

Fluoreno[2,1-*a*]fluorene: an *ortho*- Naphthoquinodimethane-Based System with Partial Diradical Character

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Part 1. Synthetic Procedures

1.1. General:

All reactions were performed under N₂. Anhydrous THF was dried and stored over activated 3 Å molecular sieves. Other solvents and commercially available reagents were used as received without further purification. Analytical thin-layer chromatography was performed on Agela Technologies silica gel plates. Melting ranges were recorded on a Vernier Melting Station apparatus. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AVANCE II HD spectrometer at 400 MHz (¹H). Chemical shifts for ¹H NMR are reported in ppm relative to residual Cl₂CHCDCl₂ (6.00 ppm). Multiplicity is indicated by one or more of the following: s (singlet); d (doublet); t (triplet); dd (doublet of doublets); br (broad). Infrared spectra were recorded on a Thermo Scientific Nicolet iS5 Fourier Transform Infrared Spectrometer (FT-IR) using the attenuated total reflectance (ATR) technique on a diamond. High-resolution mass spectra (HRMS) was performed at the Mass Spectrometry Laboratory in the School of Chemical Sciences, University of Illinois, Urbana-Champaign. Compound **1** was synthesized according to a reported procedure.¹

1.2. Fluoreno[2,1,-a]fluorene (FF-4)

To a flame-dried, three-neck round-bottom flask containing 9-bromoanthracene (386 mg, 1.5 mmol) in dry THF (10 mL) was added n-butyllithium (1.06 mL, 1.7 mmol) dropwise at -78 °C (acetone-CO_{2(s)} bath). The reaction was allowed to warm to RT while stirring, and then fluoreno[2,1-a]fluorenedione **1** (50 mg, 1.5 mmol) was added in one portion. After stirring at RT for 18 h, the reaction mixture (which had transitioned from a yellow to beige-green color) was quenched with water (~10 mL) and extracted with EtOAc. The combined organic phase was washed with water and brine, dried over MgSO₄, and concentrated *in vacuo*. The resulting crude tan solid (a diastereomeric mixture of fluorenofluorenediol) was used in the next step without any further purification.

The crude diol, which was degassed by evacuation/refill with N₂ (3 times), was dissolved in degassed (purged) CH₂Cl₂ (10 mL) in a three-neck round-bottom flask. To this solution was added SnCl₂•2H₂O (135 mg, 0.6 mmol). Three drops of concd. HCl_(aq.) were added to the mixture, and the reaction was stirred at RT for 2 h. During this time the reaction transitioned from a turbid tan color to a translucent teal. The reaction mixture was then concentrated *in vacuo*, and the crude product was purified by silica gel column eluted initially with heptane to remove excess anthracene from the previous step and then with 1:4 CH₂Cl₂/heptane to yield diradical **FF-4** as a bluish-black solid that is bright blue in dilute solution. (17 mg, 17% yield).

^1H NMR (400 MHz, 1,1,2,2-tetrachloroethane- d_2 , δ): 8.65 (s, 2H) 8.17 (d, 4H, J = 8.4 Hz), 7.91 (d, 4H, J = 8.6 Hz), 7.55 (dd-like m, 4H), 7.41 (dd-like m, 4H), 7.26 (d, 2H, J = 7.4 Hz), 6.94 (br t-like m, 2H), 6.77 (t, 2H, J = 7.4 Hz), 6.69 (d, 2H, J = 7.1 Hz), 6.26 (br d, 2H, J = 7.4 Hz), 6.14 (br d, 2H, J = 7.4). ^{13}C NMR not measured due to sparing solubility of compound. HRMS (EI/TOF) M^+ calcd. for $\text{C}_{52}\text{H}_{30}$, 654.2348; found, 654.2345.

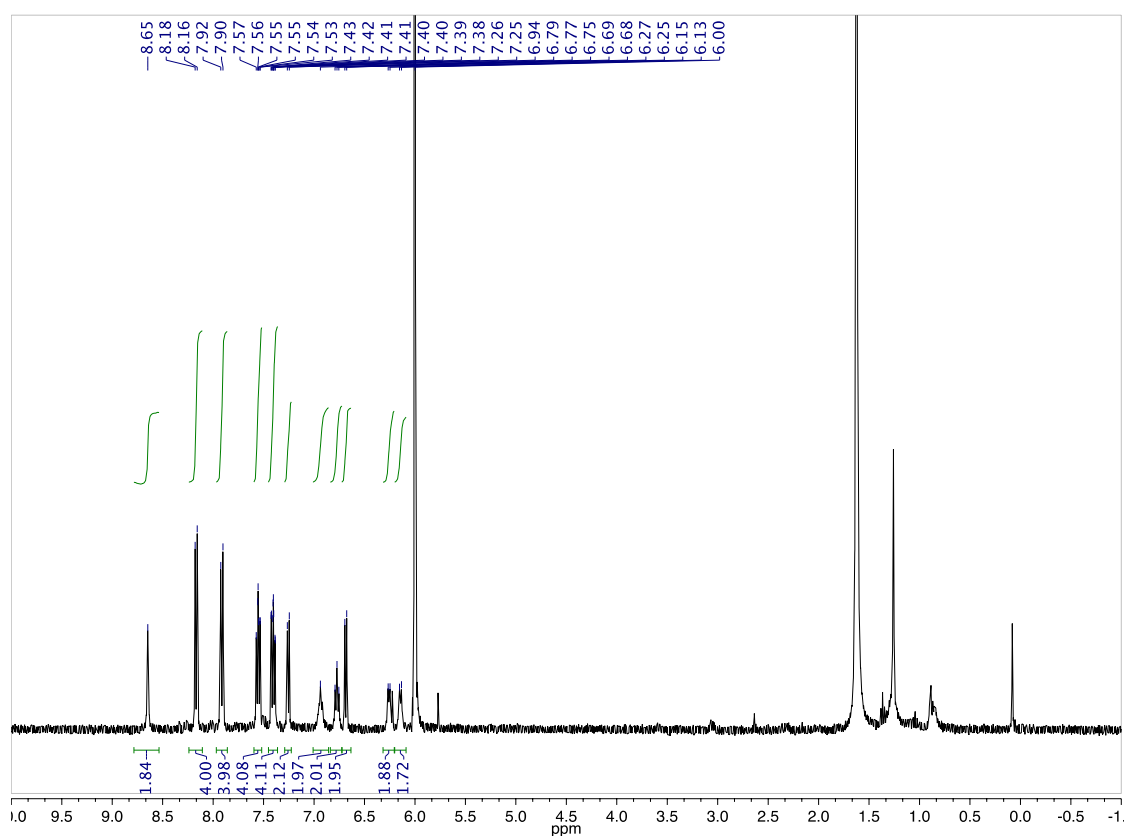


Figure S1: ^1H NMR spectrum of **FF-4** (400 MHz, 298 K, 1,1,2,2-tetrachloroethane- d_2)

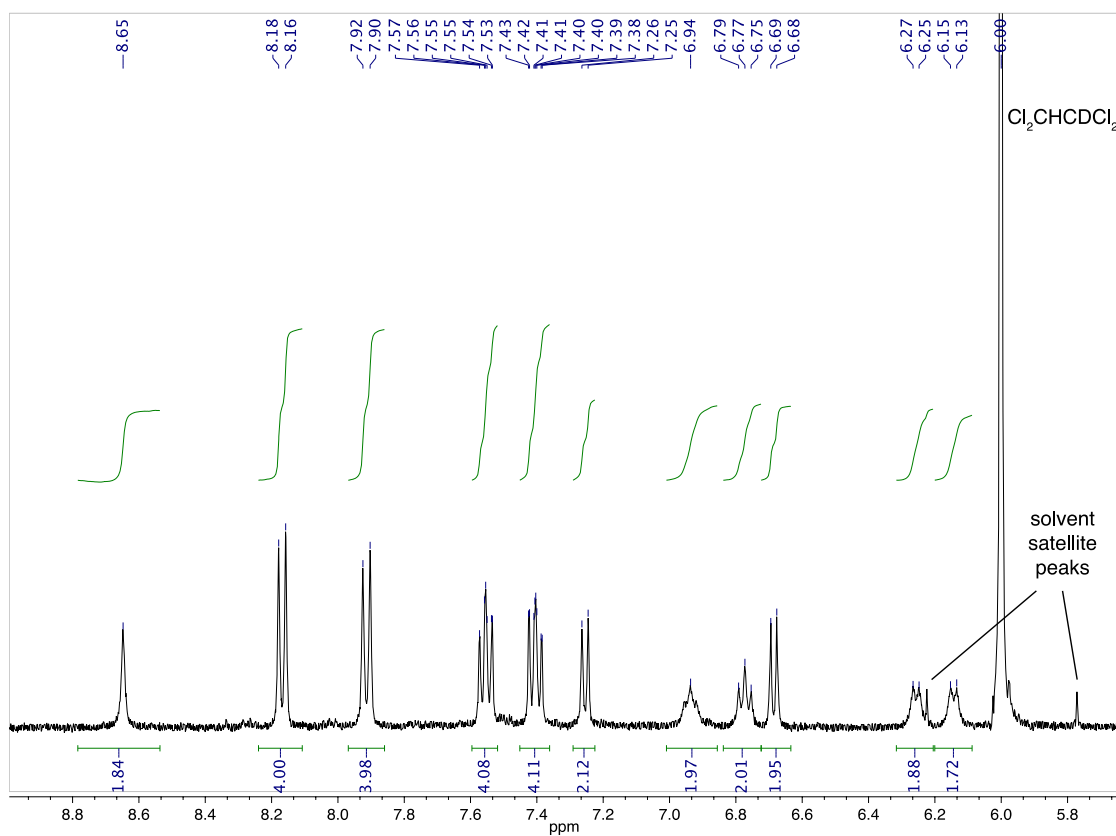


Figure S2: Aromatic region of ^1H NMR spectrum of **FF-4** (400 MHz, 298 K, 1,1,2,2-tetrachloroethane- d_2)

Part 2. Spectroscopic Measurements

2.1. Variable-Temperature NMR Spectra

Variable-temperature NMR spectra were recorded on Bruker AVANCE II HD spectrometer at 400 MHz (^1H).

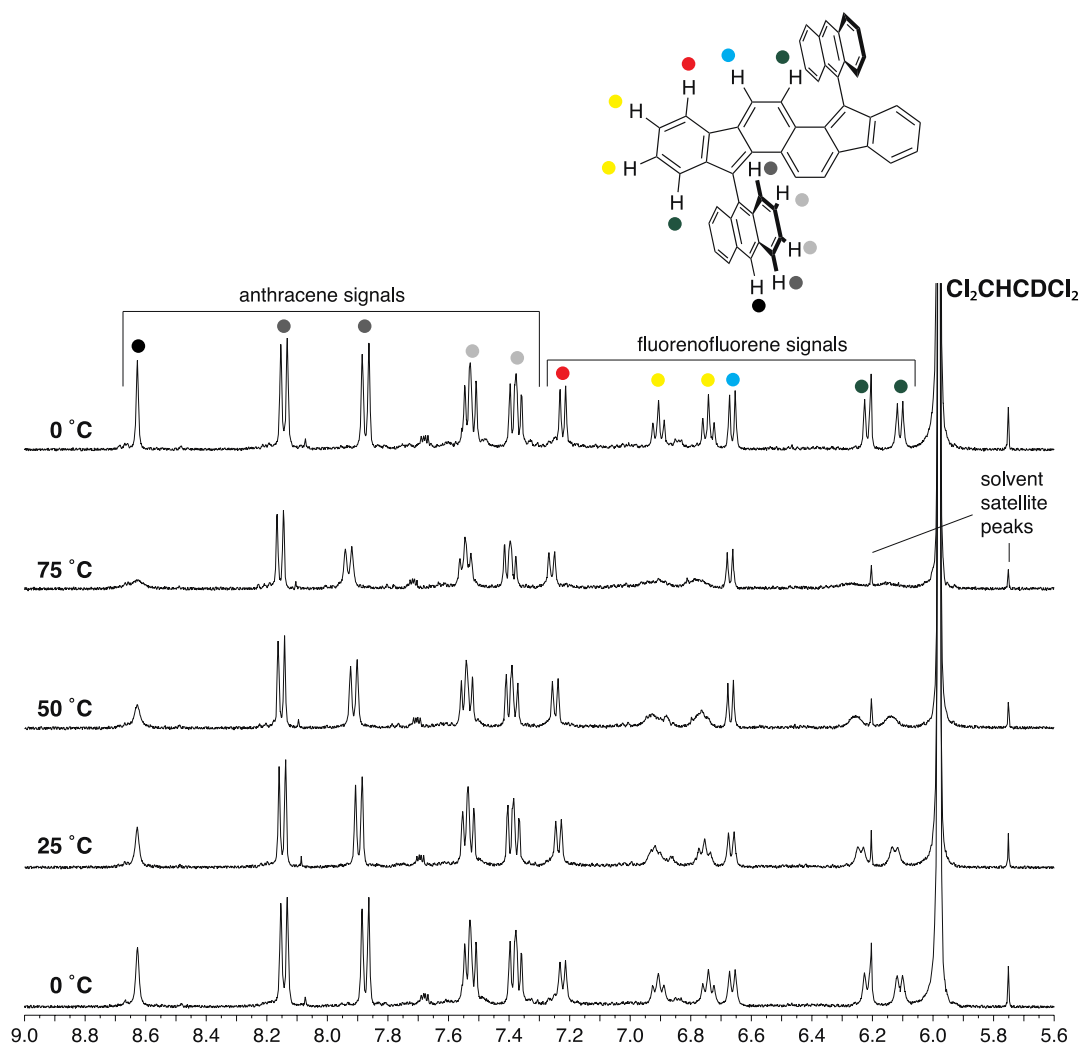


Figure S3: Tentative assignment of signals in VT-NMR experiment.

2.2. Absorption Spectrum

Absorption spectra were measured on an Agilent Technologies Cary 60 UV-vis spectrophotometer using 10 mm quartz cuvettes in spectroscopic grade dichloromethane. Molar absorptivities (ϵ) were calculated by the Beer–Lambert equation ($A = \epsilon c l$). The reported spectrum shows the average ϵ for each wavelength from three freshly prepared solutions of **FF-4** (1.01×10^{-4} M, 8.43×10^{-5} M, and 6.74×10^{-5} M).

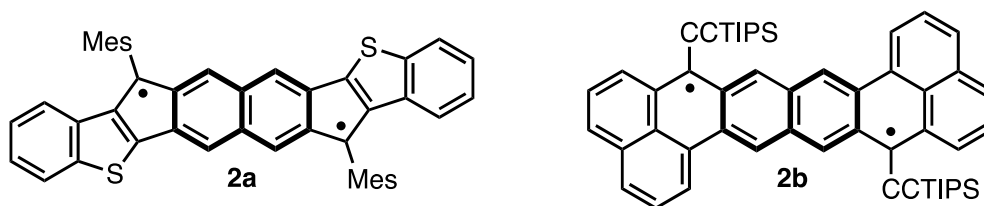
2.3. Cyclic Voltammetry

Cyclic voltammetry (CV) was performed under N_2 on a CH Instruments potentiostat (Model 760B) using a Ag/AgNO₃ reference electrode (containing a

0.01 M solution of AgNO₃ in CH₃CN), a Pt disk working electrode, and a Pt wire counter electrode. Measurements were performed in dry, degassed CH₂Cl₂ containing Bu₄NPF₆ (1.0 M) as a supporting electrolyte. Measurements were recorded at a sweep rate of 50 mV/s. The ferrocene/ferrocenium (Fc/Fc⁺) reversible oxidation was used as an internal reference standard (directly following the measurement of **FF-4**, Fc was added to the sample, which was measured immediately thereafter).

2.4 Raman measurements

The 1064 nm FT-Raman spectra were obtained with an FT-Raman accessory kit (FRA/106-S) of a Bruker Equinox 55 FT-IR interferometer. A continuous-wave Nd-YAG laser working at 1064 nm was employed for excitation. A germanium detector operating at liquid nitrogen temperature was used. Raman scattering radiation was collected in a back-scattering configuration with a standard spectral resolution of 4 cm⁻¹. 1000–3000 scans were averaged for each spectrum.



Scheme S1. Chemical structures of **2a** and **2b**.

2.5 Spectroelectrochemical Measurements.

Electrochemical experiments have been conducted in dichloromethane at room temperature by using 0.1 M tetrabutyl ammonium hexafluorophosphate, Bu₄NPF₆, as the supporting electrolyte. A glassy carbon was used as the working electrode and a Pt wire as the auxiliary electrode against a pseudo-reference electrode of Ag/0.001M AgNO₃ 0.1M Bu₄NClO₄. All redox potentials provided are referred to the Fc/Fc⁺ pair. In situ UV-Vis-NIR spectroelectrochemical studies were conducted on the Varian Cary 5000 UV-Vis-NIR Spectrophotometer. A C3 epsilon potentiostat from BASi was used for the electrolysis using a thin layer cell from a demountable omni cell from Specac. In this cell a three electrodes system was coupled to conduct in situ spectroelectrochemistry. A Pt gauze was used as the working electrode, a Pt wire was used as the counter electrode, and an Ag wire was used as the pseudoreference electrode. The spectra were collected at constant potential electrolysis and the potentials were changed in interval of 15 mV. The electrochemical medium used was 0.1 Bu₄NPF₆ in fresh distilled dichloromethane, at room temperature with sample concentrations of 10⁻³ M.

2.6 Superconducting Quantum Interference Device (SQUID) test:

Magnetic susceptibility measurements were carried out in the temperature range 200–400 K with an applied magnetic field of 0.5 T on a polycrystalline sample of compound **1** (with a mass of 36.44 mg) with a Quantum Design MPMS-XL-7 SQUID susceptometer. Susceptibility data were corrected for the sample holder and for the diamagnetic contribution of the salts using Pascal's constants. Magnetic susceptibility was fitted with Bleaney-Bowers equation after correction of a paramagnetic contamination (for example free radical).

Part 3. Quantum Chemistry Methods

All electronic structure calculations presented in this work have been done with the Q-Chem program [Mol. Phys. 113 (2015) 184–215].

3.1. Optimized Geometries

Molecular geometries have been optimized at the UB3LYP/6-311G(d,p) level. The nature has been confirmed by analysis of the vibrational modes at the structural critical points, which present no imaginary frequencies. Cartesian coordinates of optimized ground state structures of ground state singlet (S_0) and lowest triplet (T_1) states of **FF-1-4** can be found in section 2.4.

3.2. Diradical Character

The diradical character of ground state has been characterized by the ΔE_{ST} vertical and adiabatic energy gaps computed at the UB3LYP level and with the restricted active space CI spin-flip method (RASCI-SF or simply RAS-SF) [Phys. Chem. Chem. Phys. 11 (2009) 9779]. The reference configuration employed in all RAS-SF calculations corresponds to the lowest triplet ROHF state; RAS2 contains 8 electrons in 8 orbitals while RAS1 (RAS3) contains to the entire set of doubly occupied (virtual) molecular orbitals.

The diradical nature of excited singlets has been further characterized by means of the number of unpaired electrons (N_U) and by the representation of the fractional occupancy density (FOD) computed at RAS(8,8)-SF/6-31G(d) level:

$$N_U = \sum_i (1 - \text{abs}(1 - n_i))$$

$$\rho_{FOD} = \sum_i (1 - \text{abs}(1 - n_i)) |\phi_i|^2$$

where n_i corresponds to the electron occupation of the i -th natural orbital ϕ_i .

Table S1. Electronic (fractional) occupancies of highest occupied natural orbital (HONO) and lowest unoccupied natural orbital (LUNO) for the **FF-1–4** family computed at the RAS-SF/6-31G(d) level.

	HONOLUNO	
FF-1	1.69	0.31
FF-2	1.73	0.28
FF-3	1.40	0.60
FF-4	1.50	0.50

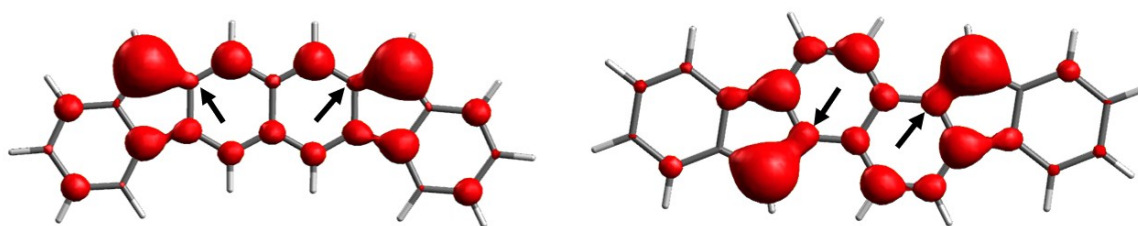


Figure S4. Representation of the FOD for the diradical singlet ground state of **FF-3** (left) and **FF-4** (right) computed at the RAS(8,8)-SF/6-31G* level. Arrows denote the key positions discussed in the text.

3.3. Absorption Spectra

Simulated absorption spectra of neutral and ionic species of **FF-4** in CH_2Cl_2 solution have been computed at the time-dependent DFT (TD-DFT) level with M06-2X and CAM-B3LYP exchange-correlation functionals and the 6-311G(d,p) basis set. Solvent effects of CH_2Cl_2 have been taken into account with the conductor-like polarized continuum model (C-PCM) [Chem. Phys. Lett. 240 (1995) 253–260.; J. Phys. Chem. A 102 (1998) 1995–2001; J. Comput. Chem. 24 (2003) 669–681]. The profiles of the simulated UV-vis absorption spectra have been obtained as the superposition of Gaussian functions centered at the computed frequencies with a 2000 cm^{-1} half-bandwidth.

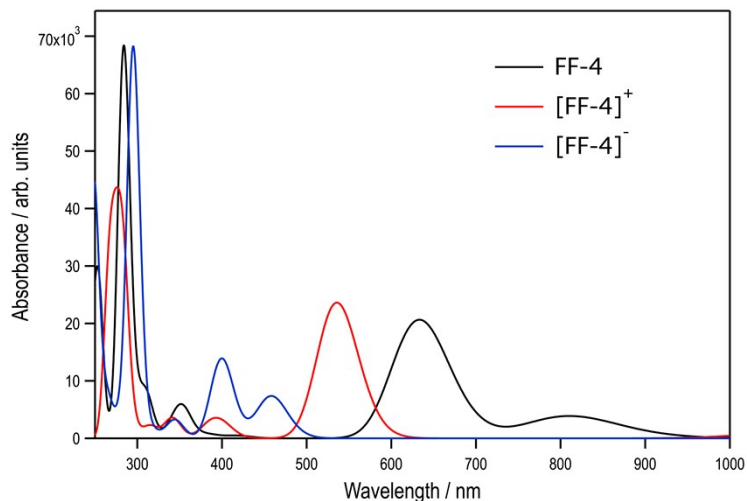


Figure S5: Simulation of the absorption spectra of **FF-4** neutral (black), cation (red) and anion (blue) species in CH_2Cl_2 solution computed at the M06-2X/6-311G(d,p) level.

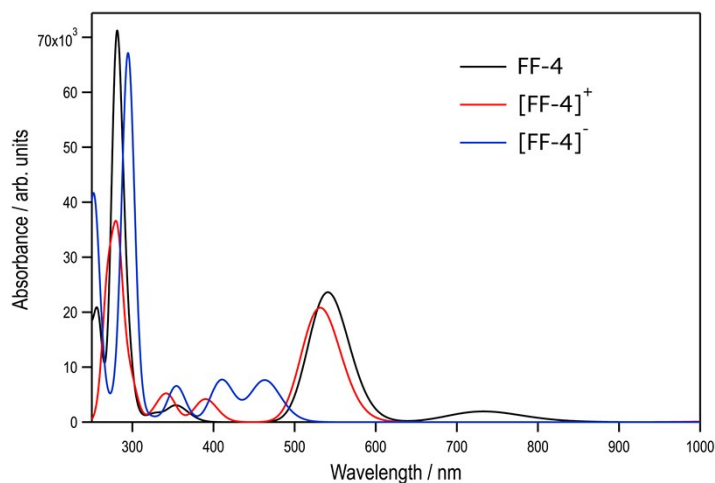


Figure S6: Simulation of the absorption spectra of **FF-4** neutral (black), cation (red) and anion (blue) species in CH_2Cl_2 solution computed at the CAM-B3LYP/6-311G(d,p) level.

3.4. Cartesian Coordinates

All molecular coordinates optimized at the UB3LYP/6-311G(d,p) level.

FF-1, ground state singlet (S_0)

H	4.064643	2.203105	0.000000
C	-0.000113	0.730754	0.000000
C	1.201158	1.418893	0.000000

C	2.430874	0.721911	0.000000
C	2.430874	-0.739512	0.000000
C	1.259759	-1.428017	0.000000
H	1.195049	2.504698	0.000000
H	1.243088	-2.513808	0.000000
C	3.744596	1.169176	0.000000
C	4.625751	0.026033	0.000000
C	6.021050	-0.064096	0.000000
C	6.614078	-1.324674	0.000000
C	5.832533	-2.485809	0.000000
C	4.436923	-2.409981	0.000000
C	3.831738	-1.160265	0.000000
H	6.633124	0.831386	0.000000
H	7.694961	-1.409659	0.000000
H	6.316604	-3.455797	0.000000
H	3.843384	-3.318039	0.000000
C	0.000113	-0.730754	0.000000
C	-1.201158	-1.418893	0.000000
C	-1.259759	1.428017	0.000000
C	-2.430874	-0.721911	0.000000
H	-1.195049	-2.504698	0.000000
C	-2.430874	0.739512	0.000000
H	-1.243088	2.513808	0.000000
C	-3.744596	-1.169176	0.000000
C	-3.831738	1.160265	0.000000
H	-4.064643	-2.203105	0.000000
C	-4.625751	-0.026033	0.000000
C	-6.021050	0.064096	0.000000
C	-6.614078	1.324674	0.000000
H	-6.633124	-0.831386	0.000000
C	-4.436923	2.409981	0.000000
C	-5.832533	2.485809	0.000000
H	-7.694961	1.409659	0.000000
H	-3.843384	3.318039	0.000000
H	-6.316604	3.455797	0.000000

FF-1, lowest triplet state (T_1)

H	4.126226	2.186263	0.000000
C	0.000513	0.719313	0.000000
C	1.239308	1.414803	0.000000
C	2.429579	0.713199	0.000000
C	2.423453	-0.731280	0.000000
C	1.239308	-1.420543	0.000000
H	1.233835	2.500210	0.000000
H	1.221771	-2.505993	0.000000
C	3.797176	1.156200	0.000000
C	4.640149	0.010498	0.000000
C	6.040477	-0.110540	0.000000
C	6.607599	-1.379320	0.000000

C	5.801549	-2.526587	0.000000
C	4.405339	-2.425003	0.000000
C	3.821376	-1.167699	0.000000
H	6.668554	0.773722	0.000000
H	7.686423	-1.486590	0.000000
H	6.266789	-3.505721	0.000000
H	3.796833	-3.323013	0.000000
C	-0.000513	-0.719313	0.000000
C	-1.239308	-1.414803	0.000000
C	-1.239308	1.420543	0.000000
C	-2.429579	-0.713199	0.000000
H	-1.233835	-2.500210	0.000000
C	-2.423453	0.731280	0.000000
H	-1.221771	2.505993	0.000000
C	-3.797176	-1.156200	0.000000
C	-3.821376	1.167699	0.000000
H	-4.126226	-2.186263	0.000000
C	-4.640149	-0.010498	0.000000
C	-6.040477	0.110540	0.000000
C	-6.607599	1.379320	0.000000
H	-6.668554	-0.773722	0.000000
C	-4.405339	2.425003	0.000000
C	-5.801549	2.526587	0.000000
H	-7.686423	1.486590	0.000000
H	-3.796833	3.323013	0.000000
H	-6.266789	3.505721	0.000000

FF-2, ground state singlet (S_0)

C	4.0798099588	0.8829837162	0.0000000000
C	3.2437873896	2.0630389127	0.0000000000
C	1.8412825758	0.2189934005	0.0000000000
C	-0.4740801778	1.8546842944	0.0000000000
C	0.7360239461	2.4632497923	0.0000000000
C	1.9257944912	1.6741084382	0.0000000000
H	-1.3670671544	2.4585260998	0.0000000000
H	0.8114903400	3.5453428910	0.0000000000
C	0.6119802245	-0.4158538301	0.0000000000
C	0.4740801778	-1.8546842944	0.0000000000
C	-1.8412825758	-0.2189934005	0.0000000000
C	-0.7360239461	-2.4632497923	0.0000000000
H	1.3670671544	-2.4585260998	0.0000000000
C	-1.9257944912	-1.6741084382	0.0000000000
H	-0.8114903400	-3.5453428910	0.0000000000
C	-4.0798099588	-0.8829837162	0.0000000000
C	-3.2437873896	-2.0630389127	0.0000000000
C	-0.6119802245	0.4158538301	0.0000000000
H	-3.6070898112	-3.0826615709	0.0000000000
H	3.6070898112	3.0826615709	0.0000000000
C	-3.2382404853	0.2716550839	0.0000000000

C	-3.8325368259	1.5293825540	0.0000000000
C	-5.4664117553	-0.7667805964	0.0000000000
C	-5.2298766772	1.6389388504	0.0000000000
H	-3.2503846508	2.4396940824	0.0000000000
C	-6.0402891609	0.5063897515	0.0000000000
H	-6.0921696061	-1.6528324854	0.0000000000
H	-5.6818835327	2.6242980087	0.0000000000
H	-7.1190267934	0.6138407125	0.0000000000
C	3.2382404853	-0.2716550839	0.0000000000
C	3.8325368259	-1.5293825540	0.0000000000
C	5.4664117553	0.7667805964	0.0000000000
C	5.2298766772	-1.6389388504	0.0000000000
H	3.2503846508	-2.4396940824	0.0000000000
C	6.0402891609	-0.5063897515	0.0000000000
H	6.0921696061	1.6528324854	0.0000000000
H	5.6818835327	-2.6242980087	0.0000000000
H	7.1190267934	-0.6138407125	0.0000000000

FF-2, lowest triplet state (T_1)

C	-0.888467	4.115970	0.000000
C	-2.057144	3.307847	0.000000
C	-0.236924	1.862020	0.000000
C	-1.831006	-0.459706	0.000000
C	-2.441329	0.767565	0.000000
C	-1.649984	1.935115	0.000000
H	-2.444423	-1.346818	0.000000
H	-3.523253	0.843663	0.000000
C	0.412444	0.595809	0.000000
C	1.831006	0.459706	0.000000
C	0.236924	-1.862020	0.000000
C	2.441329	-0.767565	0.000000
H	2.444423	1.346818	0.000000
C	1.649984	-1.935115	0.000000
H	3.523253	-0.843663	0.000000
C	0.888467	-4.115970	0.000000
C	2.057144	-3.307847	0.000000
C	-0.412444	-0.595809	0.000000
H	3.078820	-3.663650	0.000000
H	-3.078820	3.663650	0.000000
C	-0.262790	-3.254059	0.000000
C	-1.524858	-3.834400	0.000000
C	0.748919	-5.508942	0.000000
C	-1.649984	-5.232480	0.000000
H	-2.428833	-3.241999	0.000000
C	-0.528092	-6.063167	0.000000
H	1.627309	-6.145477	0.000000
H	-2.641308	-5.671471	0.000000
H	-0.653432	-7.139724	0.000000
C	0.262790	3.254059	0.000000

C	1.524858	3.834400	0.000000
C	-0.748919	5.508942	0.000000
C	1.649984	5.232480	0.000000
H	2.428833	3.241999	0.000000
C	0.528092	6.063167	0.000000
H	-1.627309	6.145477	0.000000
H	2.641308	5.671471	0.000000
H	0.653432	7.139724	0.000000

FF-3, ground state singlet (S_0)

H	4.107962	2.747316	0.000000
C	0.000000	1.266079	0.000000
C	1.232261	1.964345	0.000000
C	2.429453	1.267722	0.000000
C	2.425152	-0.181853	0.000000
C	1.238322	-0.872196	0.000000
H	1.222338	3.050061	0.000000
H	1.224295	-1.958027	0.000000
C	3.783279	1.715817	0.000000
C	4.630774	0.574964	0.000000
C	6.033499	0.460209	0.000000
C	6.604772	-0.802813	0.000000
C	5.801933	-1.957821	0.000000
C	4.410716	-1.866796	0.000000
C	3.815212	-0.608624	0.000000
H	6.656931	1.347809	0.000000
H	7.683977	-0.906348	0.000000
H	6.274671	-2.933486	0.000000
H	3.807458	-2.768315	0.000000
C	0.000000	-0.178323	0.000000
C	-1.238322	-0.872196	0.000000
C	-1.232261	1.964345	0.000000
C	-2.425152	-0.181853	0.000000
H	-1.224295	-1.958027	0.000000
C	-2.429453	1.267722	0.000000
H	-1.222338	3.050061	0.000000
C	-3.815212	-0.608624	0.000000
C	-3.783279	1.715817	0.000000
C	-4.630774	0.574964	0.000000
C	-4.410716	-1.866796	0.000000
H	-4.107962	2.747316	0.000000
C	-6.033499	0.460209	0.000000
C	-5.801933	-1.957821	0.000000
H	-3.807458	-2.768315	0.000000
C	-6.604772	-0.802813	0.000000
H	-6.656931	1.347809	0.000000
H	-6.274671	-2.933486	0.000000
H	-7.683977	-0.906348	0.000000

FF-3, lowest triplet state (T_1)

H	0.000000	4.121192	2.743875
C	0.000000	0.000000	1.295520
C	0.000000	1.236606	1.986309
C	0.000000	2.434250	1.281289
C	0.000000	2.422733	-0.167606
C	0.000000	1.237112	-0.853176
H	0.000000	1.234020	3.071634
H	0.000000	1.217058	-1.938660
C	0.000000	3.787308	1.715298
C	0.000000	4.638294	0.561217
C	0.000000	6.033092	0.440181
C	0.000000	6.600334	-0.833092
C	0.000000	5.795566	-1.976627
C	0.000000	4.398287	-1.870609
C	0.000000	3.820025	-0.611673
H	0.000000	6.663552	1.322774
H	0.000000	7.679236	-0.940132
H	0.000000	6.258266	-2.956912
H	0.000000	3.786731	-2.766605
C	0.000000	0.000000	-0.150535
C	0.000000	-1.237112	-0.853176
C	0.000000	-1.236606	1.986309
C	0.000000	-2.422733	-0.167606
H	0.000000	-1.217058	-1.938660
C	0.000000	-2.434250	1.281289
H	0.000000	-1.234020	3.071634
C	0.000000	-3.820025	-0.611673
C	0.000000	-3.787308	1.715298
C	0.000000	-4.638294	0.561217
C	0.000000	-4.398287	-1.870609
H	0.000000	-4.121192	2.743875
C	0.000000	-6.033092	0.440181
C	0.000000	-5.795566	-1.976627
H	0.000000	-3.786731	-2.766605
C	0.000000	-6.600334	-0.833092
H	0.000000	-6.663552	1.322774
H	0.000000	-6.258266	-2.956912
H	0.000000	-7.679236	-0.940132

FF-4, ground state singlet (S_0)

H	0.849262	3.600903	0.000000
C	5.759441	2.645787	0.000000
C	5.185943	3.918597	0.000000

C	3.797807	4.076505	0.000000
C	2.990085	2.938871	0.000000
C	3.579423	1.640016	0.000000
C	4.957263	1.495612	0.000000
H	6.838798	2.544741	0.000000
H	5.825941	4.793641	0.000000
H	3.358395	5.068376	0.000000
H	5.418409	0.513617	0.000000
C	1.556217	2.782237	0.000000
C	1.248049	1.412803	0.000000
C	1.248049	-1.393409	0.000000
C	2.469335	-0.709934	0.000000
C	2.479645	0.673074	0.000000
H	1.255257	-2.477170	0.000000
H	3.396762	-1.272615	0.000000
C	-0.013841	0.722981	0.000000
C	-1.248049	1.393409	0.000000
C	-1.248049	-1.412803	0.000000
C	-2.469335	0.709934	0.000000
H	-1.255257	2.477170	0.000000
C	-1.556217	-2.782237	0.000000
C	-2.479645	-0.673074	0.000000
H	-3.396762	1.272615	0.000000
H	-0.849262	-3.600903	0.000000
C	-2.990085	-2.938871	0.000000
C	-3.579423	-1.640016	0.000000
C	-3.797807	-4.076505	0.000000
C	-4.957263	-1.495612	0.000000
C	-5.185943	-3.918597	0.000000
H	-3.358395	-5.068376	0.000000
C	-5.759441	-2.645787	0.000000
H	-5.418409	-0.513617	0.000000
H	-5.825941	-4.793641	0.000000
H	-6.838798	-2.544741	0.000000
C	0.013841	-0.722981	0.000000

FF-4, lowest triplet state (T_1)

H	0.851289	3.600419	0.000000
C	5.754639	2.625826	0.000000
C	5.189103	3.902755	0.000000
C	3.802615	4.067600	0.000000
C	2.986832	2.932742	0.000000
C	3.570205	1.627860	0.000000
C	4.946542	1.478170	0.000000
H	6.833433	2.518548	0.000000
H	5.834257	4.773831	0.000000
H	3.367970	5.061487	0.000000
H	5.403941	0.494535	0.000000
C	1.560643	2.784354	0.000000

C	1.250273	1.393707	0.000000
C	1.250273	-1.407471	0.000000
C	2.458705	-0.736339	0.000000
C	2.467035	0.663169	0.000000
H	1.244802	-2.490990	0.000000
H	3.388182	-1.295203	0.000000
C	-0.007619	0.715992	0.000000
C	-1.250273	1.407471	0.000000
C	-1.250273	-1.393707	0.000000
C	-2.458705	0.736339	0.000000
H	-1.244802	2.490990	0.000000
C	-1.560643	-2.784354	0.000000
C	-2.467035	-0.663169	0.000000
H	-3.388182	1.295203	0.000000
H	-0.851289	-3.600419	0.000000
C	-2.986832	-2.932742	0.000000
C	-3.570205	-1.627860	0.000000
C	-3.802615	-4.067600	0.000000
C	-4.946542	-1.478170	0.000000
C	-5.189103	-3.902755	0.000000
H	-3.367970	-5.061487	0.000000
C	-5.754639	-2.625826	0.000000
H	-5.403941	-0.494535	0.000000
H	-5.834257	-4.773831	0.000000
H	-6.833433	-2.518548	0.000000
C	0.007619	-0.715992	0.000000

¹ Hacker, A. S.; Pavano, M.; Wood II, J. E.; Immoos, C. E.; Hashimoto, H.; Genis, S. P.; Frantz, D. K. *J. Org. Chem.* **2018**, *83*, 510.