

Fine-tune the Diradical character in Molecular systems via

Heteroatom Effect

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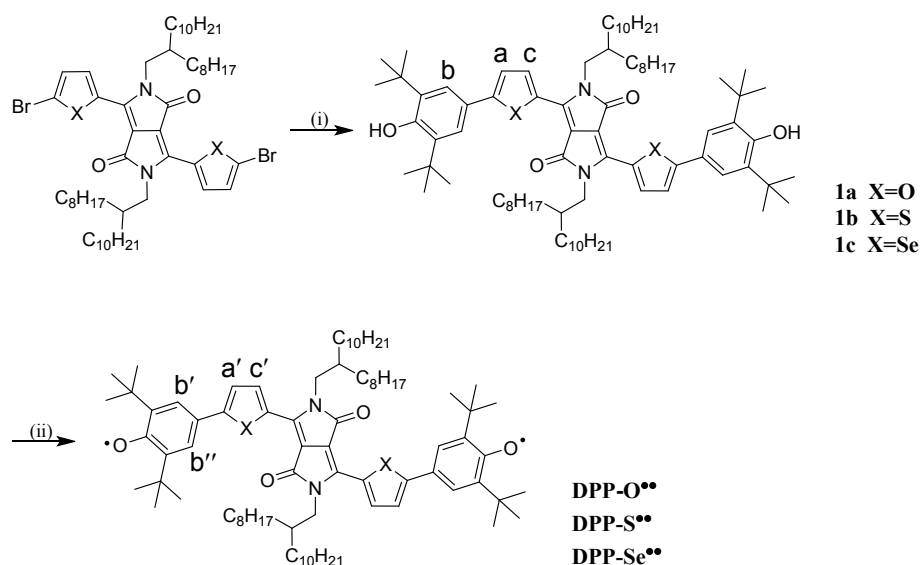
1. Instruments and Measurements.

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 reagent neutral Aluminum Oxide (200-300 mesh). Solvent toluene was freshly distilled from CaH₂ under N₂. Anhydrous Na₂SO₄ was used for drying organic extracts, and all volatiles were removed under reduced pressure. All reaction mixtures and column eluents were monitored by TLC using commercial Huanghai glass plates (HSGF 254, 2.5 x 8 cm). The plates were visualized under UV radiation at 254 and 365 nm. UV absorption spectra were recorded on a Shimadzu UV-2600 UV-VIS spectrophotometer in spectroscopy grade dichloromethane (DCM) or tetrahydrofuran (THF). NMR spectra were obtained on a Bruker AV III HD 400 MHz. 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. Cyclic voltammograms were measured on a Shanghai Chenhua CHI 660E electrochemical workstation in dry DCM with 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF₆) as the supporting electrolyte at a scan rate of 100 mV/s at room temperature under the protection of nitrogen. A gold disk was used as working electrode, platinum wire was used as counter electrode, and Ag/AgCl (3 M KCl solution) was used as reference electrode. The potential was externally calibrated after each experiment, against the ferrocene/ferrocenium couple. The film morphologies were characterized by Park XE-7 atomic force microscope (AFM). The electrical current of the devices was measured by an Agilent B2912A source meter with a probe station. For the variable temperature ESR, the ESR intensity (I) increased with increasing temperature (T), and the data was fitted by modified Bleaney-Bowers equation¹:

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

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

2. Detailed synthetic procedures



Scheme S1. The synthetic route of targeted compounds. (i) $[\text{Pd}_2(\text{dba})_3]$, $\text{P}(o\text{-tol})_3$, $n\text{Bu}_4\text{NOH}$, H_2O , Toluene, $90\text{ }^\circ\text{C}$; (ii) PbO_2 , CH_2Cl_2 , RT, 0.5 h.

Compound **1b**: Tris(dibenzylideneacetone)dipalladium(0) (31.1 mg, 0.034 mmol), 2,6-Bis(1,1-dimethylethyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) phenol (423 mg, 1.27 mmol), tri(*o*-tolyl)phosphine (31.9 mg, 0.10 mmol), 1,4-bis(5-bromothiophen-2-yl)-2,5-bis(2-octyldodecyl)pyrrolo[3,4-*c*]pyrrole-3,6-dione (500 mg, 0.49 mmol) and tetrabutylammonium hydroxide ($\text{TBAH}\cdot 30\text{H}_2\text{O}$, 1.57 g, 1.96 mmol) were suspended in a mixture of toluene (10 mL) and water (2 mL) under nitrogen. After stirring the reaction mixture at $90\text{ }^\circ\text{C}$ for 15 h, the reaction was cooled down to room temperature. Subsequently, hydrochloric acid (1 M, 60 mL) was added and the crude product was extracted with DCM (60 mL) for 3 times. The combined organic layer was dried by Na_2SO_4 and the solvent was removed under reduced pressure. The product was purified by silica gel chromatography and recrystallized from DCM/methanol solution, which affords product **1b** as a black solid.

Yield: 29 % (180 mg, 0.141 mmol). $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 9.03$ (2 H, d, J_{HH}

= 4.0 Hz), 7.50 (4 H, s), 7.34 (2 H, d, $J_{\text{HH}} = 4.0$ Hz), 5.43 (2 H, s), 4.09 (4 H, d, $J_{\text{HH}} = 8.0$ Hz), 1.50 (C(CH₃)₃), 36 H, s), 1.21-1.36 (CH₂, CH, 66 H, m), 0.83-0.90 (CH₃, 12 H, m). ¹³C NMR (100 MHz, CDCl₃): $\delta = 160.76, 153.87, 150.27, 138.74, 136.13, 135.70, 126.62, 123.86, 122.29, 122.12, 106.72, 66.93, 52.37, 45.24, 37.00, 33.40, 30.91, 30.87, 30.58, 30.31, 29.16, 29.11, 28.68, 28.62, 28.57, 28.52, 28.35, 28.33, 25.30, 21.67, 21.64, 13.10$. MALDI-TOF MS: m/z calcd for [M]⁺: 1268.93; found, 1269.21. Element analysis (%) calcd. C 77.55, H 10.16, N 2.21; found C 77.60, H 10.11, N 2.20.

Compound **1c**: The procedure was carried out similar to the synthesis of compound **1b**, which affords product **1b** as a black solid. Yield: 190 mg (0.14 mmol, 31 %). ¹H NMR (400 MHz, CDCl₃): $\delta = 8.86$ (2 H, d, $J_{\text{HH}} = 4.0$ Hz), 7.46 (2 H, d, $J_{\text{HH}} = 4.0$ Hz), 7.44 (4 H, s), 5.42 (2 H, s), 4.00 (4 H, d, $J_{\text{HH}} = 8.0$ Hz), 1.49 (C(CH₃)₃), 36 H, s), 1.21-1.36 (CH₂, CH, 66 H, m), 0.82-0.87 (CH₃, 12 H, m). ¹³C NMR (100 MHz, CDCl₃): $\delta = 161.95, 158.69, 154.94, 141.51, 138.19, 136.70, 131.46, 127.12, 125.10, 123.68, 107.92, 46.22, 37.80, 34.39, 31.92, 31.89, 31.35, 30.20, 30.09, 29.68, 29.64, 29.62, 29.56, 29.36, 29.33, 26.36, 22.69, 22.67, 14.12$. MALDI-TOF MS: m/z calcd for [M-H]⁻: 1363.82; found, 1363.19. Element analysis (%) calcd. C 72.21, H 9.46, N 2.05; found C 72.32, H 9.41, N 2.06.

Compound **DPP-O^{••}**: Tris(dibenzylideneacetone)dipalladium(0) (32.0 mg, 0.035 mmol), 2,6-Bis(1,1-dimethylethyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenol (436.6 mg, 1.315 mmol), tri(o-tolyl)phosphine (32.8 mg, 0.11 mmol), 1,4-bis(5-bromofuran-2-yl)-2,5-bis(2-octyldodecyl)pyrrolo[3,4-c]pyrrole-3,6-dione (500.0 mg, 0.506 mmol) and tetrabutylammonium hydroxide (TBAH·30H₂O, 1.60 g, 2.0 mmol) were suspended in a mixture of toluene (10 mL) and water (2 mL) under nitrogen. After stirring the reaction mixture at 90 °C for 5 h, the reaction was cooled down to room temperature. Subsequently, hydrochloric acid (1 M, 60 mL) was added and the crude product was extracted with DCM (60 mL) for 3 times. The combined organic layer was dried by Na₂SO₄ and the solvent was removed under reduced pressure. The product was purified by silica gel chromatography and recrystallized

from DCM/methanol solution, which affords product as a black solid. This black solid and excess lead (IV) oxide (3.22 g, 13.2 mmol) were suspended in DCM (20 mL). After stirring the reaction mixture at room temperature for 30 minutes the black lead oxide was filtered off and the solvent was removed under reduced pressure. The product was purified by silica gel chromatography, which affords product as a black solid. Yield: 125.6 mg (20 % for two steps). ¹H NMR (400 MHz, CDCl₃): δ = 8.86 (2 H, d, *J*_{HH} = 4.0 Hz), 7.58 (2 H, d, *J*_{HH} = 2.4 Hz), 7.35 (2 H, d, *J*_{HH} = 4.0 Hz), 7.28 (2 H, d, *J*_{HH} = 2.4 Hz), 4.18 (4 H, d, *J*_{HH} = 8.0 Hz), 1.20-1.39 (CH₂, CH, C(CH₃)₃, 102 H, m), 0.83-0.88 (CH₃, 12 H, m). ¹³C NMR (100 MHz, CDCl₃): δ = 185.47, 162.22, 161.04, 149.60, 148.43, 146.46, 133.23, 129.88, 126.27, 124.02, 123.12, 119.47, 115.38, 47.81, 37.73, 35.90, 35.64, 31.93, 31.86, 31.26, 31.23, 29.99, 29.80, 29.65, 29.63, 29.62, 29.53, 29.47, 29.35, 29.29, 26.32, 22.69, 22.64, 14.12. MALDI-TOF MS: *m/z* calcd for [M+H]⁺: 1235.96; found, 1236.59. Element analysis (%) calcd. C 79.69, H 10.28, N 2.27; found C 79.65, H 10.22, N 2.25.

Compound **DPP-S^{••}**: Lead (IV) oxide (1.57 g, 6.58 mmol) and **1b** (118.0 mg, 0.093 mmol) were suspended in DCM (10 mL). After stirring the reaction mixture at room temperature for 30 minutes the excess lead (IV) oxide was filtered off and the solvent was removed under reduced pressure. The product was purified by silica gel chromatography and recrystallized from DCM/methanol solution, which affords product as a black solid. Yield: 111.6 mg (0.088 mmol, 95 %). ¹H NMR (400 MHz, CD₂Cl₂): δ = 9.33 (2 H, d, *J*_{HH} = 8.0 Hz), 7.54 (2 H, d, *J*_{HH} = 8.0 Hz), 7.41 (2 H, d, *J*_{HH} = 4.0 Hz), 7.24 (2 H, d, *J*_{HH} = 4.0 Hz), 4.00 (4 H, d, *J*_{HH} = 8.0 Hz), 1.22-1.35 (CH₂, CH, C(CH₃)₃, 102 H, m), 0.83-0.86 (CH₃, 12 H, m). ¹³C NMR (100 MHz, CD₂Cl₂): δ = 185.43, 161.52, 154.49, 149.42, 147.26, 142.02, 132.52, 130.95, 130.04, 128.71, 127.71, 126.14, 125.47, 46.53, 38.51, 35.66, 35.53, 31.94, 31.90, 31.12, 31.08, 30.14, 30.13, 29.74, 29.65, 29.54, 29.50, 29.40, 26.15, 22.69, 13.90. MALDI-TOF MS: *m/z* calcd for [M+H]⁺: 1267.92; found, 1268.25. Element analysis (%) calcd. C 77.67, H 10.02, N 2.21; found C 77.70, H 10.08, N 2.20.

Compound **DPP-Se^{••}**: Lead (IV) oxide (1.60 g, 6.70 mmol) and **1c** (130.0 mg, 0.095

mmol) were suspended in DCM (10 mL). After stirring the reaction mixture at room temperature for 30 minutes the excess lead (IV) oxide was filtered off and the solvent was removed under reduced pressure. The product was purified by silica gel chromatography and recrystallized from DCM/methanol solution, which affords product as a black solid. Yield: 124.0 mg (0.091 mmol, 96 %). ¹H NMR (400MHz, CDCl₃): δ = 9.46 (2H, d, 4.0 Hz), 7.62 (2 H, d, *J*_{HH} = 8.0 Hz), 7.45 (2 H, d, *J*_{HH} = 4.0 Hz), 7.04 (2 H, d, *J*_{HH} = 4.0 Hz), 3.98 (4 H, d, *J*_{HH} = 4.0 Hz), 1.23-1.36 (CH₂, CH, C(CH₃)₃, 102 H, m), 0.84-0.87 (CH₃, 12 H, m). ¹³C NMR (100 MHz, CDCl₃): δ = 185.72, 162.03, 158.00, 149.97, 147.32, 144.37, 133.49, 133.32, 132.01, 130.13, 129.35, 128.60, 125.03, 46.53, 38.65, 35.70, 35.60, 31.94, 31.90, 31.23, 30.15, 29.72, 29.66, 29.64, 29.58, 29.55, 29.38, 29.37, 26.32, 22.70, 14.13. MS: *m/z* calcd for [M+H]⁺: 1361.81; found,1362.04. Element analysis (%) calcd. C 72.32, H 9.33, N 2.06; found C 72.40, H 9.27, N 2.05.

3. Variable- temperature NMR spectra

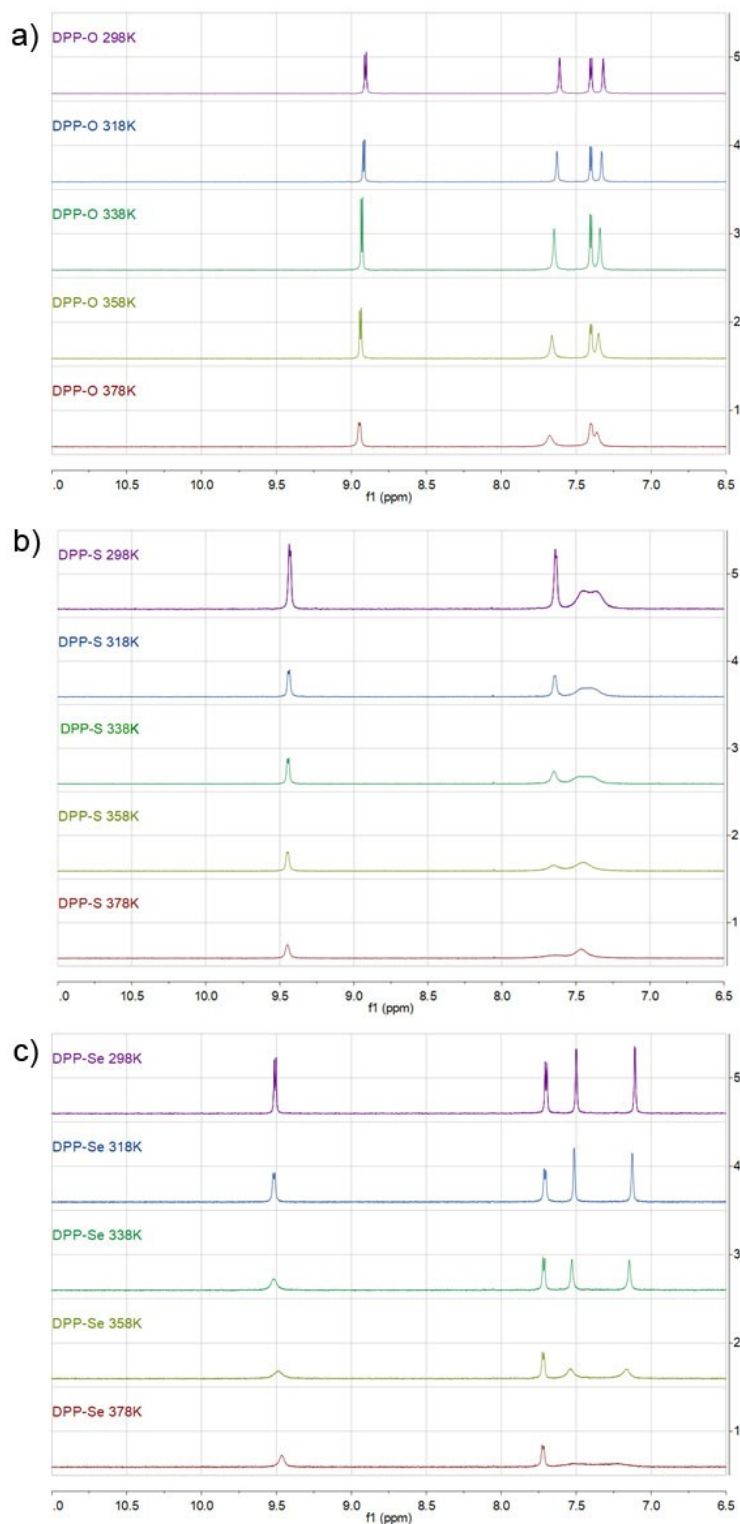


Figure S1. Variable temperature NMR spectrum of **DPP-O••** (a), **DPP-S••** (b) and **DPP-Se••** (c, 400 MHz, 1, 1, 2, 2-tetrachloroethane- d_2 , 298 K to 378 K).

4. ESR spectra

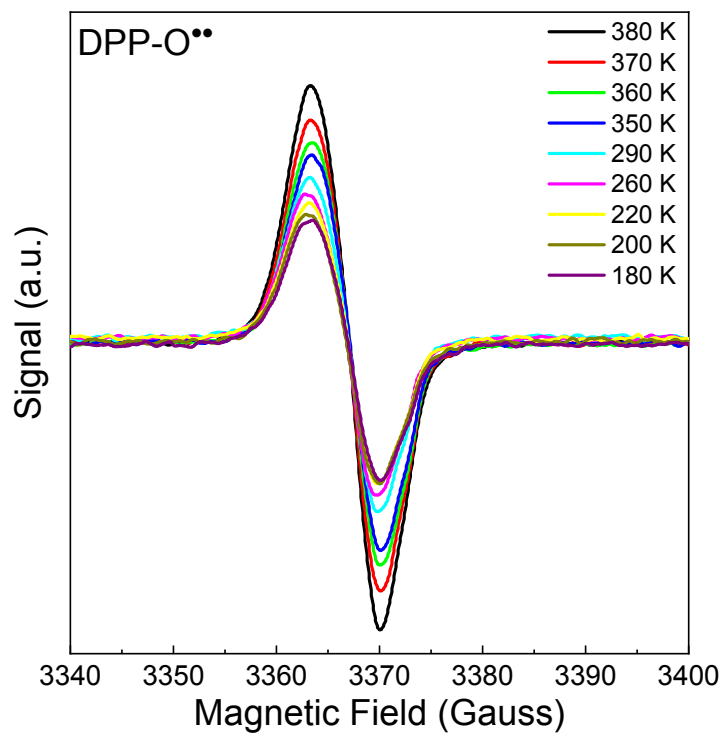


Figure S2. Variable temperature ESR spectra (180 K to 390 K) of **DPP-O^{••}**.

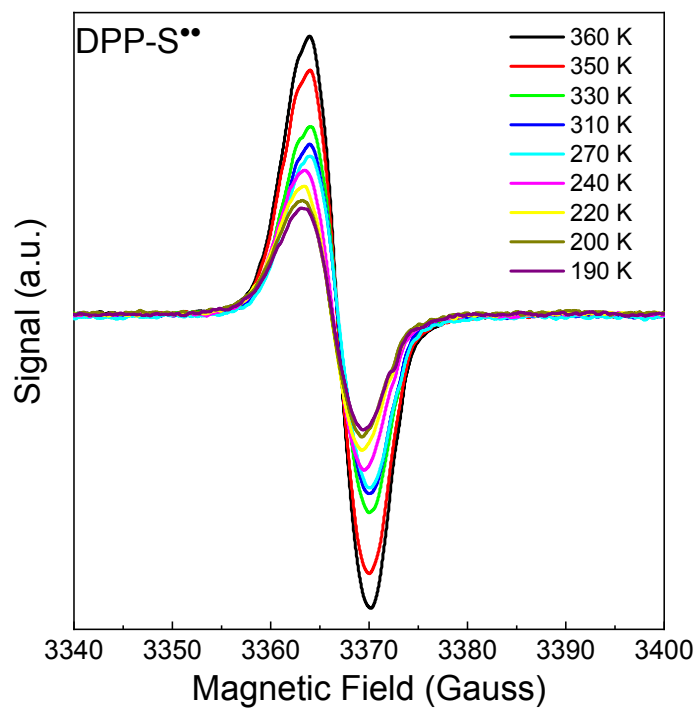


Figure S3. Variable temperature ESR spectra (180 K to 390 K) of **DPP-S^{••}**.

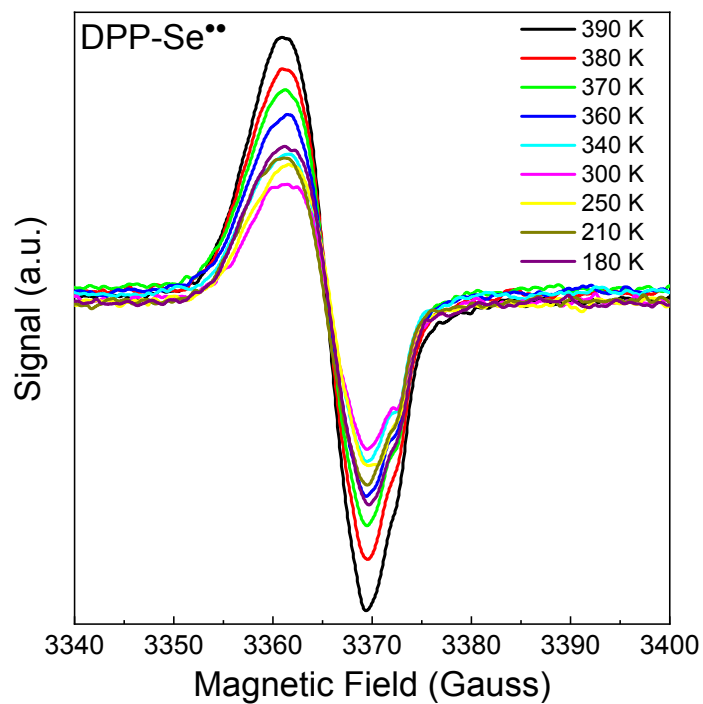


Figure S4. Variable temperature ESR spectra (180 K to 390 K) of **DPP-Se^{••}**.

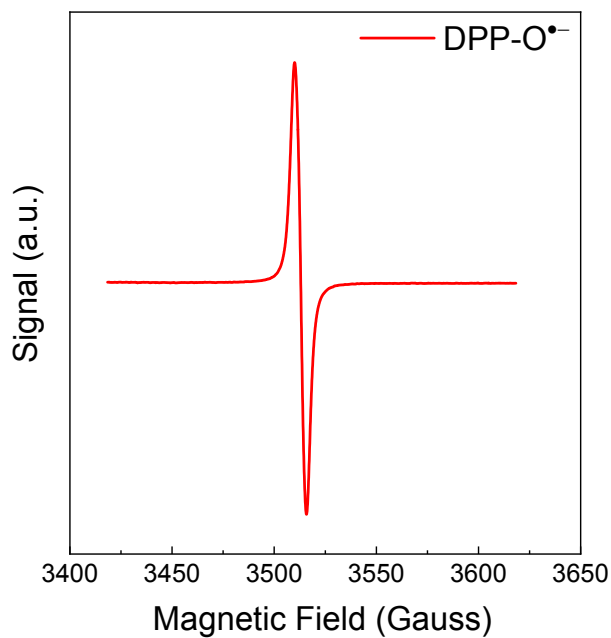


Figure S5. Room temperature ESR spectrum of **DPP-O^{•-}** in THF solution.

5. Computational details

All density functional theory calculations were performed using Gaussian 16 package² with the Becke's three-parameter hybrid exchange functional³ and the Lee-Yang-Parr correlation functional⁴ (B3LYP) employing the 6-31G* basis set^{5,6} for all atoms. The diradical character y_0 is calculated based on the natural orbital occupation number (NOON). The occupation number of lowest unoccupied natural orbital (nLUNO) is a direct measure of diradical character y_0 ⁷. A molecule with $y_0 = 0$ implies a closed-shell structure, whereas a molecule with $y_0 = 1$ indicates a pure diradical structure. The spin densities were illustrated using Multiwfn⁸ and VMD⁹. The NICS (1) ZZ value was carried out by gauge independent atomic orbital (GIAO) method¹⁰ based on the optimized geometries.

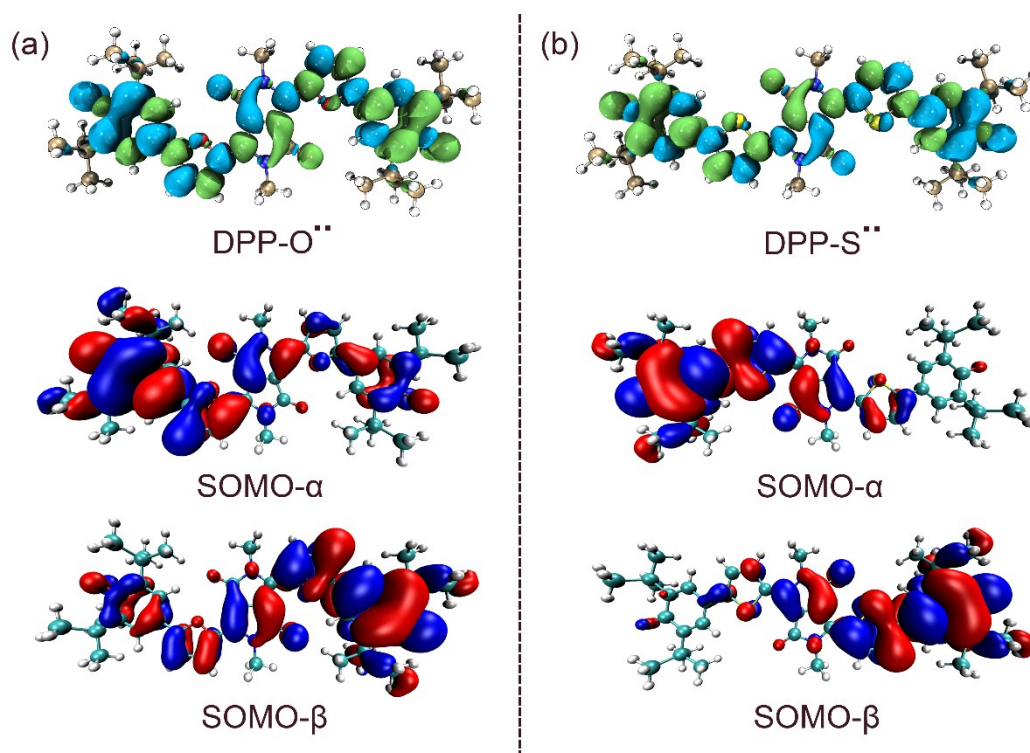


Figure S6. Spin density distribution, SOMO- α and SOMO- β of **DPP-O^{••}** (a) and **DPP-S^{••}** (b). The calculations were performed at UB3LYP/6-31G* level of theory.

6. State conversion of three diradicaloids

By adding TBAF dropwise to **1b** of tetrahydrofuran (THF) solution, the initial absorption peak decreased and shifted to the near-infrared range with the maximum absorption wavelength at 889 nm and a small band at 1083 nm appeared, meanwhile the solution changed from purple to colorless. We propose that the main band is corresponding to the dianion **DPP-S²⁻** and the small band is according to auto-reduced **DPP-S^{•-}**. At this point, the trifluoroacetic acid (TFA) solution is added, the solution changes from colorless to purple, the spectrum decreased and blue-shifted back to the absorption spectrum of **1b**, but with one smaller peak of 781 nm. This small peak can be assigned to the absorption peak of **DPP-S^{••}**, which proves that auto-reduction occurred during the titration process. We suggested that the small amount of water served as a reductant under alkaline environment and help the appearance of **DPP-S^{•-}**. To further confirm this interpretation, a titration test on **DPP-S^{••}** was performed (Figure S8). By adding TBAF dropwise to the **DPP-S^{••}** solution, the solution became to alkaline and the λ_{max} red-shifted from 781 nm to 1083 nm (**DPP-S^{•-}**) and then blue-shifted to 883 nm (**DPP-S²⁻**), which was compatible with the corresponding absorption spectrum changes of **1b**. After which TFA solution was added dropwise, the absorption band further blue shifted to 600 nm and was same with the absorption peak of **1b**. Beginning with both species, at the state of dianion **DPP-S²⁻**, the solution of Pb(OAc)₄ was added dropwise, the state of the compound will change to **DPP-S^{•-}**, and finally it will become diradical state **DPP-S^{••}**, and the corresponding absorption spectrum changes as shown in Figure S8. Similar performance was observed for furan and selenophene analogues (Figure S9, S10), and the absorption spectra of the radical anions and dianions species were exhibited clearly.

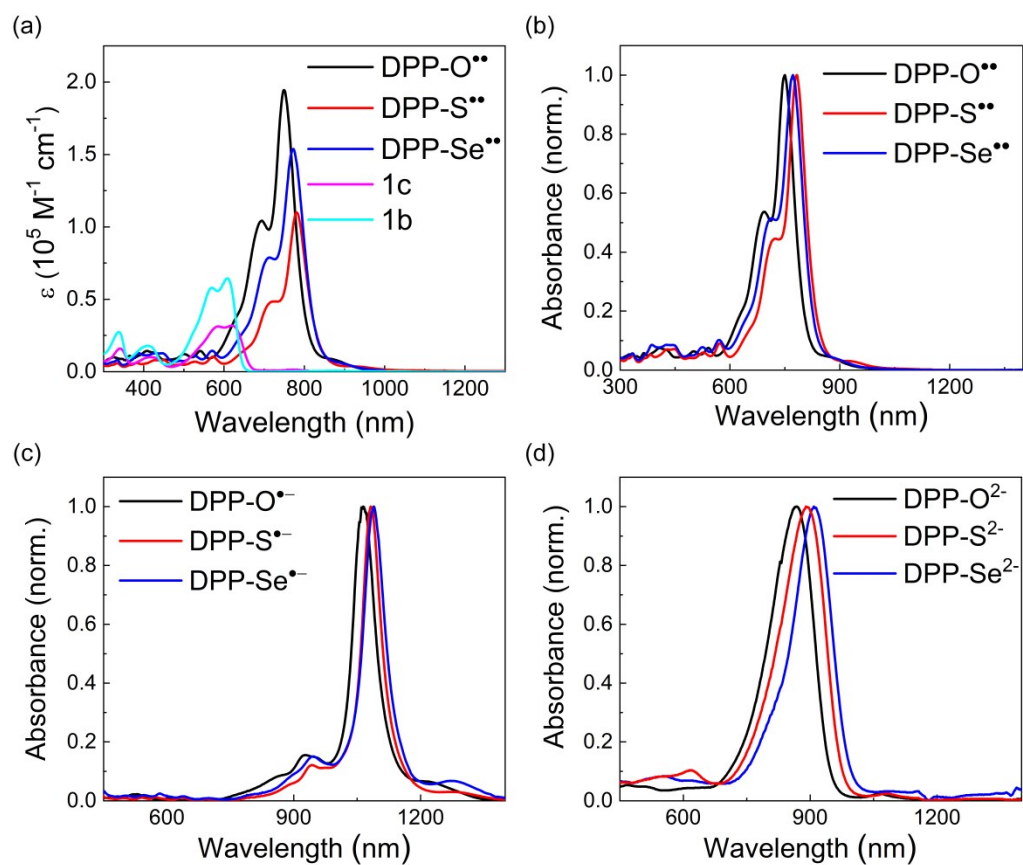


Figure S7. (a) Absorption spectra of **1b**, **1c**, **DPP-O^{••}**, **DPP-S^{••}** and **DPP-Se^{••}** in DCM at 10 μM ; Normalized absorption spectra of **DPP-O^{••}**, **DPP-S^{••}** and **DPP-Se^{••}** (b, DCM); **DPP-O^{•-}**, **DPP-S^{•-}** and **DPP-Se^{•-}** (c, THF) **DPP-O²⁻**, **DPP-S²⁻** and **DPP-Se²⁻** (d, THF).

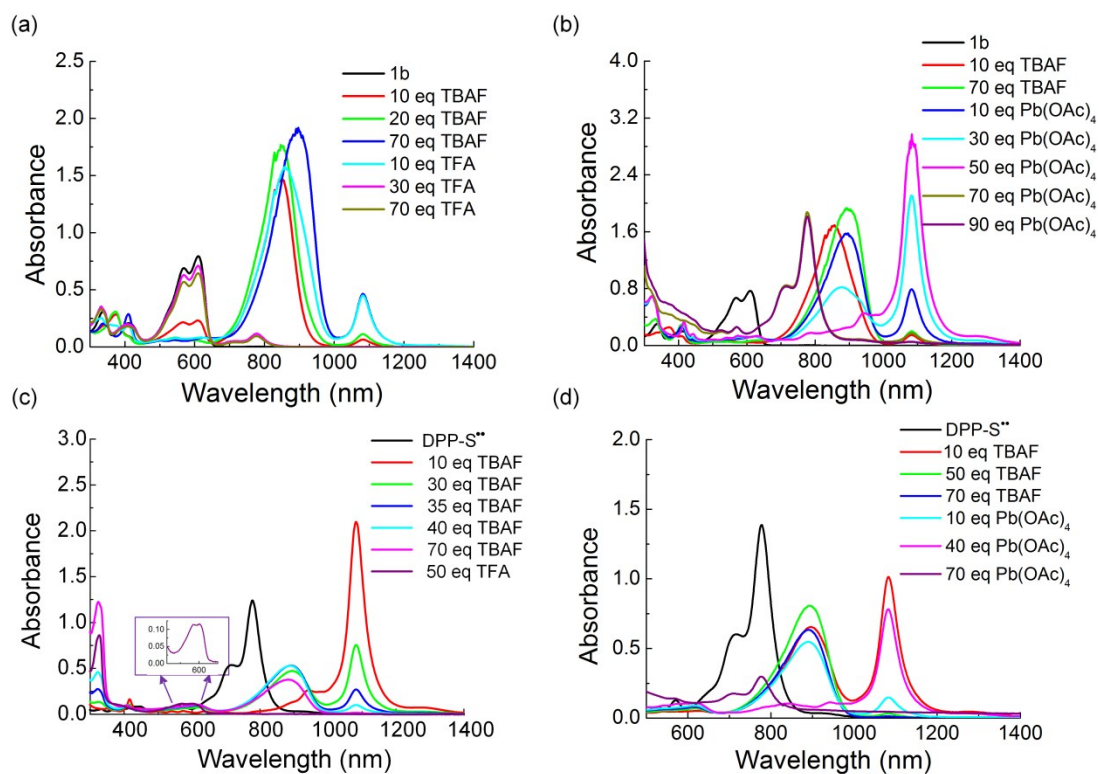


Figure S8. The absorption spectra of the ionic state conversion in the process of adding TBAF and TFA (a, c) or TBAF and Pb(OAc)₄ (b, d) dropwise to **1b** (a, b) and **DPP-S^{**}** (c, d) in THF at 10 μM.

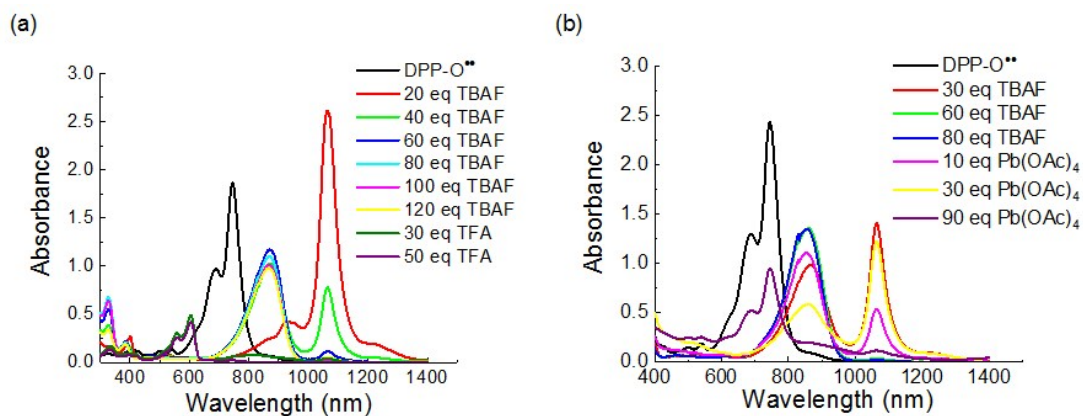


Figure S9. The absorption spectra of the ionic state conversion in the process of adding TBAF and TFA (a) or TBAF and Pb(OAc)₄ (b) dropwise to **DPP-O^{**}** in THF at 10 μM.

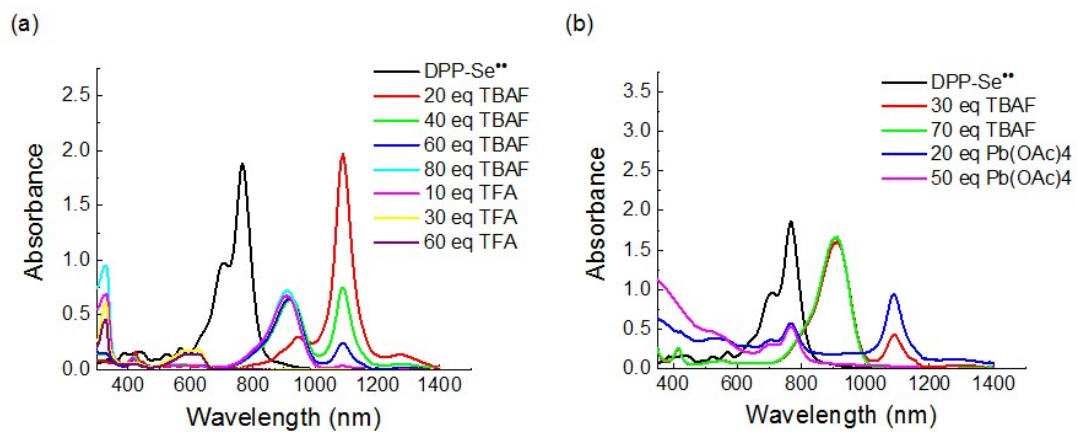


Figure S10. The absorption spectra of the ionic state conversion in the process of adding TBAF and TFA (a) or TBAF and Pb(OAc)₄ (b) dropwise to **DPP-Se**** in THF at 10 μM.

7. Electrochemical properties

Cyclic voltammetry (CV) was performed to study the electrochemical properties of these diradicaloids in dry DCM. The LUMO energy levels of **DPP-O^{••}**, **DPP-S^{••}** and **DPP-Se^{••}** were calculated to be -3.66, -3.76 and -3.72 eV.

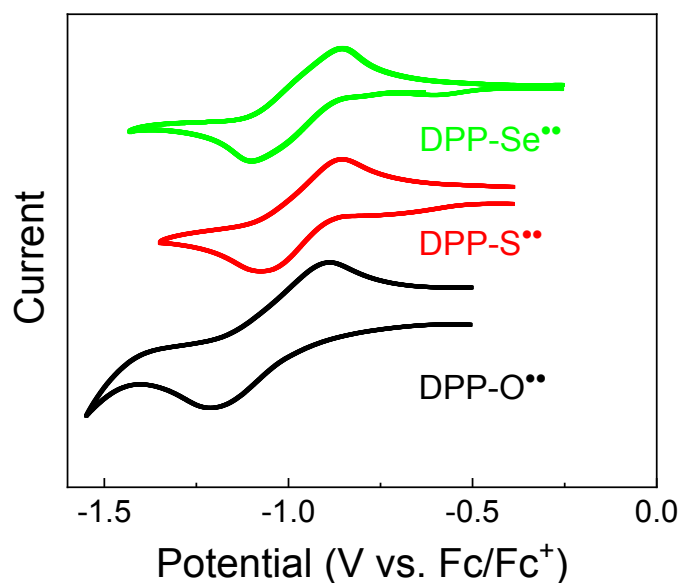


Figure S11. Cyclic voltammograms of **DPP-O^{••}**, **DPP-S^{••}** and **DPP-Se^{••}** in dry DCM with 0.1 M Bu₄NPF₆ as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 50 mV/s.

8. OFET device preparation

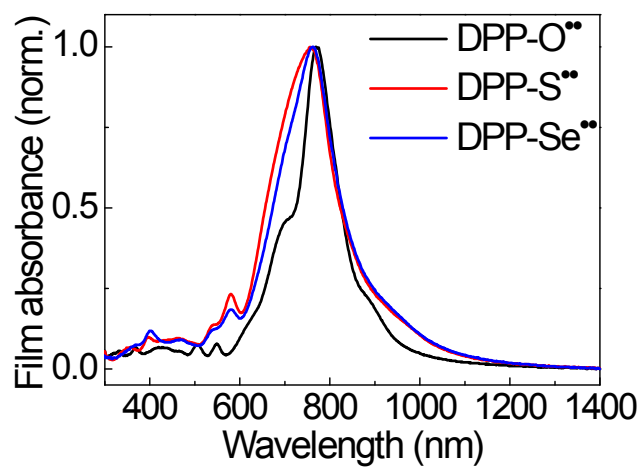


Figure S12. Normalized film absorption spectra of **DPP-O**, **DPP-S** and **DPP-Se**.

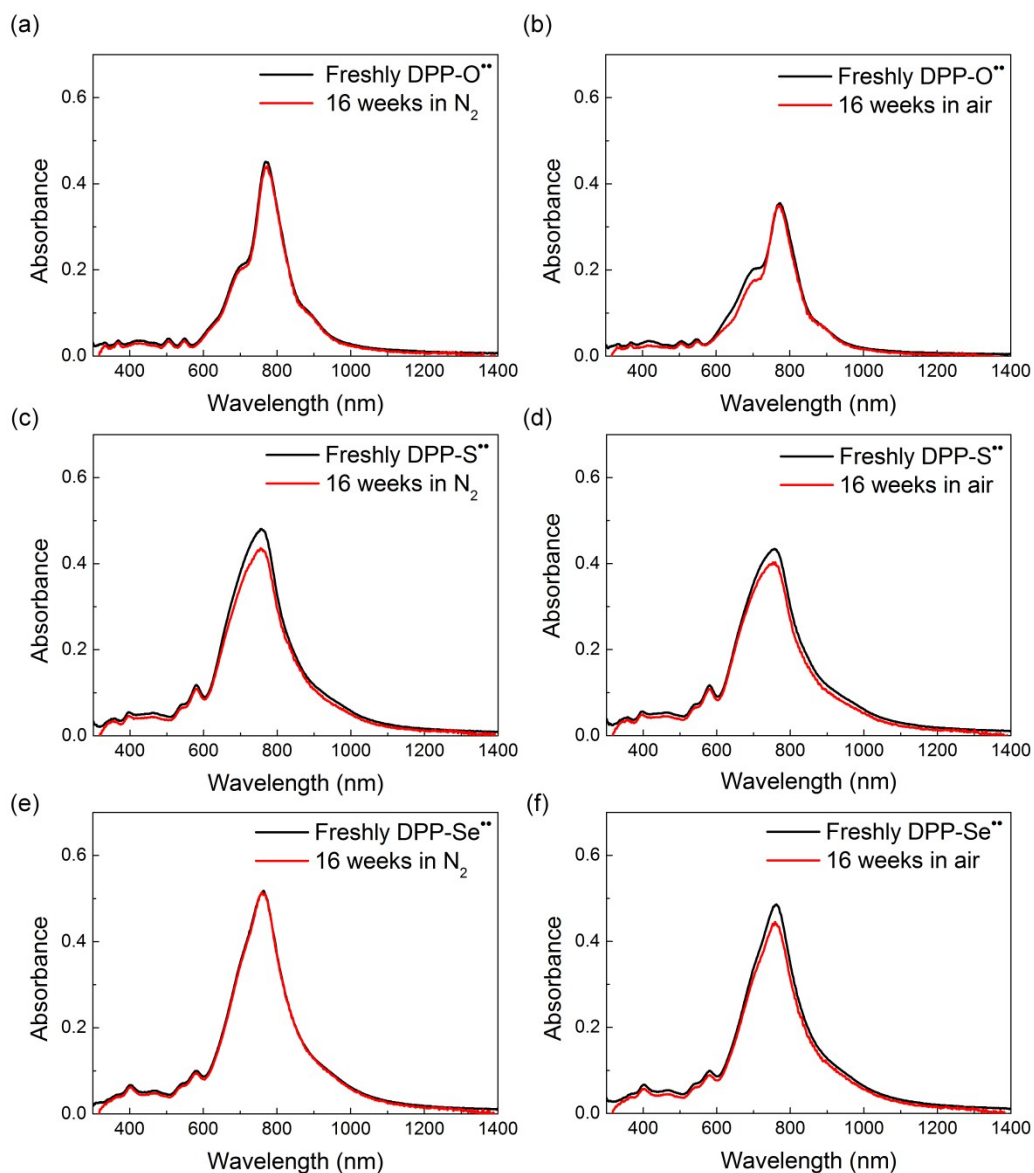


Figure S13. Film absorption spectra change of **DPP-O^{••}** (a, b), **DPP-S^{••}** (c, d), and **DPP-Se^{••}** (e, f) after being placed in nitrogen atmosphere (a, c, e) or in air (b, d, f) for 16 weeks.

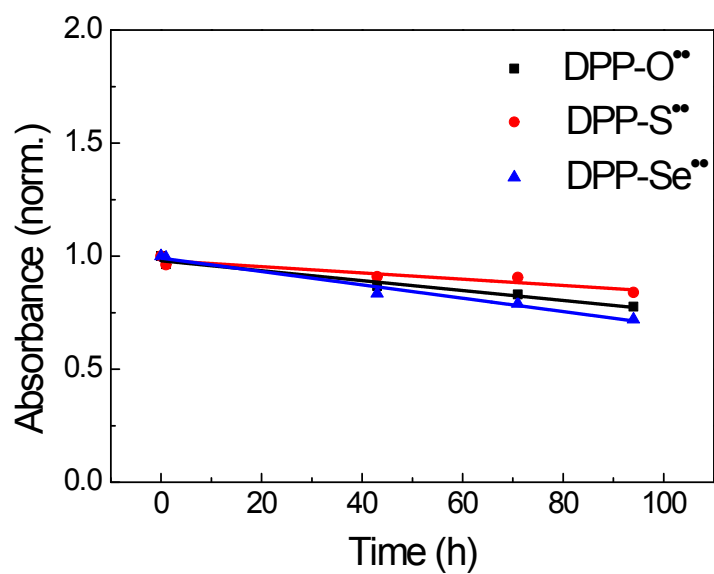


Figure S14. Normalized film absorption spectra of **DPP-O^{••}**, **DPP-S^{••}** and **DPP-Se^{••}** changes in absorption intensity of λ_{\max} under continuous illumination of a 400 W light source.

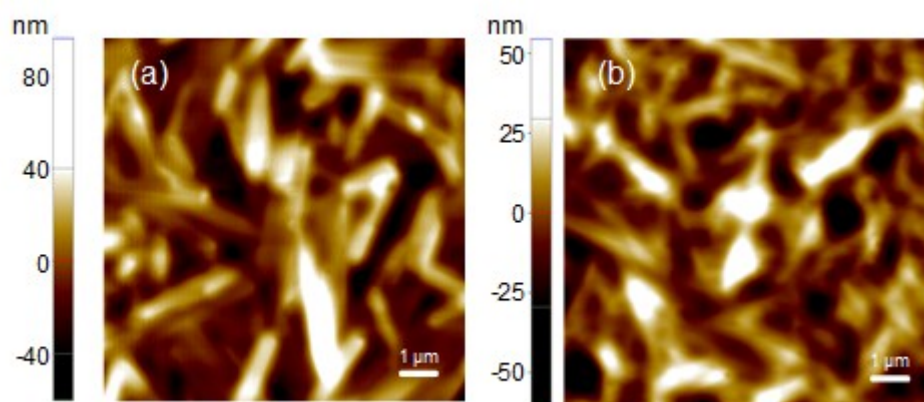


Figure S15. (a) AFM image of **DPP-S^{••}** thin film at 125°C, scale bar: 1 μ m; The root mean square height (Sq) is 20.4 nm. (b) AFM image of **DPP-Se^{••}** thin film at 125°C, scale bar: 1 μ m.

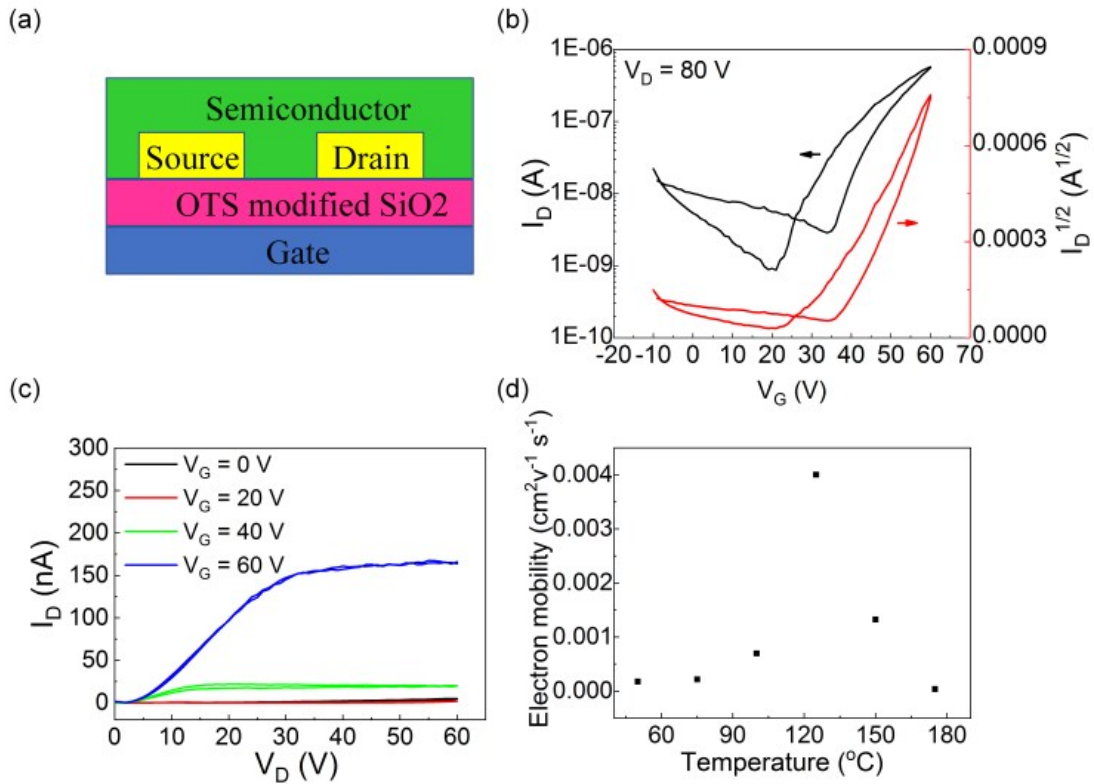


Figure S16. (a) Device structure of the OFETs; (b) Transfer characteristics (I_D - V_G) and (c) output characteristics (I_D - V_D) of a typical transistor based on **DPP-Se^{••}** with $L = 20 \mu\text{m}$ and $W = 1000 \mu\text{m}$, exhibiting an electron mobility of $4.0 \times 10^{-3} \text{ cm}^2\text{v}^{-1} \text{ s}^{-1}$ at $V_D = 80 \text{ V}$. (d) Transistor mobilities as a function of annealing temperature for **DPP-Se^{••}**

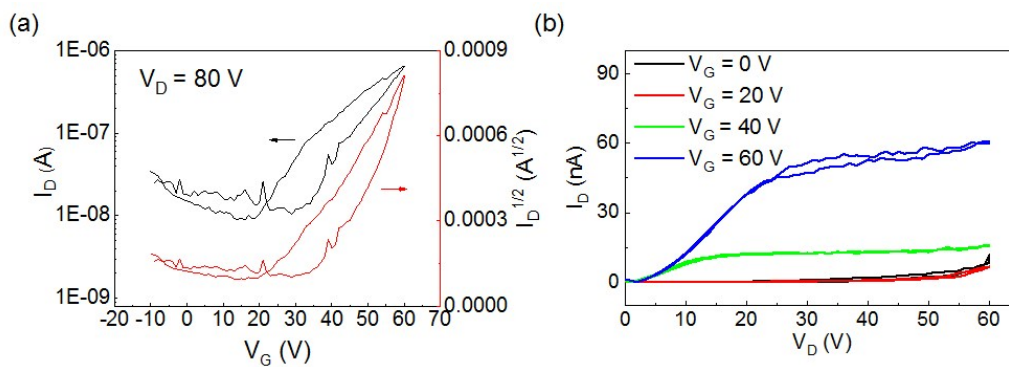


Figure S17. (a) Transfer characteristics (I_D - V_G) and (b) output characteristics (I_D - V_D) of a typical transistor based on **DPP-S^{••}** with $L=20 \mu\text{m}$ and $W=1000 \mu\text{m}$, exhibiting an electron mobility of $3.36 \times 10^{-3} \text{ cm}^2\text{v}^{-1} \text{ s}^{-1}$ at $V_D=80 \text{ V}$.

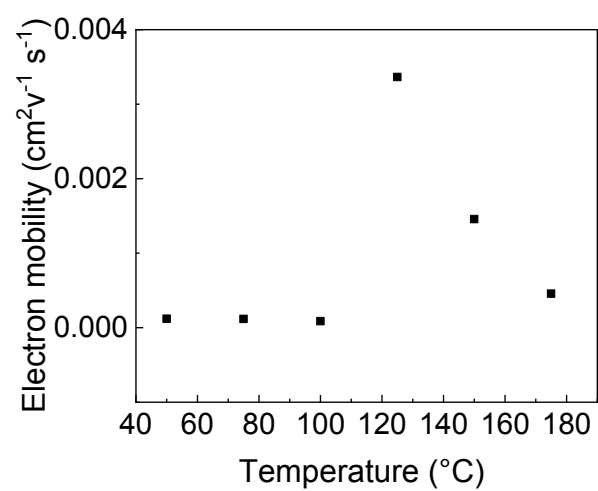


Figure S18. Transistor mobilities as a function of annealing temperature for **DPP-S**.

9. NMR spectra

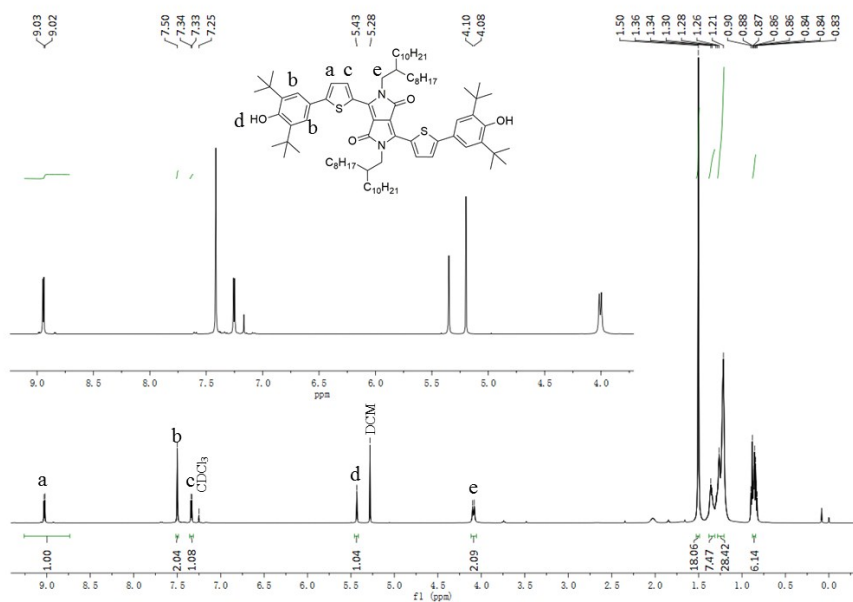


Figure S19. ¹H NMR spectrum of **1b** (400 MHz, CDCl₃, 300 K).

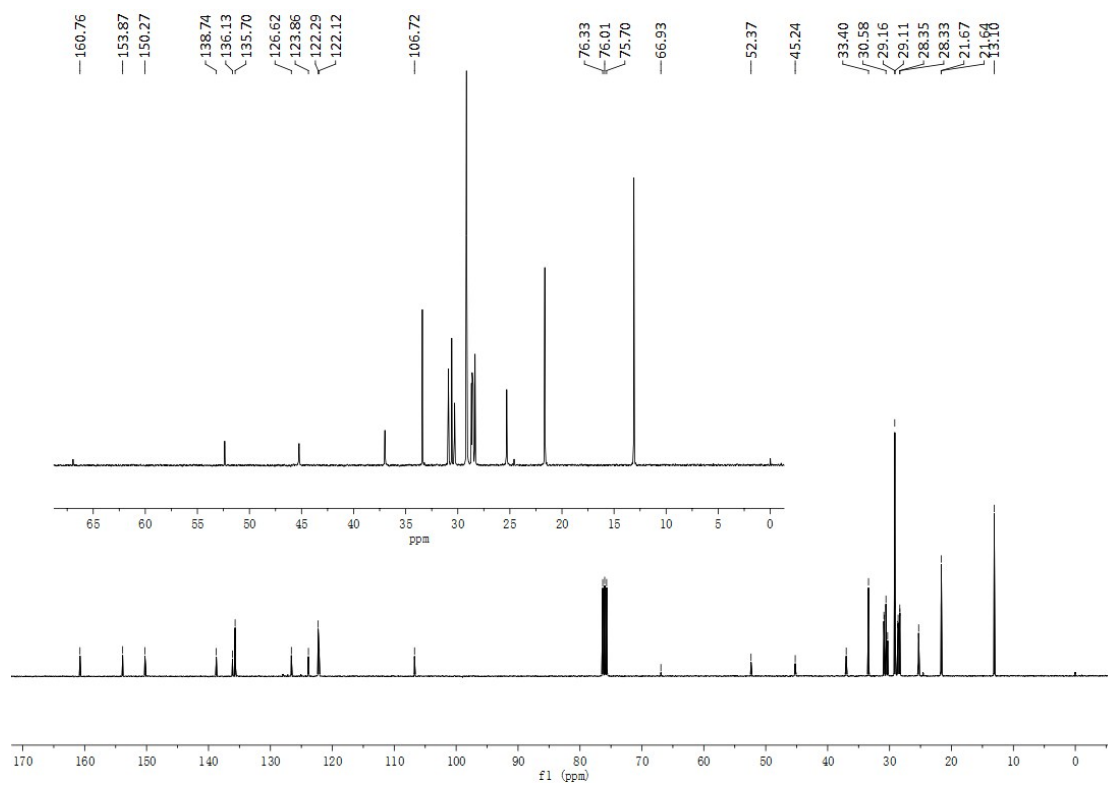


Figure S20. ¹³C NMR spectrum of **1b** (100 MHz, CD₂Cl₂, 300 K).

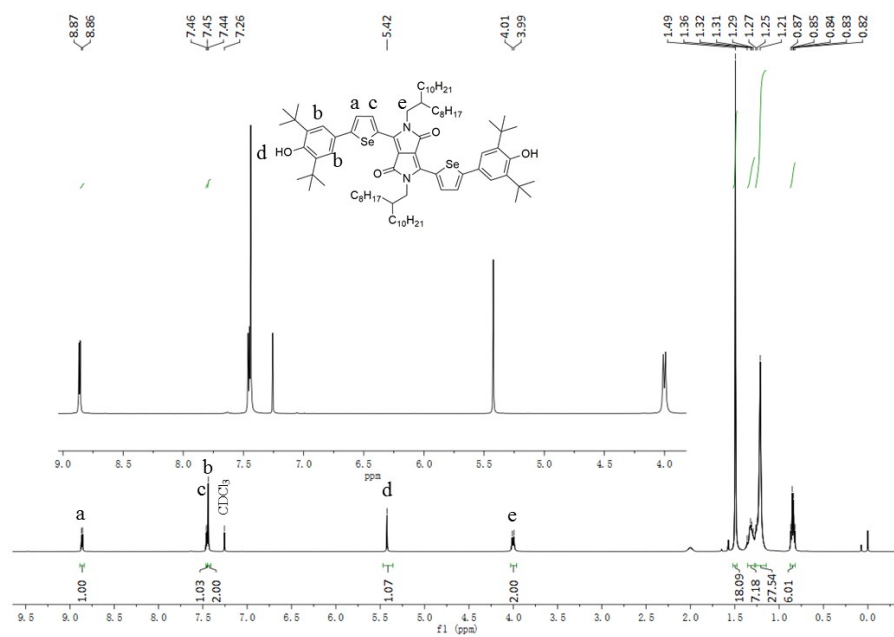


Figure S21. ¹H NMR spectrum of **1c** (400 MHz, CDCl₃, 300 K).

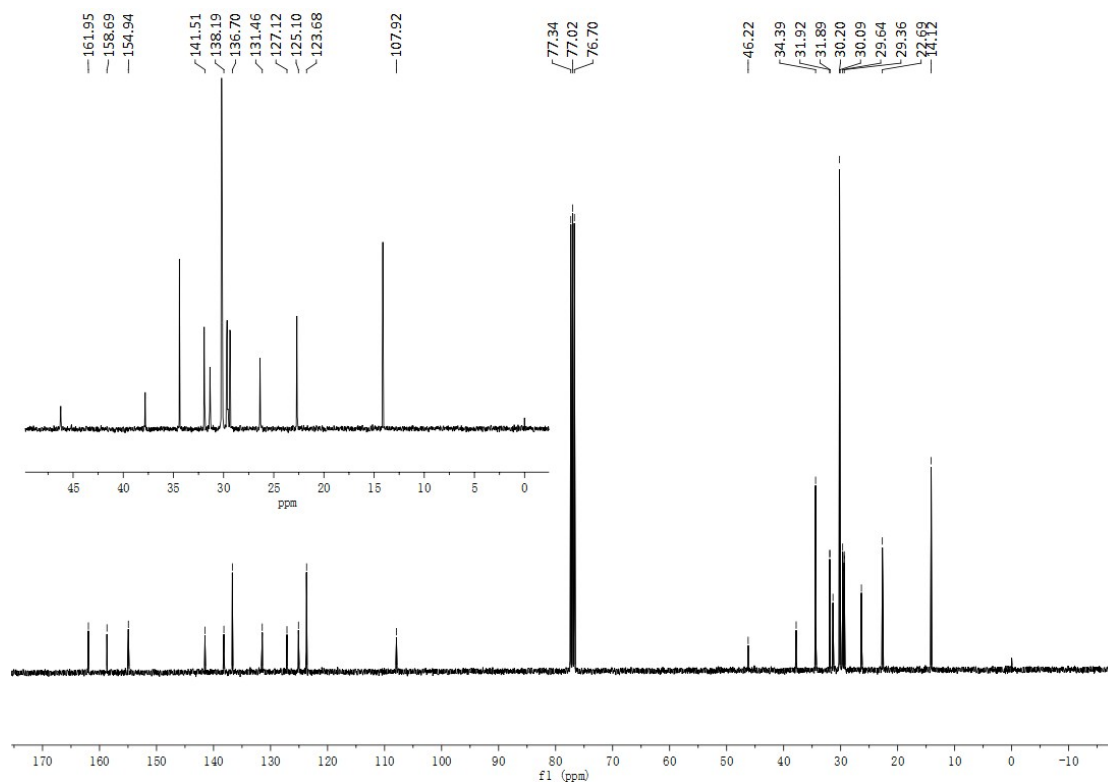


Figure S22. ¹³C NMR spectrum of **1c** (100 MHz, CDCl₃, 300 K).

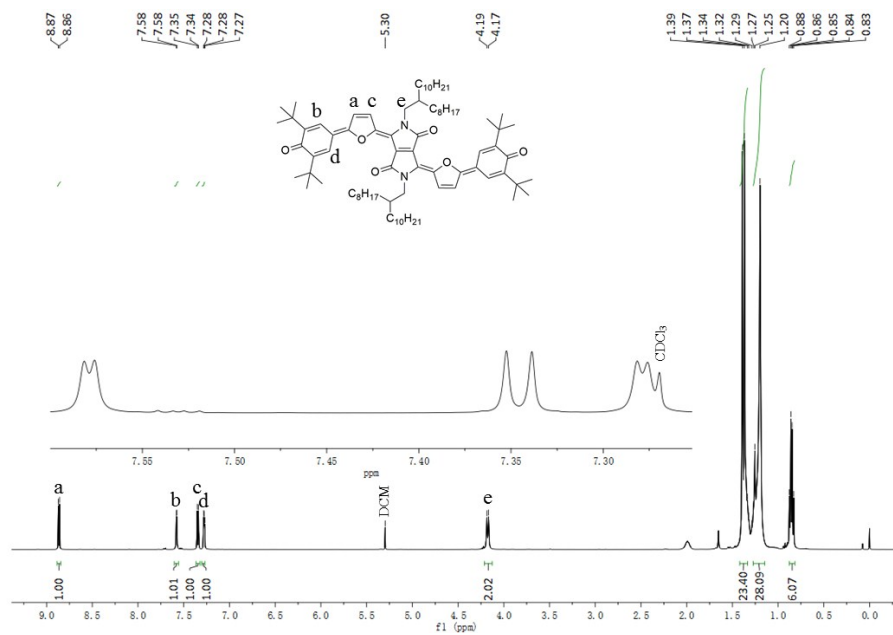


Figure S23. ¹H NMR spectrum of **DPP-O^{••}** (400 MHz, CDCl₃, 300 K).

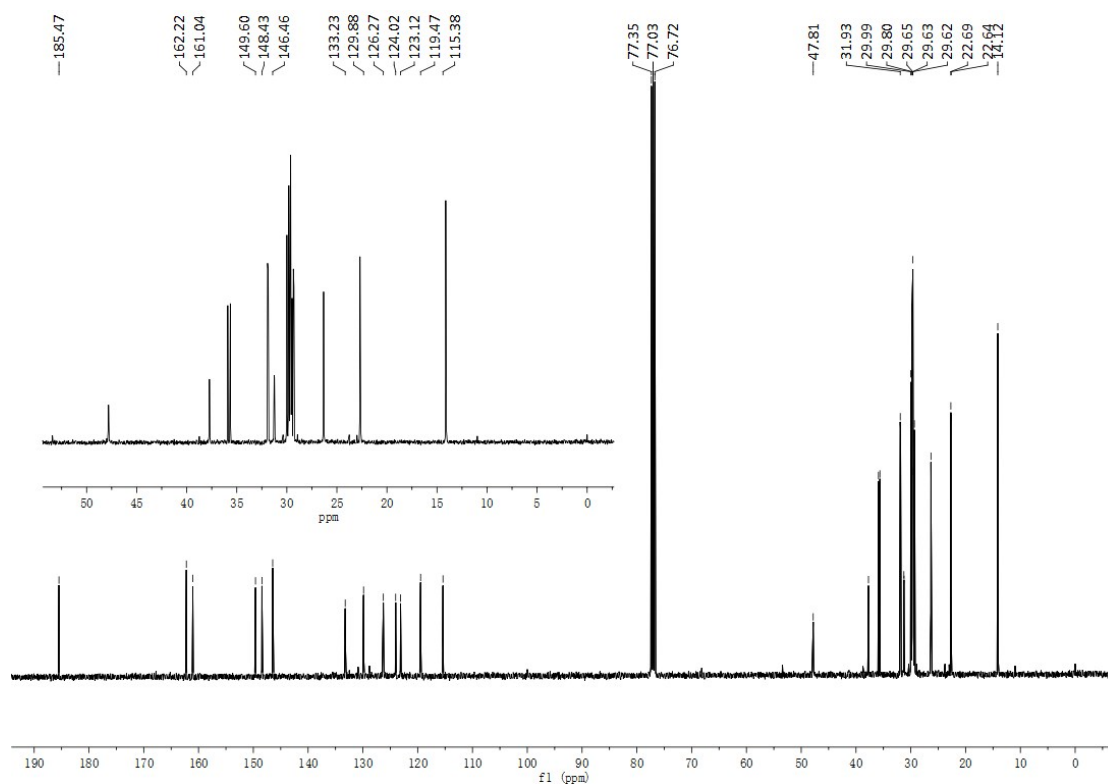


Figure S24. ¹³C NMR spectrum of **DPP-O^{••}** (100 MHz, CDCl₃, 300 K).

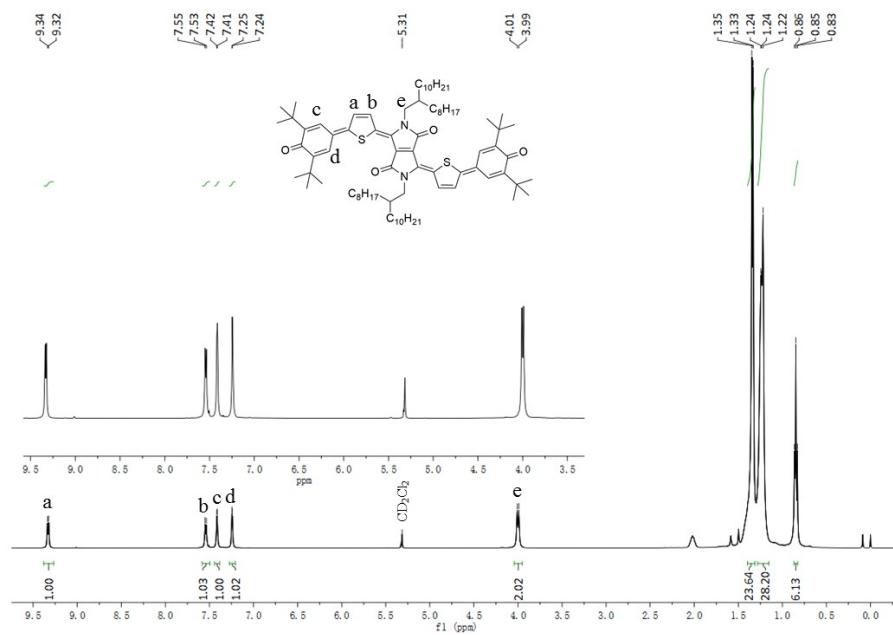


Figure S25. ¹H NMR spectrum of **DPP-S^{••}** (400 MHz, CD₂Cl₂, 300 K).

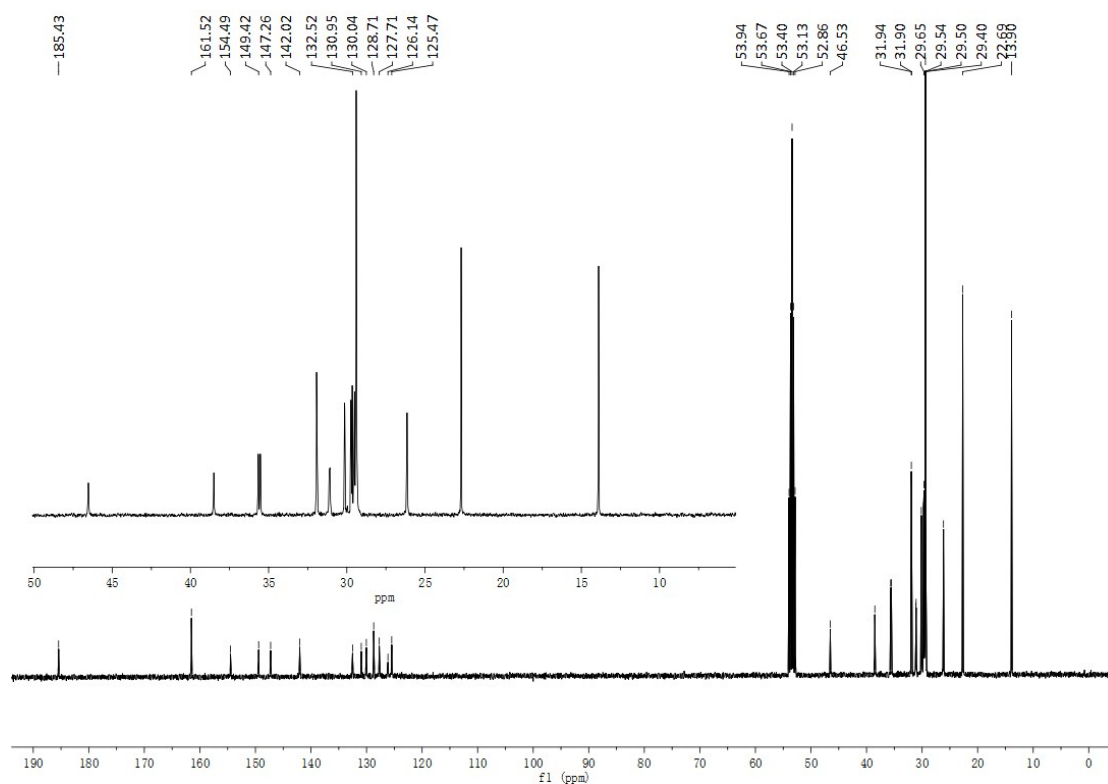


Figure S26. ¹³C NMR spectrum of **DPP-S^{••}** (100 MHz, CD₂Cl₂, 300 K).

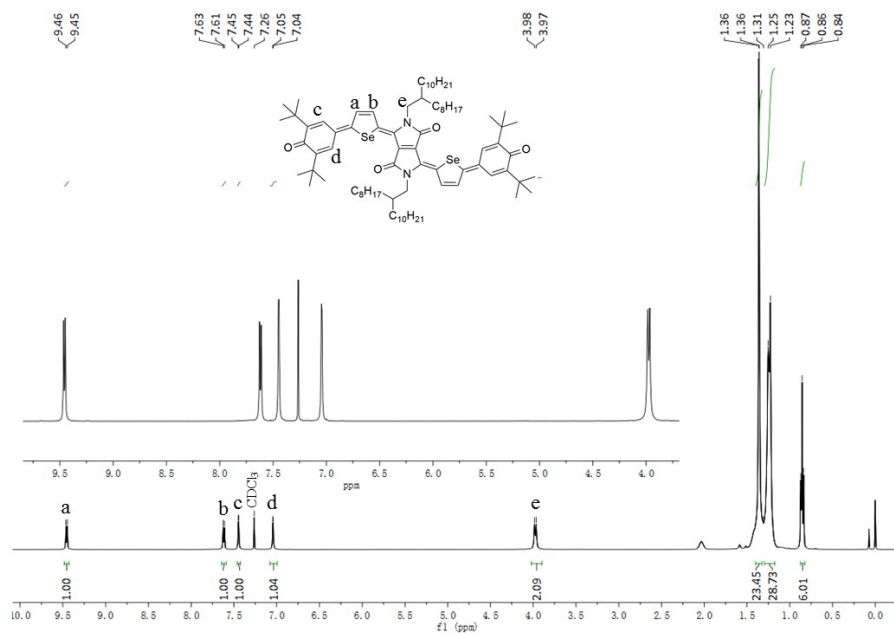


Figure S27. ¹H NMR spectrum of DPP-Se^{••} (400 MHz, CDCl₃, 300 K).

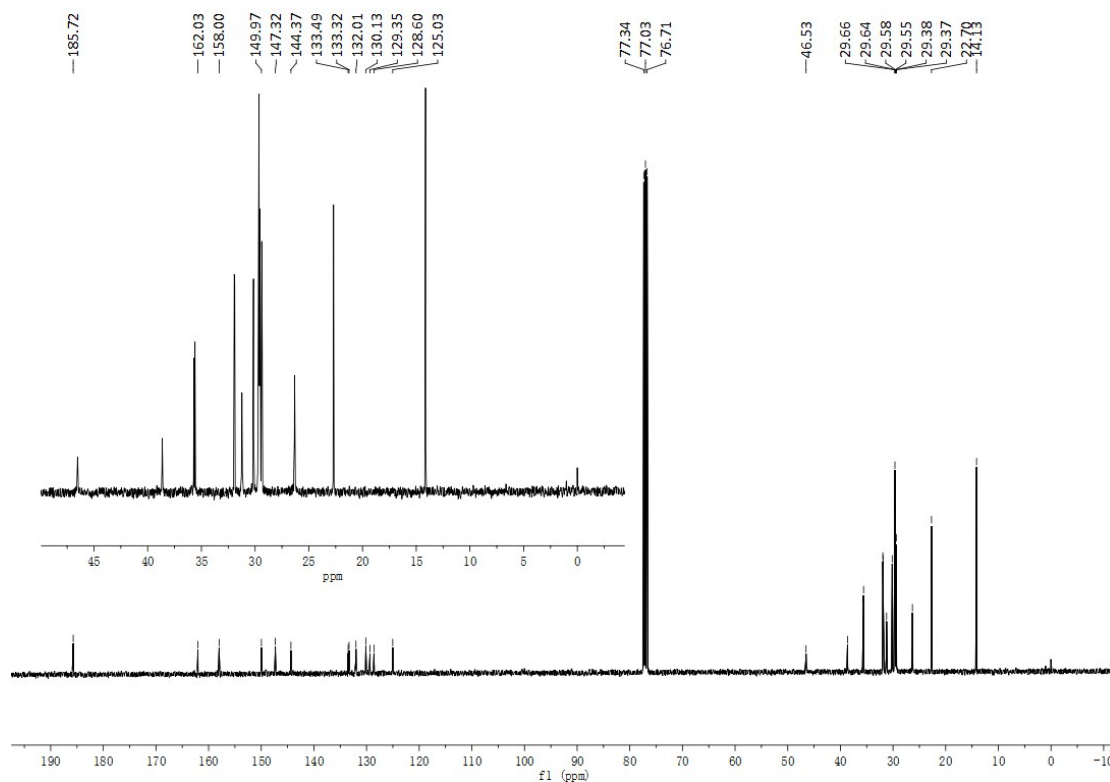


Figure S28. ¹³C NMR spectrum of DPP-Se^{••} (100 MHz, CDCl₃, 300 K).

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11. Coordinates for calculated geometries

DPP-O[•] CS

C	1.12247600	-1.38468500	0.00031100
C	0.69045500	-0.02190400	0.00034500
C	-0.69048900	0.02189100	0.00034100
C	-1.21365600	-1.35051700	0.00029300
N	-0.04265300	-2.15682100	0.00031200
C	1.21362000	1.35050600	0.00034200
N	0.04261600	2.15680900	0.00036700
C	-1.12250900	1.38467200	0.00034700
O	-2.34556100	-1.80963000	0.00028200
O	2.34552400	1.80962300	0.00032700
C	-0.14755600	-3.60205400	0.00035800
C	0.14750400	3.60204200	0.00043500
H	0.31354800	-4.03477500	-0.89462600
H	0.31355200	-4.03468800	0.89538800
H	-1.21374000	-3.83494600	0.00036700
H	-0.31361100	4.03476800	-0.89454400
H	-0.31361100	4.03465700	0.89547100
H	1.21368400	3.83494700	0.00044700
C	2.42126500	-1.86735200	0.00027000
C	3.01123100	-3.16300800	0.00029000
C	4.37352000	-2.99307800	0.00020300
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C	4.63756400	-1.59415500	0.00013000
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C	-2.42128700	1.86734400	0.00029900
C	-3.01124200	3.16300300	0.00029400
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H	-2.48113000	4.10246400	0.00029200
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C	7.08599700	-1.52973900	-0.00003600
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H	-7.09448200	-3.05588500	2.17474700
C	-7.59848600	-3.40959700	-1.26762000

H	-8.64327300	-3.09852600	-1.30265300
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H	-8.92566100	3.47430600	-0.88981900
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C	-10.43116200	1.19968600	-1.26748100
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C	-10.43130500	1.19959700	1.26708800
H	-11.39304300	1.72742800	1.26865000
H	-10.62260300	0.12656500	1.30119900
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DPP-O" OS

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H	4.79236800	-1.02777800	0.00001600
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C	-9.62689000	-1.57050500	0.00000200
C	-10.43038000	-1.18246400	-1.26729400
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H	-10.61928900	-0.10896100	-1.30014600
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H	-7.07180200	3.04958900	2.17542700
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H	-8.61948800	3.10736100	-1.30127000
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H	-7.07231600	3.04962900	-2.17536600

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H	-5.44423000	4.48788100	-0.00012600
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C	9.46517000	3.10391100	0.00014600
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H	11.39310100	1.70831700	1.26987100
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C	5.42030400	-3.39200100	0.00017500
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H	4.85787900	-3.07207200	-0.88332800
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C	7.57176200	-3.40881200	1.26750800
H	7.52251200	-4.50474400	1.27052800
H	8.61939200	-3.10731800	1.30148900
H	7.07216200	-3.04951500	2.17547700
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H	7.07194300	-3.04970500	-2.17531600
H	8.61926100	-3.10742800	-1.30147900
H	7.52238600	-4.50485300	-1.27028500
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O	9.28918800	-1.29261700	0.00015300

DPP-O* OT

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C	1.09528600	1.37504900	-0.00012300

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O	-2.37050200	1.79020100	0.00001700
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C	-0.18016700	3.58749400	0.00015300
H	-0.27595000	-4.02521100	0.89465800
H	-0.27598300	-4.02531600	-0.89489300
H	1.24925300	-3.80747300	-0.00015400
H	0.27608300	4.02519600	0.89495200
H	0.27591400	4.02545900	-0.89460300
H	-1.24922200	3.80754100	0.00029100
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C	-2.97379100	-3.18545300	0.00016600
C	-4.36790100	-3.01983000	0.00014600
H	-2.44197200	-4.12351000	0.00028300
C	-4.61907800	-1.64897000	-0.00002200
H	-5.10844000	-3.80623900	0.00029000
C	2.41580100	1.91059700	-0.00010200
C	2.97382200	3.18551000	-0.00017500
C	4.36793400	3.01988000	-0.00015900
H	2.44200400	4.12356900	-0.00027000
C	4.61909500	1.64901700	-0.00010000
H	5.10847900	3.80628200	-0.00019400
C	-5.81943700	-0.87137600	-0.00005800
C	-7.08052000	-1.53111700	-0.00000800
C	-5.75932300	0.54937800	-0.00016400
C	-8.26622600	-0.84280300	0.00011600
H	-7.08564600	-2.61450500	-0.00012200
C	-6.89903400	1.31953300	-0.00002800
H	-4.77715700	1.00759800	-0.00034800
C	-8.21643000	0.63976400	0.00033000
C	5.81944100	0.87140600	-0.00007500
C	7.08054200	1.53111800	-0.00000200
C	5.75929000	-0.54934500	-0.00013000
C	8.26623000	0.84277200	0.00011300
H	7.08570100	2.61450600	-0.00005600
C	6.89898300	-1.31952800	-0.00001600
H	4.77711100	-1.00753600	-0.00025800
C	8.21639700	-0.63979300	0.00021000
C	-9.62693300	-1.55679100	0.00012100
C	-10.42880000	-1.16479100	-1.26722200
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H	-9.88725100	-1.45436400	-2.17605600
C	-10.42846900	-1.16539000	1.26786100

H	-9.88668800	-1.45541000	2.17641100
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H	-8.94346800	-3.45347500	-0.89009800
H	-8.94330000	-3.45391200	0.88928200
H	-10.46550200	-3.55263000	-0.00027900
C	-6.84281700	2.85502600	-0.00017900
C	-7.54344900	3.40802500	1.26768200
H	-7.48427200	4.50340400	1.27114900
H	-8.59372200	3.11579600	1.30113800
H	-7.04728800	3.04399400	2.17560300
C	-7.54445100	3.40779800	-1.26757800
H	-8.59475900	3.11559000	-1.30014200
H	-7.48526200	4.50317400	-1.27129400
H	-7.04902500	3.04359600	-2.17583400
C	-5.39260500	3.37664900	-0.00080000
H	-4.83163800	3.05330400	0.88218300
H	-4.83232700	3.05309300	-0.88414800
H	-5.40994600	4.47263100	-0.00092100
C	9.62696700	1.55669500	0.00019300
C	9.47223300	3.09094400	-0.00001600
H	8.94360900	3.45352800	-0.88979700
H	8.94345800	3.45375600	0.88958400
H	10.46565600	3.55247900	0.00001500
C	10.42848400	1.16507700	1.26787500
H	10.61445000	0.09102500	1.29986600
H	11.39256100	1.68839400	1.27107000
H	9.88674500	1.45503200	2.17647100
C	10.42879500	1.16477400	-1.26719800
H	10.61478600	0.09071700	-1.29888400
H	9.88727500	1.45450600	-2.17599800
H	11.39286500	1.68810200	-1.27027500
C	6.84274300	-2.85501900	-0.00010400
C	5.39252500	-3.37662800	-0.00044400
H	4.83172500	-3.05326300	0.88263900
H	4.83208400	-3.05307700	-0.88369100
H	5.40984900	-4.47260900	-0.00055500
C	7.54359800	-3.40798100	1.26765000
H	7.48440600	-4.50335900	1.27116600
H	8.59388100	-3.11576700	1.30090300
H	7.04760700	-3.04391100	2.17564800
C	7.54414300	-3.40785100	-1.26761000
H	7.04855100	-3.04368100	-2.17578900

H	8.59444500	-3.11564800	-1.30037900
H	7.48494300	-4.50322600	-1.27127100
O	-3.42525000	-0.98808000	-0.00015300
O	3.42526500	0.98813700	-0.00002100
O	-9.27543600	1.30457900	0.00081400
O	9.27539100	-1.30463200	0.00048900

DPP-S^o CS

C	1.40796600	1.11191100	0.00025900
C	0.67782900	-0.12232700	0.00019600
C	-0.67782000	0.12242600	0.00019300
C	-0.88840700	1.56969400	0.00033200
N	0.42186900	2.11395700	0.00034400
C	0.88841500	-1.56959300	0.00021800
N	-0.42185900	-2.11385400	0.00017500
C	-1.40795700	-1.11180700	0.00017600
O	-1.90734200	2.24675400	0.00042900
O	1.90735700	-2.24665000	0.00026300
C	0.58392100	3.55613900	0.00073400
C	-0.58391500	-3.55603400	0.00016800
C	2.78682600	1.30580500	0.00017400
C	-2.78681400	-1.30572700	0.00019600
C	-3.53023800	-2.52816500	0.00025800
C	-4.88904000	-2.36864000	0.00018200
C	-5.32759500	-1.01061000	0.00007100
S	-3.92154600	0.06182300	0.00007200
C	3.53028000	2.52822700	-0.00011800
C	4.88907800	2.36866900	-0.00022000
C	5.32760100	1.01062700	-0.00002300
S	3.92152900	-0.06177400	0.00031500
H	1.11226100	3.89917000	0.89637800
H	1.11163500	3.89976100	-0.89505600
H	-0.42351500	3.97578700	0.00120300
H	-1.11191400	-3.89937000	0.89589900
H	0.42352000	-3.97568600	0.00014400
H	-1.11197200	-3.89934900	-0.89553500
H	-3.06346100	-3.50132100	0.00033800
H	-5.57622000	-3.20572200	0.00024600
H	3.06353200	3.50139600	-0.00036300
H	5.57627100	3.20573900	-0.00050500
C	6.64306800	0.53166400	-0.00009200
C	6.92436200	-0.87781600	0.00004500

C	7.75841100	1.44101500	-0.00033300
C	8.18816900	-1.38647400	0.00010200
H	6.07747500	-1.55507600	0.00005900
C	9.05606500	1.02658800	-0.00028600
H	7.54155000	2.50116500	-0.00057100
C	9.33827700	-0.43656000	0.00014200
C	-6.64307100	-0.53166900	-0.00000900
C	-7.75839800	-1.44104100	-0.00024600
C	-6.92438800	0.87780300	0.00006800
C	-9.05605800	-1.02664000	-0.00025100
H	-7.54151100	-2.50118600	-0.00048800
C	-8.18820400	1.38644000	0.00008800
H	-6.07751300	1.55507800	0.00012300
C	-9.33829200	0.43651000	0.00016200
C	8.46335200	-2.89841900	0.00018000
C	10.23325000	2.01603500	-0.00061400
C	9.26627200	-3.28784400	-1.26728400
H	9.44926900	-4.36940000	-1.26910900
H	8.70249800	-3.04228100	-2.17551800
H	10.22672600	-2.77235200	-1.30131200
C	9.26576100	-3.28783300	1.26796100
H	9.44872600	-4.36939300	1.26987400
H	10.22620100	-2.77234300	1.30236500
H	8.70163300	-3.04224000	2.17597000
C	7.15912900	-3.72045000	-0.00008200
H	6.54665500	-3.52713600	0.88845700
H	6.54699500	-3.52709500	-0.88884800
H	7.40760900	-4.78735900	-0.00005600
C	11.09993000	1.80456500	-1.26795200
H	10.50919600	1.97508300	-2.17631900
H	11.93216100	2.51926100	-1.27021600
H	11.50896700	0.79423900	-1.30186400
C	11.09975600	1.80571100	1.26701700
H	10.50889500	1.97699500	2.17515900
H	11.50882200	0.79543000	1.30187900
H	11.93194700	2.52045800	1.26876400
C	9.75416800	3.48145700	-0.00131100
H	9.16015400	3.72225800	-0.89127100
H	9.16011300	3.72310200	0.88839300
H	10.62573600	4.14500100	-0.00160100
C	-8.46341200	2.89838300	0.00010700
C	-7.15919600	3.72043100	-0.00017200
H	-6.54675100	3.52719000	0.88840400
H	-6.54702300	3.52702100	-0.88890000

H	-7.40768200	4.78733700	-0.00022700
C	-9.26584600	3.28784700	1.26786300
H	-9.44886000	4.36940000	1.26970300
H	-10.22626500	2.77232300	1.30229600
H	-8.70169500	3.04234500	2.17588100
C	-9.26631200	3.28773800	-1.26738600
H	-10.22675300	2.77222500	-1.30142000
H	-9.44931900	4.36929300	-1.26925200
H	-8.70251200	3.04215300	-2.17559700
C	-10.23321600	-2.01611900	-0.00062000
C	-9.75407200	-3.48152500	-0.00123100
H	-9.15997900	-3.72234400	-0.89113400
H	-9.16007600	-3.72311500	0.88852800
H	-10.62561500	-4.14510100	-0.00156100
C	-11.09979700	-1.80578800	1.26696400
H	-11.50889600	-0.79552000	1.30178200
H	-11.93196900	-2.52055800	1.26867900
H	-10.50897100	-1.97704100	2.17513100
C	-11.09982000	-1.80473500	-1.26801400
H	-11.50892900	-0.79444000	-1.30198500
H	-10.50901500	-1.97522900	-2.17633800
H	-11.93199900	-2.51949300	-1.27031700
O	10.50585800	-0.85684000	0.00051300
O	-10.50587800	0.85676500	0.00057200

DPP-S OS**

C	-1.39325500	-1.11011900	-0.00005500
C	-0.68726600	0.11882400	-0.00004300
C	0.68726600	-0.11882400	-0.00003800
C	0.90471300	-1.55749600	-0.00006800
N	-0.41049300	-2.10915800	-0.00006800
C	-0.90471300	1.55749600	-0.00008900
N	0.41049200	2.10915800	-0.00007900
C	1.39325400	1.11011900	-0.00005200
O	1.92208400	-2.23934700	-0.00009100
O	-1.92208400	2.23934700	-0.00012500
C	-0.56729900	-3.55181500	-0.00014900
C	0.56729900	3.55181400	-0.00020300
C	-2.78958800	-1.32542800	-0.00003000
C	2.78958800	1.32542700	-0.00000800
C	3.51706100	2.53841200	0.00004800
C	4.89055000	2.37909100	0.00007100
C	5.31937900	1.03408400	0.00002700
S	3.92050100	-0.03586900	-0.00004200

C	-3.51706100	-2.53841200	-0.00001900
C	-4.89055100	-2.37909100	-0.00000500
C	-5.31937900	-1.03408400	-0.00001200
S	-3.92050100	0.03586900	-0.00003900
H	-1.09379500	-3.89771900	0.89543300
H	-1.09386200	-3.89760900	-0.89573200
H	0.44235400	-3.96632800	-0.00021000
H	1.09374600	3.89775300	0.89539400
H	-0.44235400	3.96632800	-0.00033100
H	1.09391000	3.89757400	-0.89577100
H	3.05076200	3.51180200	0.00007700
H	5.57552700	3.21809100	0.00012100
H	-3.05076200	-3.51180300	-0.00002200
H	-5.57552700	-3.21809100	0.00000800
C	-6.65007800	-0.53885300	-0.00000300
C	-7.76189600	-1.44130400	0.00003600
C	-6.91856800	0.86590000	-0.00002500
C	-9.06227800	-1.01930400	0.00005200
H	-7.54986100	-2.50235200	0.00005700
C	-8.18459500	1.38322300	-0.00000600
H	-6.06924700	1.53976600	-0.00005800
C	-9.33457500	0.44123200	0.00002500
C	6.65007800	0.53885400	0.00003500
C	6.91856800	-0.86590000	-0.00001900
C	7.76189600	1.44130500	0.00009100
C	8.18459600	-1.38322200	-0.00000500
H	6.06924800	-1.53976600	-0.00007500
C	9.06227800	1.01930500	0.00010600
H	7.54986000	2.50235300	0.00012200
C	9.33457600	-0.44123100	0.00007200
C	-10.24233100	-2.00502600	0.00010400
C	-8.44902200	2.89707700	-0.00002600
C	-11.10819000	-1.79093400	1.26769300
H	-11.94142600	-2.50439100	1.27051300
H	-10.51767100	-1.96176900	2.17610900
H	-11.51550100	-0.77988800	1.30086700
C	-11.10819300	-1.79106500	-1.26750600
H	-11.94142800	-2.50452400	-1.27025000
H	-11.51550700	-0.78002300	-1.30078200
H	-10.51767700	-1.96199300	-2.17590600
C	-9.76827800	-3.47223200	0.00017700
H	-9.17523700	-3.71577900	-0.88959700
H	-9.17524200	-3.71569300	0.88997700
H	-10.64239800	-4.13237300	0.00020700

C	-9.24904600	3.29186200	1.26771000
H	-8.68776800	3.04082800	2.17597200
H	-9.42281900	4.37489900	1.27037600
H	-10.21378100	2.78435300	1.30090000
C	-9.24920200	3.29180000	-1.26768100
H	-8.68803500	3.04072900	-2.17600000
H	-10.21393900	2.78428300	-1.30073000
H	-9.42298400	4.37483500	-1.27037300
C	-7.13928100	3.71058900	-0.00012600
H	-6.52813200	3.51367900	0.88846700
H	-6.52825000	3.51364800	-0.88879500
H	-7.38115800	4.77898400	-0.00012900
C	10.24233100	2.00502600	0.00015800
C	9.76828200	3.47223400	0.00012400
H	9.17528300	3.71573000	-0.88969100
H	9.17520400	3.71574600	0.88988400
H	10.64240300	4.13237200	0.00015800
C	11.10825300	1.79098800	-1.26739900
H	11.94149300	2.50444200	-1.27014300
H	11.51556200	0.77994200	-1.30059800
H	10.51778000	1.96186800	-2.17583600
C	11.10813100	1.79100700	1.26780000
H	11.51544100	0.77996300	1.30105100
H	11.94136700	2.50446400	1.27061800
H	10.51756900	1.96189400	2.17617800
C	8.44902200	-2.89707600	-0.00007600
C	7.13927900	-3.71058600	-0.00028100
H	6.52808400	-3.51371400	0.88828900
H	6.52829600	-3.51360500	-0.88897300
H	7.38115500	-4.77898200	-0.00031800
C	9.24926900	-3.29174500	-1.26770600
H	10.21400800	-2.78422700	-1.30068200
H	9.42304900	-4.37478000	-1.27043700
H	8.68814900	-3.04063400	-2.17604400
C	9.24897700	-3.29192000	1.26768500
H	10.21371300	-2.78441600	1.30094700
H	8.68765300	-3.04092200	2.17592800
H	9.42274400	-4.37495700	1.27031300
O	-10.50440100	0.86864100	0.00010200
O	10.50440200	-0.86863800	0.00005800

DPP-S" OT

C	1.37927700	-1.10544100	0.07512600
C	0.69768200	0.11629400	0.05682700

C	-0.69765200	-0.11635200	0.05688000
C	-0.92048800	-1.54711900	0.06146000
N	0.40243300	-2.10409100	0.07724000
C	0.92049200	1.54707200	0.06135200
N	-0.40241900	2.10403100	0.07721300
C	-1.37926400	1.10536900	0.07521400
O	-1.93330600	-2.23614200	0.04352600
O	1.93330900	2.23609900	0.04329100
C	0.55821600	-3.54607800	0.03321400
C	-0.55822300	3.54601600	0.03308500
C	2.79374100	-1.34192700	0.09600400
C	-2.79371100	1.34185500	0.09618400
C	-3.50489700	2.54101200	0.20926600
C	-4.89322100	2.38249200	0.19629900
C	-5.31214900	1.05493000	0.07272800
S	-3.91973200	-0.00825400	-0.02206400
C	3.50493700	-2.54110900	0.20876200
C	4.89325900	-2.38256500	0.19580100
C	5.31217600	-1.05497600	0.07254600
S	3.91972500	0.00822400	-0.02193800
H	1.15395200	-3.85619100	-0.83100200
H	1.01195700	-3.93215300	0.95236500
H	-0.44933200	-3.95590100	-0.05858300
H	-1.15421300	3.85602500	-0.83099200
H	0.44929600	3.95583700	-0.05903000
H	-1.01170500	3.93218300	0.95232500
H	-3.03764200	3.50874100	0.31163400
H	-5.57656800	3.21833200	0.28415700
H	3.03770300	-3.50887500	0.31085700
H	5.57662800	-3.21841700	0.28338200
C	6.65733500	-0.54421600	0.02730000
C	7.76603700	-1.43948800	0.05289900
C	6.91249400	0.85447500	-0.04441000
C	9.06863100	-1.01093600	0.01185800
H	7.55864500	-2.50028700	0.10134600
C	8.18006100	1.37945700	-0.08908600
H	6.06042200	1.52435100	-0.05886400
C	9.33052000	0.44577000	-0.06210900
C	-6.65732500	0.54420400	0.02738000
C	-6.91251300	-0.85447600	-0.04438200
C	-7.76600800	1.43949800	0.05290600
C	-8.18009300	-1.37943300	-0.08906700
H	-6.06046200	-1.52437800	-0.05883500
C	-9.06861400	1.01097300	0.01183200

H	-7.55860800	2.50029900	0.10125700
C	-9.33053200	-0.44573100	-0.06197900
C	10.25169000	-1.99195700	0.03896700
C	8.43330600	2.89314100	-0.16364300
C	11.09688300	-1.83486900	-1.25095700
H	11.93108500	-2.54691400	-1.23400800
H	10.49258400	-2.04788700	-2.14117300
H	11.50172200	-0.82592300	-1.33674200
C	11.13650800	-1.71538200	1.28141700
H	11.97131400	-2.42653700	1.30509700
H	11.54161900	-0.70313700	1.25959800
H	10.56079000	-1.84363000	2.20615900
C	9.78355200	-3.45918400	0.11559000
H	9.20529200	-3.66238900	1.02491900
H	9.17814300	-3.74668100	-0.75236900
H	10.66046400	-4.11532400	0.13331400
C	9.21077500	3.23291400	-1.46120400
H	8.63787800	2.93492200	-2.34772400
H	9.37553700	4.31583800	-1.51779500
H	10.17896000	2.73146100	-1.48520400
C	9.25071300	3.35159800	1.07134800
H	8.70645800	3.13864800	1.99944400
H	10.21994300	2.85322100	1.11166700
H	9.41548900	4.43483600	1.02121200
C	7.11815100	3.69793700	-0.18070500
H	6.49449800	3.45616600	-1.04924400
H	6.52233300	3.53977100	0.72578300
H	7.35315900	4.76647200	-0.23471700
C	-10.25164800	1.99202600	0.03882100
C	-9.78347800	3.45925800	0.11516100
H	-9.20527000	3.66264400	1.02448300
H	-9.17801000	3.74655400	-0.75282300
H	-10.66037500	4.11542400	0.13270000
C	-11.13644800	1.71569600	1.28134100
H	-11.97122700	2.42688400	1.30491100
H	-11.54158200	0.70345800	1.25970800
H	-10.56070400	1.84409100	2.20604700
C	-11.09688300	1.83473600	-1.25105600
H	-11.50174900	0.82578600	-1.33665600
H	-11.93106700	2.54680300	-1.23420600
H	-10.49260500	2.04759000	-2.14132600
C	-8.43336500	-2.89310800	-0.16366900
C	-7.11822200	-3.69792500	-0.18099700
H	-6.49469400	-3.45608900	-1.04960800

H	-6.52226500	-3.53985500	0.72541600
H	-7.35325800	-4.76645100	-0.23506700
C	-9.25059000	-3.35163700	1.07141800
H	-10.21980800	-2.85325000	1.11191400
H	-9.41537600	-4.43487000	1.02123200
H	-8.70619600	-3.13875000	1.99944600
C	-9.21105200	-3.23278200	-1.46112400
H	-10.17922100	-2.73128700	-1.48494500
H	-8.63828600	-2.93476900	-2.34772100
H	-9.37587100	-4.31569400	-1.51774300
O	10.50210000	0.87922400	-0.10101800
O	-10.50212100	-0.87918200	-0.10064200

DPP-Se^{••} CS

C	1.44230600	-1.06727500	-0.00053500
C	0.67281100	0.14228800	-0.00050100
C	-0.67280700	-0.14240500	-0.00049900
C	-0.83803900	-1.59304300	-0.00061100
N	0.48405300	-2.09969100	-0.00064900
C	0.83804600	1.59292900	-0.00056700
N	-0.48404900	2.09957100	-0.00052500
C	-1.44229600	1.06715800	-0.00049100
O	-1.84299000	-2.29552900	-0.00071200
O	1.84299100	2.29542300	-0.00063200
C	0.68922100	-3.53672200	-0.00106700
C	-0.68924400	3.53659400	-0.00075300
H	1.22797600	-3.86311500	-0.89655700
H	1.22752900	-3.86369700	0.89451400
H	-0.30466300	-3.98756900	-0.00145400
H	-1.22775700	3.86314800	-0.89633800
H	-1.22781900	3.86337900	0.89473300
H	0.30462500	3.98747300	-0.00079600
C	-2.82427100	1.20341700	-0.00037900
C	-3.60954000	2.39846700	-0.00036600
C	-4.96945500	2.24383000	-0.00025300
H	-3.15919700	3.38040100	-0.00040600
C	-5.46303500	0.90587500	-0.00013600
H	-5.63568600	3.09897700	-0.00022300
C	2.82429000	-1.20351200	-0.00036000
C	3.60959000	-2.39854600	-0.00021000
C	4.96950600	-2.24387300	-0.00001900
H	3.15929000	-3.38049700	-0.00018900
C	5.46305400	-0.90591200	0.00000000
H	5.63574100	-3.09901600	0.00011400

C	6.79781200	-0.49493000	0.00016800
C	7.87671300	-1.44850500	0.00033000
C	7.13956300	0.90183000	0.00015900
C	9.18987900	-1.08698200	0.00036400
H	7.61725400	-2.49896200	0.00042000
C	8.42141200	1.35980600	0.00027900
H	6.32227500	1.61538000	0.00003400
C	9.53198900	0.36370200	0.00034100
C	-6.79779900	0.49493600	0.00000900
C	-7.13959400	-0.90181800	0.00009300
C	-7.87667100	1.44855200	0.00009900
C	-8.42145400	-1.35975100	0.00025800
H	-6.32231900	-1.61538500	0.00004100
C	-9.18984500	1.08706900	0.00033700
H	-7.61716700	2.49899800	-0.00004500
C	-9.53200400	-0.36360500	0.00038500
Se	3.99699100	0.30738400	-0.00025400
Se	-3.99699600	-0.30746200	-0.00017900
C	10.32605700	-2.12331200	0.00048300
C	11.20048800	-1.94787600	1.26797800
H	12.00249500	-2.69631500	1.27014000
H	11.65098700	-0.95534200	1.30229400
H	10.60314100	-2.09413000	2.17624300
C	11.20061900	-1.94788800	-1.26696700
H	10.60333400	-2.09422500	-2.17525600
H	11.65107400	-0.95533800	-1.30127200
H	12.00264900	-2.69630000	-1.26901200
C	9.78773300	-3.56796700	0.00042600
H	9.18431600	-3.78478900	0.89019600
H	9.18431600	-3.78468400	-0.88936400
H	10.63154900	-4.26645700	0.00040000
C	8.75605000	2.85945600	0.00030100
C	9.57314100	3.21713100	1.26787100
H	10.51233400	2.66384800	1.30205300
H	9.79900300	4.29054000	1.26965200
H	9.00001300	2.99408900	2.17605600
C	9.57326000	3.21722900	-1.26717200
H	9.00027000	2.99410400	-2.17542200
H	9.79896600	4.29066900	-1.26891300
H	10.51253100	2.66407500	-1.30123000
C	7.48433100	3.73096900	0.00026800
H	6.86541400	3.56154800	-0.88879200
H	6.86532800	3.56150200	0.88926000
H	7.77311500	4.78764000	0.00030800

C	-10.32599700	2.12342800	0.00045500
C	-11.20036800	1.94793300	1.26802600
H	-10.60293700	2.09418400	2.17623200
H	-12.00237300	2.69637200	1.27025200
H	-11.65085400	0.95539600	1.30232500
C	-9.78763700	3.56807000	0.00052800
H	-9.18407800	3.78471300	0.89024100
H	-9.18434900	3.78493700	-0.88931900
H	-10.63143300	4.26658300	0.00073100
C	-11.20062400	1.94809200	-1.26691700
H	-11.65112900	0.95556200	-1.30123800
H	-12.00262400	2.69653800	-1.26890400
H	-10.60341400	2.09440600	-2.17526200
C	-8.75613200	-2.85939000	0.00035000
C	-7.48442600	-3.73092100	0.00026100
H	-6.86555700	-3.56154100	-0.88884200
H	-6.86536800	-3.56143100	0.88920900
H	-7.77322600	-4.78758900	0.00035200
C	-9.57318000	-3.21708400	1.26794900
H	-9.79890000	-4.29052000	1.26977800
H	-9.00006800	-2.99391600	2.17611200
H	-10.51244200	-2.66391900	1.30210200
C	-9.57338800	-3.21711600	-1.26709900
H	-10.51258600	-2.66383700	-1.30118300
H	-9.00037800	-2.99411000	-2.17536800
H	-9.79925000	-4.29052500	-1.26880800
O	10.71529600	0.73643100	0.00045000
O	-10.71532000	-0.73629200	0.00045000

DPP-Se^{II} OS

C	-1.42961300	-1.06595000	-0.00005500
C	-0.68105300	0.13958600	-0.00007100
C	0.68105200	-0.13959000	-0.00006400
C	0.85221300	-1.58265500	-0.00003400
N	-0.47455000	-2.09549200	-0.00003500
C	-0.85221400	1.58265100	-0.00013800
N	0.47454900	2.09548800	-0.00023200
C	1.42961200	1.06594600	-0.00020900
O	1.85570800	-2.28945200	0.00002200
O	-1.85570900	2.28944800	-0.00006900
C	-0.67542600	-3.53300700	0.00004200
C	0.67542500	3.53300300	0.00014600
H	-1.21279000	-3.86175100	0.89550900
H	-1.21283200	-3.86183200	-0.89536900

H	0.32042400	-3.97966300	0.00004100
H	1.21336900	3.86144100	0.89537200
H	1.21225200	3.86213400	-0.89550500
H	-0.32042400	3.97965900	0.00089300
C	2.82755000	1.21940200	-0.00038600
C	3.59868200	2.40588200	-0.00105800
C	4.97174500	2.25092000	-0.00102300
H	3.14918100	3.38823300	-0.00171400
C	5.45571000	0.92419900	-0.00034800
H	5.63622600	3.10753600	-0.00166600
C	-2.82755200	-1.21940500	-0.00004200
C	-3.59868300	-2.40588500	-0.00003500
C	-4.97174600	-2.25092300	-0.00001000
H	-3.14918200	-3.38823700	-0.00005600
C	-5.45571100	-0.92420200	0.00000400
H	-5.63622700	-3.10753900	-0.00001700
C	6.80439600	0.49983500	-0.00024200
C	7.13519100	-0.89318800	-0.00026700
C	7.88022500	1.44737900	-0.00004800
C	8.41935000	-1.35829100	-0.00019000
H	6.31596500	-1.60419500	-0.00051700
C	9.19615900	1.07967100	0.00012900
H	7.62484600	2.49876300	0.00016100
C	9.52999600	-0.36897400	0.00001100
C	-6.80439600	-0.49983600	0.00002200
C	-7.88022700	-1.44737900	0.00010600
C	-7.13519000	0.89318700	-0.00004000
C	-9.19616000	-1.07966900	0.00012400
H	-7.62485000	-2.49876300	0.00017000
C	-8.41934800	1.35829200	-0.00002900
H	-6.31596400	1.60419300	-0.00010500
C	-9.52999500	0.36897600	0.00004200
Se	-3.99606000	0.28658900	-0.00001100
Se	3.99606000	-0.28659200	0.00036600
C	8.74498700	-2.85991400	-0.00031000
C	9.56020400	-3.22231500	1.26721800
H	9.77841500	-4.29727800	1.26954200
H	10.50325000	-2.67555100	1.30045000
H	8.98925100	-2.99469100	2.17561900
C	9.56014700	-3.22212800	-1.26792700
H	8.98916500	-2.99434100	-2.17626900
H	10.50320600	-2.67538300	-1.30110500
H	9.77833200	-4.29709600	-1.27043400
C	7.46838800	-3.72450100	-0.00034000

H	6.85034200	-3.55207300	0.88869600
H	6.85031800	-3.55198400	-0.88934200
H	7.75172400	-4.78262200	-0.00039800
C	10.33472700	2.11312400	0.00051900
C	11.20888700	1.93541300	-1.26699200
H	10.61190800	2.08192100	-2.17543500
H	12.01180000	2.68282800	-1.26947000
H	11.65792200	0.94219200	-1.30049000
C	11.20857700	1.93476900	1.26815100
H	11.65760200	0.94153000	1.30125600
H	12.01149600	2.68217500	1.27120500
H	10.61138000	2.08081900	2.17652400
C	9.80046800	3.55940800	0.00081700
H	9.19795400	3.77832800	-0.88897700
H	9.19762400	3.77783800	0.89050800
H	10.64649000	4.25519700	0.00116100
C	-8.74498100	2.85991700	-0.00010700
C	-7.46837900	3.72449900	-0.00035800
H	-6.85017600	3.55206700	0.88856800
H	-6.85046600	3.55198200	-0.88946900
H	-7.75171100	4.78262100	-0.00036300
C	-9.55998900	3.22233400	1.26755100
H	-9.77817500	4.29730200	1.26991000
H	-10.50304300	2.67559300	1.30093300
H	-8.98889600	2.99469700	2.17586100
C	-9.56034800	3.22212000	-1.26759500
H	-10.50339900	2.67535200	-1.30062800
H	-9.77855700	4.29708200	-1.27005900
H	-8.98950200	2.99435200	-2.17602700
C	-10.33473100	-2.11311900	0.00023300
C	-9.80047700	-3.55940500	0.00037300
H	-9.19781800	-3.77817600	-0.88935900
H	-9.19778000	-3.77798800	0.89012600
H	-10.64650100	-4.25519100	0.00046300
C	-11.20872500	-1.93495600	1.26779300
H	-12.01164700	-2.68235900	1.27063900
H	-10.61163200	-2.08114900	2.17621100
H	-11.65774700	-0.94171800	1.30099900
C	-11.20874700	-1.93521100	-1.26734900
H	-11.65777500	-0.94198300	-1.30074700
H	-10.61166600	-2.08158200	-2.17574800
H	-12.01166400	-2.68262100	-1.27003400
O	-10.71556400	0.74758300	-0.00000100
O	10.71556400	-0.74757900	0.00007100

DPP-Se²⁺ OT

C	-1.41254300	1.06494000	0.00040900
C	-0.69252600	-0.13554100	0.00005800
C	0.69249200	0.13558600	0.00010900
C	0.87272800	1.56918100	0.00067100
N	-0.46147100	2.09093500	0.00064400
C	-0.87276600	-1.56913400	0.00038700
N	0.46143500	-2.09089100	0.00042900
C	1.41250800	-1.06489800	0.00026900
O	1.87316700	2.28147200	0.00101000
O	-1.87320600	-2.28142300	0.00069700
C	-0.65599800	3.52908900	0.00120000
C	0.65596100	-3.52904500	0.00118800
H	-1.19114200	3.86167100	-0.89417100
H	-1.19193900	3.86076100	0.89642500
H	0.34274800	3.96955700	0.00180600
H	1.19085100	-3.86180500	-0.89427100
H	1.19215200	-3.86054400	0.89632400
H	-0.34278500	-3.96951300	0.00212800
C	2.83109400	-1.24202000	0.00012400
C	3.58440300	-2.41881400	-0.00045800
C	4.97409000	-2.26366500	-0.00061800
H	3.13523500	-3.40137500	-0.00091400
C	5.44600600	-0.94977700	-0.00016300
H	5.63665100	-3.12191500	-0.00112700
C	-2.83112800	1.24205000	0.00028900
C	-3.58444800	2.41884000	-0.00009100
C	-4.97413200	2.26367700	-0.00026900
H	-3.13528800	3.40140300	-0.00033400
C	-5.44603900	0.94978300	-0.00001700
H	-5.63670100	3.12192100	-0.00057900
C	6.81151700	-0.50709400	-0.00020000
C	7.12765600	0.88188000	-0.00017000
C	7.88447600	-1.44653300	-0.00028300
C	8.41401300	1.35699600	-0.00031400
H	6.30527400	1.58883500	-0.00007300
C	9.20339000	-1.07005200	-0.00036000
H	7.63471000	-2.49918400	-0.00024100
C	9.52585700	0.37682300	-0.00042900
C	-6.81154000	0.50708300	-0.00007000
C	-7.88451400	1.44650500	-0.00013800
C	-7.12766600	-0.88189200	-0.00003900
C	-9.20341800	1.07001700	-0.00035300

H	-7.63477000	2.49916500	-0.00001900
C	-8.41401400	-1.35703400	-0.00015400
H	-6.30527200	-1.58883400	0.00011700
C	-9.52588100	-0.37687100	-0.00049400
Se	-3.99379600	-0.25795200	0.00044800
Se	3.99378100	0.25797200	0.00047200
C	8.72733800	2.86099100	-0.00027800
C	9.54007400	3.22953400	-1.26783400
H	9.74835300	4.30641800	-1.27075600
H	10.48801300	2.69120600	-1.29991600
H	8.97186400	2.99607900	-2.17644500
C	9.53975300	3.22947800	1.26749500
H	8.97133000	2.99600100	2.17595800
H	10.48769300	2.69115000	1.29976400
H	9.74810000	4.30635800	1.27053000
C	7.44417100	3.71609400	-0.00045000
H	6.82749600	3.53936800	-0.88951600
H	6.82729200	3.53946300	0.88849800
H	7.72000000	4.77615900	-0.00045400
C	10.34569100	-2.09866700	-0.00040700
C	11.21910300	-1.91639200	1.26725300
H	10.62267100	-2.06370700	2.17587600
H	12.02412000	-2.66145800	1.27040600
H	11.66493200	-0.92168800	1.29934600
C	11.21890800	-1.91638800	-1.26816700
H	11.66496600	-0.92177900	-1.30018000
H	12.02375400	-2.66164700	-1.27163000
H	10.62229600	-2.06337600	-2.17672900
C	9.81801600	-3.54750500	-0.00032500
H	9.21653000	-3.76908800	0.88939600
H	9.21646300	-3.76919300	-0.88998900
H	10.66749800	-4.23901900	-0.00033400
C	-8.72727900	-2.86105100	-0.00011700
C	-7.44407800	-3.71610100	0.00014500
H	-6.82721000	-3.53955300	-0.88882700
H	-6.82740000	-3.53924800	0.88918600
H	-7.71986100	-4.77617800	0.00027600
C	-9.53962300	-3.22963300	-1.26792500
H	-9.74790600	-4.30652600	-1.27092300
H	-10.48758300	-2.69134800	-1.30025200
H	-8.97116100	-2.99615800	-2.17636200
C	-9.54005100	-3.22960900	1.26740100
H	-10.48806200	-2.69140300	1.29939400
H	-9.74820400	-4.30651800	1.27037600

H	-8.97193500	-2.99604000	2.17604200
C	-10.34568100	2.09866900	-0.00050800
C	-9.81789100	3.54746000	-0.00021800
H	-9.21653800	3.76893900	0.88963200
H	-9.21615800	3.76914800	-0.88975000
H	-10.66731200	4.23904900	-0.00031000
C	-11.21866300	1.91661100	-1.26850600
H	-12.02354500	2.66182600	-1.27193300
H	-10.62186400	2.06386000	-2.17690000
H	-11.66465200	0.92198700	-1.30081400
C	-11.21934600	1.91631100	1.26692700
H	-11.66550000	0.92173900	1.29867900
H	-10.62303200	2.06314600	2.17571200
H	-12.02412400	2.66163800	1.27019600
O	-10.71383700	-0.76363000	-0.00094500
O	10.71382200	0.76357700	-0.00057900