Electronic supplementary information (ESI)

Intramolecular *versus* intermolecular electronic interaction between [5,6]-open and [6,6]-closed C_{60} adducts with exTTF

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Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C. J.; Ochterski, W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J. and Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Experimental Section

Spectroscopy: All NMR spectra were recorded respectively on a spectrometer (AV 300 or AV 500; Bruker) with a CryoProbe system, locked on deuterated solvents and referenced to the solvent peak. The 1D (^{1}H, ^{13}C and DEPT135) and 2D experiments (COSY, HMQC, and HMBC) were performed using standard experimental procedures from the Bruker library. Absorption spectra of all samples were recorded in toluene with a spectrometer (UV-3150; Shimadzu Corp.) using a quartz cell and 1-nm resolution. Matrix-assisted laser desorption-ionization time-of flight (MALDI-TOF) mass spectra were recorded with a mass spectrometer (BIFLEX-III; Bruker) using 1,1,4,4-tetraphenyl-1,3-butadiene as the matrix. Measurements were taken in both positive and negative ion modes.

Steady-state emission: Spectra were recorded on a fluorometer (vis detection, FluoroMax 3; Horiba Jobin Yvon, Inc.) and on a spectrometer (NIR detection, Fluorolog; Horiba Jobin Yvon, Inc.). Measurements were conducted at room temperature (r.t.).

Time resolved absorption: Femtosecond transient absorption studies were performed with 387 nm and 530 nm laser pulses (1 kHz, 150 fs pulse width) from an amplified Ti:Sapphire laser system (Clark-MXR, Inc.) with laser energy of 200 nJ. Nanosecond laser flash photolysis experiments were performed with a (355 and) 532 nm laser pulse from a Quanta-Ray CDR Nd:YAG system (6 ns pulse width) in a front face excitation geometry.

Time resolved emission: Fluorescence lifetimes were measured using a Fluorolog (Horiba Jobin Yvon, Inc.).

Electrochemistry: Differential pulse voltammetry (DPV) and cyclic voltammetry (CV) were conducted in *o*-DCB (CW-50 BAS Inc.). A conventional three-electrode cell consisting of a platinum working electrode, a platinum counter-electrode, and a saturated calomel reference electrode (SCE) or $Ag^{0/+}$ electrode was used for both measurements. 0.1 M $(n\text{-Bu})_4NPF_6$ was used as the supporting electrolyte. All potentials were corrected against Fc/Fc^{+}. DPV and CV were measured at respective scan rates of 20 and 50 $mV \bullet s^{-1}$.

Materials: [5,6]-$PC_{61}BM$ (**4a**), [6,6]-$PC_{61}BM$ (**4b**)[S1] and exTTF-OH[S2] were synthesized and characterized according to a procedure explained in the literature. C_{60} (>99.5%) was purchased from MTR Ltd. The other chemicals, all of which were of reagent grade, were purchased from Wako Pure Chemical Industries Ltd.

High pressure liquid chromatography: Preparative and analytical HPLC were performed respectively on a preparative Buckyprep column (ø20×100 mm; Cosmosil) and Buckyprep column (ø4.6×100 mm; Cosmosil). Toluene was used as eluent.

Synthesis of exTTF-$CH_2OCOC_3H_6COPh$ (1): exTTF-OH (40.0 mg, 9.8×10^{-2} mmol) and 4-benzoylbutyric acid (20.6 mg, 1.1 mmol) were dissolved in dry dichloroethane (5 mL). Then, *N, N*-dimethyl-4-aminopyridine (DMAP) (13.2 mg, 1.1 mmol) and *N, N*-dicyclohexylcarbodiimide (DCC) (40.3 mg, 2.0 mmol) were added to the solution and stirred for 1 h at r.t. The reaction crude was subjected to the silica chromatography using chloroform as an eluent. The solvent was removed under reduced pressure and the target compound was obtained as yellow solid (97% yield). MALDI-TOF MS: found *m/z* 584.38 [M^{-}] (calculated for $C_{32}H_{24}O_3S_4$: 584.06); UV-vis ($CHCl_3$): λ_{max} 278, 366, 412, 432 nm; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.90 (d, J = 7.2 Hz, 2H, *o*-PhH), 7.68–7.64 (m, 4H, ArH), 7.50 (t, J = 14.7 Hz, 1H, *p*-PhH), 7.39 (t, J = 15.3 Hz, 2H, *m*-PhH), 7.28–7.23 (m, 3H, ArH), 7.26 (m, 1H, $CHCl_3$), 6.23 (m, 4H, SCH), 5.17 (s, 2H, OCH_2),

3.02 (t, J = 14.4 Hz, 2H, OC=OCH_2), 2.51 (t, J = 14.4 Hz, 2H, C=OCH_2), 2.10 (m, J = 28.5 Hz, 2H, CH_2); ^{13}C NMR (75 MHz, CDCl_3): δ 199.3 (Phc=O), 173.0 (OC=O), 136.6, 136.2, 136.1, 135.6, 135.2, 135.1, 133.4, 132.9, 128.5, 127.9, 125.9, 125.6, 125.0, 124.8, 124.6, 121.5 (aromatic), 117.1 (SCH), 117.0 (SCH), 66.0 (CH_2O), 37.3 (OC=OC), 33.3 (Phc=OC), 19.3 (CH_2).

Synthesis of exTTF-CH_2OCOC$_3$H$_6$C(NNHTs)Ph (2):

exTTF-CH_2OCOC$_3$H$_6$COPh (9) (33.0 mg, 5.7 × 10^{-2} mmol) and *p*-toluenesulfonyl hydrazide (52.6 mg, 0.3 mmol) was mixed in a glass vessel and $C_2H_4Cl_2$ (1.0 mL) was added. The solution was degassed using freeze–thaw methods three times and then stirred overnight at 85 °C. The solvent was removed under reduced pressure. Then the solid was solved in toluene and filtered. The filtrate was concentrated under reduced pressure and subjected to silica chromatography using toluene/acetone = 201/1 (v/v) as eluents. The solvent was removed under reduced pressure and the target compound was obtained as a yellow solid (71%).

MALDI-TOF MS: found *m/z* 752.12 [M^-] (calculated for $C_{39}H_{32}O_4N_2S_5$: 752.10); ^{1}H NMR (300 MHz, CDCl_3): δ 9.29 (s, 1H, NH), 7.89 (d, J = 7.9 Hz, 2H, *o*-PhH), 7.88–7.67 (m, 4H, ArH), 7.65–7.62 (m, 2H, *m*-PhH), 7.40–7.36 (m, 1H, *p*-PhH), 7.340–7.23 (m, 6H, ArH), 7.12 (d, J = 7.2 Hz, 1H, ArH), 6.29–6.27 (m, 4H, SCH), 5.29 (d, J = 3.3 Hz, 2H, OCH_2), 2.6 (t, J = 8.0 Hz, 2H, N=CCH_2), 2.38–2.33 (m, 3H, PhcCH_3), 2.38–2.33 (m, 2H, C=OCH_2), 1.73–1.64 (m, 2H, CH_2); ^{13}C NMR (75 MHz, CDCl_3): δ 174.3 (C=O), 153.5 (C=N), 143.6 (CSO_2), 136.5, 136.1, 136.0, 135.8, 135.6, 135.2, 133.0, 129.7, 129.6, 129.5(2C), 129.0, 128.4(2C), 128.2, 127.9, 127.9, 126.6, 126.2, 126.1, 126.0(2C), 125.3, 125.2, 125.1, 124.9(2C) (aromatic), 117.3 (SCH), 117.2 (SCH), 117.1 (SCH), 67.0 (CH_2O), 32.3 (OC=OC), 25.8 (N=C), 21.5 (PhcCH_3), 21.0 (CH_2).

Synthesis of [5,6]-open C$_{61}$Phc$_3$H$_6$COOCH$_2$-exTTF (3a):

Compound **2** (9.4 mg, 13 μmol) and NaOMe (1.0 mg, 19 μmol) were dissolved in pyridine (70 μL) and stirred for 10 min at r.t. under argon atmosphere. Then, C_{60} (3.0 mg, 4.2 mmol) in 2.0 mL *o*-DCB was added to it. The mixture was stirred at 75 °C for 20 h under argon. The reaction mixture was separated using HPLC (Buckyprep column, toluene). The fraction containing the target compound was dried under reduced pressure, then dispersed in acetone/hexane = 1/3 (v/v) and filtered using a 0.45 μm PTFE membrane filter. **2** was obtained as a black solid as the residue. Yield: 73% based on consumed C_{60}; MALDI-TOF MS: found *m/z* 1288.15 [M^-] (calculated for $C_{92}H_{24}O_2S_4$: 1288.07); UV-vis ($CHCl_3$): λ_{max} 265, 325, 334, 365, 420, 427, 537, 599 nm; ^{1}H NMR (500 MHz, CDCl_3): δ 7.93 (dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 2H, *o*-PhH), 7.70–7.65 (m, 4H, ArH), 7.56–7.52 (m, 2H, *m*-PhH), 7.41 (tt, J_1 = 7.0 Hz, J_2 = 1.0 Hz, 1H, *p*-PhH), 7.29 (dd, J_1 = 7.3 Hz, J_2 = 3.3 Hz, 2H, ArH), 7.22 (dd, J_1 = 8.0 Hz, J_2 = 1.5 Hz, 1H, ArH), 6.33–6.29 (m, 4H, SCH), 5.12 (s, 2H, OCH_2), 2.22 (td, J_1 = 7.1 Hz, J_2 = 1.6 Hz, 2H, C=OCH_2), 1.65–1.62 (m, 2H, PhcCH_2), 1.51–1.48 (m, 2H, CH_2); ^{1}H NMR (300 MHz, CS_2): δ 7.85 (d, J = 7.2 Hz, 2H, *o*-PhH), 7.53–7.44 (m, 4H, ArH), 7.53–7.44 (m, 2H, *m*-PhH), 7.34 (t, J = 7.3 Hz, 1H, *m*-PhH), 7.16 (dd, J_1 = 7.4 Hz, J_2 = 3.3 Hz, 2H, ArH), 7.07 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H, ArH), 6.23–6.22 (m, 4H, SCH), 4.97–4.96 (m, 2H, OCH_2), 2.10 (t, J = 6.8 Hz, 2H, C=OCH_2), 1.61–1.56 (m, 2H, PhcCH_2), 1.52–1.45 (m, 2H, CH_2); ^{13}C NMR (125 MHz, CDCl_3): δ 172.8, 147.3 (2C), 146.4, 145.1 (2C), 144.6 (2C), 144.5, 144.2 (2C), 143.9 (2C), 143.7 (2C), 143.6, 143.6 (2C), 143.5 (2C), 143.0 (4C), 143.0 (2C), 142.9 (2C), 142.7 (2C), 142.5, 142.3 (2C), 142.0 (4C), 141.9 (2C), 141.8 (2C), 141.2 (2C), 140.9 (2C), 140.4 (2C), 139.7 (2C), 139.6 (2C), 138.7 (2C),

138.2 (2C), 138.1 (2C), 137.9 (2C), 136.6, 136.1, 136.0, 135.6, 135.2, 135.2, 135.0 (2C), 133.4, 130.7, 128.6, 127.7, 126.1 (2C), 125.6, 125.1, 125.0, 124.9, 124.5, 121.8, 121.7, 117.3, 117.3, 117.1, 66.2, 60.9, 35.2, 34.2, 20.0.

Synthesis of [6,6]-closed $C_{61}Phc_3H_6COOCH_2$-exTTF (3b): 3a (21 mg, 16 μmol) was dissolved in dry toluene (30.0 mL) and then degassed using freeze–pump–thaw cycles under reduced pressures. The solution was refluxed under argon atmosphere for 10 h. The reaction crude was subjected to preparative HPLC with Buckyprep Column, and the target compound was isolated from the unreacted starting materials and byproducts. Yield: 99%. MALDI-TOF MS: *m/z* 1288.18 [M^-] (calculated for $C_{92}H_{24}O_2S_4$: 1288.07); UV-vis ($CHCl_3$): λ_{max} 261, 318, 365, 418, 433, 483, 695 nm; ^{1}H NMR (500 MHz, CS_2 with acetone-d_6 capillary): δ 7.81 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 2H, *o*-PhH), 7.51–7.47 (m, 4H, ArH), 7.46–7.43 (m, 2H, *m*-PhH), 7.39–7,36 (m, 1H, *p*-PhH), 7.15 (dd, J_1 = 5.5 Hz, J_2 = 3.5 Hz, 2H, ArH), 7.10 (dd, J_1 = 8.0 Hz, J_2 = 1.5 Hz, 1H, ArH), 6.23–6.19 (m, 4H, SC*H*), 5.02 (s, 2H, OCH_2), 2.86-2.83 (m, 2H, PhcCH_2), 2.49 (t, J = 7.0 Hz, 2H, C=OCH_2), 2.15–2.10 (m, 2H, CH_2CH_2CO_2R); ^{13}C NMR (125 MHz, CS_2 with acetone-d_6 capillary): δ 170.5, 148.1, 147.2, 145.3, 144.8 (2C), 144.7 (2C), 144.7 (2C), 144.6 (4C), 144.4, 144.3 (2C), 144.3, 144.2 (2C), 144.0 (2C), 144.0 (2C), 143.7 (2C), 143.3 (2C), 143.3 (2C), 142.6 (2C), 142.6 (2C), 142.6, 142.6 (2C), 142.5 (2C), 142.5, 142.5 (2C), 141.7 (2C), 141.7 (2C), 141.7 (2C), 141.6 (2C), 140.6 (2C), 140.3 (2C), 137.7 (2C), 137.3 (2C), 136.4, 136.4, 136.2, 135.1, 134.8, 134.7, 133.4, 131.6, 128.7, 127.9, 125.8 (2C), 125.5, 124.8, 124.6, 124.6, 124.3, 121.4, 121.3, 117.1, 117.0, 116.9, 79.3 (bridgehead C), 65.4, 51.5, 33.5, 33.3, 22.3.

Titration experiments of 4a or 4b, in combination with exTTF-OH: 1.4×10^{-4} M solution of exTTF-OH (5.7 mg, 14 μmol) and 7.0×10^{-4} M solutions of **4a** and **4b** were prepared respectively in chloroform.

To the quartz cell (1.0 cm of light path), mixed solutions of exTTF-OH and **4a** or **4b** were added to various ratios ([exTTF]/[**4a** or **4b**] = 0.0, 0.5, 1.0, 1.5, 2.0, and 2.5). The absorbance data were recorded and compensated with the absorption of added **4a** or **4b**. Consequently, obtained spectra only reflect the absorption change by the addition of **4a** or **4b**, with charge transfer bands attributable to the interaction between exTTF-OH and **4a** or **4b**.

Theoretical calculations: Calculations were conducted using the hybrid density functional theory (DFT) at the M06-2X level[S3], as implemented in the Gaussian 09 software package.[S4] 6-31G(d) basis set for C, H, O, and S.[S5]

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S1 J. C. Hummelen , B. W. Knight, F. LePeq, F. Wudl, J. Yao and C. L. Wilkins, *J. Org. Chem.*, 1995, **60**, 532–538.

S2 E. M. Pérez, L. Sánchez, G. Fernández and N. Martín, *J. Am. Chem. Soc.*, 2006, **128**, 7172–7173.

S4 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

S5 M. J. Frisch,et al., GAUSSIAN 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.

S6 (a) R. Ditchfie, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*,1971, **54**, 724–728; (b) W. J. Hehre, R. Ditchfie and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257–2261.

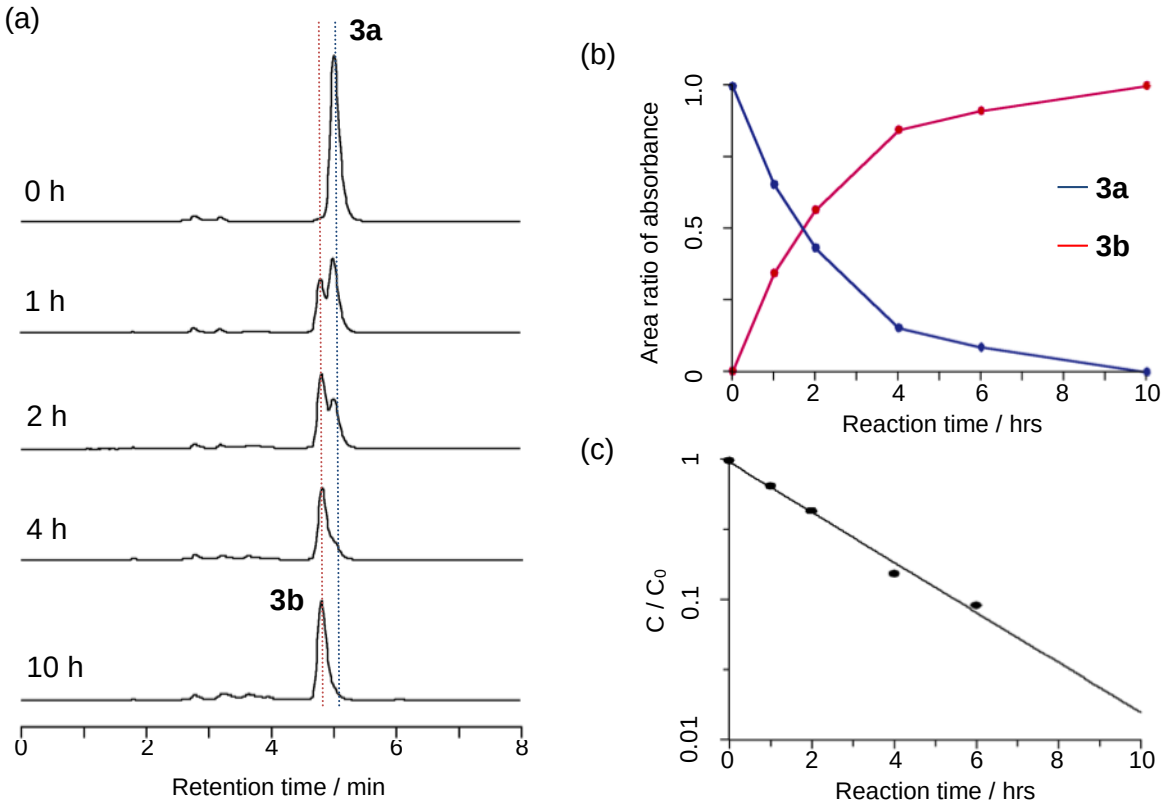

Fig. S1. (a) HPLC profiles of the thermal conversion of **3b** from **3a** by heating in refluxing toluene. Conditions: Buckprep column (ϕ4.6 × 250 mm); eluent, toluene; flow rate, 1.0 mL/min; wavelength, 330 nm; temperature, 40°C. HPLC profiles of the reaction mixtures. (b) Comparison of area change of **3a** and **3b** in the HPLC profile. (c) Single logarithmic plot of decrease ratio of **3a** vs.reaction time. Linear approximation: $y = 0.971\ e^{-0.411x}$, $R^2 = 0.987$. Half-life of **3a** is 1.69 hrs.

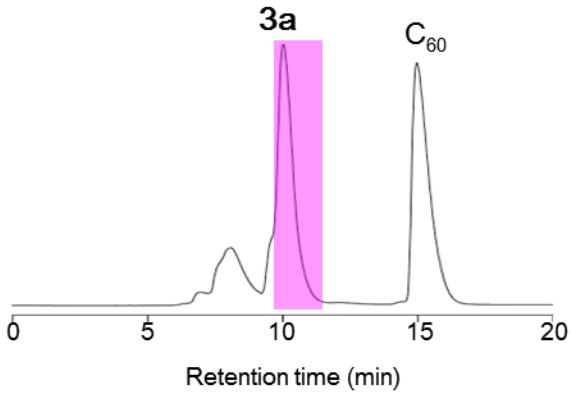

Fig. S2 Preparative HPLC profile for the isolation of **3a**. Conditions: Buckprep column (ϕ20 × 250 mm); eluent, toluene; flow rate, 9.99 mL/min; wavelength, 330 nm; temperature, r.t.

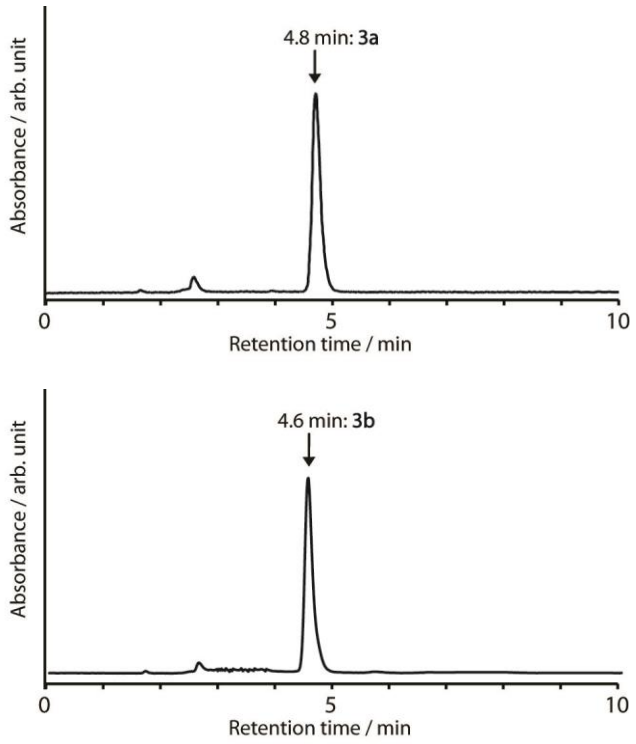

Fig. S3. HPLC profiles of isolated **3a** (upper) and **3b** (lower). Conditions: Buckprep column (ϕ4.6 × 250 mm); eluent, toluene; flow rate, 1.0 mL/min; wavelength, 330 nm; temperature, 40°C.

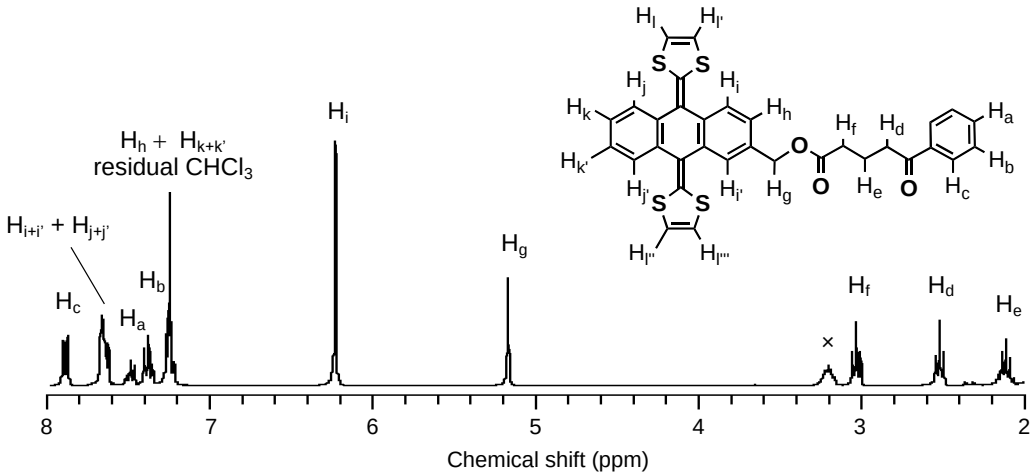

Fig. S4 ^{1}H NMR spectrum of **1** in $CDCl_3$ at 300 MHz.

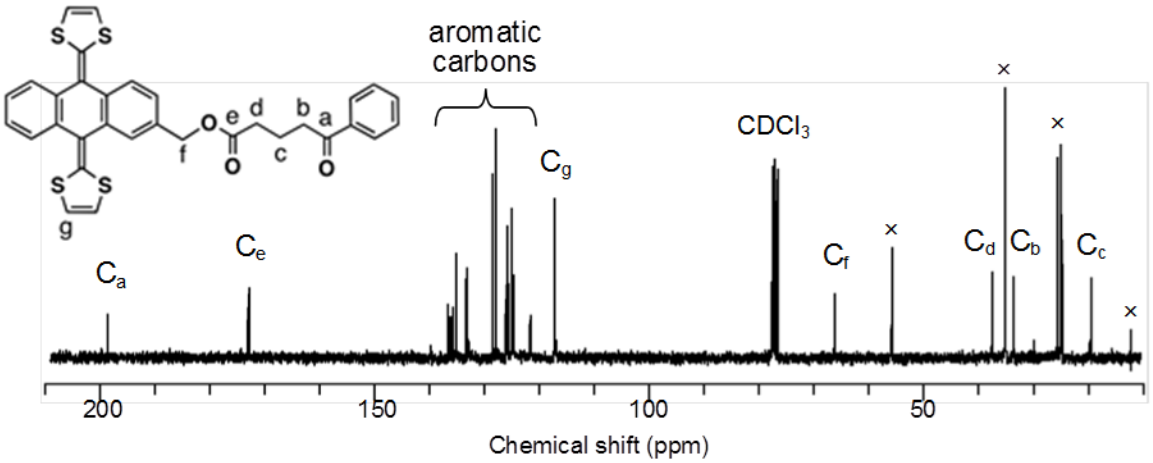

Fig. S5 ^{13}C NMR spectrum of **1** in $CDCl_3$ at 75 MHz.

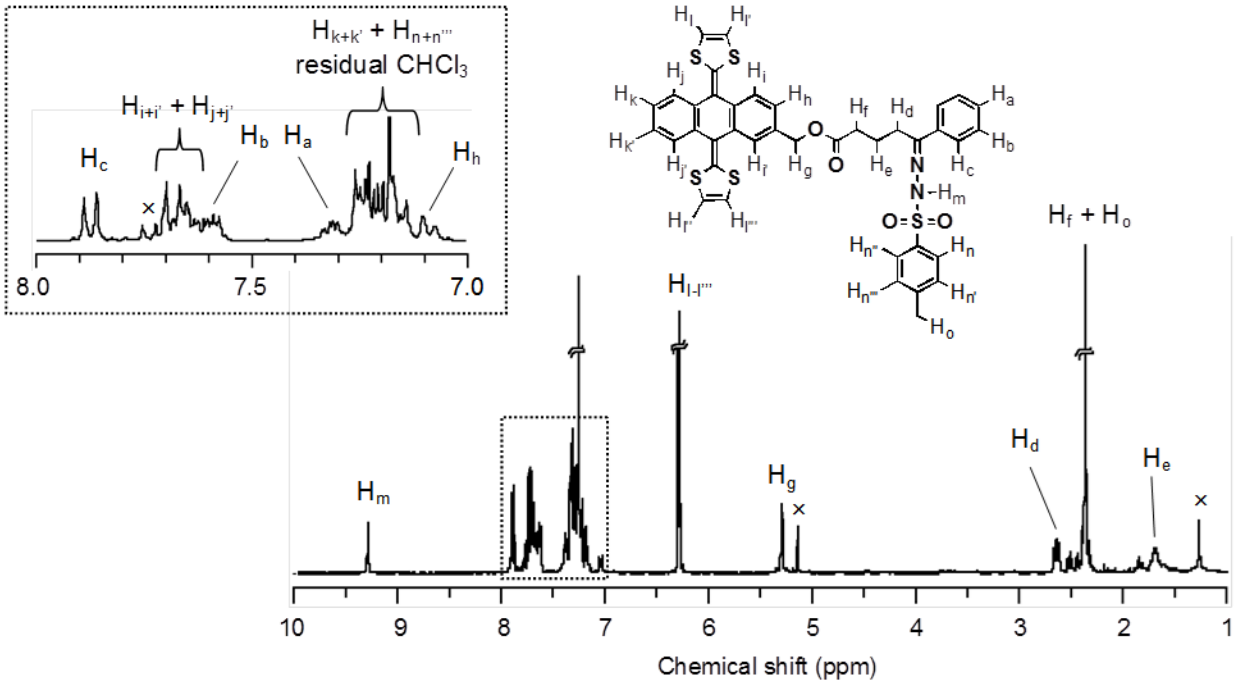

Fig. S6 ^{1}H NMR spectra of **2** in $CDCl_3$ at 300 MHz.

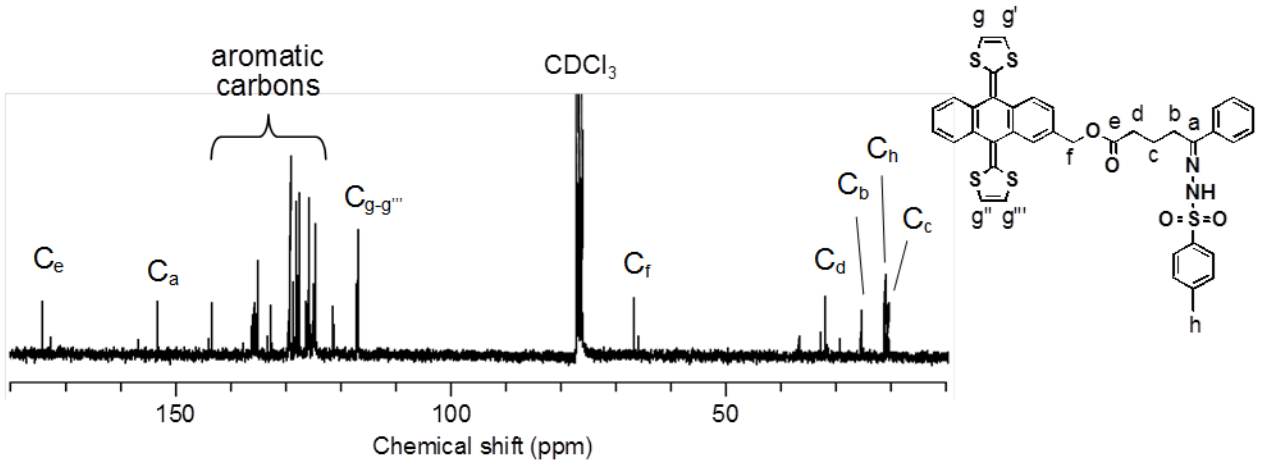

Fig. S7 ^{13}C NMR spectrum of **2** in $CDCl_3$ at 75 MHz.

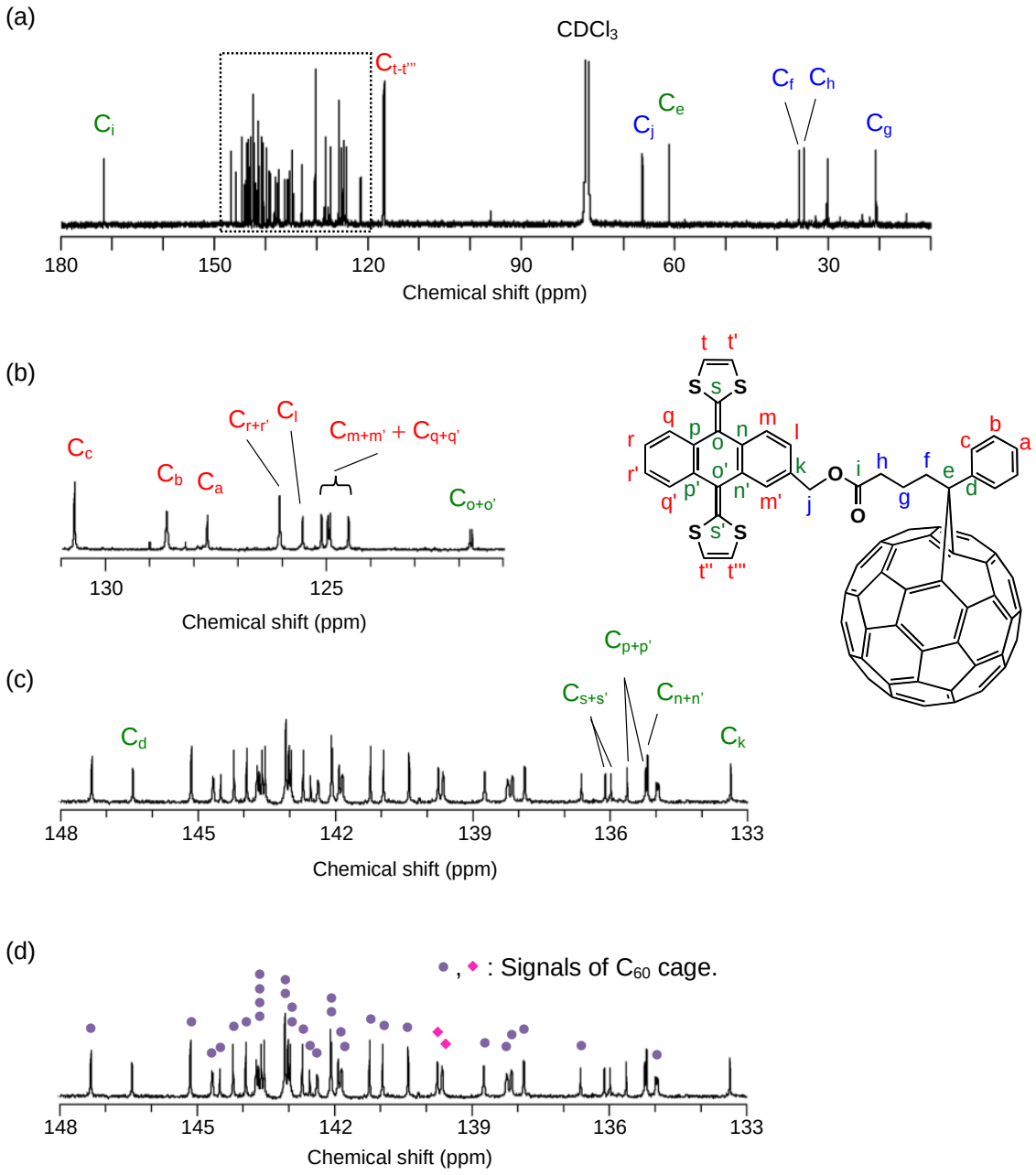

Fig. S8 ^{13}C NMR spectra of **3a** in $CDCl_3$, (a) in 10-180 ppm. (b) in 121-131 ppm. (c) Carbon peaks in 133-148 ppm were attributed to the structure of substituent. (d) 32 sp^2 carbon peaks in 133-148 ppm were attributed to the C_{60} cage. Pink square marks indicate the bridgehead carbon atoms on the C_{60} cage.

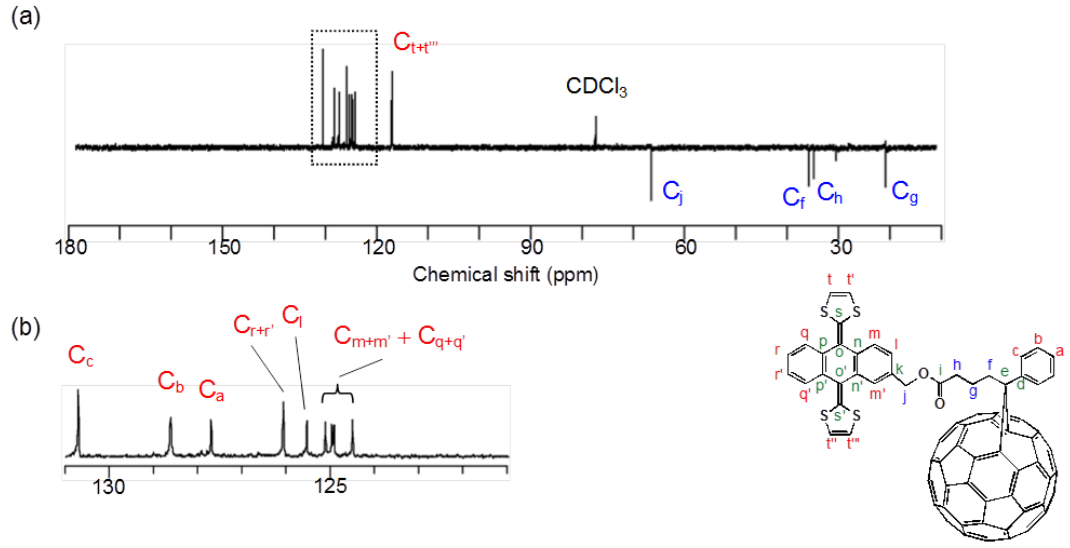

Fig. S9 DEPT135 spectra of **3a** in $CDCl_3$, (a) in 10-180 ppm. (b) in 121-131 ppm.

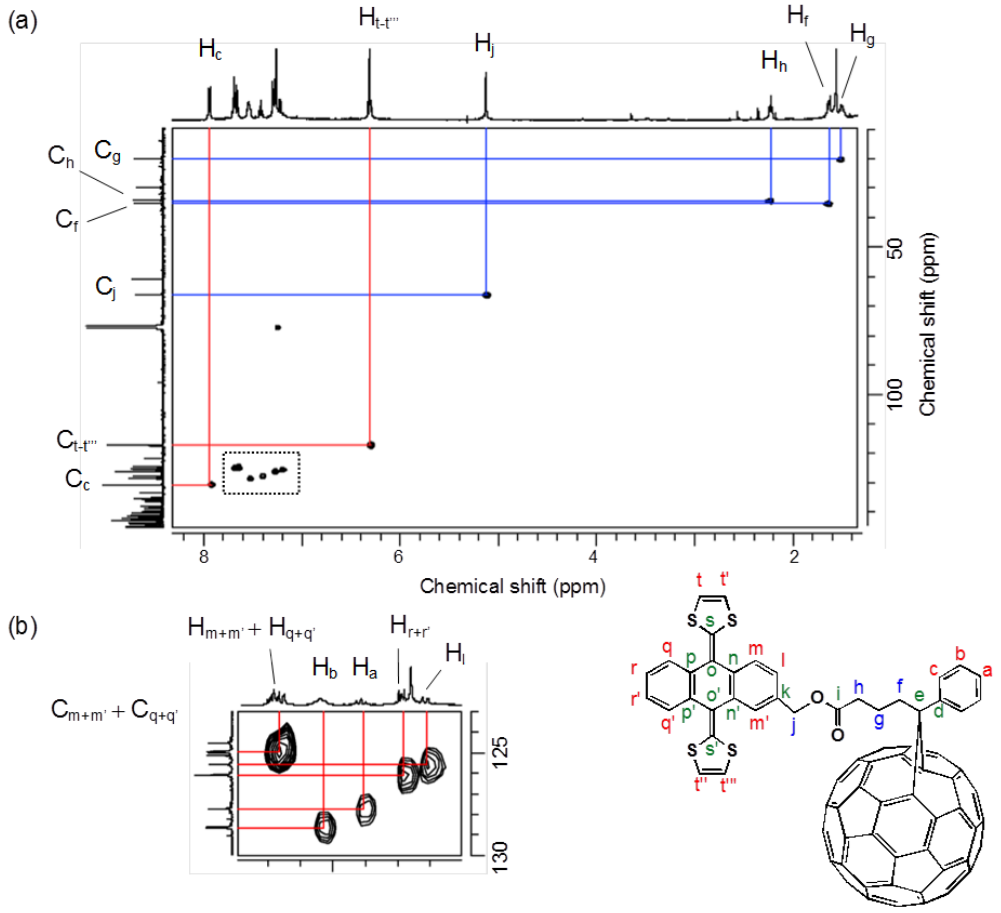

Fig. S10 HMQC spectra of **3a** in $CDCl_3$. (a) Full spectra and (b) expanded spectra of dotted line square in (a).

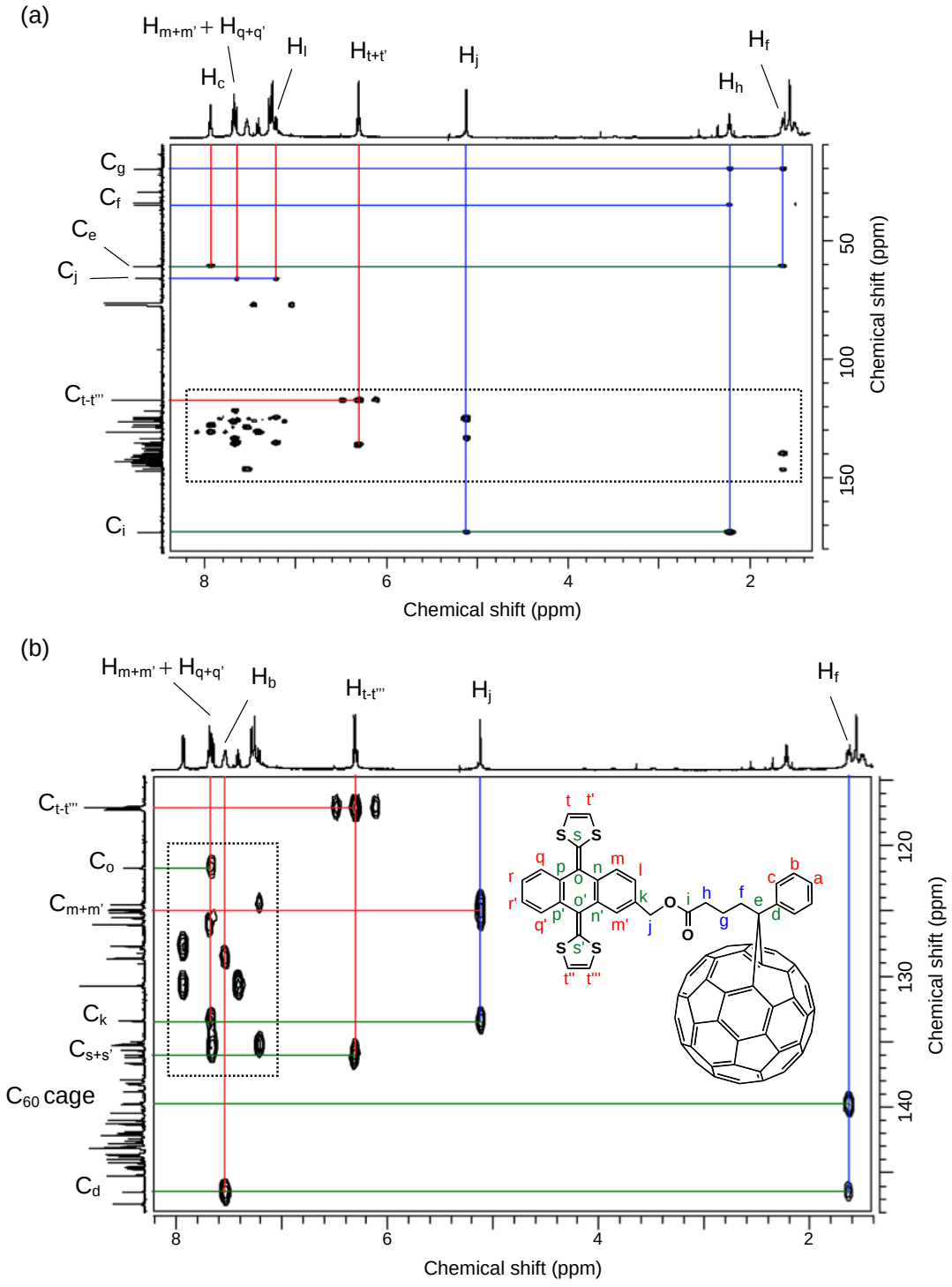

Fig. S11 HMBC spectra of **3a** in $CDCl_3$. (a) Full spectra and (b) expanded spectra of dotted line square in (a).

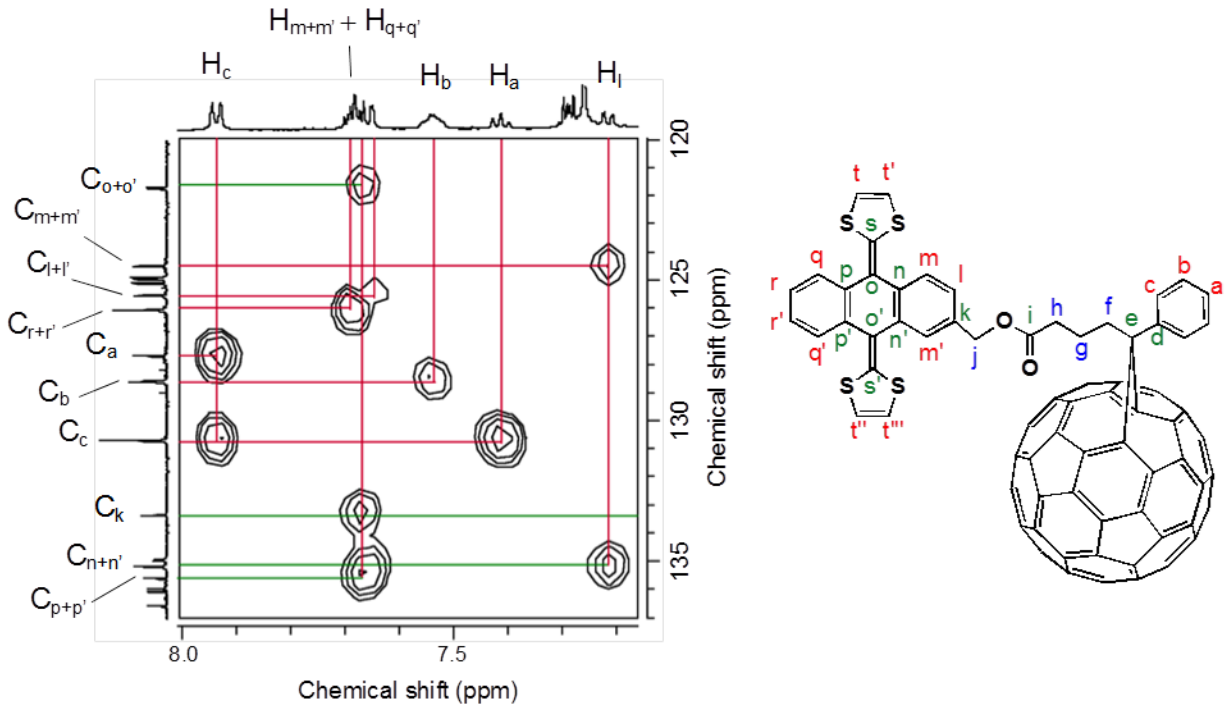

Fig. S12 Expanded HMBC spectra of **3a** in $CDCl_3$ of the dotted line square in Fig. S11b.

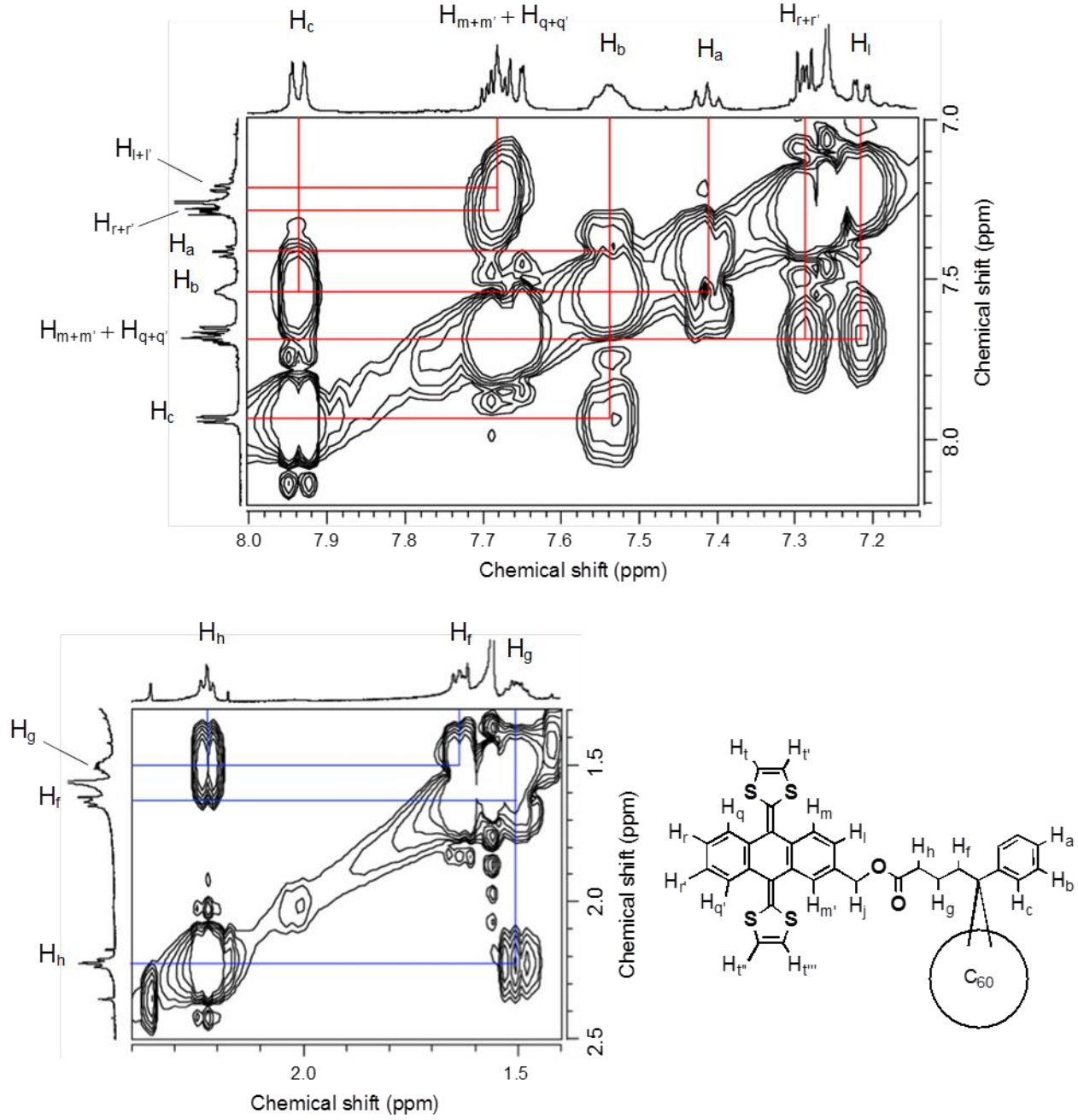

Fig. S13 ^{1}H-^{1}H COSY spectra of **3a** in $CDCl_3$.

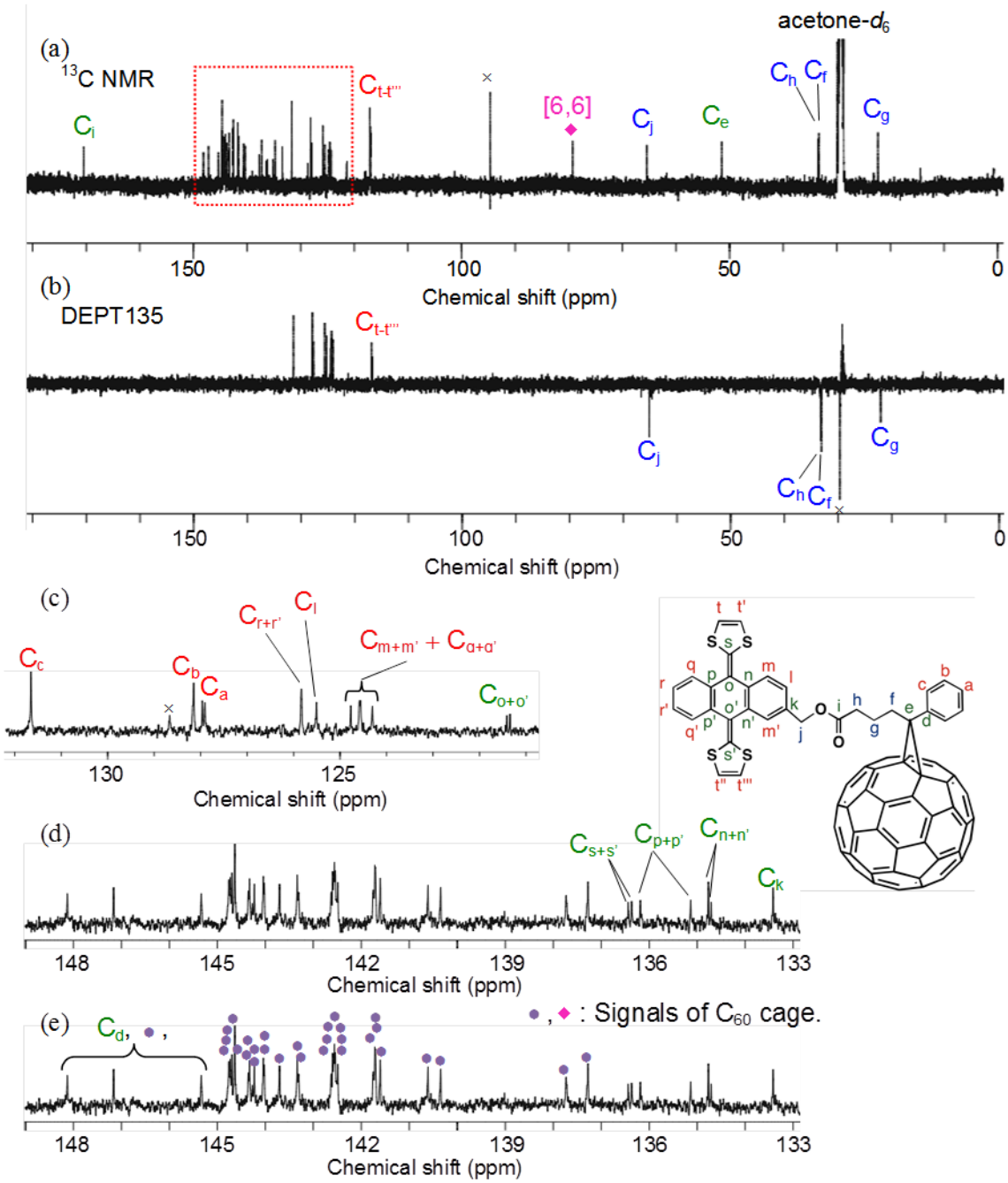

Fig. S14 ^{13}C NMR spectra of **3b** in CS_2 with acetone-d_6 capillary, (a) in 0-180 ppm. Pink square marks indicate the bridgehead carbon atoms on the C_{60} cage. (b) DEPT135 spectrum. (c) in 121-132 ppm. (d) Carbon peaks in 133-149 ppm were attributed to the structure of substituent. (e) 31 sp^2 carbon peaks in 133-149 ppm were attributed to the C_{60} cage.

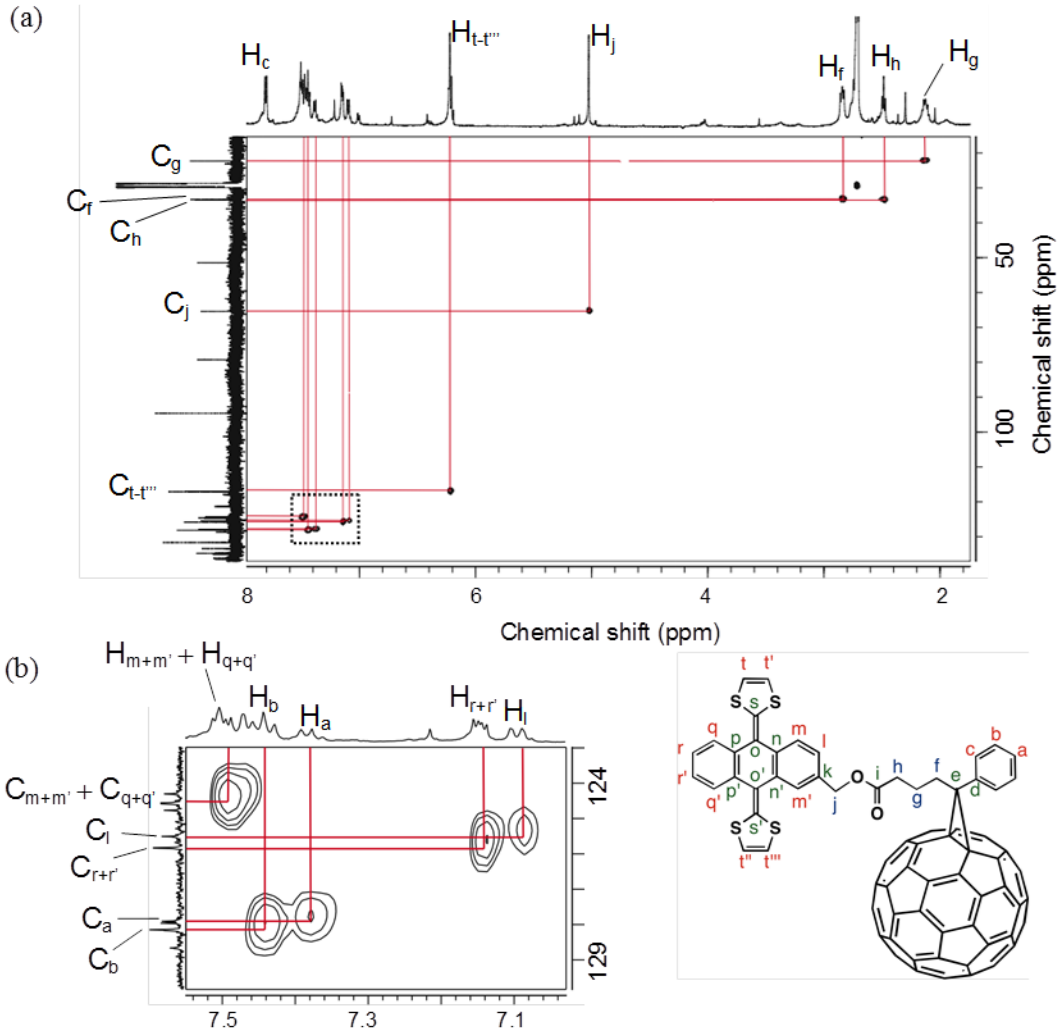

Fig. S15 (a) HSQC spectra of **3b** in CS_2 with acetone-d_6 capillary and (b) expanded spectra of dotted line square in (a).

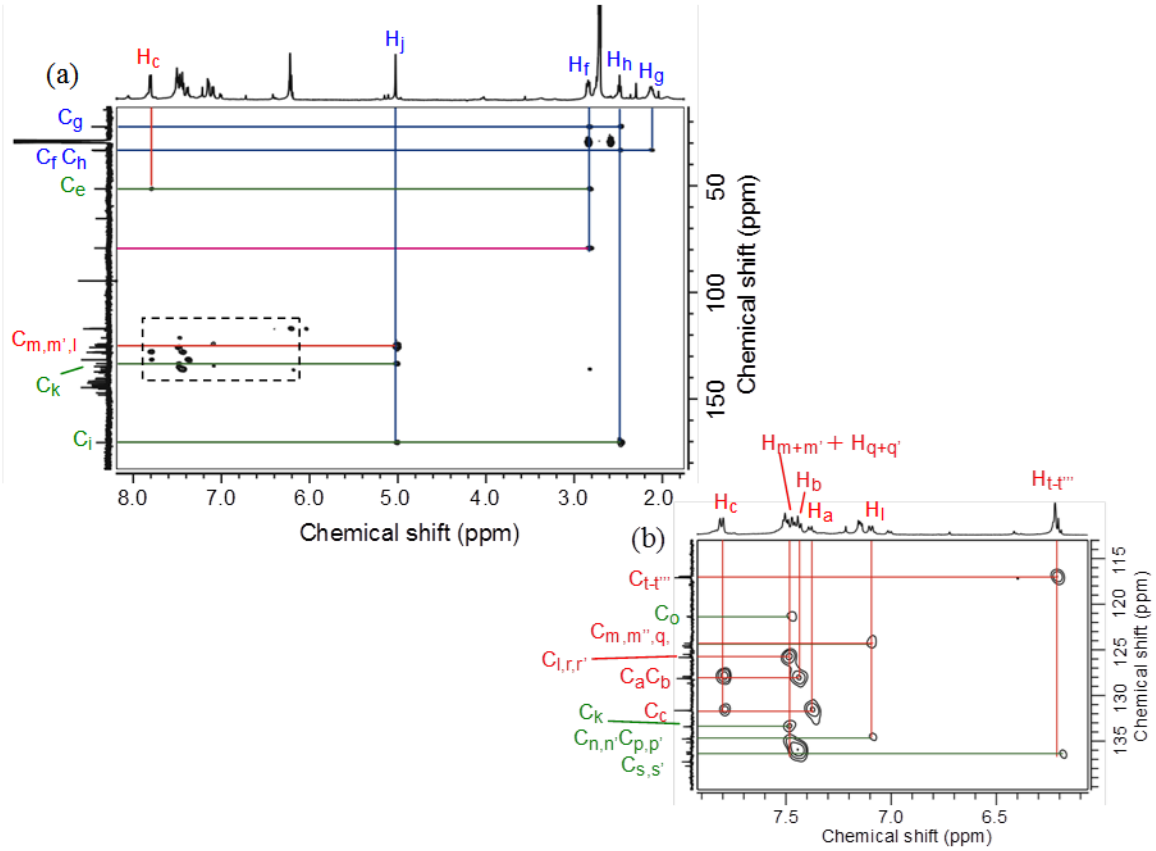

Fig. S16 (a) HMBC spectra of **3b** in CS_2 with acetone-d_6 capillary and (b) expanded spectra of dashed line square in (a).

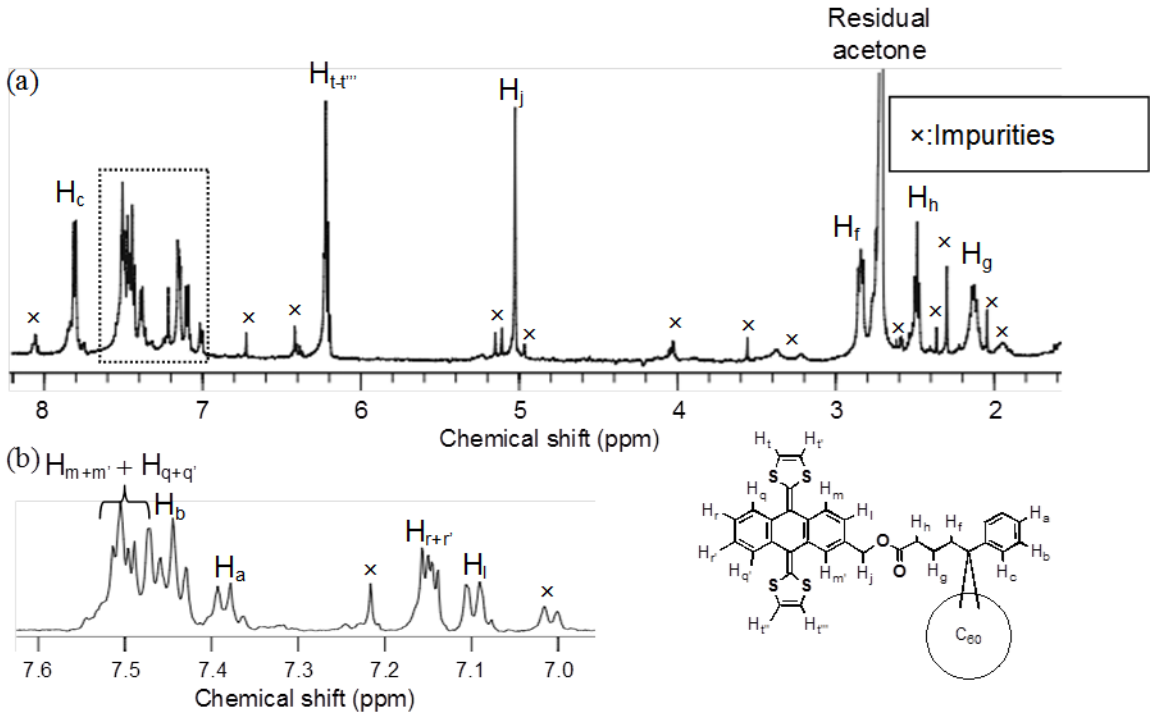

Fig. S17 ^{1}H NMR spectra of **3b** in CS_2 with acetone-d_6 capillary, (a) in 1.6-8.2 and (b) in 6.95-7.64 ppm.

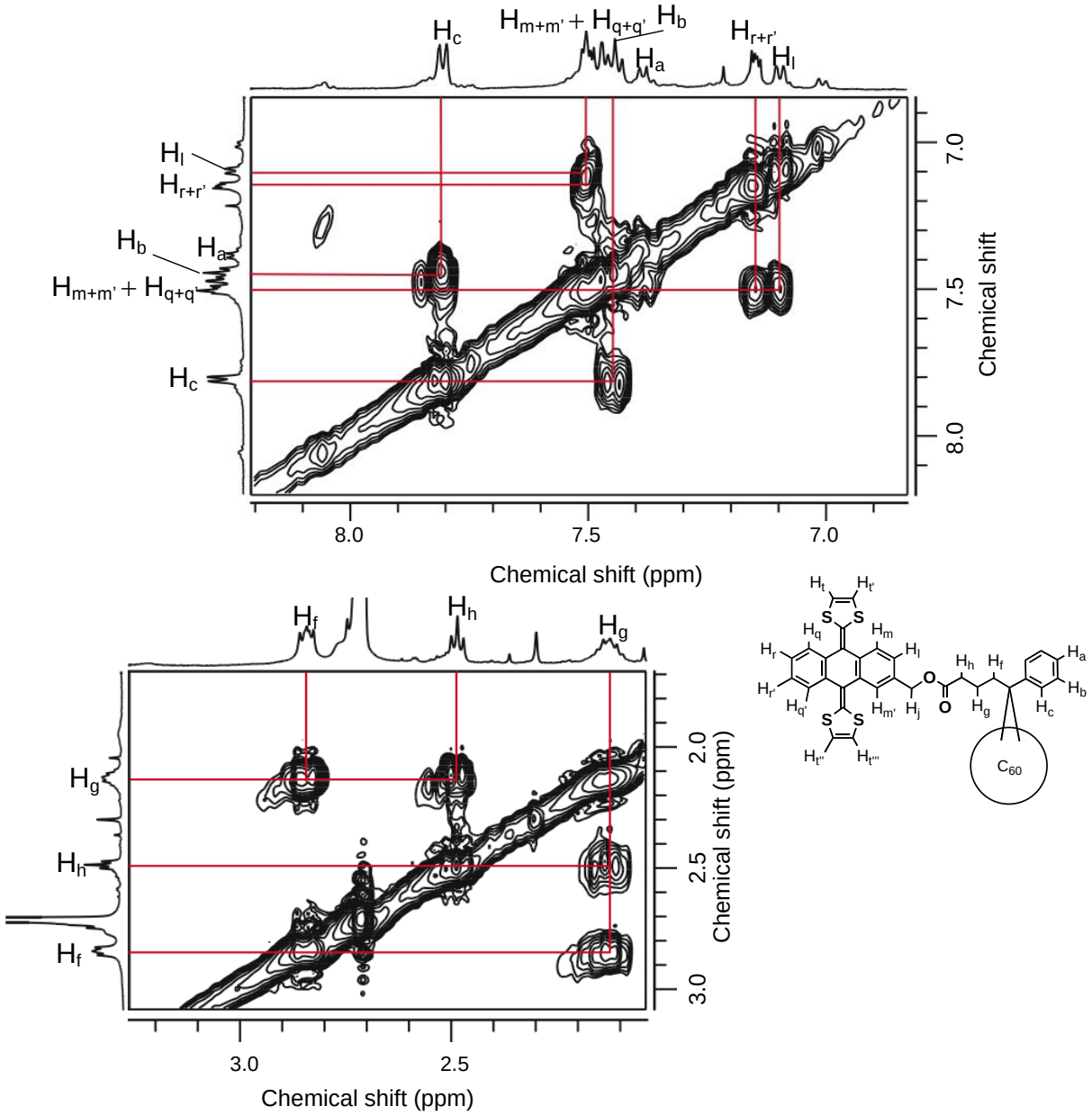

Fig. S18 ^{1}H-^{1}H COSY spectra of **3b** in CS_2 with acetone-d_6 capillary.

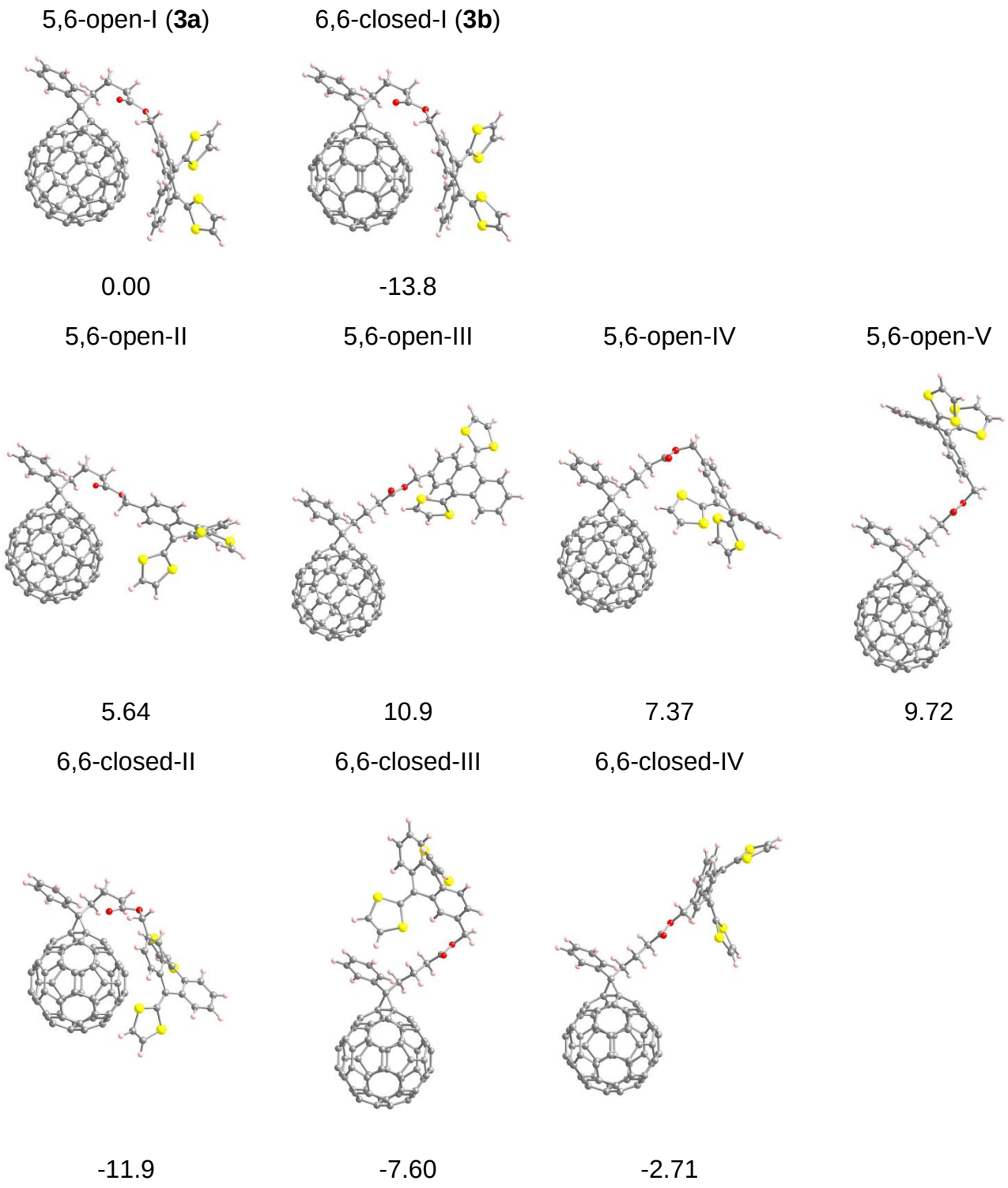

Fig. S19 Optimized structures and the relative energies (kcal mol^{-1}) of possible conformers of **3a** and **3b**, calculated at the M06-2X/6-31G(d) level of theory. The two structures in the first row are also appeared in Fig. 5.

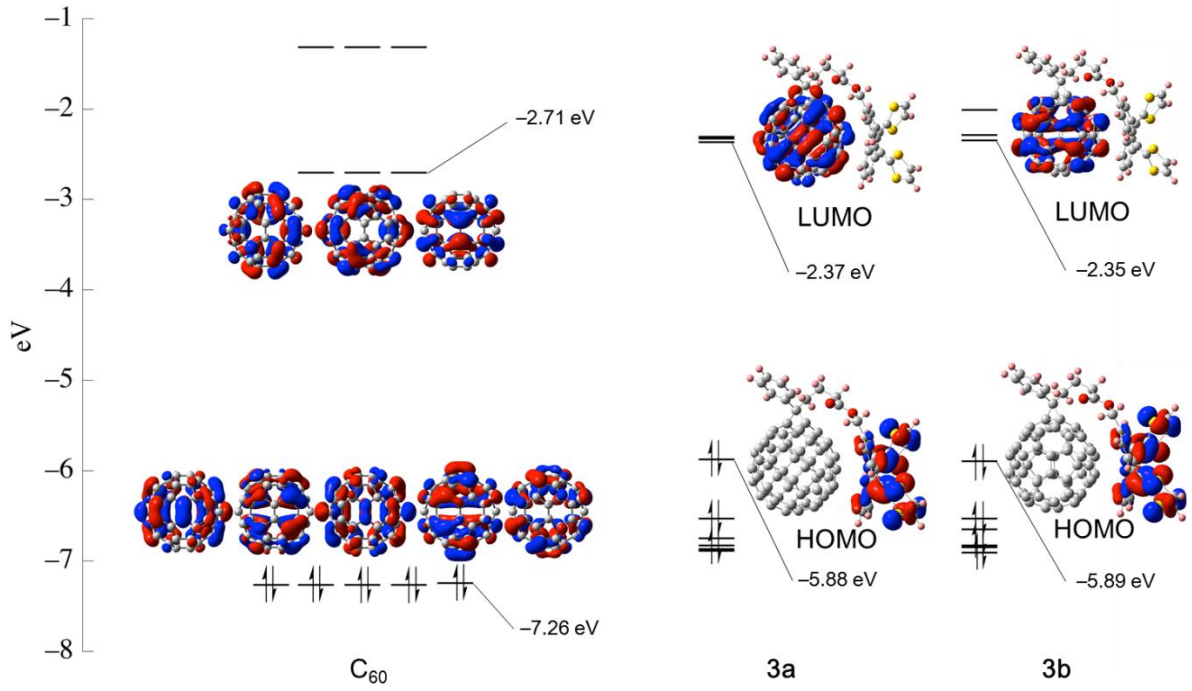

Fig. S20. Energy diagrams of pristine C_{60} and the most stable structures of **3a** and **3b**, calculated at the M06-2X/6-31G(d) level of theory.

Table S1. Redox Potentials of **3a** and **3b** as well as references exTTF, C_{60} and **4b** (in mV *versus* $Ag/AgNO_3$).[a]

Compound	$E_{pa,\ ox}^{(1)}$	$E_{1/2,red}^{(1)}$	$E_{1/2,red}^{(2)}$	$E_{1/2,red}^{(3)}$
exTTF	+394	–	–	–
C_{60}	–	-706	-1085	-1532
4b	–	-791	-1167	-1663
3a	+439	-776	-1146	-1618
3b	+393	-785	-1155	-1648

[a] Conditions: Glassy carbon working electrode (3 mm ϕ), platinum wire counter electrode, and $Ag/AgNO_3$ reference electrode, supporting electrolyte, 0.05 M $TBAPF_6$ in *o*-DCB. CV: scan rate, 100 mV s^{-1}.

Table S2. Cartesian coordinates (Å) of **3a** and **3b** at the M06-2X/6-31G(d) level of theory

5,6-open-I (**3a**)

C 4.808912 0.662903 -0.691880
C 5.546498 -1.150517 0.649621
C 4.632339 -2.830922 2.188716
C 5.395871 -0.684213 -0.710998
C 5.368067 -2.484263 0.985811
C 5.025765 -3.441405 -0.044836
C 4.892858 -3.010661 -1.356429
C 3.812637 -3.520828 -2.179293
C 5.088206 -1.610290 -1.693199
C 0.260537 -3.875214 1.949383
C 3.882226 1.000649 -1.692346
C -0.652466 -3.537923 0.959051
C 5.028888 -0.119937 1.508668
C 2.548969 -4.116292 2.428493
C 2.019315 -3.063967 3.275775
C 2.146882 0.100592 -3.038773
C 1.599842 1.141414 -2.209041
C -0.873601 -2.857667 -1.280267
C -1.403047 -1.804702 -0.433581
C 4.128383 -1.829071 3.007703
C 0.042402 -1.142065 -2.788167
C -0.471231 -0.136692 -1.979896
C 4.652992 1.025993 0.720185
C 1.461227 -4.616687 1.608022
C 0.606938 -2.910324 2.975317
C 3.551234 -0.006785 -2.710744
C 2.653412 1.757037 -1.446446
C -0.406885 -3.928135 -0.418416
C -1.258343 -2.221486 0.949062
C 4.347757 -0.436710 2.668993
C 3.825740 -4.000244 1.894398
C 2.790657 -1.946291 3.552254

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C -0.162349 -2.532820 -2.428986
C -1.200977 -0.477587 -0.775655
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C 2.188112 -0.626146 3.521639
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C 0.852529 -4.684931 -0.622237

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6,6-closed-II

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