

Supporting Information for
Synthesis and Properties of the 5,10,15-Trimesityltruxen-5-yl Radical

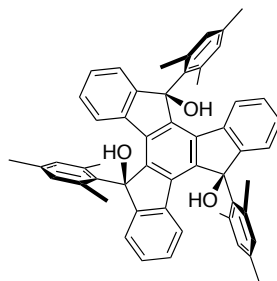
Derik K. Frantz, Joseph J. Walish, and Timothy M. Swager*

Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139

1. Synthetic Procedures

1.1. General:

All synthetic procedures were performed under argon. Anhydrous THF was dried by passage through solvent purification columns containing activated alumina and was stored over activated 3 Å molecular sieves according to a literature procedure.¹ Other solvents and commercially available reagents were used as received without further purification. Analytical thin-layer chromatography was performed with J.T Baker Baker-flex silica gel IB-F sheets. Melting ranges were recorded on a Mel-Temp II apparatus. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AVANCE III spectrometer at 400 MHz (¹H) or 100 MHz (¹³C). Chemical shifts for ¹H NMR are reported in ppm relative to residual CHDCl₂ (5.30 ppm). Chemical shifts for ¹³C NMR are reported in ppm relative to CD₂Cl₂ (53.8 ppm). Multiplicity is indicated by one or more of the following: s (singlet); d (doublet); td (triplet of doublets). Infrared spectra were recorded on a Thermo Scientific Nicolet 6700 Fourier Transform Infrared Spectrometer (FT-IR) using the attenuated total reflectance (ATR) technique on a Ge crystal. Percent transmittance of peaks is indicated relative to that of the strongest peak (normalized to 0%): *s* (0–33%); *m* (33–67%); *w* (67–100%). High resolution mass spectra were performed by the Department of Chemistry Instrumentation Facility (DCIF) and measured on a Bruker Daltonics APEXIV 4.7 Tesla Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR-MS) using electrospray ionization (ESI). Routine mass spectra were recorded on a Waters LCT Premier electrospray-ionization time-of-flight mass spectrometer (ESI-TOF-MS). Solution phase electron paramagnetic resonance (EPR) spectroscopy was carried out on a Bruker EMX EPR spectrometer using a Gunn diode to generate monochromatic microwave radiation in the X-band region.



1.2. (*syn*)-5,10,15-tris(2,4,6-trimethylphen-1-yl)truxen-5,10,15-triol (4):

In a 250-mL, two-neck round-bottom flask, a solution of 2-bromomesitylene (5.18 g, 26.0 mmol) in dry THF (80 mL) was cooled to –78 °C (CO_{2(s)}–acetone bath) and *tert*-

¹ Williams, D. B. G.; Lawton, M. J. *Org. Chem.* **2010**, 75, 8351.

butyllithium (31 mL, 1.7 mol/L in pentane, 53 mmol) was added steadily over 4 min while stirring. The reaction mixture was allowed to warm to 22 °C and was stirred at that temperature for 10 min, after which it was added by cannula to a stirring suspension of truxene5,10,15-trione (**3**) (1.00 g, 2.6 mmol) in THF (40 mL) at 0 °C. The resulting reaction mixture was allowed to warm to r.t. and was stirred for 18 h, after which H₂O (~80 mL) was added under argon flow. EtOAc was added and the phases were separated. The aqueous phase was extracted with EtOAc and the combined organic phase was dried with MgSO₄ and concentrated *in vacuo*. The resulting residue was suspended in CH₂Cl₂ (~20 mL) and hexane (~100 mL) was added, forming a colorless precipitate, which was filtered (fraction 1). The filtrate was concentrated and the CH₂Cl₂–hexane precipitation method was repeated, affording additional precipitate (fraction 2). NMR showed that the fractions contained the same product, each with a small amount of a mesitylene impurity. The fractions were combined and triturated with hexane (10 mL) for 15 min at 22 °C and filtered, affording triol **4** as a colorless precipitate (1.09 g, 56%)

mp (~2 °C/min) 265–270 °C (decomp. to black solid) (Slow discoloration begins at 240 °C.)

¹H NMR (400 MHz, CD₂Cl₂, δ) 7.31 (d, 3H, ³J = 7.6 Hz), 7.26 (d, 3H, ³J = 7.6 Hz), 7.13 (td, 3H, ³J = 7.5 Hz, ⁴J = 1.1 Hz), 7.07 (s, 3H), 7.04 (td, 3H, ³J = 7.5 Hz, ⁴J = 1.1 Hz), 6.55 (s, 3H), 2.99 (s, 9H), 2.41 (s, 3H), 2.21 (s, 9H), 1.57 (s, 9H) (Note that rotation of the mesityl groups about the truxene framework is blocked, which is evidenced by two distinct signals for both the *ortho* methyl groups and the *meta* protons of the mesityl group.);

¹³C NMR (100 MHz, CD₂Cl₂, δ) 149.9, 147.8, 138.2, 137.8, 137.1, 136.8, 136.1, 135.3, 133.3, 131.3, 129.1, 128.8, 125.6, 124.7, 86.7, 26.3, 22.8, 20.6.

IR (neat) 3559w, 3450–3150w (broad), 2968w, 2922w, 1609w, 1471m, 1455w, 1379w, 1265w, 1129w, 1044m, 1026m, 1005m, 917m, 853m, 818w, 763m 746s, 643m;

HRMS (ESI) Calcd. for C₅₄H₄₈O₃Na (M+Na⁺) 767.3496, found 767.3480.

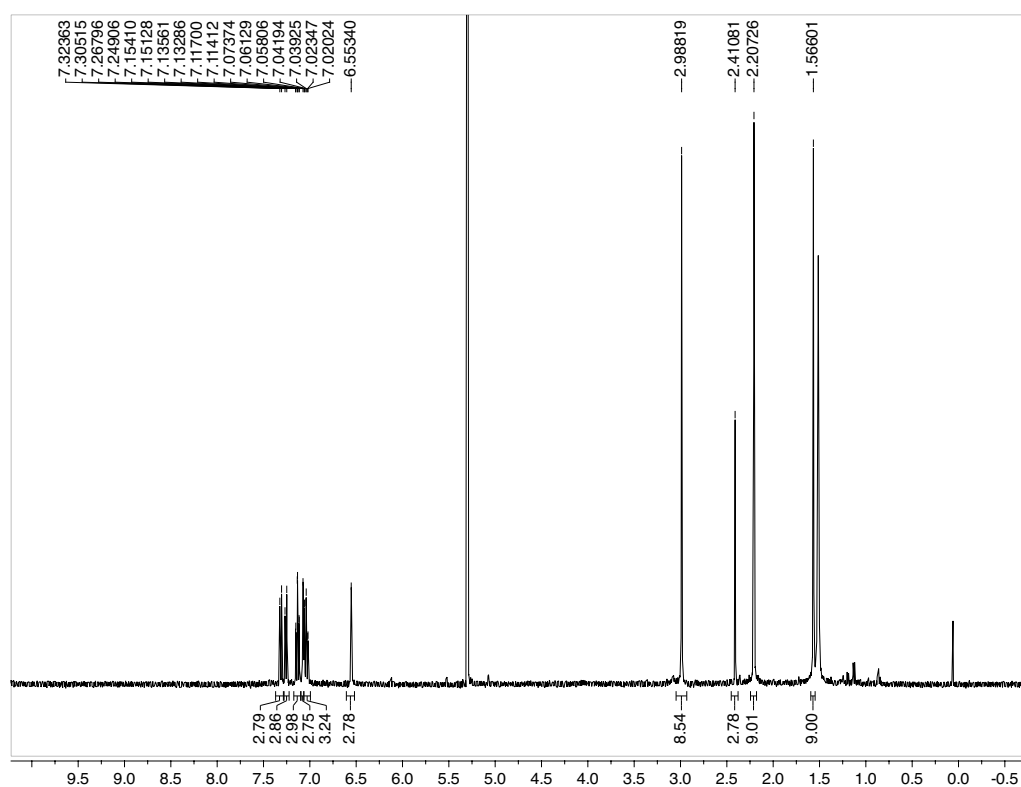


Figure S1: ^1H NMR (400 MHz) spectrum of compound **4**. Residual solvent peak at 5.32 ppm and water from solvent at 1.52 ppm.

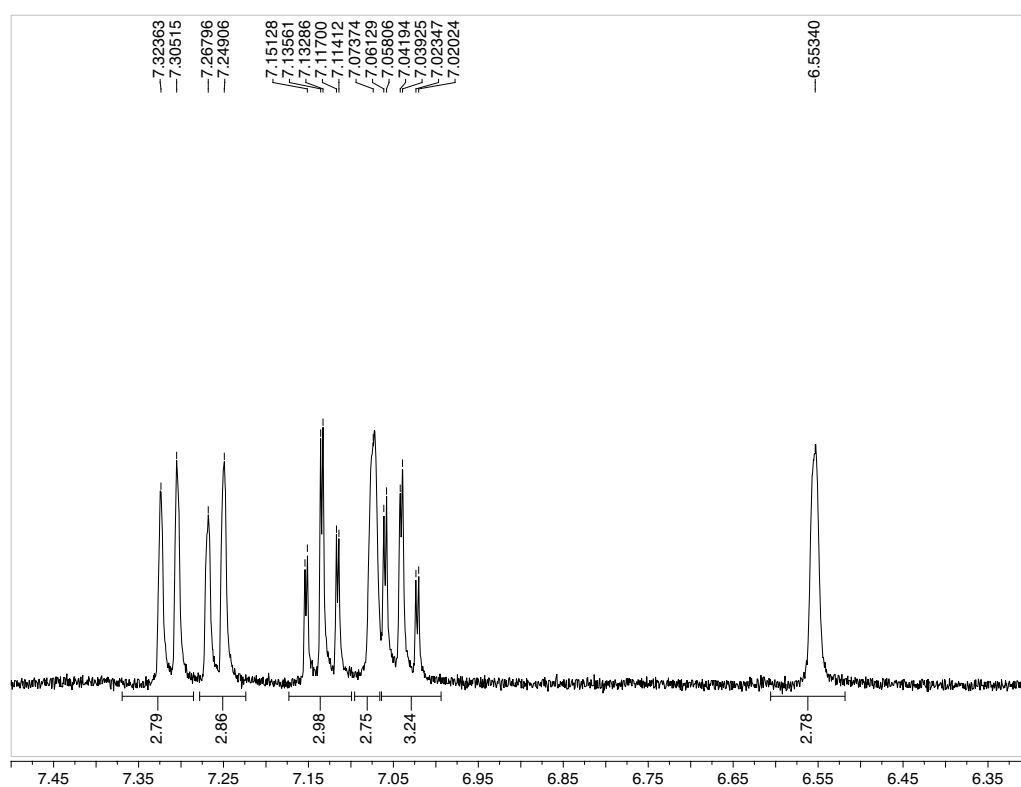


Figure S2: aromatic region of ^1H NMR (400 MHz) spectrum of compound **4**.

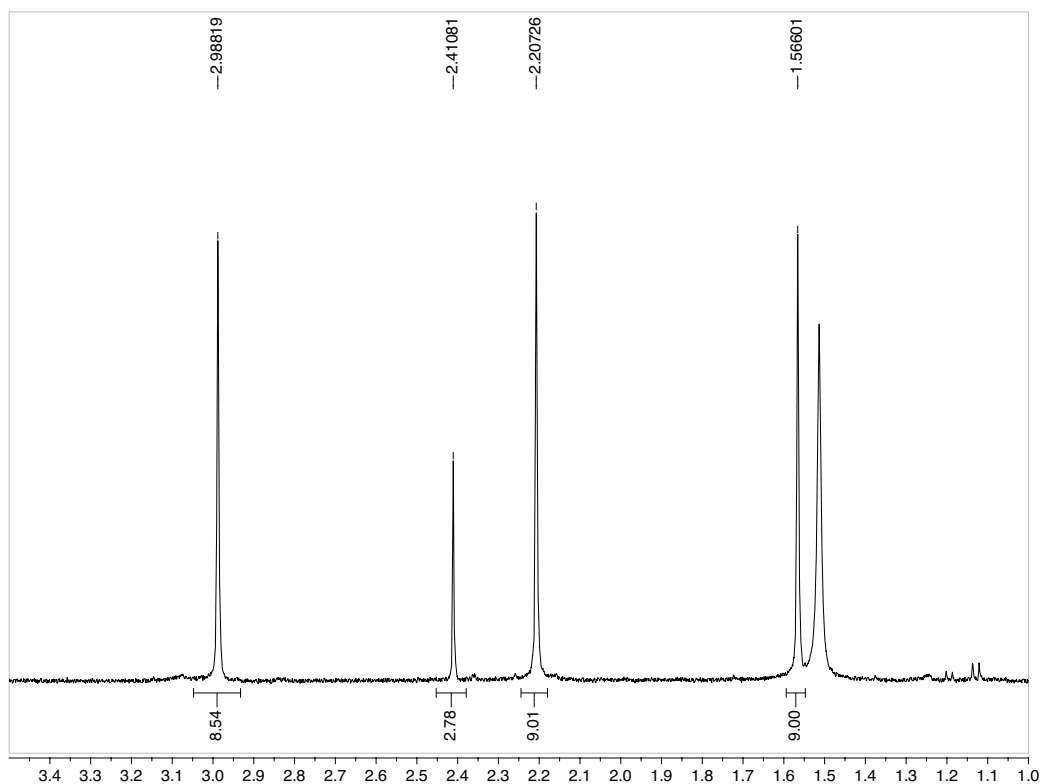


Figure S3: aliphatic region of ^1H NMR (400 MHz) spectrum of compound **4**. Water from solvent is present at 1.52 ppm.

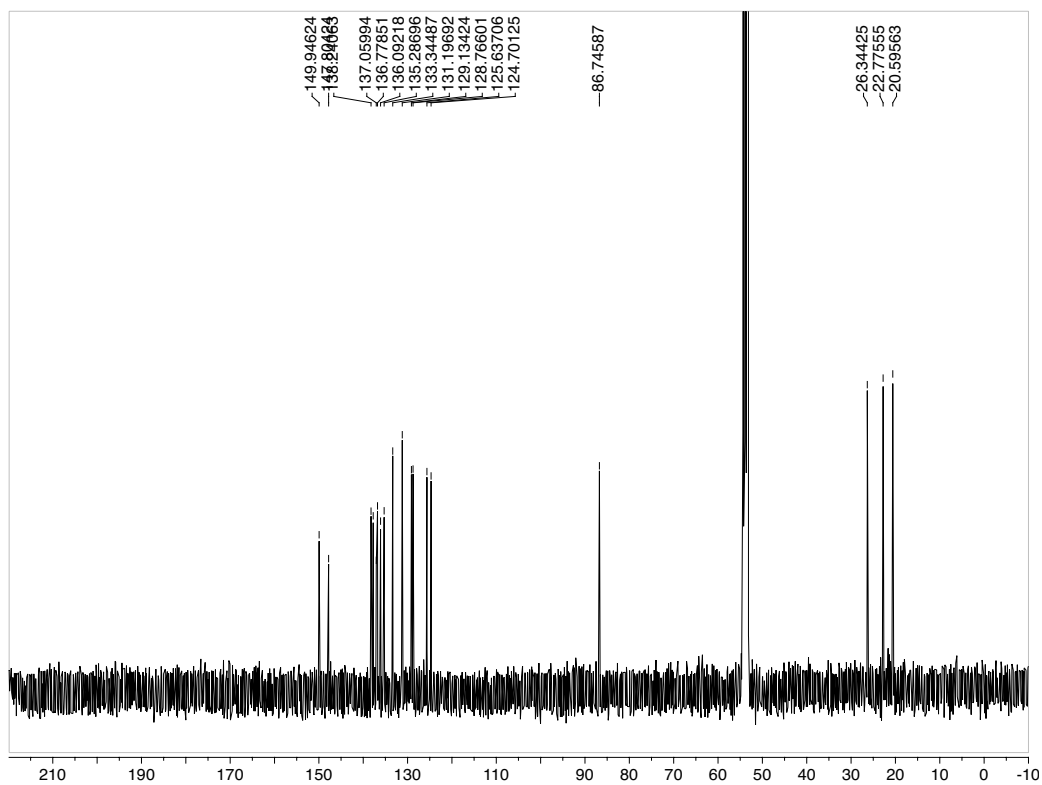


Figure S4: ^{13}C NMR (100 MHz) spectrum of compound **4**. Residual solvent peak at 53.8 ppm.

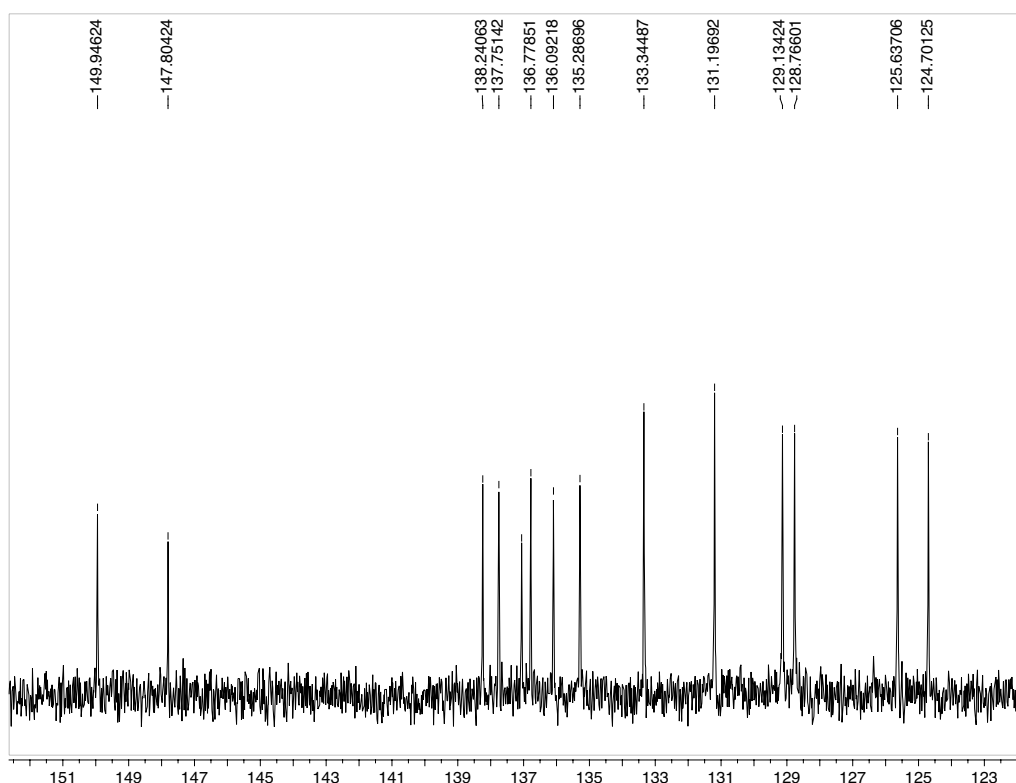
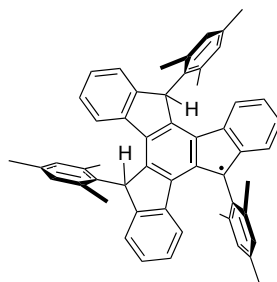


Figure S4: aromatic region of ^{13}C NMR (100 MHz) spectrum of compound **4**.



1.3. 5,10,15-tris(2,4,6-trimethylphenyl)truxen-5-yl (**5**):

A 25-mL, two-neck round-bottom flask was charged with triol **4** (100 mg, 134 μmol) and anhydrous SnCl_2 (181 mg, 955 μmol). CH_2Cl_2 (5 mL) was added while stirring and concentrated HCl (0.08 mL) was added immediately thereafter. The dark reaction mixture was allowed to stir for 2 h, after which hexane (5 mL) was added. The solution was charged onto a pre-packed silica column and the column was eluted with 1:1 CH_2Cl_2 –hexane. Fractions containing a bright green product were concentrated, affording **5** (48 mg, 52%) as a dark green film. A very dark material with red/purple coloration remained on the top of the column. As the green radical slowly oxidizes, it can be freshly re-purified by silica plug with 1:1 CH_2Cl_2 –hexane, leaving dark material on the baseline.

Rf 0.83 (silica, 1:1 CH_2Cl_2 –hexane);

mp (not measured: product exists as non-crystalline film)

IR (neat): 2958_w, 2918_w, 2858_w, 1610_w, 1465_m, 1377_w, 1155_w, 1027_w, 851_m, 741_s.

HRMS (ESI) Calcd. for C₅₄H₄₇ 695.3672, found 695.3684.

EPR (9.823 GHz, CH₂Cl₂ [degassed by purging with Ar])

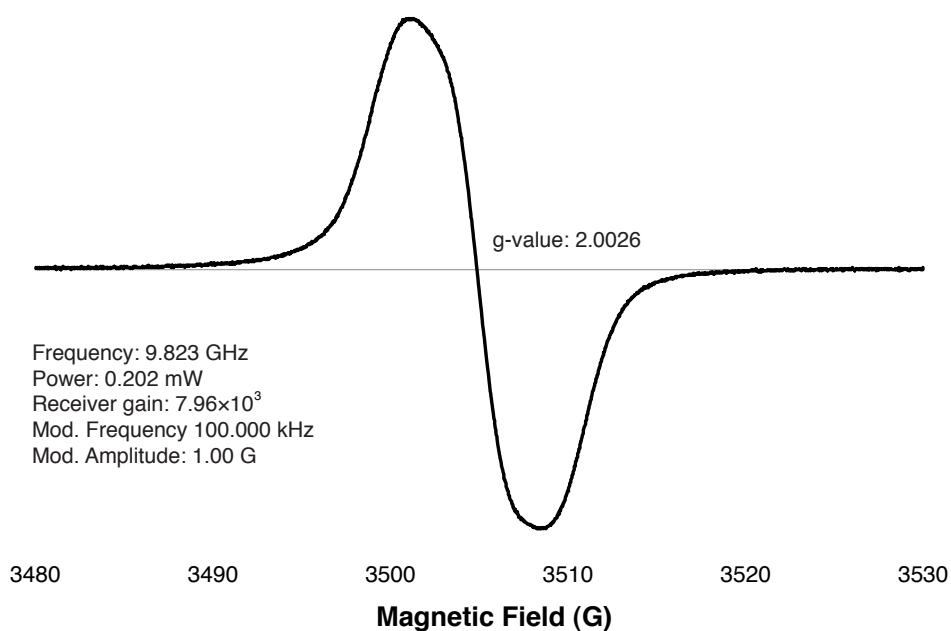


Figure S6: Solution-phase EPR spectrum of radical **5** in degassed CH₂Cl₂ at 9.823 GHz.

1.4. Synthesis of Derivative of **5** with Deuterated Methanetriyl Groups:

Triol **4** (25 mg, 34 mmol) was dissolved in a mixture of CH₂Cl₂ (1 mL) and CD₃OD (1 mL, 99.5% D). The mixture was stirred for 5 min and the solvent was removed *in vacuo*. To the deuterium-exchanged triol residue was added dry CH₂Cl₂ (2 mL) and a solution of SnCl₂ (anhydrous, 45 mg, 240 mmol) in 35% DCl in D₂O (99% D). The reaction was stirred for 15 minutes and the contents of the reaction were placed on a SiO₂ column. Elution with 1:1 CH₂Cl₂/hexane afforded deuterated radicals **5**-(D,D) (74% by MS) and **5**-(H,D) (26% by MS) (87% total deuteration of methanetriyl moieties) as a green film.

2. Absorption Spectrum

Absorption spectra of **5** were measured on a Cary 400 UV-Vis spectrophotometer. Measurements were conducted using 10 mm quartz cuvettes and degassed (argon purged) CH₂Cl₂ as solvent. Molar extinction coefficients were measured in triplicate, using three separately and freshly prepared solutions (5.02 × 10⁻⁵ M, 3.65 × 10⁻⁵ M, and 3.54 × 10⁻⁵ M) and calculated according to the Beer–Lambert law ($\epsilon = Acl$).

Standard deviation of ϵ remains below 1.8% for all values with λ greater than 300 and ϵ greater than 1000. The spectrum shown in Figure 4B in letter shows ϵ as the average of the three solutions.

3. Cyclic Voltammetry

Cyclic voltammetry (CV) measurements of **5** were performed under N₂ in a glove box on an Eco Chemie Autolab potentiostat (Model PGSTAT20) using a Ag/AgNO₃ reference electrode (containing a solution of 0.01 M AgNO₃, 0.1 Bu₄NPF₆ in CH₃CN), a Pt button working electrode, and a Pt wire counter electrode. Measurements were performed at a sweep rate of 50 mV/s in dry, degassed CH₂Cl₂ with Bu₄NPF₆ (0.1 M) as electrolyte. The ferrocene/ferrocenium (Fc/Fc⁺) couple was used as an internal standard, measured directly after measurement of pure **5**, and compared to the reduction peak of **5**, as the Fc/Fc⁺ oxidation peak overlaps with the oxidation peak of compound **5**. The HOMO energy level was calculated by the equation:

$$E_{\text{HOMO}} \text{ (eV)} = - [E_{\text{onset}} - E_{\text{onset}}(\text{Fc/Fc}^+)] - 4.80 \text{ eV},$$

where E_{onset} is the onset oxidation potential for the oxidation of **4** and $E_{\text{onset}}(\text{Fc/Fc}^+)$ is the onset oxidation potential for the Fc/Fc⁺ couple. The value −4.80 is the HOMO energy of ferrocene compared to the vacuum level.

4. Determination of Half-Life of Radical **5** under Air

Radical **4** was freshly prepared by a short silica column (1:1 CH₂Cl₂/hexane) and was dissolved in non-degassed CH₂Cl₂ (4×10^{-5} mol/L) and an absorption spectrum (Agilent 845x UV-Vis spectrophotometer) was measured immediately thereafter (0 h). The cuvette was allowed to stand uncapped under air and absorption spectra were collected every few hours (Figure 5 in letter, Table S1). Prior to collection of each spectrum, CH₂Cl₂ was added to the cuvette up to a marker line to ensure roughly constant total concentration of **5** and its oxidation products. The peak at 403 nm steadily decreased upon reaction with oxygen reduction of absorption at this wavelength was used to determine decay of **5** under air.

Table S1. Kinetic data from oxidation of radical **5** under air.

t (min)	t (h)	Absorbance at 403 nm (Abs)	Abs* ^(a)	−ln(Abs*−Abs ₀ *)
0	0.0	0.624	0.543	0.000
235	3.9	0.411	0.330	0.498
474	7.0	0.287	0.206	0.969
716	11.9	0.198	0.117	1.535
985	16.4	0.158	0.077	1.953
1290	21.5	0.123	0.042	2.559
1590	26.5	0.102	0.021	3.253

^(a)Abs* is defined as Abs − 0.080, this number being the extrapolated value for Abs after radical **5** is completely consumed (Abs_∞, see text).

The oxidized product(s) also absorb at 403 nm; therefore, the first order decay equation must include a limit for $t \rightarrow \infty$ (Abs_∞) and follow $\text{Abs} = \text{Abs}_0 e^{-kt} + \text{Abs}_\infty$. A value of Abs_∞ = 0.080 gives the best line fit for the exponential decay and was used in the determination of Abs* (Abs* = Abs − Abs_∞), which was shown in the kinetic plots in Figure 5B in the letter.

The mass spectrum (ESI-TOF, positive mode) of the material in the cuvette after 26.5 h exposure to air showed only a very small peak from **5**⁺. The major peak at 711 could be attributable to [**5**+O]⁺, the peak at 727 to [**5**+O₂]⁺, the peak at 743 to [**5**+O₃]⁺, and the peak at 792 to [**5**+O₆H]⁺. The structures of the products giving rise to these peaks are unclear and were not investigated further.

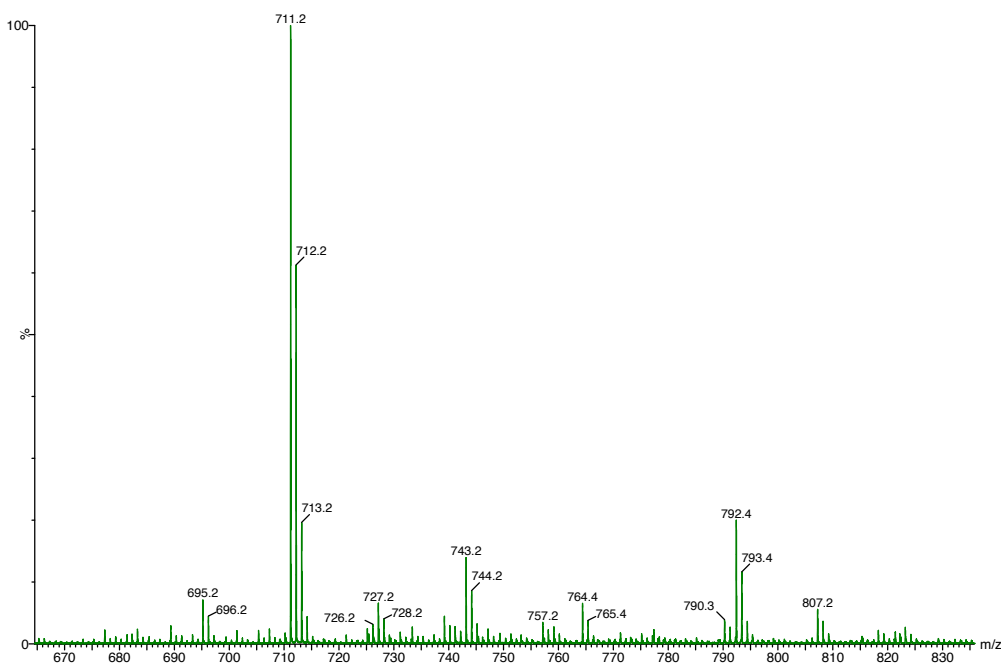


Figure S7. ESI-TOF MS spectrum of material after exposing **5** to air for 26.5 h.

5. High-Field EPR Measurement

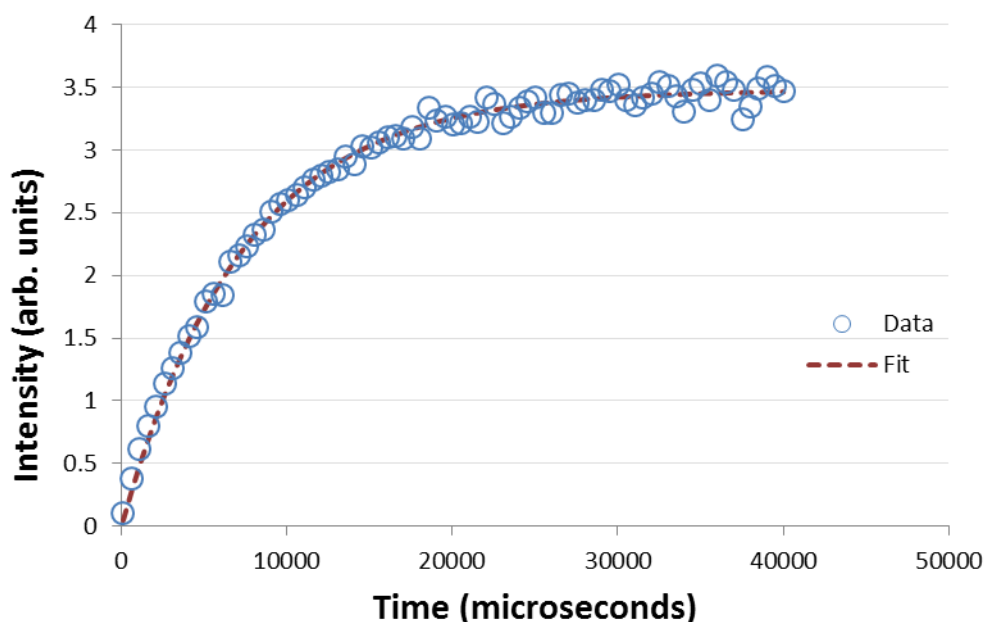


Figure S8. High-field EPR measurement (saturation recovery) and least-squares fit of the electron T_1 of radical **5**.

EPR measurements were conducted on a custom-made 140 GHz spectrometer in the Francis Bitter Magnet Laboratory. Radical **5** was dissolved in toluene at a concentration of 1 mM. The frozen powder pattern shown in figure 3 (bold, black line) was recorded at 80K using a Hahn echo ($\pi/2$ pulse = 20 ns, π pulse = 40 ns, pulse separation = 200 ns). The magnetic field was swept from 4993 mT to 4996.5 mT and data were collected at 71 equally-spaced point utilizing 100 transients per point. Ten powder patterns were collected and averaged to improve the signal-to-noise ratio.

The powder pattern data shown for the trityl and SA-BDPA samples were extracted from reference 8 in the main text. The peak positions of these radicals were adjusted to the field location specified in the supporting information of that text.

The spin-lattice relaxation time (T_1) was measured with a saturation recovery experiment. At a field position corresponding to the center of the EPR line (4994.75 mT), a saturation pulse with a duration of 1 ms was applied and the intensity of the Hahn echo ($\pi/2$ pulse = 35 ns, π pulse = 70 ns, pulse separation = 200 ns, repetition time 50 ms) was recorded after a recovery delay. This recovery delay was varied to perform the saturation recovery experiment: 100 samples were taken at each of the 81 equally-spaced data points from 100 microseconds to 40 milliseconds. These data were then fit to the equation $y = A - Ae^{(-x/T_1)}$ using the least-squares method. From the least-squares fit, the value of the electron T_1 was determined to be 7.3 milliseconds.

6. Calculations

6.1 General Remarks

Density functional calculations on radical **5**, both *syn* and *anti* diastereomers, were carried out using the Spartan² software package. B3LYP calculations were performed in the 6-31G(d) basis set.

6.2 Geometric Coordinates and Spin Densities for Calculated Structures

5 (*anti* configuration) (B3LYP/6-31G*)

E = -2086.123808850 (Hartrees)

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	0.659557	-1.192496	0.382975
2 C	-0.843713	1.036501	-0.469770
3 C	-0.702573	-1.330411	0.092885
4 C	1.288412	0.082253	0.351284
5 C	0.555655	1.213815	-0.110909
6 C	-1.462883	-0.190799	-0.314617
7 C	-1.603532	-2.490726	0.152115
8 C	-3.749633	-4.291018	0.173927
9 C	-1.389600	-3.827013	0.514550
10 C	-2.901315	-2.075366	-0.211171
11 C	-3.972734	-2.959894	-0.190546
12 C	-2.463644	-4.717278	0.518363
13 H	-0.401558	-4.181469	0.770067
14 H	-4.974135	-2.619456	-0.438997
15 H	-2.294361	-5.754164	0.796575
16 H	-4.578420	-4.993703	0.191560
17 C	-1.349483	2.326690	-0.956149
18 C	-1.669371	4.990753	-1.784612
19 C	-0.272194	3.252473	-0.874545
20 C	-2.575784	2.748029	-1.462154
21 C	-2.729289	4.079934	-1.872467
22 C	-0.432536	4.583608	-1.286134

² Shao, Y.; Molnar, L. F.; Jung, Y.; Kussmann, J.; Ochsenfeld, C.; Brown, S. T.; Gilbert, A. T. B.; Slipchenko, L. V.; Levchenko, S. V.; O'Neill, D. P.; DiStasio Jr. R. A.; Lochan, R. C.; Wang, T.; Beran, G. T. O.; Besley, N. A.; Herbert, J. M.; Lin, C. Y.; Van Voorhis, T.; Chien, S. H.; Sodt, A.; Steele, R. P.; Rassolov, V. A.; Maslen, P. E.; Korambath, P. P.; Adamson, R. D.; Austin, B.; Baker, J. Byrd, E. F. C.; Dachsel, H.; Doerksen, R. J.; Dreuw, A.; Dunietz, B. D.; Dutoi, A. D.; Furlani, T. R.; Gwaltney, S. R.; Heyden, A.; Hirata, S.; Hsu, C.-P.; Kedziora, G.; Khalliulin, R. Z.; Klunzinger, P.; Lee, A. M.; Lee, A. S.; Liang, W. Z.; Lotan, I.; Nair, N.; Peters, B.; Proynov, E. I.; Pieniazek, P. A.; Rhee, Y. M.; Ritchie, J.; Rosta, E.; Sherrill, C. D.; Simmonett, A. C.; Subotnik, J. E.; Woodcock III, H. L.; Zhang, W.; Bell, A. T.; Chakraborty, A. T.; Chipman, D. M.; Keil, F. J.; Warshel, A.; Hehre, W. J.; Schaefer, J. F.; Kong, J.; Krylov, A. I.; Gill, P. M. W.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* **2006**, 8, 3172.

23	H	-3.418928	2.073770	-1.525298
24	H	-3.689862	4.406936	-2.261704
25	H	0.398831	5.279662	-1.216936
26	H	-1.811474	6.018714	-2.107542
27	C	2.677846	-0.083591	0.829109
28	C	5.172077	-1.000300	1.748217
29	C	3.724786	0.824107	1.051415
30	C	2.898756	-1.449236	1.107630
31	C	4.134568	-1.912992	1.543888
32	C	4.957700	0.359136	1.509780
33	H	4.298020	-2.973610	1.714544
34	H	5.761066	1.071925	1.676341
35	H	6.141923	-1.348785	2.093459
36	C	1.636959	-2.260463	0.873568
37	H	1.265779	-2.589173	1.852745
38	C	-2.909831	-0.601686	-0.595396
39	C	0.896732	2.591114	-0.350181
40	C	1.904302	-3.527752	0.048791
41	C	2.502068	-5.917465	-1.370636
42	C	2.044420	-4.758608	0.733360
43	C	2.105769	-3.497798	-1.351140
44	C	2.391425	-4.689481	-2.025751
45	C	2.335302	-5.923976	0.013342
46	H	2.542110	-4.649101	-3.103236
47	H	2.437956	-6.861725	0.556401
48	C	2.154952	3.357741	-0.166237
49	C	4.485320	4.922431	0.150400
50	C	3.101464	3.432880	-1.209915
51	C	2.360367	4.089750	1.025350
52	C	3.522383	4.853287	1.162941
53	C	4.250610	4.209992	-1.028041
54	H	3.677247	5.408693	2.086471
55	H	4.981711	4.260163	-1.833004
56	H	3.596948	1.880665	0.876838
57	H	-3.030630	-0.546080	-1.685266
58	C	-4.080448	0.169144	0.025630
59	C	-6.332760	1.525370	1.102700
60	C	-5.222369	0.419421	-0.773312
61	C	-4.094165	0.564861	1.381897
62	C	-5.213140	1.239682	1.884297
63	C	-6.319423	1.091594	-0.223509
64	H	-5.207067	1.543303	2.929484
65	H	-7.188082	1.276077	-0.853311
66	C	-2.956601	0.276646	2.338150
67	H	-2.669661	-0.780151	2.326564
68	H	-3.252546	0.527540	3.361759
69	H	-2.060016	0.857317	2.098033
70	C	-7.509956	2.285366	1.667214
71	H	-8.455688	1.944054	1.231707
72	H	-7.426864	3.360578	1.458505

73 H	-7.576524	2.169974	2.754305
74 C	-5.310951	-0.011561	-2.226634
75 H	-5.140776	-1.086394	-2.356511
76 H	-4.580206	0.506433	-2.862330
77 H	-6.303456	0.214407	-2.627133
78 C	2.059313	-2.222457	-2.165008
79 H	2.353305	-2.425682	-3.199474
80 H	2.742694	-1.464008	-1.768426
81 H	1.060018	-1.776188	-2.183181
82 C	1.889424	-4.882056	2.239048
83 H	2.104569	-5.906214	2.558776
84 H	0.871030	-4.648379	2.577295
85 H	2.566548	-4.218932	2.789046
86 C	2.785433	-7.187933	-2.137284
87 H	1.880418	-7.566200	-2.631037
88 H	3.154016	-7.980514	-1.477817
89 H	3.534487	-7.024878	-2.920423
90 C	2.891822	2.685000	-2.507259
91 H	2.805883	1.605040	-2.340848
92 H	3.726799	2.855159	-3.194144
93 H	1.969767	3.003480	-3.007669
94 C	1.349718	4.038688	2.148824
95 H	1.153914	3.007436	2.465110
96 H	0.386517	4.464155	1.841822
97 H	1.703915	4.598460	3.019924
98 C	5.748011	5.732311	0.334709
99 H	6.461077	5.216592	0.991647
100 H	5.538364	6.706485	0.791586
101 H	6.251903	5.909435	-0.620925

Ground-State Mulliken Net Atomic Charges

Atom	Charge (a.u.)	Spin (a.u.)

1 C	0.007315	-0.089805
2 C	-0.030733	0.130343
3 C	0.027246	0.177833
4 C	0.005809	0.195589
5 C	0.036432	-0.167830
6 C	0.030920	-0.063437
7 C	0.064035	-0.045535
8 C	-0.130679	0.053156
9 C	-0.174364	0.049088
10 C	0.122022	0.047504
11 C	-0.204327	-0.026682
12 C	-0.151814	-0.025155
13 H	0.149841	-0.002342
14 H	0.135473	0.000977

15 H	0.126307	0.000923
16 H	0.127213	-0.002560
17 C	0.059678	0.111116
18 C	-0.134596	-0.065312
19 C	0.084906	-0.127015
20 C	-0.173830	-0.048907
21 C	-0.152548	0.151750
22 C	-0.201276	0.155270
23 H	0.148391	0.001867
24 H	0.125449	-0.007452
25 H	0.138468	-0.006718
26 H	0.125388	0.002204
27 C	0.057853	-0.043020
28 C	-0.131587	0.046402
29 C	-0.179777	0.043357
30 C	0.120972	0.042087
31 C	-0.202266	-0.023561
32 C	-0.145595	-0.022246
33 H	0.134066	0.000870
34 H	0.125714	0.000815
35 H	0.125730	-0.002233
36 C	-0.366484	0.002126
37 H	0.172069	-0.001706
38 C	-0.365260	0.000445
39 C	-0.091530	0.575378
40 C	0.080522	-0.001514
41 C	0.207317	0.000197
42 C	0.126683	0.000276
43 C	0.133984	0.000329
44 C	-0.246327	-0.000145
45 C	-0.255902	-0.000116
46 H	0.112323	-0.000017
47 H	0.111078	-0.000013
48 C	-0.109715	-0.048352
49 C	0.213650	0.002249
50 C	0.202314	0.016879
51 C	0.189213	0.016927
52 C	-0.265543	-0.001654
53 C	-0.270861	-0.001591
54 H	0.114908	0.001136
55 H	0.114878	0.001138
56 H	0.164942	-0.001882
57 H	0.175521	-0.001325
58 C	0.083977	-0.000883
59 C	0.207237	0.000013
60 C	0.122132	0.000008
61 C	0.136402	0.000146
62 C	-0.248443	-0.000008
63 C	-0.252697	0.000005
64 H	0.112436	-0.000014

65 H	0.110857	-0.000008
66 C	-0.545613	0.000371
67 H	0.169215	-0.000089
68 H	0.148147	-0.000186
69 H	0.177820	0.000139
70 C	-0.532094	0.000001
71 H	0.155097	-0.000001
72 H	0.164758	0.000002
73 H	0.155787	0.000000
74 C	-0.550151	-0.000052
75 H	0.165408	-0.000035
76 H	0.164817	-0.000008
77 H	0.157315	-0.000058
78 C	-0.546337	0.000120
79 H	0.147793	-0.000204
80 H	0.172651	-0.000085
81 H	0.175351	-0.000098
82 C	-0.551834	0.000023
83 H	0.157331	-0.000070
84 H	0.164322	0.000030
85 H	0.165972	-0.000022
86 C	-0.532489	-0.000013
87 H	0.164380	0.000012
88 H	0.153494	0.000000
89 H	0.157870	0.000004
90 C	-0.536513	0.000016
91 H	0.171805	-0.000012
92 H	0.150125	0.000492
93 H	0.169157	-0.000219
94 C	-0.534073	0.000120
95 H	0.168719	-0.000119
96 H	0.170772	-0.000019
97 H	0.150055	0.000571
98 C	-0.532403	-0.000140
99 H	0.163491	0.000103
100 H	0.158685	0.000063
101 H	0.155659	-0.000003

Sum of atomic charges = 0.000000

Sum of spin charges = 1.000000

5 (*syn* configuration) (B3LYP/6-31G*)

E = -2086.123451918 (Hartrees)

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	0.062741	1.326897	0.577629

2 C	-0.161928	-1.483278	0.406190
3 C	1.177795	0.512420	0.812249
4 C	-1.208553	0.757969	0.291741
5 C	-1.348908	-0.658357	0.244550
6 C	1.067416	-0.906566	0.673312
7 C	2.550492	0.828144	1.235641
8 C	5.238116	0.841898	2.030027
9 C	3.185177	2.041587	1.533142
10 C	3.276705	-0.374729	1.357060
11 C	4.613558	-0.374095	1.737453
12 C	4.522651	2.038496	1.930062
13 H	2.662510	2.981340	1.430517
14 H	5.172080	-1.304513	1.795730
15 H	5.013457	2.982224	2.152903
16 H	6.282359	0.855729	2.330895
17 C	-0.576968	-2.889011	0.309355
18 C	-1.995875	-5.303836	0.107804
19 C	-1.988342	-2.894673	0.127915
20 C	0.108633	-4.098821	0.377827
21 C	-0.605860	-5.300819	0.275359
22 C	-2.697323	-4.100946	0.035003
23 H	1.184665	-4.128595	0.485604
24 H	-0.066642	-6.243070	0.325565
25 H	-3.776372	-4.092039	-0.091950
26 H	-2.530141	-6.247267	0.033245
27 C	-2.174491	1.861371	0.107144
28 C	-3.515030	4.319010	-0.136553
29 C	-3.525353	1.892063	-0.272272
30 C	-1.509508	3.083269	0.340209
31 C	-2.164004	4.303351	0.218075
32 C	-4.182889	3.117252	-0.384285
33 H	-1.627225	5.235090	0.374076
34 H	-5.229467	3.129734	-0.677400
35 H	-4.039920	5.265688	-0.234478
36 C	-0.050925	2.849169	0.692471
37 H	0.081579	3.079774	1.757434
38 C	2.396831	-1.574630	1.036401
39 H	2.204630	-2.108691	1.975412
40 C	-2.476976	-1.537658	0.093039
41 C	3.086485	-2.568178	0.093322
42 C	4.485771	-4.416075	-1.550731
43 C	3.678761	-3.726803	0.652304
44 C	3.222504	-2.331625	-1.293009
45 C	3.907760	-3.262203	-2.082119
46 C	4.358824	-4.625479	-0.177404
47 H	3.993711	-3.070268	-3.150117
48 H	4.800146	-5.515578	0.267253
49 C	0.879023	3.787761	-0.086956
50 C	2.525558	5.644423	-1.473742
51 C	1.381554	4.939116	0.568764

52	C	1.173376	3.599201	-1.455333
53	C	1.994157	4.524452	-2.112311
54	C	2.194196	5.836875	-0.131587
55	H	2.215606	4.362008	-3.165497
56	H	2.574530	6.713498	0.389423
57	C	-3.936253	-1.277481	0.016895
58	C	-6.735333	-0.907316	-0.103100
59	C	-4.608286	-1.361927	-1.222272
60	C	-4.669671	-1.030131	1.199552
61	C	-6.051607	-0.844784	1.115789
62	C	-5.993834	-1.166850	-1.258169
63	H	-6.608869	-0.647909	2.029985
64	H	-6.505520	-1.218754	-2.217363
65	H	-4.066475	0.984178	-0.487867
66	C	2.664296	-1.101402	-1.973589
67	H	3.028234	-0.178362	-1.509052
68	H	1.570377	-1.074328	-1.934907
69	H	2.963502	-1.081673	-3.026086
70	C	3.589441	-4.058124	2.131081
71	H	4.162109	-4.964181	2.351249
72	H	2.556063	-4.244179	2.452264
73	H	3.983912	-3.258910	2.769188
74	C	5.248961	-5.384196	-2.423976
75	H	6.309266	-5.105774	-2.495088
76	H	4.850252	-5.403851	-3.444102
77	H	5.207633	-6.403316	-2.024170
78	C	-3.978402	-0.953113	2.541755
79	H	-3.311670	-0.084626	2.601936
80	H	-3.362471	-1.840388	2.726967
81	H	-4.709113	-0.870465	3.352130
82	C	-3.849691	-1.614002	-2.506474
83	H	-3.075511	-0.854492	-2.668385
84	H	-4.525156	-1.595745	-3.367399
85	H	-3.342503	-2.585560	-2.494364
86	C	-8.234292	-0.724399	-0.160587
87	H	-8.559201	0.124767	0.451824
88	H	-8.758796	-1.612122	0.217400
89	H	-8.577482	-0.552579	-1.185852
90	C	0.621329	2.446453	-2.265651
91	H	1.007934	1.480548	-1.925413
92	H	0.893019	2.562484	-3.319628
93	H	-0.471233	2.393687	-2.208538
94	C	1.078228	5.249374	2.024093
95	H	1.521680	6.209341	2.305113
96	H	1.487029	4.493650	2.707761
97	H	0.002591	5.313862	2.226070
98	C	3.431899	6.609407	-2.201470
99	H	4.487983	6.420832	-1.965625
100	H	3.220107	7.648117	-1.922450
101	H	3.319477	6.521227	-3.287193

Ground-State Mulliken Net Atomic Charges

Atom	Charge (a.u.)	Spin (a.u.)
1 C	0.011214	-0.090293
2 C	-0.025885	0.130990
3 C	0.026469	0.179731
4 C	0.003775	0.194044
5 C	0.038044	-0.167679
6 C	0.025063	-0.063570
7 C	0.062308	-0.045844
8 C	-0.130196	0.053541
9 C	-0.174355	0.049385
10 C	0.123459	0.047941
11 C	-0.204188	-0.026928
12 C	-0.151880	-0.025345
13 H	0.150204	-0.002343
14 H	0.134902	0.000989
15 H	0.126215	0.000929
16 H	0.126957	-0.002579
17 C	0.055599	0.110066
18 C	-0.134931	-0.064489
19 C	0.086836	-0.125619
20 C	-0.178605	-0.048329
21 C	-0.153067	0.149896
22 C	-0.201256	0.153225
23 H	0.153921	0.001838
24 H	0.125878	-0.007357
25 H	0.138294	-0.006634
26 H	0.125431	0.002174
27 C	0.057373	-0.042453
28 C	-0.131854	0.045775
29 C	-0.177693	0.042811
30 C	0.118776	0.041456
31 C	-0.201504	-0.023154
32 C	-0.147088	-0.021790
33 H	0.134038	0.000853
34 H	0.126560	0.000798
35 H	0.125795	-0.002204
36 C	-0.363011	0.002161
37 H	0.172904	-0.001699
38 C	-0.364602	0.000351
39 H	0.176491	-0.001196
40 C	-0.091442	0.573109
41 C	0.078723	-0.001039
42 C	0.206133	0.000090
43 C	0.123299	0.000093
44 C	0.137835	0.000231

45 C	-0.248241	-0.000060
46 C	-0.252224	-0.000032
47 H	0.112983	-0.000014
48 H	0.111312	-0.000007
49 C	0.078227	-0.001578
50 C	0.207201	0.000352
51 C	0.123500	0.000420
52 C	0.135594	0.000474
53 C	-0.249867	-0.000236
54 C	-0.251372	-0.000195
55 H	0.112501	-0.000013
56 H	0.110918	-0.000008
57 C	-0.103352	-0.050428
58 C	0.213287	0.005763
59 C	0.180283	0.019351
60 C	0.204559	0.019703
61 C	-0.265556	-0.003233
62 C	-0.269648	-0.003478
63 H	0.114814	0.001192
64 H	0.114706	0.001165
65 H	0.163631	-0.001850
66 C	-0.553632	0.000175
67 H	0.174728	-0.000058
68 H	0.178849	0.000023
69 H	0.149176	-0.000116
70 C	-0.550230	-0.000065
71 H	0.156881	-0.000057
72 H	0.166572	-0.000029
73 H	0.164848	-0.000034
74 C	-0.531907	-0.000007
75 H	0.164210	0.000006
76 H	0.157165	0.000003
77 H	0.154908	0.000002
78 C	-0.534914	-0.000270
79 H	0.172913	0.000290
80 H	0.168073	-0.000314
81 H	0.149219	0.000412
82 C	-0.534383	0.000053
83 H	0.167211	0.000140
84 H	0.150097	0.000552
85 H	0.171127	0.000321
86 C	-0.532833	-0.000410
87 H	0.158990	0.000188
88 H	0.164391	0.000267
89 H	0.154808	0.000001
90 C	-0.555091	0.000088
91 H	0.183339	-0.000096
92 H	0.147783	-0.000233
93 H	0.172974	-0.000028
94 C	-0.550142	0.000019

95 H	0.157120	-0.000070
96 H	0.164557	0.000033
97 H	0.165727	-0.000015
98 C	-0.532397	-0.000024
99 H	0.164003	0.000019
100 H	0.156181	0.000006
101 H	0.155482	0.000002

Sum of atomic charges = 0.000000

Sum of spin charges = 1.000000