 | -0.01580100 |
| H | -5.03731200 | 2.81542600 | 1.22096200 |
| H | -4.62665100 | 5.25588000 | 0.95357300 |
| H | -3.08426900 | 6.07020200 | -0.82135500 |
| H | -1.97474300 | 4.43533600 | -2.33393100 |
| H | -2.40032300 | 2.00937500 | -2.07061700 |
| H | 2.40082300 | 2.00960000 | 2.07099700 |
| H | 1.97539700 | 4.43561800 | 2.33414700 |
| H | 3.08460000 | 6.07026000 | 0.82110100 |
| H | 4.62651500 | 5.25568200 | -0.95411100 |
| H | 5.03702200 | 2.81517700 | -1.22132200 |
| H | 7.71131900 | 1.05878900 | 0.01660800 |
| H | 10.13108200 | 0.55270100 | -0.19906100 |
| H | 10.89488900 | -1.80503600 | -0.41360700 |
| H | 9.22291100 | -3.64732700 | -0.41121000 |
| H | 6.79885100 | -3.12217500 | -0.19720400 |

**Nap_CS**

| | | | |
|---|---|---|---|
| C | -1.26730600 | 1.92152600 | -1.10372700 |
| C | -2.27949200 | 1.02537100 | -0.63258100 |
| C | -1.84893500 | -0.26234900 | -0.12770000 |
| C | -0.50063900 | -0.49424100 | 0.19811800 |
| C | 0.50070500 | 0.49408700 | -0.19821300 |
| C | 0.05467200 | 1.65767900 | -0.90252700 |
| N | -3.55564400 | 1.37918300 | -0.68558200 |
| C | -4.46122000 | 0.47401500 | -0.20016200 |
| N | -4.20057400 | -0.77690000 | 0.09578000 |
| N | -2.88989600 | -1.18273100 | -0.02119200 |
| C | -0.05457200 | -1.65779900 | 0.90247000 |
| C | 1.26741600 | -1.92162800 | 1.10370100 |
| C | 2.27956800 | -1.02545700 | 0.63256300 |
| C | 1.84898000 | 0.26220100 | 0.12762800 |
| N | 3.55577400 | -1.37916100 | 0.68560100 |
| C | 4.46125600 | -0.47397600 | 0.20018500 |

| | | | |
|---|---|---|---|
| N | 4.20055800 | 0.77688300 | -0.09576000 |
| N | 2.88993300 | 1.18261500 | 0.02112700 |
| C | 5.86342600 | -0.93254000 | 0.03828500 |
| C | 2.75732600 | 2.60212400 | 0.14149800 |
| C | -2.75740900 | -2.60224400 | -0.14138300 |
| C | -5.86332500 | 0.93268300 | -0.03840200 |
| C | 6.85803500 | -0.06886500 | -0.44910700 |
| C | 8.16739500 | -0.51677500 | -0.59744400 |
| C | 8.50451300 | -1.83217500 | -0.26452900 |
| C | 7.52084900 | -2.69544400 | 0.21985600 |
| C | 6.20803900 | -2.25075900 | 0.37179300 |
| C | 3.48775400 | 3.43774900 | -0.71024800 |
| C | 3.39620200 | 4.82145500 | -0.56252500 |
| C | 2.58495000 | 5.37604700 | 0.42880900 |
| C | 1.86836600 | 4.53420000 | 1.28386000 |
| C | 1.95467500 | 3.15084100 | 1.14966900 |
| C | -1.95461000 | -3.15116400 | -1.14933200 |
| C | -1.86841200 | -4.53454400 | -1.28337400 |
| C | -2.58526600 | -5.37623900 | -0.42840100 |
| C | -3.39667500 | -4.82145400 | 0.56270000 |
| C | -3.48812000 | -3.43772800 | 0.71027300 |
| C | -6.85813200 | 0.06901700 | 0.44864000 |
| C | -8.16745500 | 0.51704400 | 0.59688200 |
| C | -8.50437300 | 1.83256600 | 0.26421500 |
| C | -7.52053900 | 2.69582000 | -0.21983100 |
| C | -6.20775400 | 2.25100700 | -0.37166900 |
| H | -1.59963000 | 2.81879100 | -1.61482100 |
| H | 0.78765100 | 2.35324700 | -1.29103700 |
| H | -0.78752700 | -2.35336400 | 1.29102100 |
| H | 1.59972200 | -2.81888300 | 1.61482000 |
| H | 6.59249500 | 0.95088600 | -0.70536700 |
| H | 8.92846700 | 0.16149100 | -0.97430400 |
| H | 9.52759600 | -2.17972800 | -0.38217500 |
| H | 7.77507600 | -3.71917300 | 0.48181800 |
| H | 5.43687400 | -2.91168600 | 0.75043300 |
| H | 4.12316400 | 2.99596800 | -1.46919700 |
| H | 3.96223100 | 5.46676000 | -1.22863200 |
| H | 2.51528200 | 6.45429800 | 0.53929100 |
| H | 1.24732500 | 4.95484100 | 2.06978400 |
| H | 1.40561500 | 2.49731000 | 1.81943800 |
| H | -1.40534100 | -2.49777200 | -1.81906500 |
| H | -1.24724000 | -4.95530900 | -2.06912700 |
| H | -2.51569200 | -6.45450900 | -0.53875100 |
| H | -3.96291700 | -5.46663600 | 1.22874600 |

| | | | |
|---|---|---|---|
| H | -4.12363600 | -2.99582000 | 1.46905400 |
| H | -6.59275300 | -0.95082500 | 0.70469500 |
| H | -8.92866800 | -0.16121200 | 0.97347000 |
| H | -9.52743600 | 2.18020300 | 0.38179300 |
| H | -7.77459000 | 3.71963900 | -0.48160900 |
| H | -5.43647000 | 2.91194700 | -0.75004700 |

**Nap_OS**

| | | | |
|---|---|---|---|
| C | 1.27505700 | -1.93169800 | -1.06432100 |
| C | 2.27937200 | -1.02284500 | -0.62103300 |
| C | 1.85856400 | 0.24896700 | -0.12521500 |
| C | 0.49384800 | 0.49408700 | 0.19207700 |
| C | -0.49386000 | -0.49407300 | -0.19206700 |
| C | -0.05201000 | -1.66642300 | -0.87875100 |
| N | 3.57453700 | -1.38149600 | -0.69333000 |
| C | 4.46557800 | -0.49365000 | -0.19148200 |
| N | 4.20530000 | 0.75947100 | 0.14150700 |
| N | 2.89920900 | 1.17165600 | 0.02223500 |
| C | 0.05199600 | 1.66642900 | 0.87877400 |
| C | -1.27507200 | 1.93170000 | 1.06435100 |
| C | -2.27938600 | 1.02285000 | 0.62105600 |
| C | -1.85857500 | -0.24895500 | 0.12522400 |
| N | -3.57455200 | 1.38149300 | 0.69336400 |
| C | -4.46559100 | 0.49364800 | 0.19151000 |
| N | -4.20530900 | -0.75946700 | -0.14149600 |
| N | -2.89921500 | -1.17164700 | -0.02223700 |
| C | -5.87331300 | 0.94328800 | 0.03713100 |
| C | -2.77608000 | -2.58960700 | 0.12239300 |
| C | 2.77609100 | 2.58961400 | -0.12243000 |
| C | 5.87329700 | -0.94329400 | -0.03709300 |
| C | -6.86552100 | 0.07331900 | -0.44257100 |
| C | -8.17840100 | 0.51441600 | -0.58518700 |
| C | -8.52041000 | 1.82787800 | -0.25161800 |
| C | -7.53868400 | 2.69732700 | 0.22692400 |
| C | -6.22296300 | 2.26006600 | 0.37097300 |
| C | -3.50241000 | -3.43213900 | -0.72628600 |
| C | -3.41870400 | -4.81374200 | -0.56005500 |
| C | -2.61970200 | -5.35894800 | 0.44709000 |
| C | -1.90766900 | -4.51037700 | 1.29829500 |
| C | -1.98625100 | -3.12785400 | 1.14548300 |
| C | 1.98630100 | 3.12784600 | -1.14555800 |
| C | 1.90774100 | 4.51036600 | -1.29840700 |

| | | | |
|---|---|---|---|
| C | 2.61975900 | 5.35895000 | -0.44720100 |
| C | 3.41872500 | 4.81375800 | 0.55998100 |
| C | 3.50240800 | 3.43215700 | 0.72624800 |
| C | 6.86550700 | -0.07332400 | 0.44260300 |
| C | 8.17838500 | -0.51442500 | 0.58522900 |
| C | 8.52038900 | -1.82789300 | 0.25167600 |
| C | 7.53866100 | -2.69734300 | -0.22686000 |
| C | 6.22294300 | -2.26007800 | -0.37091900 |
| H | 1.61074000 | -2.84167800 | -1.55051800 |
| H | -0.78208800 | -2.36960600 | -1.25673700 |
| H | 0.78207100 | 2.36960900 | 1.25677000 |
| H | -1.61075400 | 2.84167300 | 1.55056100 |
| H | -6.59633900 | -0.94591500 | -0.69651500 |
| H | -8.93806100 | -0.16848200 | -0.95646100 |
| H | -9.54601500 | 2.16988000 | -0.36367500 |
| H | -7.79725400 | 3.71989600 | 0.48913800 |
| H | -5.45211600 | 2.92520700 | 0.74309200 |
| H | -4.12668900 | -2.99652200 | -1.49792300 |
| H | -3.98045000 | -5.46539600 | -1.22353000 |
| H | -2.55633100 | -6.43605500 | 0.57185000 |
| H | -1.29601500 | -4.92389900 | 2.09522600 |
| H | -1.44341600 | -2.46788900 | 1.81389700 |
| H | 1.44347800 | 2.46787200 | -1.81397300 |
| H | 1.29611800 | 4.92387600 | -2.09536700 |
| H | 2.55640600 | 6.43605300 | -0.57198900 |
| H | 3.98046000 | 5.46542100 | 1.22345600 |
| H | 4.12666000 | 2.99655200 | 1.49791300 |
| H | 6.59632900 | 0.94591400 | 0.69653400 |
| H | 8.93804600 | 0.16847300 | 0.95649800 |
| H | 9.54599200 | -2.16989900 | 0.36374100 |
| H | 7.79722700 | -3.71991600 | -0.48906200 |
| H | 5.45209400 | -2.92522000 | -0.74303300 |

**Nap_T**

| | | | |
|---|---|---|---|
| C | -1.27614100 | 1.92762400 | -1.06453900 |
| C | -2.27528200 | 1.00918700 | -0.64244100 |
| C | -1.86282600 | -0.24475400 | -0.14137700 |
| C | -0.48752900 | -0.49502900 | 0.18450300 |
| C | 0.48759700 | 0.49508800 | -0.18415700 |
| C | 0.05290600 | 1.66924000 | -0.87273700 |
| N | -3.58830200 | 1.36969200 | -0.73274600 |
| C | -4.46239200 | 0.50797100 | -0.19465300 |

| | | | |
|---|---|---|---|
| N | -4.20014800 | -0.74450900 | 0.18537200 |
| N | -2.90268000 | -1.16687700 | 0.04918800 |
| C | -0.05276600 | -1.66918100 | 0.87307500 |
| C | 1.27629100 | -1.92758100 | 1.06478500 |
| C | 2.27540700 | -1.00913500 | 0.64262700 |
| C | 1.86289600 | 0.24480200 | 0.14168500 |
| N | 3.58845900 | -1.36962400 | 0.73274600 |
| C | 4.46241600 | -0.50791500 | 0.19441700 |
| N | 4.20011000 | 0.74457400 | -0.18552800 |
| N | 2.90271900 | 1.16697700 | -0.04889000 |
| C | 5.87264100 | -0.95230900 | 0.03795200 |
| C | 2.78849300 | 2.58223500 | 0.11379600 |
| C | -2.78846400 | -2.58220700 | -0.11312600 |
| C | -5.87267700 | 0.95229700 | -0.03869800 |
| C | 6.85937400 | -0.08266100 | -0.45236900 |
| C | 8.17333100 | -0.52107200 | -0.59854700 |
| C | 8.52083400 | -1.83018100 | -0.25569100 |
| C | 7.54412500 | -2.69929500 | 0.23504900 |
| C | 6.22800100 | -2.26540700 | 0.38065000 |
| C | 3.53457100 | 3.42964300 | -0.71404400 |
| C | 3.45534000 | 4.80903900 | -0.53478200 |
| C | 2.64238500 | 5.34860500 | 0.46526200 |
| C | 1.91132900 | 4.49608100 | 1.29504800 |
| C | 1.98410000 | 3.11425700 | 1.12896000 |
| C | -1.98420700 | -3.11448500 | -1.12824900 |
| C | -1.91145100 | -4.49635700 | -1.29398000 |
| C | -2.64239600 | -5.34865400 | -0.46387000 |
| C | -3.45523000 | -4.80882500 | 0.53613600 |
| C | -3.53444300 | -3.42938200 | 0.71503400 |
| C | -6.85938800 | 0.08285400 | 0.45203900 |
| C | -8.17342100 | 0.52120000 | 0.59772600 |
| C | -8.52103200 | 1.83004100 | 0.25395500 |
| C | -7.54435400 | 2.69895100 | -0.23719900 |
| C | -6.22815100 | 2.26512400 | -0.38230800 |
| H | -1.61301900 | 2.84156700 | -1.54275800 |
| H | 0.78344600 | 2.37656600 | -1.23992700 |
| H | -0.78326700 | -2.37649500 | 1.24034700 |
| H | 1.61318000 | -2.84154000 | 1.54296500 |
| H | 6.58622900 | 0.93425300 | -0.71070900 |
| H | 8.92918000 | 0.16134000 | -0.97835200 |
| H | 9.54702000 | -2.16988200 | -0.36957600 |
| H | 7.80757600 | -3.71880600 | 0.50417500 |
| H | 5.45988900 | -2.92967400 | 0.76019500 |
| H | 4.16731400 | 2.99815900 | -1.48087700 |

| | | | |
|---|---|---|---|
| H | 4.03092300 | 5.46457100 | -1.18233800 |
| H | 2.58327700 | 6.42474500 | 0.60005400 |
| H | 1.28842400 | 4.90478500 | 2.08568000 |
| H | 1.43005400 | 2.45082200 | 1.78429500 |
| H | -1.43023500 | -2.45121800 | -1.78382100 |
| H | -1.28864200 | -4.90526800 | -2.08458200 |
| H | -2.58330500 | -6.42483200 | -0.59837100 |
| H | -4.03072900 | -5.46419100 | 1.18393400 |
| H | -4.16709500 | -2.99768800 | 1.48182700 |
| H | -6.58616100 | -0.93385500 | 0.71109500 |
| H | -8.92924600 | -0.16105200 | 0.97786700 |
| H | -9.54727900 | 2.16968900 | 0.36746100 |
| H | -7.80788400 | 3.71825200 | -0.50703700 |
| H | -5.46007300 | 2.92925500 | -0.76215600 |