Supporting Information

Muonium addition to the C=S sulfur in the conformationally regulated thiobenzophenone

Tetsuya Fujino,[a] Masaya Morisaki,[a] Shoichiro Nishimura,[b] Jumpei G. Nakamura,[b] Akihiro Koda,[b] Shigekazu Ito*[a,b]

[a] *Department of Chemical Science and Engineering, School of Materials and Chemical Technology, Institute of Science Tokyo (Science Tokyo), 2-12-1-H113 Ookayama, Meguro-ku, Tokyo 152-8552, Japan. E-mail: ito@mct.isct.ac.jp*

[b] *Muon Science Laboratory, Institute of Materials Structure Science, High Energy Acceleration Research Organization (KEK), 203-1 Shirakata, Tokai-mura, Naka-gun, Ibaraki 319-1106, Japan*

Synthesis of thioketones

General

All experiments were conducted under an inert atmosphere (nitrogen or argon) unless otherwise noted. ^{1}H NMR and ^{13}C NMR spectra were measured on an Avance Neo (400 MHz) spectrometer. Chemical shifts of ^{1}H NMR were expressed in parts per million downfield from $CHCl_3$ and MeCN as internal standards (δ = 7.26 and 2.05) in $CDCl_3$ and in acetonitrile-d_3. Chemical shifts of ^{13}C NMR were expressed in parts per million relative to the central line of the triplet (δ = 77.10) for $CDCl_3$ and the singlet (δ = 118.26) in acetonitrile-d_3. Important NMR data were tabulated in the following order: multiplicity (s: singlet, d: doublet, t: triplet, q: quartet, m: multiplet, br: broad) and coupling constant *J* (Hz). UV-Vis spectra were measured on a Hitachi U4100 spectrometer.

Analytical thin-layer chromatography (TLC) was performed on a glass plate pre-coated with silica gel (Merck Kieselgel 60 F254, layer thickness 0.25 mm). Visualization was accomplished by UV light (254 nm) and anisaldehyde. Column chromatography was performed on KANTO Silica Gel 60N (spherical, neutral).

Dichloromethane (dehydrate) chloroform(dehydrate), tetrahydrofuran (dehydrate), diethyl ether (dehydrate), ethyl acetate (dehydrate), acetonitrile (dehydrate), ethanol (dehydrate), phosphoryl chloride and hydrochloric acid were purchased from Kanto Chemical Co., Inc.

Thiodibenzosuberone (10,11-dihydro-5*H*-dibenzo[*a*,*d*][7]annulene-5-thione) 4[46]

Lawesson's reagent (0.57 g, 1.4 mmol) was added to a toluene solution (10 ml) of dibenzosuberone (2.0 mmol, 0.42 g), and the mixture was then heated to reflux for 3.5 h before removal of the solvent in vacuo. The residue was purified by column chromatography (silica gel, hexane), thereby affording **4** (0.21 g, 46%) as a purple solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, 2H, *J* = 7.8, 1.2 Hz), 7.35 (td, 2H, *J* = 7.5, 1.6 Hz), 7.19 (td, 2H, *J* = 7.6, 1.2 Hz), 7.11 (d, 2H, *J* = 7.4 Hz), 3.18 (s, 4H).

3-Phenethylphthalide 7[47]

(2-Bromoethyl)benzene (2.0 ml, 15 mmol) was added to magnesium turnings (0.36 g, 15 mmol) in THF (15 ml) under nitrogen slowly. The reaction was stirred for 30 min at room temperature before being cooled to 0 °C. A THF solution (15 ml) of phthalaldehydic acid (1.4 g, 9.3 mmol) was added to the stirring mixture at 0 °C. The mixture was stirred for 1 h at room temperature. The reaction was quenched with aqueous HCl and extracted with EtOAc. The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4 and filtered. After removal of the solvents in vacuo, the residue was purified by column

chromatography (silica gel, hexane/EtOAc = 100:1) affording 3-phenethylphthalide **7** (1.2 g, 5.1 mmol, 55%) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, 1H, *J* = 7.7 Hz), 7.66 (td, 1H, *J* = 7.5, 1.1 Hz), 7.52 (t, 1H, *J* = 7.5 Hz), 7.41 (dd, 1H, *J* = 7.7, 0.82 Hz), 7.32-7.28 (m, 2H), 7.23-7.19 (m, 3H), 5.47 (dd, 1H, *J* = 8.8, 3.5 Hz), 2.87-2.82 (m, 2H), 2.39-2.31 (m, 1H), 2.08-1.99 (m, 1H).

2-(3-Phenylpropyl)benzoic acid 8[47]

3-Phenethylphthalide **7** (1.2 g, 5.0 mmol) was added to hydriodic acid (57wt%, 8 ml) under nitrogen. The mixture was hen heated to reflux for 24 h prior to being extracted with hexane (10 ml x 2) and EtOAc (10 ml). The combined organic layer was washed with sat. KI aq. and dried over Na_2SO_4 and filtered. After removal of the solvents in vacuo, the crude was used in the next reaction without any purification.

Dibenzo[*a*,*d*]cycloocten-12(5*H*)-one (10)[47]

Oxalyl chloride (0.79 ml, 10 mmol) and DMF (4 drops) were added to a CH_2Cl_2 (20 ml) solution of the crude material containing **8** (0.80 g) at 0 °C. The mixture was stirred at room temperature for 3 h. After removal of the solvents in vacuo, $AlCl_3$ (2.0 g, 15 mmol) and CH_2Cl_2 (20 ml) were added to the mixture under nitrogen at 0 °C. The mixture was stirred for 18 h. The reaction was quenched with aqueous HCl and extracted with CH_2Cl_2. The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4, and filtered. After removal of the solvents in vacuo, the residue was purified by column chromatography (silica gel, hexane/EtOAc = 50:1), affording dibenzo[*a*,*d*]cycloocten-12(5*H*)-one **10** (0.11 g, 0.48 mmol) as a yellow solid (22% from **7**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, 2H, *J* = 7.9, 1.4 Hz), 7.50 (td, 2H, *J* = 7.4, 1.5 Hz), 7.37 (td, 2H, *J* = 7.9, 1.3 Hz), 7.18 (dd, 2H, *J* = 7.6, 1.1 Hz), 2.64 (t, 4H, *J* = 6.3 Hz), 1.84-1.78 (m, 2H).

Dibenzo[*a*,*d*]cycloocten-12(5*H*)-thione (5)

Lawesson's reagent (0.20 g, 0.50 mmol) was added to a toluene solution (5.0 ml) of **10** (0.50 mmol, 0.11 g), and the mixture was then heated to reflux for 3 h before removal of the solvent in vacuo. The residue was purified by column chromatography (silica gel, hexane), affording dibenzo[*a*,*d*]cycloocten-12(5*H*)-thione (**5**) (0.073 g, 62%) as a greenish blue solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, 2H, *J* = 8.1, 1.2 Hz), 7.46 (td, 2H, *J* = 7.2, 1.2 Hz), 7.27-7.23 (m, *J* = 1.2 Hz, 2H, overlap with $CHCl_3$), 7.08 (dd, 2H, *J* = 7.6, 1.2 Hz),

2.62 (t, 4H, J = 6.4 Hz), 1.84-1.77 (m, 2H); (acetonitrile-d_3) δ 7.91 (dd, 2H, J = 8.0, 0.8 Hz), 7.37 (td, 2H, J = 7.6, 1.2 Hz), 7.13 (td, 2H, J = 8.1, 1.1 Hz), 7.01 (dd, 2H, J = 7.6, 0.8 Hz), 2.43 (t, 4H, J = 6.3 Hz), 1.66-1.60 (m, 2H); $^{13}C\{^1H\}$ NMR (101 MHz, acetonitrile-d_3) δ 147.8, 137.4, 132.4, 132.3, 129.3, 125.9, 33.6, 30.3, (101 MHz, in $CDCl_3$) δ 266.9 (C=S). FAB-MS calcd for $C_{16}H_{14}S$ [M^+] 238.08, found 238.07.
*ESI-MS and APCI-MS did not show the corresponding m/z signal.

_o_-Allylbromobenzene (11)[48]

0.1 M vinylmagnesium bromide in THF (30 mL, 30 mmol) was added to a suspension of **10** (7.3 g, 30 mmol), CuI (0.57 g, 3.0 mmol) and 2,2'-bipyridine (0.47 g, 3.0 mmol) in toluene (50 mL) at –78 °C. The mixture was stirred for 24 h. The reaction was quenched with HCl aq. and extracted with EtOAc. The combined organic layer was washed with brine (20 mL) and dried over Na_2SO_4, and filtered. After removal of the solvents in vacuo, the residue was purified by column chromatography (silica gel, hexane), affording *o*-allylbromobenzene (**11**) (4.2 g, 22 mmol, 74%) as a colorless liquid.
^1H NMR (400 MHz, $CDCl_3$) δ 7.56-7.53 (m, 1H), 7.27-7.21 (m, 2H), 7.10-7.06 (m, 1H), 5.98 (ddt, 1H, J = 16.7, 10.2, 6.5 Hz), 5.14-5.05 (m, 2H), 3.52 (dt, 2H, J = 6.5, 1.4 Hz).

_o_-Allylbenzaldehyde (12)[49]

o-Allylbromobenzene (**11**) (2.6 ml, 13 mmol) was added to magnesium turnings (0.36 g, 15 mmol) in THF (25 ml) under nitrogen slowly. The reaction was stirred for 45 min at room temperature before being cooled to 0 ℃. DMF (1.5 ml, 1.9 mmol) was added to the stirring mixture at 0 °C. The mixture was stirred for 18 h at room temperature. The reaction was quenched with HCl aq. and extracted with EtOAc. The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4, and filtered. After removal of the solvents in vacuo, the residue was purified by column chromatography (silica gel, hexane/EtOAc = 30:1), affording *o*-allylbenzaldehyde (**12**) (1.4 g, 9.3 mmol, 71%) as a yellow oil.
^1H NMR (400 MHz, $CDCl_3$) δ 10.26 (s, 1H), 7.85 (dd, 1H, J = 7.7, 1.4 Hz), 7.53 (td, 1H, J = 7.5, 1.7 Hz), 7.40 (td, 1H, J = 7.5, 0.93 Hz), 7.30 (d, 2H, J = 7.6 Hz), 6.04 (ddt, 1H, J = 17.3, 10.1, 6.5 Hz), 5.09 (dq, 1H, J = 10.1, 1.5 Hz), 4.99 (dq, 1H, J = 17.1, 1.7 Hz), 3.83 (dt, 2H, J = 3.4, 1.4 Hz).

Bis(2-allylphenyl)methanol (13)

o-Allylbromobenzene (**11**) (1.1 ml, 8 mmol) was added to magnesium turnings (0.20 g, 8.2 mmol) in THF (20 ml) under nitrogen slowly. The reaction was stirred for 45 min at

room temperature before being cooled to 0 °C. A THF solution (8 ml) of *o*-allylbenzaldehyde (**12**) (1.0 g, 8.2 mmol) was added to the stirring mixture at 0 °C. The mixture was stirred for 18 h at room temperature. The reaction was quenched with HCl aq. and extracted with EtOAc. The combined organic layer was washed with brine (20 mL) and dried over Na_2SO_4 and filtered. After removal of the solvents in vacuo, the residue was purified by column chromatography (silica gel, hexane/EtOAc = 20:1), thereby affording bis(2-allylphenyl)methanol (1.7 g, 6.3 mmol, 92%) as a colorless solid.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.19 (m, 8H), 6.27 (s, 1H), 5.94 (ddt, 2H, *J* = 17.1, 10.1, 6.3 Hz), 5.06 (dq, 2H, *J* = 10.1, 1.5 Hz), 4.99 (dq, 2H, *J* = 17.1, 1.7 Hz), 3.43-3.32 (m, 4H), 2.07 (br, 1H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 140.8, 137.6, 137.4, 130.1, 127.9, 127.2, 126.7, 116.1, 69.5, 36.8.

Bis(2-allylphenyl)methanone (14)

A CH_2Cl_2 (9.0 ml) solution of oxalyl chloride (0.51 ml, 6.0 mmol) was added dropwise to a CH_2Cl_2 (9.0 ml) solution of DMSO (0.64 ml, 9.0 mmol) for 15 min at –78 °C. After that, a CH_2Cl_2 (4.5 ml) solution of **13** (0.79 g, 3.0 mmol) was added to the mixture at –78 °C. Triethylamine (2.1 ml, 15 mmol) was added to the mixture at –78 °C prior to being stirred at room temperature for 60 min. The reaction was quenched with HCl aq. and extracted with EtOAc. The combined organic layer was washed with brine (20 mL) and dried over Na_2SO_4, and filtered. After removal of the solvents in vacuo, the residue was purified by column chromatography (silica gel, hexane/EtOAc = 20:1), affording bis(2-allylphenyl)methanone (**14**) (0.68 g, 2.6 mmol, 86%) as a yellow oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (td, 2H, *J* = 7.6, 1.6 Hz), 7.33 (dd, 2H, *J* = 7.7, 0.6 Hz), 7.28 (dd, 2H, *J* = 7.7, 1.4 Hz), 7.21 (td, 2H, *J* = 7.5, 1.2 Hz), 5.97 (ddt, 2H, *J* = 16.7, 10.3, 6.6 Hz), 5.04-4.98 (m, 4H), 3.60 (d, 4H, *J* = 6.6 Hz); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 200.4, 140.4, 138.9, 137.2, 131.3, 130.8 (x2), 125.8, 116.1, 37.7.

(*Z*)-5,8-Dihydro-13*H*-dibenzo[*a*,*d*][9]annulen-13-one (15)

Grubbs Catalyst® M204 (4.6 mg, 5.4 μmol) was added to a toluene (20 ml) solution of **14** (0.13 g, 0.50 mmol). The mixture was stirred for 18 h at 80 °C. After removal of the solvent in vacuo, the residue was purified by column chromatography (silica gel, hexane/EtOAc = 100:1), affording (*Z*)-5,8-dihydro-13*H*-dibenzo[*a*,*d*][9]annulen-13-one (**15**) (0.056 g, 0.24 mmol, 47%) as a colorless solid.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, 2H, *J* = 7.6, 1.4 Hz), 7.40 (td, 2H, *J* = 7.5, 1.7 Hz), 7.29 (td, 2H, *J* = 7.5, 1.2 Hz), 7.16 (dd, 2H, *J* = 7.6, 0.73 Hz), 5.69-5.66 (m, 4H), 3.3 (dd, 2H, *J* = 5.1 Hz); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 201.9, 141.1, 138.7, 131.3,

130.2, 129.9, 127.5, 126.6, 33.0.

5,6,7,8-Tetrahydro-13*H*-dibenzo[*a*,*d*][9]annulen-13-one (16)[51,52]

Pd/C (0.032 g, 0.30 mmol) was added to a methanol (20 ml) solution of **15** (0.22 g, 0.91 mmol) under hydrogen with a balloon. The mixture was stirred for 12 h at room temperature under hydrogen. After filtering the organic layer and removal of the solvent in vacuo, the residue was purified by column chromatography (silica gel, hexane/EtOAc = 100:1), affording 5,6,7,8-tetrahydro-13*H*-dibenzo[*a*,*d*][9]annulen-13-one (**16**) (0.19 g, 0.78 mmol, 86%) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, 2H, *J* = 7.6, 1.3 Hz), 7.37 (td, 2H, *J* = 7.5, 1.5 Hz), 7.27 (td, 2H, *J* = 7.5, 1.2 Hz), 7.17 (dd, 2H, *J* = 7.6, 0.53 Hz), 2.67-2.63 (m, 4H), 1.73-1.70 (m, 4H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 203.4, 141.6, 141.2, 131.0, 130.7, 126.7, 126.2, 33.0, 27.1.

5,6,7,8-Tetrahydro-13*H*-dibenzo[*a*,*d*][9]annulen-13-thione (6)

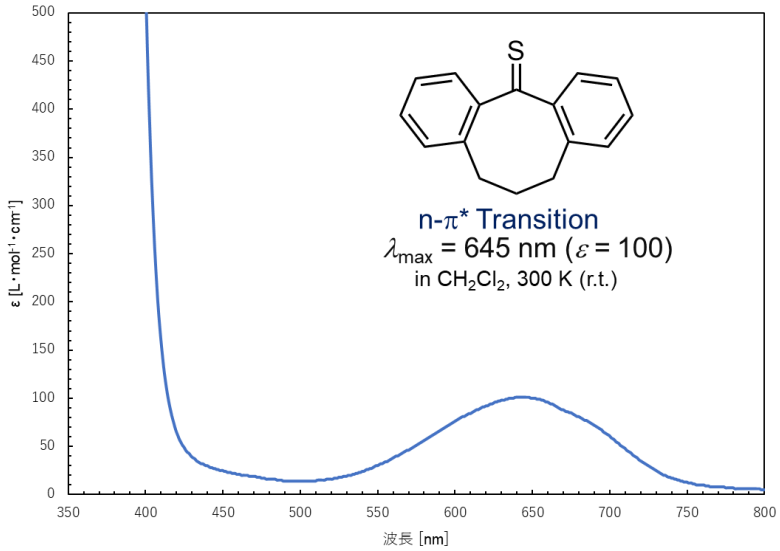
Lawesson's reagent (0.26 g, 0.63 mmol) was added to a toluene solution (6 ml) of **16** (0.86 mmol, 0.21 g), and the mixture was then heated to reflux for 3.5 h before removal of the solvent in vacuo. The residue was purified by column chromatography (silica gel, hexane), affording 5,6,7,8-tetrahydro-13*H*-dibenzo[*a*,*d*][9]annulen-13-thione (**6**) (0.062 g, 28%) as a blue amorphous solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dd, 2H, *J* = 7.7, 1.3 Hz), 7.31 (td, 2H, *J* = 7.5, 1.5 Hz), 7.19 (td, 2H, *J* = 7.6, 1.3 Hz), 7.11 (dd, 2H, *J* = 7.5, 0.7 Hz), 2.70 (br, 4H), 1.70 (br, 4H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 249.4, 150.6, 140.2, 130.5, 130.3, 126.9, 125.9, 33.4, 28.3. HRMS (ESI$^+$) calcd for $C_{17}H_{16}SK$ [M^++K] 0291.0610, found 291.0979.

Physical properties of thioketones

UV-Vis Spectra

Dibenzo[*a*,*d*]cycloocten-12(5*H*)-thione (**5**)



5,6,7,8-tetrahydro-13H-dibenzo[a,d][9]annulen-13-thione (**6**)

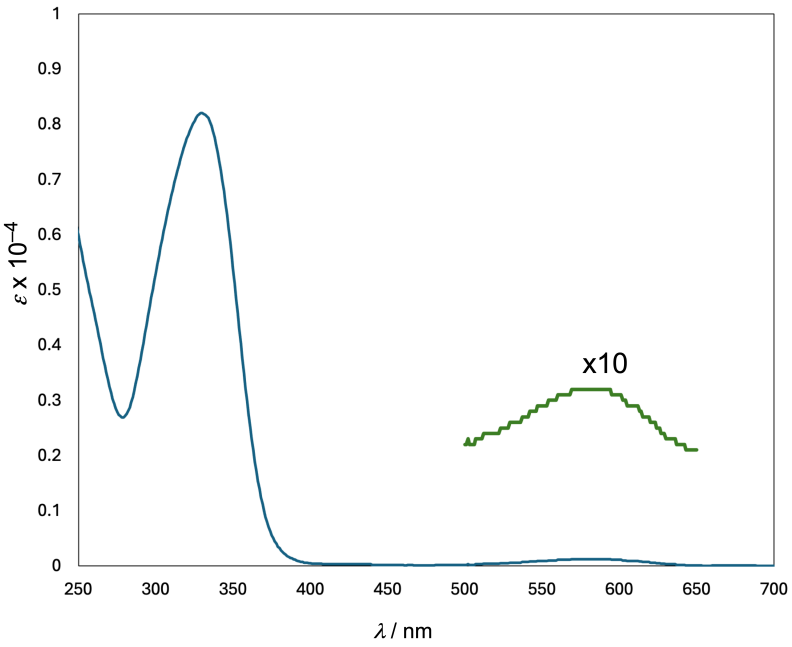


Table S1. Typical physical properties of cyclic thioketones **4**–**6** and acyclic **1**

Compound	^{13}C NMR (C=S) / δ	n-π* λ_{max} / nm	Refs.
4	246.7	593	53
5	266.7[a)]	645[b)]	This work
6	249.4[a)]	582[b)]	This work
1	238.7	610	54-56

a) In $CDCl_3$, 300 K.

b) In CH_2Cl_2, 300 K.

A brief description of μLCR (ALC-μSR)

In muon *avoided* level-crossing resonance (μLCR) measurements, the magnetic field is oriented parallel to the muon beam polarization, and the positron rate is measured in the forward and backward directions (Figure S1a). The difference in the rates is the muon asymmetry $A(t)$, which is proportional to the longitudinal muon spin polarization (Eq. 2 in the main text). For the coupled spin system of a muoniated free radical, there are some fields where the mixing of a pair of spin states results in an avoided crossing. If the mixed states involve different muon spin orientations, there is a partial loss of spin polarization at the resonance field. In Figure S1b, M is the sum of the spin quantum numbers of the muon (μ), electron (e), and I=1/2 nucleus (k). For Δ_1 (ΔM=±1) transitions, the resonant state involves an exchange of the muon spin. The level-crossing is avoided by indirect coupling of both Zeeman states to a third one. This avoided resonance occurs at a magnetic field according to Eq. 3 in the main text. The anisotropic motion of the muoniated radicals normally promotes the Δ_1 transitions.

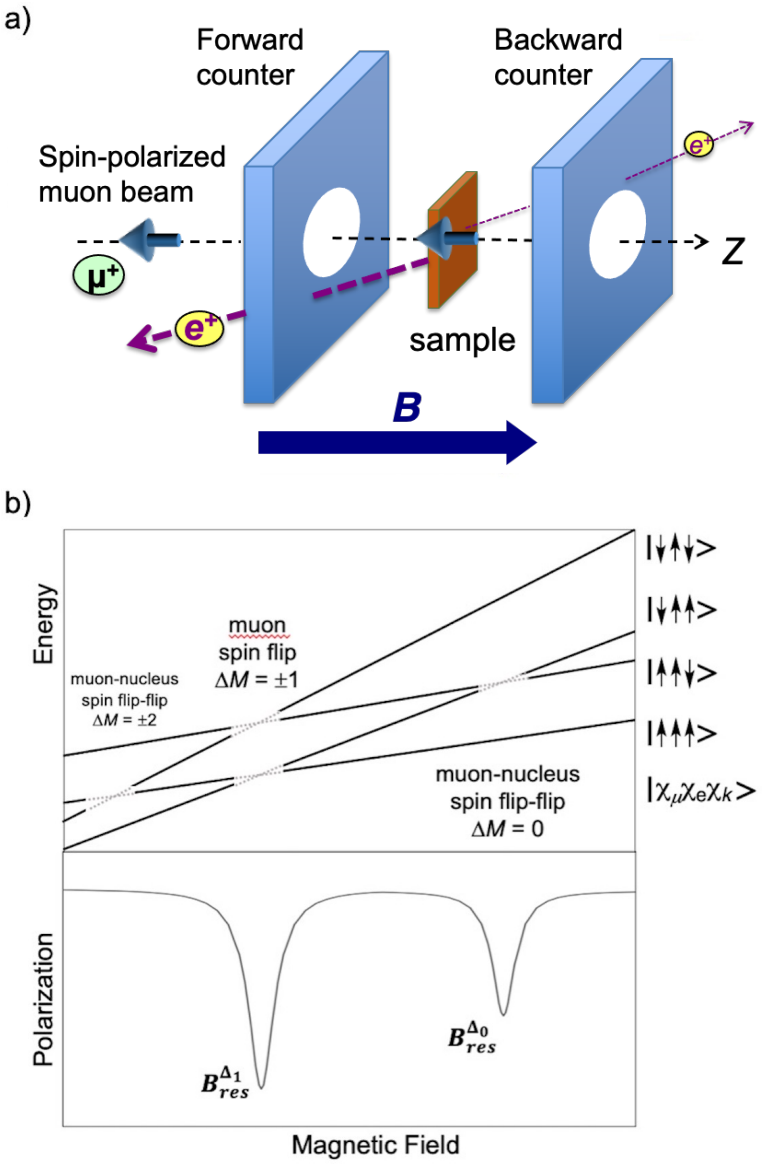
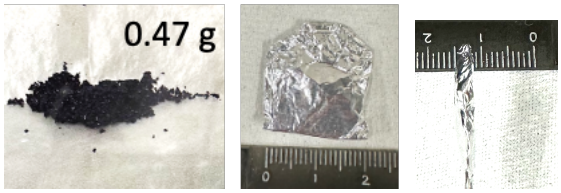


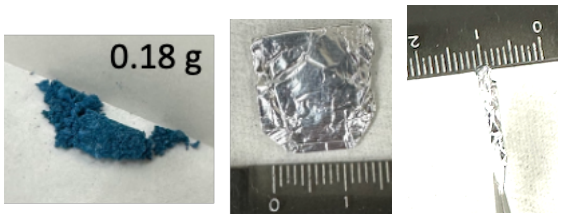
Fig. S1 a) A schematic of μLCR geometry. The longitudinal external field is denoted as *B*. b) Top panel: Energy diagram for a three-spin system [muon (μ), electron (e), $I = 1/2$ nucleus (k)]. Bottom panel: LCR resonances occur when states with opposite muon spin become near degenerate in energy. A transition with $\Delta M = \pm 2$, a muon-nucleus spin flip-flip transition, is usually very weak and negligible.

Samples for µLCR measurement

4



5



6

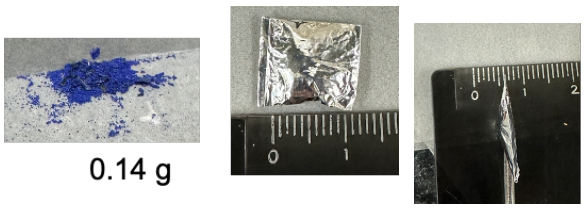
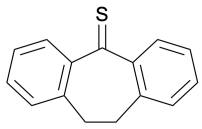


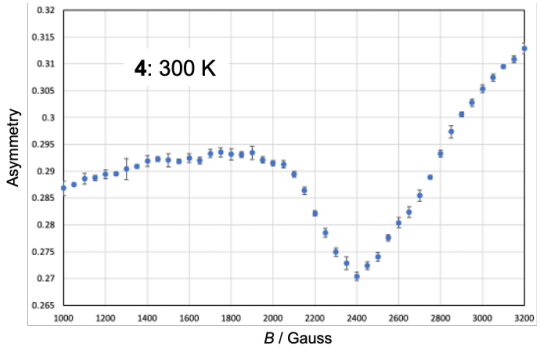
Fig. S2 Pelletized samples **4**–**6** for µLCR measurements.

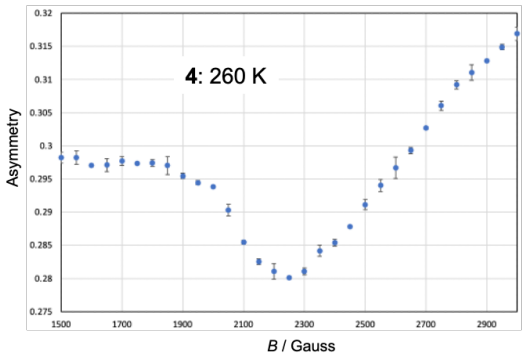
Fig. S3 The Microstat probe with the sample of **6**.

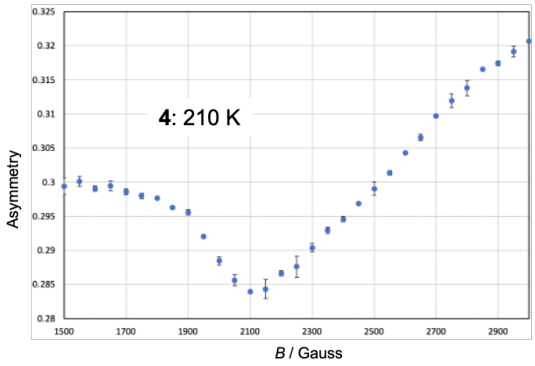
Raw μLCR spectra before subtracting Ag background, baseline corrections, and normalization

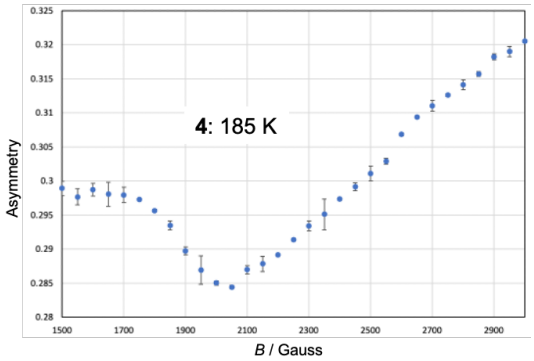


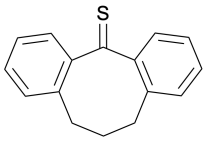
4



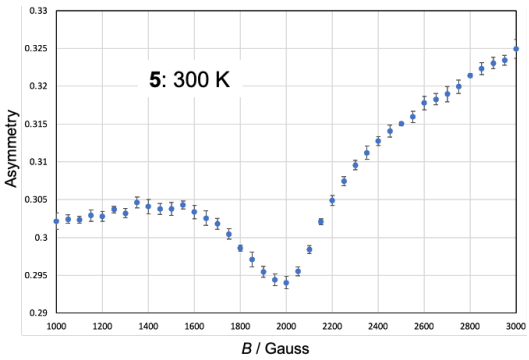


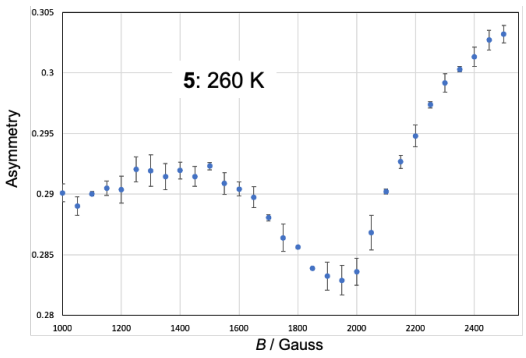


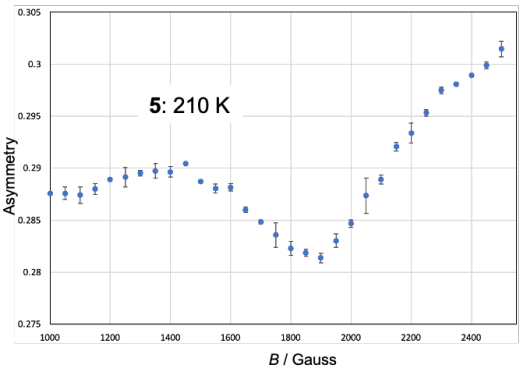


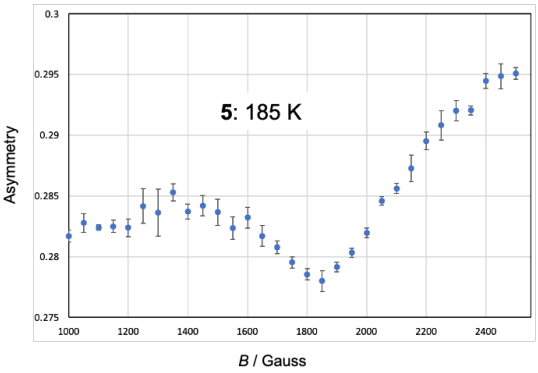

S

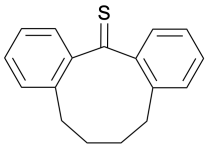
5


5: 300 K
Asymmetry
B / Gauss

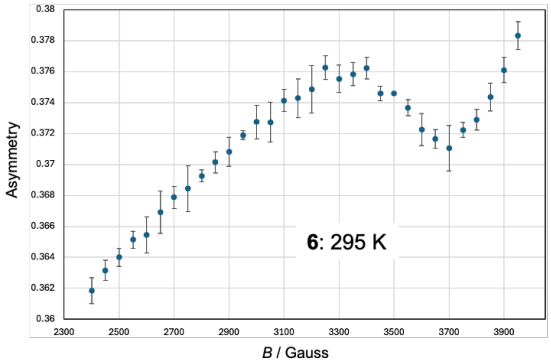

5: 260 K
Asymmetry
B / Gauss

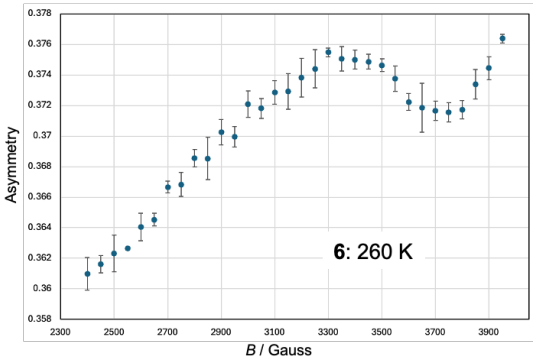

5: 210 K
Asymmetry
B / Gauss

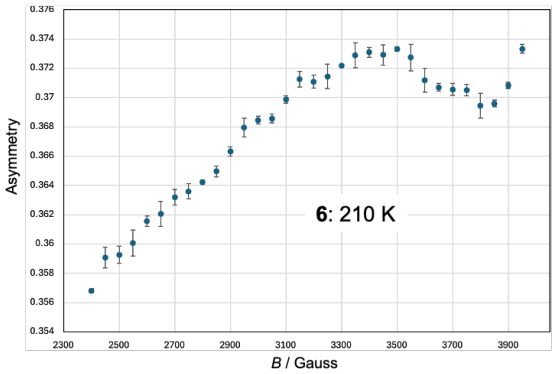

5: 185 K
Asymmetry
B / Gauss

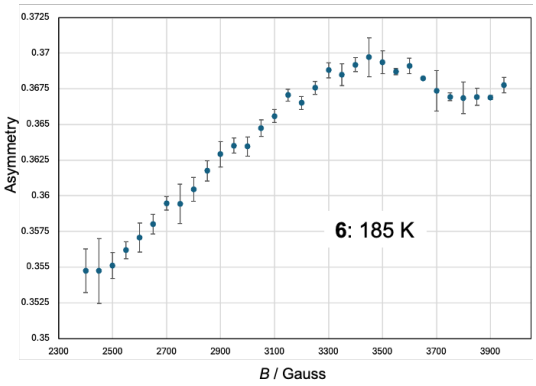

S

6


Asymmetry
B / Gauss
6: 295 K


Asymmetry
B / Gauss
6: 260 K


Asymmetry
B / Gauss
6: 210 K


Asymmetry
B / Gauss
6: 185 K

Analyzing the temperature dependence of the μLCR spectra

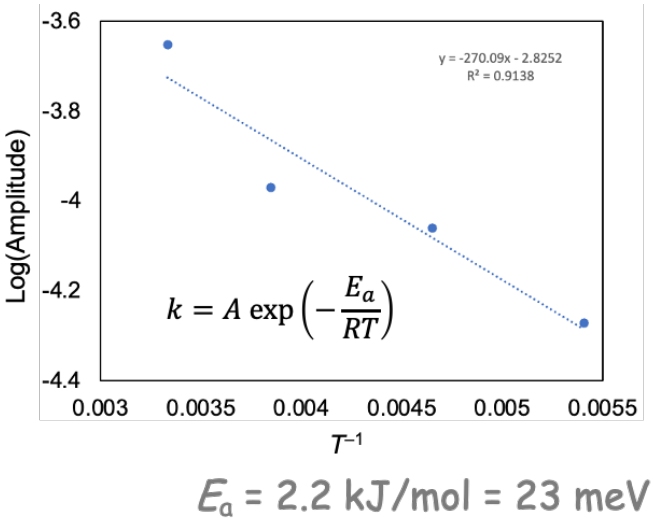


Fig. S4 An Arrhenius plot of the μLCR amplitudes and reciprocal temperature for **4Mu**, showing a least-squares regression line.

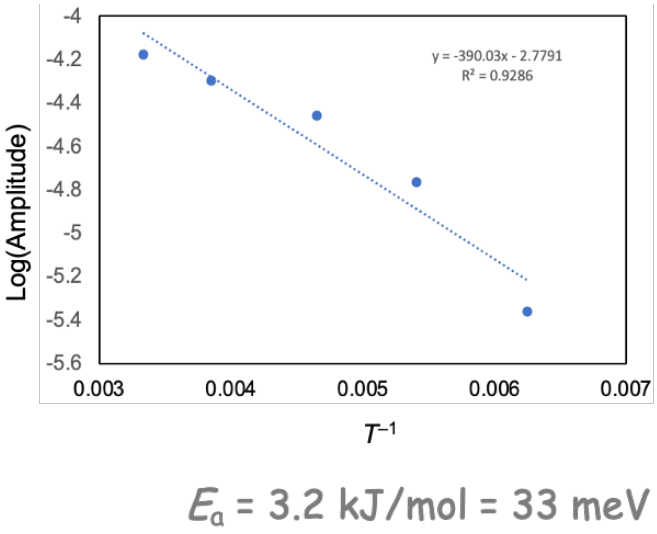


Fig. S5 An Arrhenius plot of the μLCR amplitudes and reciprocal temperature for **5Mu**, showing a least-squares regression line.

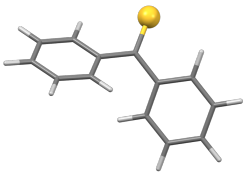
DFT calculation data

The structures of cyclic thioketones **4**–**6** and acyclic thiobenzophenone **1** were optimized at the B3LYP/def2-SVP level by using the Gaussian 09 software package. The structure of **1Mu** was optimized at the UB3LYP/def2-SVP level, and its vibrational averaging was conducted with Fermi keyword by using the Gaussian 16 software package.

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT, 2010.

Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

1

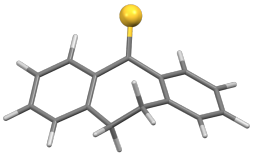


E(RB3LYP) = -899.122167918 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.276977	0.155906	0.026244
2	6	0	0.000000	0.918975	0.000000
3	6	0	-2.600464	-1.735727	-0.818062
4	6	0	-1.276977	0.155906	-0.026244
5	1	0	-2.666372	-2.664143	-1.390978
6	6	0	-1.382281	-1.057943	-0.737852
7	6	0	-3.730641	-1.228721	-0.170771
8	16	0	0.000000	2.571558	0.000000
9	1	0	-4.681514	-1.765046	-0.225278
10	6	0	-3.639308	-0.029664	0.546451
11	6	0	1.382281	-1.057943	0.737853
12	1	0	-4.518141	0.370186	1.058581
13	6	0	-2.430555	0.660147	0.608838
14	1	0	-2.356064	1.603648	1.152555
15	6	0	2.430554	0.660147	-0.608839
16	1	0	2.356063	1.603647	-1.152557
17	6	0	3.639308	-0.029664	-0.546452
18	1	0	4.518140	0.370185	-1.058583
19	6	0	3.730641	-1.228721	0.170770
20	1	0	4.681514	-1.765046	0.225277
21	6	0	2.600464	-1.735726	0.818062
22	1	0	2.666372	-2.664142	1.390979
23	1	0	-0.508739	-1.458024	-1.255649
24	1	0	0.508739	-1.458023	1.255650

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.189202 (Hartree/Particle)
Thermal correction to Energy= 0.200216
Thermal correction to Enthalpy= 0.201160
Thermal correction to Gibbs Free Energy= 0.150940
Sum of electronic and zero-point Energies= -898.932965
Sum of electronic and thermal Energies= -898.921952
Sum of electronic and thermal Enthalpies= -898.921008
Sum of electronic and thermal Free Energies= -898.971228

4

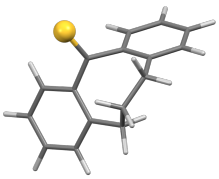


E(RB3LYP) = -976.487395027 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.214356	-2.382387	0.463261
2	6	0	-0.019018	1.005708	0.328742
3	6	0	-1.305405	0.310565	0.016746
4	6	0	-1.518553	-1.094913	0.048871
5	6	0	3.791494	-0.684729	-0.740499
6	6	0	3.418473	0.577433	-1.211330
7	6	0	2.181435	1.111766	-0.854796
8	6	0	1.283873	0.383546	-0.051566
9	6	0	1.658770	-0.891107	0.422871
10	6	0	2.916529	-1.403282	0.076959
11	6	0	-2.383242	1.141553	-0.379151
12	6	0	-2.781604	-1.586786	-0.329631
13	1	0	4.764683	-1.106872	-1.003672
14	1	0	4.095109	1.151424	-1.849191
15	1	0	1.890997	2.107006	-1.196214
16	6	0	-3.615536	0.629396	-0.760471
17	6	0	-3.818212	-0.754130	-0.739169
18	1	0	-4.413771	1.305589	-1.075727
19	1	0	-4.780965	-1.180928	-1.031860
20	16	0	0.004444	2.512832	1.003686
21	1	0	-2.213175	2.218645	-0.390174
22	1	0	-2.949986	-2.666952	-0.287312
23	6	0	-0.520477	-2.146421	0.504871
24	6	0	0.705824	-1.673063	1.287960
25	1	0	-0.176345	-2.709560	-0.382453
26	1	0	1.221272	-2.553577	1.701035
27	1	0	-1.072281	-2.876799	1.120232
28	1	0	0.382889	-1.064132	2.150658

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.224915 (Hartree/Particle)
Thermal correction to Energy= 0.237013
Thermal correction to Enthalpy= 0.237957
Thermal correction to Gibbs Free Energy= 0.186059
Sum of electronic and zero-point Energies= -976.262480
Sum of electronic and thermal Energies= -976.250382
Sum of electronic and thermal Enthalpies= -976.249438
Sum of electronic and thermal Free Energies= -976.301336

5

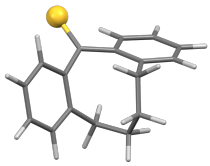


E(RB3LYP) = -1015.76004126 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.360607	-0.356621	0.025669
2	6	0	0.090824	-0.880537	0.597387
3	6	0	-3.195032	0.798007	-0.392156
4	6	0	-1.191965	-0.517285	-0.094780
5	1	0	-3.819712	1.646274	-0.097336
6	6	0	-1.992389	0.575608	0.297987
7	6	0	-3.607741	-0.028676	-1.438112
8	16	0	0.055740	-1.932981	1.857810
9	1	0	-4.551109	0.170449	-1.952699
10	6	0	-2.804269	-1.103480	-1.825299
11	6	0	1.548423	1.011820	-0.311812
12	1	0	-3.109147	-1.757646	-2.645951
13	6	0	-1.602813	-1.340504	-1.157472
14	1	0	-0.972090	-2.182821	-1.452425
15	6	0	2.409692	-1.273259	-0.194361
16	1	0	2.252838	-2.314324	0.094021
17	6	0	3.610611	-0.877817	-0.777482
18	1	0	4.400474	-1.611910	-0.954081
19	6	0	3.793678	0.462202	-1.126194
20	1	0	4.732029	0.793476	-1.578406
21	6	0	2.777374	1.386329	-0.876350
22	1	0	2.942660	2.440486	-1.116451
23	1	0	-0.255720	2.092280	-0.789430
24	6	0	0.528409	2.097561	-0.011857
25	6	0	-0.124423	2.016727	1.391180
26	6	0	-1.586922	1.500782	1.425549
27	1	0	1.041838	3.064428	-0.121718
28	1	0	-1.755802	0.991165	2.390511
29	1	0	-2.277245	2.358996	1.414886
30	1	0	-0.113580	3.017498	1.851162
31	1	0	0.508342	1.394202	2.041564

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253054 (Hartree/Particle)
Thermal correction to Energy= 0.266565
Thermal correction to Enthalpy= 0.267509
Thermal correction to Gibbs Free Energy= 0.212284
Sum of electronic and zero-point Energies= -1015.506987
Sum of electronic and thermal Energies= -1015.493476
Sum of electronic and thermal Enthalpies= -1015.492532
Sum of electronic and thermal Free Energies= -1015.547757

6

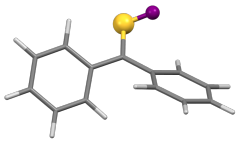


E(RB3LYP) = -1055.04356192 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.317487	0.638794	0.018201
2	6	0	0.000004	1.351105	-0.000002
3	6	0	-2.886770	-1.052276	-0.785661
4	6	0	-1.317480	0.638798	-0.018203
5	1	0	-3.088732	-1.943955	-1.386521
6	6	0	-1.575622	-0.545080	-0.763253
7	6	0	-3.926447	-0.458144	-0.073951
8	16	0	0.000006	3.009505	-0.000002
9	1	0	-4.931151	-0.887331	-0.109224
10	6	0	-3.669918	0.690374	0.681659
11	6	0	1.575621	-0.545091	0.763244
12	1	0	-4.467732	1.168778	1.254905
13	6	0	-2.389644	1.230795	0.691159
14	1	0	-2.187874	2.139667	1.259044
15	6	0	2.389657	1.230794	-0.691148
16	1	0	2.187894	2.139673	-1.259024
17	6	0	3.669928	0.690366	-0.681649
18	1	0	4.467747	1.168772	-1.254885
19	6	0	3.926447	-0.458163	0.073947
20	1	0	4.931149	-0.887358	0.109218
21	6	0	2.886765	-1.052294	0.785651
22	1	0	3.088721	-1.943979	1.386505
23	6	0	-0.517657	-1.310863	-1.526206
24	6	0	0.517653	-1.310863	1.526204
25	6	0	0.039895	-2.552969	-0.769762
26	6	0	-0.039925	-2.552962	0.769768
27	1	0	0.307590	-0.646423	-1.804850
28	1	0	-0.957468	-1.655469	-2.475911
29	1	0	1.087364	-2.695294	-1.080998
30	1	0	-0.497526	-3.452974	-1.113246
31	1	0	0.497474	-3.452977	1.113260
32	1	0	-1.087398	-2.695260	1.081003
33	1	0	-0.307582	-0.646411	1.804857
34	1	0	0.957469	-1.655473	2.475905

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.282647 (Hartree/Particle)
Thermal correction to Energy= 0.297035
Thermal correction to Enthalpy= 0.297979
Thermal correction to Gibbs Free Energy= 0.241061
Sum of electronic and zero-point Energies= -1054.760915
Sum of electronic and thermal Energies= -1054.746527
Sum of electronic and thermal Enthalpies= -1054.745583
Sum of electronic and thermal Free Energies= -1054.802501

1Mu



E(UB3LYP) = -899.704907731 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.003628	0.782467	0.020867
2	6	0	1.284664	0.101012	0.026185
3	6	0	1.440588	-1.153877	0.673409
4	6	0	2.441562	0.673806	-0.562343
5	6	0	2.676510	-1.793331	0.720498
6	1	0	0.581247	-1.608650	1.169035
7	6	0	3.674396	0.025851	-0.514655
8	1	0	2.353241	1.626643	-1.087993
9	6	0	3.803514	-1.211521	0.125832
10	1	0	2.765537	-2.752000	1.238517
11	1	0	4.542916	0.488036	-0.991524
12	1	0	4.771852	-1.716318	0.164394
13	6	0	-1.290528	0.102406	-0.015702
14	6	0	-1.426553	-1.175036	-0.624366
15	6	0	-2.468046	0.696205	0.511452
16	6	0	-2.659165	-1.819145	-0.684219
17	1	0	-0.553435	-1.645663	-1.079001
18	6	0	-3.697029	0.044558	0.448025
19	1	0	-2.398237	1.672928	0.993622
20	6	0	-3.804664	-1.218173	-0.146951
21	1	0	-2.730878	-2.796752	-1.168465
22	1	0	-4.581624	0.524559	0.875072
23	1	0	-4.770758	-1.726393	-0.196056
24	16	0	-0.056275	2.551084	-0.027551
25	1	0	1.090830	2.784918	0.655011

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.196670 (Hartree/Particle)
Thermal correction to Energy= 0.208337
Thermal correction to Enthalpy= 0.209281
Thermal correction to Gibbs Free Energy= 0.157450
Sum of electronic and zero-point Energies= -899.508238
Sum of electronic and thermal Energies= -899.496571
Sum of electronic and thermal Enthalpies= -899.495627
Sum of electronic and thermal Free Energies= -899.547457

Vibrational averaging

[Input (inpart)]

freq=(anharmonic,readanharm) ub3lyp/def2svp

0 2

C	-0.00362800	0.78246700	0.02086700		
C	1.28466400	0.10101200	0.02618500		
C	1.44058800	-1.15387700	0.67340900		
C	2.44156200	0.67380600	-0.56234300		
C	2.67651000	-1.79333100	0.72049800		
H	0.58124700	-1.60865000	1.16903500		
C	3.67439600	0.02585100	-0.51465500		
H	2.35324100	1.62664300	-1.08799300		
C	3.80351400	-1.21152100	0.12583200		
H	2.76553700	-2.75200000	1.23851700		
H	4.54291600	0.48803600	-0.99152400		
H	4.77185200	-1.71631800	0.16439400		
C	-1.29052800	0.10240600	-0.01570200		
C	-1.42655300	-1.17503600	-0.62436600		
C	-2.46804600	0.69620500	0.51145200		
C	-2.65916500	-1.81914500	-0.68421900		
H	-0.55343500	-1.64566300	-1.07900100		
C	-3.69702900	0.04455800	0.44802500		
H	-2.39823700	1.67292800	0.99362200		
C	-3.80466400	-1.21817300	-0.14695100		
H	-2.73087800	-2.79675200	-1.16846500		
H	-4.58162400	0.52455900	0.87507200		
H	-4.77075800	-1.72639300	-0.19605600		
S	-0.05627500	2.55108400	-0.02755100		
H(Iso=0.113429,NMagM=8.890597)			**1.09083000**	**2.78491800**	**0.65501100**

Property=Fermi

[Output (in part)]

Fermi contact terms

Property at reference geometry

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	0.12595	141.59457	50.52446	47.23086
2	C(13)	-0.04217	-47.40424	-16.91501	-15.81235
3	C(13)	0.03056	34.36027	12.26060	11.46135
4	C(13)	0.02984	33.54469	11.96958	11.18930
5	C(13)	-0.01765	-19.83958	-7.07926	-6.61777
6	H(1)	-0.00182	-8.13201	-2.90170	-2.71255
7	C(13)	-0.01801	-20.24346	-7.22337	-6.75249
8	H(1)	-0.00201	-8.99274	-3.20883	-2.99965
9	C(13)	0.02628	29.53849	10.54007	9.85298
10	H(1)	0.00090	4.00644	1.42960	1.33641
11	H(1)	0.00100	4.48445	1.60016	1.49585
12	H(1)	-0.00204	-9.13727	-3.26040	-3.04786
13	C(13)	-0.04484	-50.41021	-17.98762	-16.81504
14	C(13)	0.03244	36.46518	13.01168	12.16348
15	C(13)	0.03114	35.00866	12.49196	11.67763
16	C(13)	-0.01978	-22.23551	-7.93418	-7.41697
17	H(1)	-0.00204	-9.12684	-3.25668	-3.04439
18	C(13)	-0.02024	-22.75472	-8.11945	-7.59016
19	H(1)	-0.00213	-9.51201	-3.39412	-3.17287
20	C(13)	0.02937	33.01428	11.78032	11.01238
21	H(1)	0.00099	4.42673	1.57957	1.47660
22	H(1)	0.00107	4.76857	1.70154	1.59062
23	H(1)	-0.00228	-10.17464	-3.63056	-3.39389
24	S(33)	0.02124	7.29368	2.60257	2.43291
25	**H(1)**	**0.00332**	**47.18926**	**16.83830**	**15.74064**

Temperature: 0K

Isotropic Fermi Contact Couplings

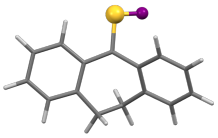
	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	0.14219	159.85229	57.03927	53.32099
2	C(13)	-0.05200	-58.45798	-20.85926	-19.49948
3	C(13)	0.04055	45.58966	16.26752	15.20707
4	C(13)	0.03958	44.49665	15.87751	14.84248
5	C(13)	-0.02166	-24.34648	-8.68743	-8.12111
6	H(1)	-0.00241	-10.75668	-3.83825	-3.58804
7	C(13)	-0.02197	-24.70177	-8.81421	-8.23963
8	H(1)	-0.00255	-11.38982	-4.06417	-3.79923
9	C(13)	0.03043	34.21162	12.20756	11.41177
10	H(1)	0.00122	5.44380	1.94248	1.81586
11	H(1)	0.00134	6.01060	2.14473	2.00492
12	H(1)	-0.00211	-9.44518	-3.37028	-3.15057
13	C(13)	-0.04809	-54.06061	-19.29017	-18.03268
14	C(13)	0.03482	39.14386	13.96750	13.05699
15	C(13)	0.03394	38.15251	13.61377	12.72631
16	C(13)	-0.01591	-17.88142	-6.38053	-5.96460
17	H(1)	-0.00207	-9.23078	-3.29377	-3.07906
18	C(13)	-0.01657	-18.63237	-6.64849	-6.21509
19	H(1)	-0.00221	-9.88692	-3.52790	-3.29792
20	C(13)	0.02537	28.52128	10.17710	9.51368
21	H(1)	0.00074	3.30422	1.17903	1.10217
22	H(1)	0.00083	3.72394	1.32879	1.24217
23	H(1)	-0.00170	-7.59540	-2.71023	-2.53355
24	S(33)	0.02680	9.20582	3.28486	3.07073
25	**H(1)**	**0.00660**	**93.93226**	**33.51737**	**31.33243**

Temperature: 298K

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	0.16789	188.74250	67.34802	62.95772
2	C(13)	-0.07479	-84.08229	-30.00265	-28.04683
3	C(13)	0.05931	66.67388	23.79090	22.24001
4	C(13)	0.05707	64.16240	22.89474	21.40227
5	C(13)	-0.02887	-32.45429	-11.58050	-10.82559
6	H(1)	-0.00369	-16.49636	-5.88631	-5.50259
7	C(13)	-0.02907	-32.67799	-11.66032	-10.90020
8	H(1)	-0.00376	-16.81523	-6.00009	-5.60896
9	C(13)	0.03356	37.72807	13.46231	12.58473
10	H(1)	0.00176	7.85230	2.80189	2.61924
11	H(1)	0.00194	8.67745	3.09633	2.89449
12	H(1)	-0.00208	-9.27856	-3.31082	-3.09499
13	C(13)	-0.05471	-61.49938	-21.94451	-20.51399
14	C(13)	0.03264	36.69208	13.09265	12.23916
15	C(13)	0.03225	36.25358	12.93618	12.09289
16	C(13)	-0.00160	-1.79534	-0.64062	-0.59886
17	H(1)	-0.00181	-8.07314	-2.88070	-2.69291
18	C(13)	-0.00286	-3.21628	-1.14765	-1.07284
19	H(1)	-0.00210	-9.37389	-3.34484	-3.12679
20	C(13)	0.00553	6.21549	2.21784	2.07326
21	H(1)	-0.00024	-1.08507	-0.38718	-0.36194
22	H(1)	-0.00012	-0.52511	-0.18737	-0.17516
23	H(1)	0.00011	0.51193	0.18267	0.17076
24	S(33)	0.02737	9.40035	3.35428	3.13562
25	**H(1)**	**0.00781**	**111.09204**	**39.64040**	**37.05632**

4Mu



E(UB3LYP) = -977.585993814035 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.044756	2.649412	0.536475
2	6	0	0.023194	0.896470	0.157394
3	6	0	1.326410	0.273364	-0.004478
4	6	0	2.473747	1.116524	-0.080389
5	6	0	3.754034	0.635072	-0.297141
6	6	0	3.964440	-0.737193	-0.438547
7	6	0	2.868407	-1.591416	-0.340966
8	6	0	1.563313	-1.135413	-0.130302
9	6	0	0.494364	-2.200232	0.000037
10	6	0	-0.610128	-1.881770	1.024797
11	6	0	-1.653086	-0.987426	0.414041
12	6	0	-2.959357	-1.454322	0.248315
13	6	0	-3.943712	-0.685786	-0.372607
14	6	0	-3.610355	0.580349	-0.854139
15	6	0	-2.318732	1.066952	-0.688945
16	6	0	-1.307477	0.309301	-0.048633
17	1	0	-1.219613	2.712032	0.997644
18	1	0	2.352729	2.189727	0.015829
19	1	0	4.585313	1.332388	-0.355971
20	1	0	4.960679	-1.136894	-0.604792
21	1	0	3.026688	-2.664868	-0.418713
22	1	0	0.988852	-3.137698	0.280180
23	1	0	0.019621	-2.389158	-0.973926
24	1	0	-0.160182	-1.419503	1.913505
25	1	0	-1.081131	-2.814535	1.353706
26	1	0	-3.207186	-2.445814	0.620735
27	1	0	-4.952070	-1.074378	-0.484830
28	1	0	-4.351795	1.188715	-1.365148
29	1	0	-2.068380	2.042542	-1.092442

Zero-point correction= 0.233418 (Hartree/Particle)
Thermal correction to Energy= 0.246170
Thermal correction to Enthalpy= 0.247114
Thermal correction to Gibbs Free Energy= 0.193238
Sum of electronic and zero-point Energies= -977.352576
Sum of electronic and thermal Energies= -977.339824
Sum of electronic and thermal Enthalpies= -977.338880
Sum of electronic and thermal Free Energies= -977.392756

Vibrational averaging

[Input (inpart)]

freq=(anharmonic,readanharm) ub3lyp/6-31g(d)

0 2

S	0.04476	2.64941	0.53648	
C	0.02319	0.89647	0.15739	
C	1.32641	0.27336	-0.00448	
C	2.47375	1.11652	-0.08039	
C	3.75403	0.63507	-0.29714	
C	3.96444	-0.73719	-0.43855	
C	2.86841	-1.59142	-0.34097	
C	1.56331	-1.13541	-0.1303	
C	0.49436	-2.20023	0.00004	
C	-0.61013	-1.88177	1.0248	
C	-1.65309	-0.98743	0.41404	
C	-2.95936	-1.45432	0.24832	
C	-3.94371	-0.68579	-0.37261	
C	-3.61036	0.58035	-0.85414	
C	-2.31873	1.06695	-0.68895	
C	-1.30748	0.3093	-0.04863	
H(Iso=0.113429,NMagM=8.890597)	**-1.21961**	**2.71203**	**0.99764**	
H	2.35273	2.18973	0.01583	
H	4.58531	1.33239	-0.35597	
H	4.96068	-1.13689	-0.60479	
H	3.02669	-2.66487	-0.41871	
H	0.98885	-3.1377	0.28018	
H	0.01962	-2.38916	-0.97393	
H	-0.16018	-1.4195	1.91351	
H	-1.08113	-2.81454	1.35371	
H	-3.20719	-2.44581	0.62074	
H	-4.95207	-1.07438	-0.48483	
H	-4.3518	1.18872	-1.36515	
H	-2.06838	2.04254	-1.09244	

Property=Fermi

[Output (in part)]

Fermi contact terms

Property at reference geometry

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	S(33)	0.01230	4.22349	1.50704	1.40880
2	C(13)	0.08099	91.04671	32.48773	30.36991
3	C(13)	-0.02964	-33.31597	-11.88797	-11.11301
4	C(13)	0.02240	25.17839	8.98428	8.39861
5	C(13)	-0.01349	-15.16264	-5.41041	-5.05771
6	C(13)	0.02059	23.14919	8.26021	7.72174
7	C(13)	-0.01442	-16.20765	-5.78329	-5.40629
8	C(13)	0.02191	24.63381	8.78996	8.21695
9	C(13)	-0.00035	-0.39624	-0.14139	-0.13217
10	C(13)	-0.00051	-0.57059	-0.20360	-0.19033
11	C(13)	0.02114	23.77093	8.48206	7.92913
12	C(13)	-0.00791	-8.88744	-3.17126	-2.96453
13	C(13)	0.01277	14.35647	5.12275	4.78880
14	C(13)	-0.00818	-9.19539	-3.28114	-3.06725
15	C(13)	0.01802	20.25960	7.22913	6.75787
16	C(13)	-0.02453	-27.58143	-9.84174	-9.20018
17	**H(1)**	**0.00153**	**21.82610**	**7.78810**	**7.28040**
18	H(1)	-0.00270	-12.07842	-4.30988	-4.02893
19	H(1)	0.00116	5.16992	1.84476	1.72450
20	H(1)	-0.00287	-12.81291	-4.57196	-4.27393
21	H(1)	0.00123	5.49794	1.96180	1.83391
22	H(1)	0.00172	7.69527	2.74586	2.56687
23	H(1)	0.00476	21.29532	7.59870	7.10336
24	H(1)	0.00086	3.86617	1.37955	1.28962
25	H(1)	0.00000	-0.00351	-0.00125	-0.00117
26	H(1)	0.00080	3.57705	1.27638	1.19317
27	H(1)	-0.00178	-7.97779	-2.84667	-2.66110
28	H(1)	0.00103	4.58240	1.63511	1.52852
29	H(1)	-0.00184	-8.22583	-2.93518	-2.74384

Temperature: 0K

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	S(33)	0.02133	7.32555	2.61394	2.44354
2	C(13)	0.09872	110.98192	39.60111	37.01958
3	C(13)	-0.03013	-33.87485	-12.08739	-11.29943
4	C(13)	0.01926	21.65608	7.72743	7.22369
5	C(13)	-0.00392	-4.40777	-1.57280	-1.47027
6	C(13)	0.00963	10.82486	3.86258	3.61079
7	C(13)	-0.00404	-4.54734	-1.62260	-1.51683
8	C(13)	0.01704	19.15262	6.83413	6.38862
9	C(13)	0.00391	4.39953	1.56986	1.46753
10	C(13)	-0.00452	-5.08251	-1.81357	-1.69534
11	C(13)	0.03747	42.12898	15.03267	14.05272
12	C(13)	-0.02015	-22.65331	-8.08326	-7.55633
13	C(13)	0.02496	28.05812	10.01183	9.35918
14	C(13)	-0.02049	-23.02965	-8.21755	-7.68186
15	C(13)	0.03486	39.18558	13.98239	13.07090
16	C(13)	-0.04196	-47.16726	-16.83045	-15.73330
17	H(1)	0.00505	71.79278	25.61745	23.94749
18	**H(1)**	**-0.00200**	**-8.95704**	**-3.19609**	**-2.98775**
19	H(1)	-0.00001	-0.05203	-0.01857	-0.01736
20	H(1)	-0.00094	-4.19045	-1.49526	-1.39778
21	H(1)	-0.00001	-0.03622	-0.01292	-0.01208

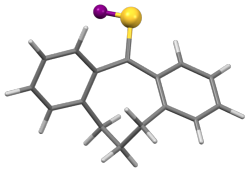
22	H(1)	0.00180	8.04616	2.87107	2.68391
23	H(1)	0.00404	18.06817	6.44717	6.02689
24	H(1)	0.00196	8.77795	3.13219	2.92801
25	H(1)	0.00027	1.19664	0.42699	0.39915
26	H(1)	0.00248	11.09406	3.95864	3.70058
27	H(1)	-0.00318	-14.21503	-5.07227	-4.74162
28	H(1)	0.00281	12.54251	4.47548	4.18373
29	H(1)	-0.00381	-17.03482	-6.07845	-5.68220

Temperature: 298K

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	S(33)	0.03317	11.39435	4.06579	3.80075
2	C(13)	0.14180	159.41110	56.88184	53.17382
3	C(13)	-0.02971	-33.39949	-11.91777	-11.14087
4	C(13)	-0.00319	-3.58102	-1.27780	-1.19450
5	C(13)	0.03376	37.95695	13.54398	12.66107
6	C(13)	-0.03849	-43.26586	-15.43834	-14.43194
7	C(13)	0.03705	41.65220	14.86254	13.89368
8	C(13)	-0.00861	-9.67762	-3.45321	-3.22810
9	C(13)	0.02014	22.63902	8.07817	7.55156
10	C(13)	-0.01879	-21.12264	-7.53708	-7.04575
11	C(13)	0.09217	103.61233	36.97146	34.56135
12	C(13)	-0.06397	-71.91403	-25.66071	-23.98794
13	C(13)	0.06589	74.07057	26.43022	24.70728
14	C(13)	-0.06456	-72.57468	-25.89645	-24.20831
15	C(13)	0.08938	100.47848	35.85322	33.51601
16	C(13)	-0.10416	-117.10078	-41.78447	-39.06062
17	**H(1)**	**0.00853**	**121.40559**	**43.32053**	**40.49654**
18	H(1)	0.00095	4.23501	1.51116	1.41265
19	H(1)	-0.00473	-21.14138	-7.54377	-7.05201
20	H(1)	0.00643	28.72792	10.25084	9.58260
21	H(1)	-0.00503	-22.46807	-8.01717	-7.49454
22	H(1)	0.00096	4.29218	1.53156	1.43172
23	H(1)	-0.00028	-1.23319	-0.44003	-0.41135
24	H(1)	0.00609	27.20726	9.70823	9.07537
25	H(1)	0.00127	5.68444	2.02835	1.89613
26	H(1)	0.00829	37.05788	13.22317	12.36118
27	H(1)	-0.00823	-36.77728	-13.12305	-12.26758
28	H(1)	0.00892	39.89124	14.23419	13.30629
29	H(1)	-0.01097	-49.05259	-17.50318	-16.36218

5Mu



E(UB3LYP) = -1016.89725440 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.054959	2.831313	0.054478
2	6	0	0.012534	1.041409	0.030287
3	6	0	-1.319396	0.429404	-0.027853
4	6	0	-2.373574	1.127515	-0.676702
5	6	0	-3.685342	0.673066	-0.672063
6	6	0	-4.009050	-0.507124	-0.002107
7	6	0	-2.989996	-1.227427	0.618857
8	6	0	-1.657485	-0.803357	0.612753
9	6	0	-0.621463	-1.727635	1.203018
10	6	0	-0.018720	-2.624779	0.100154
11	6	0	0.568082	-1.804691	-1.068819
12	6	0	1.629955	-0.849308	-0.579242
13	6	0	2.957205	-1.283678	-0.643649
14	6	0	4.021525	-0.536153	-0.142375
15	6	0	3.749258	0.689230	0.466727
16	6	0	2.443896	1.151487	0.538424
17	6	0	1.337530	0.425836	0.009603
18	1	0	-1.137421	3.029986	0.654872
19	1	0	-2.137745	2.033260	-1.224486
20	1	0	-4.451248	1.239706	-1.194984
21	1	0	-5.033464	-0.867682	0.028372
22	1	0	-3.229164	-2.157686	1.130004
23	1	0	-1.085507	-2.361559	1.967455
24	1	0	0.176158	-1.165133	1.698101
25	1	0	-0.796199	-3.296512	-0.286605
26	1	0	0.768087	-3.254831	0.534819
27	1	0	-0.236361	-1.273953	-1.587019
28	1	0	1.010437	-2.493494	-1.797657
29	1	0	3.156649	-2.247024	-1.108310
30	1	0	5.039201	-0.908611	-0.218941
31	1	0	4.551634	1.285114	0.893527
32	1	0	2.255836	2.094634	1.037130

Zero-point correction=	0.262879 (Hartree/Particle)
Thermal correction to Energy=	0.276472
Thermal correction to Enthalpy=	0.277416
Thermal correction to Gibbs Free Energy=	0.221960
Sum of electronic and zero-point Energies=	-1016.634376
Sum of electronic and thermal Energies=	-1016.620783
Sum of electronic and thermal Enthalpies=	-1016.619839
Sum of electronic and thermal Free Energies=	-1016.675294

Vibrational averaging

[Input (inpart)]

freq=(anharmonic,readanharm) ub3lyp/6-31g(d)

0 2

S		0.05498	2.83131	0.05444
C		0.01253	1.04141	0.03031
C		-1.3194	0.4294	-0.02786
C		-2.37358	1.12754	-0.67668
C		-3.68535	0.67309	-0.67205
C		-4.00906	-0.50712	-0.00214
C		-2.99	-1.22745	0.6188
C		-1.65749	-0.80339	0.61271
C		-0.62148	-1.72769	1.20295
C		-0.01871	-2.62478	0.10006
C		0.56811	-1.80464	-1.06887
C		1.62997	-0.84928	-0.57924
C		2.95722	-1.28366	-0.64361
C		4.02152	-0.53615	-0.14227
C		3.74924	0.68922	0.46686
C		2.44387	1.15147	0.53853
C		1.33753	0.42583	0.00965
H(Iso=0.113429,NMagM=8.890597)		**-1.13738**	**3.03001**	**0.65486**
H		-2.13776	2.0333	-1.22443
H		-4.45125	1.23976	-1.19495
H		-5.03347	-0.86768	0.02833
H		-3.22918	-2.15773	1.12991
H		-1.08554	-2.36165	1.96735
H		0.17613	-1.16521	1.69808
H		-0.79617	-3.29651	-0.28674
H		0.7681	-3.25484	0.53472
H		-0.23633	-1.27388	-1.58705
H		1.01046	-2.49341	-1.79774
H		3.15668	-2.24698	-1.10831
H		5.0392	-0.9086	-0.21881
H		4.5516	1.28509	0.89371
H		2.25579	2.0946	1.03725

Property=Fermi

[Output (in part)]

Fermi contact terms

Property at reference geometry

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	S(33)	0.01317	4.52262	1.61378	1.50859
2	C(13)	0.07931	89.16420	31.81600	29.74197
3	C(13)	-0.02633	-29.59553	-10.56042	-9.87201
4	C(13)	0.01692	19.02525	6.78868	6.34614
5	C(13)	-0.01026	-11.53194	-4.11488	-3.84664
6	C(13)	0.01538	17.29525	6.17137	5.76907
7	C(13)	-0.01047	-11.77452	-4.20144	-3.92756
8	C(13)	0.02417	27.16722	9.69394	9.06201
9	C(13)	-0.00399	-4.48664	-1.60094	-1.49658
10	C(13)	0.00544	6.11803	2.18307	2.04076
11	C(13)	-0.00460	-5.16843	-1.84423	-1.72400
12	C(13)	0.02468	27.74010	9.89836	9.25310
13	C(13)	-0.01290	-14.50063	-5.17418	-4.83689
14	C(13)	0.01887	21.21120	7.56868	7.07529
15	C(13)	-0.01292	-14.52930	-5.18442	-4.84645
16	C(13)	0.01843	20.71413	7.39132	6.90949
17	C(13)	-0.02863	-32.18852	-11.48567	-10.73694
18	**H(1)**	**0.00206**	**29.37990**	**10.48348**	**9.80008**
19	H(1)	-0.00216	-9.63305	-3.43731	-3.21324
20	H(1)	0.00113	5.06014	1.80558	1.68788
21	H(1)	-0.00215	-9.59241	-3.42281	-3.19968
22	H(1)	0.00089	3.98355	1.42143	1.32877
23	H(1)	0.00074	3.31182	1.18174	1.10470
24	H(1)	0.00074	3.28918	1.17366	1.09715
25	H(1)	0.00056	2.50427	0.89358	0.83533
26	H(1)	0.00044	1.97207	0.70368	0.65781
27	H(1)	0.00109	4.87840	1.74073	1.62726
28	H(1)	0.00073	3.26715	1.16580	1.08980
29	H(1)	0.00105	4.68315	1.67107	1.56213
30	H(1)	-0.00262	-11.70547	-4.17680	-3.90452
31	H(1)	0.00123	5.51772	1.96886	1.84051
32	H(1)	-0.00252	-11.24658	-4.01306	-3.75146

Temperature: 0K

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	S(33)	0.02020	6.93855	2.47585	2.31445
2	C(13)	0.10281	115.58171	41.24243	38.55391
3	C(13)	-0.04293	-48.26376	-17.22171	-16.09906
4	C(13)	0.02981	33.50696	11.95612	11.17672
5	C(13)	-0.01800	-20.23371	-7.21989	-6.74924
6	C(13)	0.02224	25.00275	8.92160	8.34002
7	C(13)	-0.01799	-20.22498	-7.21678	-6.74633
8	C(13)	0.03652	41.05224	14.64846	13.69355
9	C(13)	-0.00583	-6.55309	-2.33831	-2.18588
10	C(13)	0.00684	7.69151	2.74452	2.56561
11	C(13)	-0.00357	-4.01883	-1.43402	-1.34054
12	C(13)	0.02227	25.04008	8.93492	8.35247
13	C(13)	-0.00533	-5.99670	-2.13977	-2.00028
14	C(13)	0.01033	11.60966	4.14262	3.87257
15	C(13)	-0.00594	-6.67546	-2.38197	-2.22669
16	C(13)	0.01776	19.96216	7.12299	6.65866
17	C(13)	-0.03390	-38.11379	-13.59995	-12.71339
18	**H(1)**	**0.00604**	**85.98363**	**30.68110**	**28.68105**

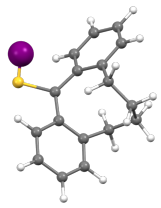
19	H(1)	-0.00361	-16.12529	-5.75390	-5.37882
20	H(1)	0.00235	10.49170	3.74370	3.49966
21	H(1)	-0.00277	-12.35969	-4.41024	-4.12275
22	H(1)	0.00198	8.86265	3.16242	2.95626
23	H(1)	0.00101	4.49351	1.60340	1.49887
24	H(1)	0.00113	5.04094	1.79873	1.68148
25	H(1)	0.00052	2.33611	0.83358	0.77924
26	H(1)	0.00053	2.38956	0.85265	0.79707
27	H(1)	0.00092	4.13421	1.47519	1.37902
28	H(1)	0.00058	2.60042	0.92789	0.86741
29	H(1)	0.00015	0.69205	0.24694	0.23084
30	H(1)	-0.00106	-4.75754	-1.69761	-1.58694
31	H(1)	0.00037	1.67207	0.59664	0.55774
32	H(1)	-0.00212	-9.45994	-3.37554	-3.15550

Temperature: 298K

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	S(33)	0.02514	8.63382	3.08076	2.87993
2	C(13)	0.16894	189.91649	67.76693	63.34932
3	C(13)	-0.10119	-113.75353	-40.59009	-37.94409
4	C(13)	0.06999	78.68441	28.07655	26.24629
5	C(13)	-0.04367	-49.09122	-17.51697	-16.37507
6	C(13)	0.04135	46.49007	16.58881	15.50742
7	C(13)	-0.04297	-48.31094	-17.23854	-16.11479
8	C(13)	0.07508	84.40067	30.11626	28.15303
9	C(13)	-0.01189	-13.36540	-4.76911	-4.45822
10	C(13)	0.00847	9.52310	3.39808	3.17656
11	C(13)	0.00115	1.29388	0.46169	0.43159
12	C(13)	0.00692	7.78114	2.77650	2.59551
13	C(13)	0.02650	29.79448	10.63141	9.93837
14	C(13)	-0.03028	-34.04078	-12.14660	-11.35478
15	C(13)	0.02398	26.95843	9.61944	8.99236
16	C(13)	0.00626	7.03442	2.51006	2.34643
17	C(13)	-0.05049	-56.76366	-20.25468	-18.93432
18	**H(1)**	**0.01087**	**154.69928**	**55.20055**	**51.60212**
19	H(1)	-0.00867	-38.76676	-13.83295	-12.93120
20	H(1)	0.00629	28.10109	10.02717	9.37351
21	H(1)	-0.00478	-21.35236	-7.61905	-7.12238
22	H(1)	0.00555	24.81646	8.85513	8.27788
23	H(1)	0.00184	8.22007	2.93313	2.74192
24	H(1)	0.00229	10.22900	3.64996	3.41203
25	H(1)	0.00027	1.20758	0.43089	0.40280
26	H(1)	0.00088	3.93145	1.40284	1.31139
27	H(1)	-0.00028	-1.24415	-0.44394	-0.41500
28	H(1)	-0.00010	-0.45255	-0.16148	-0.15095
29	H(1)	-0.00355	-15.87500	-5.66459	-5.29533
30	H(1)	0.00523	23.37448	8.34060	7.79689
31	H(1)	-0.00328	-14.65807	-5.23036	-4.88941
32	H(1)	0.00001	0.04701	0.01677	0.01568

6Mu



E(UB3LYP) = -1056.20031344 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.324005	0.609142	-0.015805
2	6	0	-0.004709	1.243580	0.018392
3	6	0	2.920287	-1.081120	0.721990
4	6	0	1.315046	0.608569	0.012067
5	1	0	3.135257	-1.981517	1.294286
6	6	0	1.609683	-0.591326	0.730446
7	6	0	3.951202	-0.451998	0.026101
8	16	0	-0.061372	3.025806	-0.013758
9	1	0	4.956458	-0.863849	0.044919
10	6	0	3.670971	0.714629	-0.687714
11	6	0	-1.600910	-0.602697	-0.723661
12	1	0	4.452387	1.218793	-1.250241
13	6	0	2.383082	1.232937	-0.684509
14	1	0	2.173586	2.125343	-1.265190
15	6	0	-2.412057	1.242428	0.643989
16	1	0	-2.220903	2.151342	1.203445
17	6	0	-3.697643	0.720990	0.624744
18	1	0	-4.493898	1.235291	1.156318
19	6	0	-3.957505	-0.461726	-0.070464
20	1	0	-4.960395	-0.878504	-0.103320
21	6	0	-2.909151	-1.098703	-0.731810
22	1	0	-3.108256	-2.010009	-1.292449
23	6	0	0.569389	-1.356759	1.518390
24	6	0	-0.549247	-1.376615	-1.488268
25	6	0	-0.005704	-2.612340	0.796016
26	6	0	0.017455	-2.624179	-0.746259
27	1	0	-0.247930	-0.689765	1.794804
28	1	0	1.022897	-1.686641	2.461298
29	1	0	-1.035174	-2.757403	1.144298
30	1	0	0.551192	-3.498947	1.125566
31	1	0	-0.545891	-3.511915	-1.061613
32	1	0	1.045691	-2.782194	-1.092797
33	1	0	0.270531	-0.713203	-1.764895
34	1	0	-0.991934	-1.718286	-2.432108
35	1	0	1.121250	3.259696	0.595935

Zero-point correction= 0.291612 (Hartree/Particle)
Thermal correction to Energy= 0.306665
Thermal correction to Enthalpy= 0.307610
Thermal correction to Gibbs Free Energy= 0.249080
Sum of electronic and zero-point Energies= -1055.908701
Sum of electronic and thermal Energies= -1055.893648
Sum of electronic and thermal Enthalpies= -1055.892704
Sum of electronic and thermal Free Energies= -1055.951233

Vibrational averaging

[Input (inpart)]

freq=(anharmonic,readanharm) ub3lyp/6-31g(d)

0 2

C	-1.32401	0.60914	-0.01581
C	-0.00471	1.24358	0.01839
C	2.92029	-1.08112	0.72199
C	1.31505	0.60857	0.01207
H	3.13526	-1.98152	1.29429
C	1.60968	-0.59133	0.73045
C	3.9512	-0.452	0.0261
S	-0.06137	3.02581	-0.01376
H	4.95646	-0.86385	0.04492
C	3.67097	0.71463	-0.68771
C	-1.60091	-0.6027	-0.72366
H	4.45239	1.21879	-1.25024
C	2.38308	1.23294	-0.68451
H	2.17359	2.12534	-1.26519
C	-2.41206	1.24243	0.64399
H	-2.2209	2.15134	1.20345
C	-3.69764	0.72099	0.62474
H	-4.4939	1.23529	1.15632
C	-3.95751	-0.46173	-0.07046
H	-4.9604	-0.8785	-0.10332
C	-2.90915	-1.0987	-0.73181
H	-3.10826	-2.01001	-1.29245
C	0.56939	-1.35676	1.51839
C	-0.54925	-1.37662	-1.48827
C	-0.0057	-2.61234	0.79602
C	0.01746	-2.62418	-0.74626
H	-0.24793	-0.68977	1.7948
H	1.0229	-1.68664	2.4613
H	-1.03517	-2.7574	1.1443
H	0.55119	-3.49895	1.12557
H	-0.54589	-3.51192	-1.06161
H	1.04569	-2.78219	-1.0928
H	0.27053	-0.7132	-1.7649
H	-0.99193	-1.71829	-2.43211
H(Iso=0.113429,NMagM=8.890597)	**1.12125**	**3.2597**	**0.59594**

Property=Fermi

[Output (in part)]

Fermi contact terms

Property at reference geometry

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.02798	-31.45555	-11.22412	-10.49244
2	C(13)	0.08275	93.02972	33.19532	31.03137
3	C(13)	-0.01036	-11.64294	-4.15449	-3.88367
4	C(13)	-0.02667	-29.98135	-10.69809	-10.00070
5	H(1)	0.00096	4.27158	1.52421	1.42485
6	C(13)	0.02301	25.86454	9.22911	8.62748
7	C(13)	0.01483	16.67714	5.95082	5.56290
8	S(33)	0.01357	4.66136	1.66329	1.55486
9	H(1)	-0.00208	-9.27558	-3.30976	-3.09400
10	C(13)	-0.00981	-11.02713	-3.93475	-3.67825
11	C(13)	0.02393	26.89844	9.59803	8.97235
12	H(1)	0.00116	5.16544	1.84316	1.72300
13	C(13)	0.01826	20.52785	7.32485	6.84735
14	H(1)	-0.00210	-9.36502	-3.34167	-3.12384
15	C(13)	0.01845	20.74329	7.40172	6.91922
16	H(1)	-0.00218	-9.73060	-3.47212	-3.24578
17	C(13)	-0.01089	-12.24417	-4.36903	-4.08422
18	H(1)	0.00119	5.33986	1.90539	1.78118
19	C(13)	0.01617	18.17567	6.48553	6.06275
20	H(1)	-0.00225	-10.07760	-3.59594	-3.36153
21	C(13)	-0.01124	-12.63252	-4.50760	-4.21376
22	H(1)	0.00104	4.63510	1.65392	1.54610
23	C(13)	-0.00388	-4.35836	-1.55517	-1.45379
24	C(13)	-0.00426	-4.79175	-1.70981	-1.59835
25	C(13)	0.00372	4.18563	1.49354	1.39617
26	C(13)	0.00426	4.78795	1.70846	1.59709
27	H(1)	0.00033	1.48226	0.52891	0.49443
28	H(1)	0.00108	4.80744	1.71542	1.60359
29	H(1)	0.00040	1.77751	0.63426	0.59291
30	H(1)	-0.00013	-0.57733	-0.20601	-0.19258
31	H(1)	-0.00015	-0.65019	-0.23200	-0.21688
32	H(1)	0.00037	1.66066	0.59256	0.55394
33	H(1)	0.00038	1.69123	0.60347	0.56413
34	H(1)	0.00122	5.44673	1.94353	1.81683
35	**H(1)**	**0.00231**	**32.86369**	**11.72658**	**10.96215**

Temperature: 0K

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.03651	-41.04325	-14.64525	-13.69055
2	C(13)	0.11765	132.25895	47.19328	44.11684
3	C(13)	-0.01606	-18.04960	-6.44055	-6.02070
4	C(13)	-0.04233	-47.58387	-16.97911	-15.87227
5	H(1)	0.00196	8.76878	3.12892	2.92495
6	C(13)	0.03036	34.13344	12.17966	11.38569
7	C(13)	0.02035	22.87287	8.16161	7.62957
8	S(33)	0.01495	5.13490	1.83226	1.71282
9	H(1)	-0.00278	-12.44124	-4.43934	-4.14995
10	C(13)	-0.01555	-17.47995	-6.23728	-5.83068
11	C(13)	0.02247	25.26451	9.01501	8.42733
12	H(1)	0.00222	9.90967	3.53602	3.30551
13	C(13)	0.02618	29.42887	10.50095	9.81641
14	H(1)	-0.00261	-11.66109	-4.16097	-3.88972
15	C(13)	0.01646	18.50926	6.60456	6.17403

16	H(1)	-0.00122	-5.44428	-1.94266	-1.81602
17	C(13)	-0.00550	-6.17829	-2.20457	-2.06086
18	H(1)	0.00061	2.71470	0.96867	0.90553
19	C(13)	0.01131	12.71960	4.53867	4.24280
20	H(1)	-0.00155	-6.93801	-2.47565	-2.31427
21	C(13)	-0.00729	-8.18975	-2.92231	-2.73181
22	H(1)	0.00077	3.45091	1.23137	1.15110
23	C(13)	-0.00434	-4.87452	-1.73935	-1.62597
24	C(13)	-0.00305	-3.42715	-1.22289	-1.14317
25	C(13)	0.00496	5.57852	1.99056	1.86080
26	C(13)	0.00364	4.08699	1.45834	1.36327
27	H(1)	0.00042	1.85887	0.66329	0.62005
28	H(1)	0.00130	5.80348	2.07082	1.93583
29	H(1)	0.00042	1.87194	0.66795	0.62441
30	H(1)	-0.00011	-0.47085	-0.16801	-0.15706
31	H(1)	-0.00007	-0.29126	-0.10393	-0.09715
32	H(1)	0.00042	1.87423	0.66877	0.62518
33	H(1)	0.00026	1.15407	0.41180	0.38496
34	H(1)	0.00100	4.45798	1.59072	1.48702
35	**H(1)**	**0.00665**	**94.61986**	**33.76272**	**31.56179**

Temperature: 298K

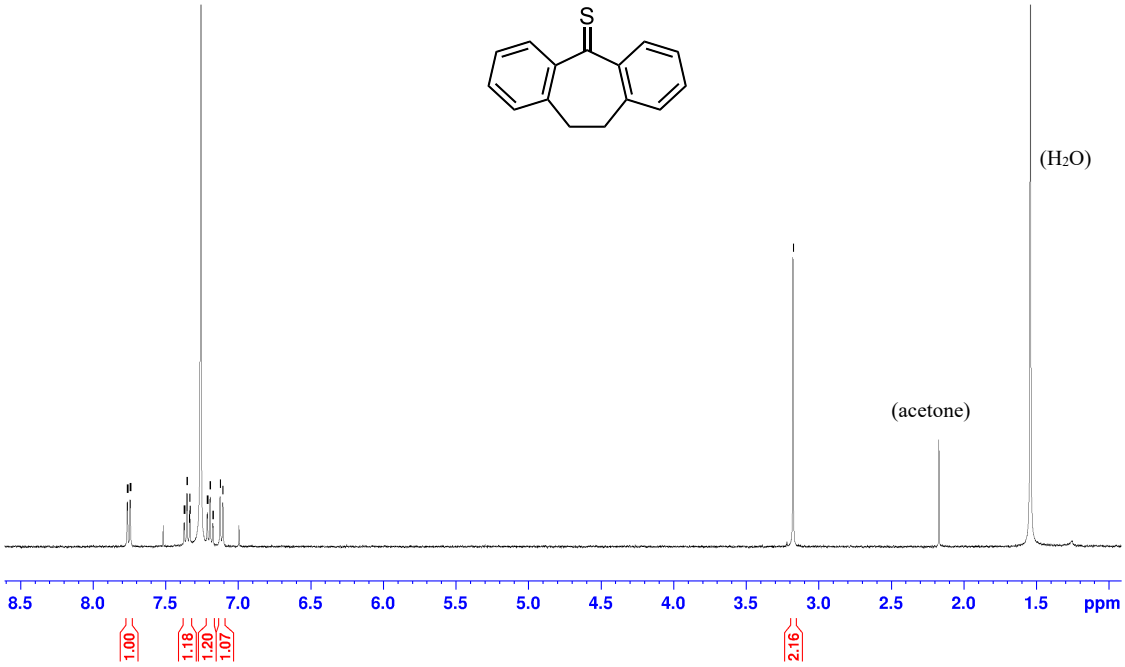
Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.05945	-66.82829	-23.84600	-22.29152
2	C(13)	0.20152	226.54825	80.83805	75.56836
3	C(13)	-0.03064	-34.43985	-12.28899	-11.48790
4	C(13)	-0.08586	-96.52386	-34.44211	-32.19689
5	H(1)	0.00454	20.29865	7.24306	6.77090
6	C(13)	0.04744	53.32743	19.02855	17.78812
7	C(13)	0.03177	35.71609	12.74439	11.91361
8	S(33)	0.00010	0.03542	0.01264	0.01182
9	H(1)	-0.00462	-20.65446	-7.37002	-6.88959
10	C(13)	-0.03029	-34.04689	-12.14878	-11.35682
11	C(13)	0.01382	15.53977	5.54498	5.18351
12	H(1)	0.00491	21.95821	7.83524	7.32447
13	C(13)	0.04410	49.57497	17.68958	16.53643
14	H(1)	-0.00399	-17.82068	-6.35886	-5.94434
15	C(13)	0.00439	4.93565	1.76116	1.64636
16	H(1)	0.00194	8.69029	3.10091	2.89877
17	C(13)	0.01290	14.50153	5.17451	4.83719
18	H(1)	-0.00147	-6.57558	-2.34633	-2.19338
19	C(13)	-0.00898	-10.09144	-3.60088	-3.36614
20	H(1)	0.00091	4.04768	1.44431	1.35016
21	C(13)	0.00708	7.96244	2.84120	2.65599
22	H(1)	-0.00034	-1.51943	-0.54217	-0.50683
23	C(13)	-0.00513	-5.76436	-2.05687	-1.92278
24	C(13)	0.00123	1.37830	0.49181	0.45975
25	C(13)	0.00748	8.41051	3.00108	2.80544
26	C(13)	0.00016	0.17775	0.06343	0.05929
27	H(1)	0.00046	2.04209	0.72867	0.68117
28	H(1)	0.00178	7.96479	2.84203	2.65677
29	H(1)	0.00044	1.97954	0.70635	0.66031
30	H(1)	-0.00004	-0.17043	-0.06082	-0.05685
31	H(1)	0.00018	0.79707	0.28441	0.26587
32	H(1)	0.00051	2.27430	0.81153	0.75862
33	H(1)	-0.00033	-1.48288	-0.52913	-0.49463
34	H(1)	0.00005	0.23677	0.08449	0.07898
35	**H(1)**	**0.00970**	**137.95520**	**49.22585**	**46.01690**

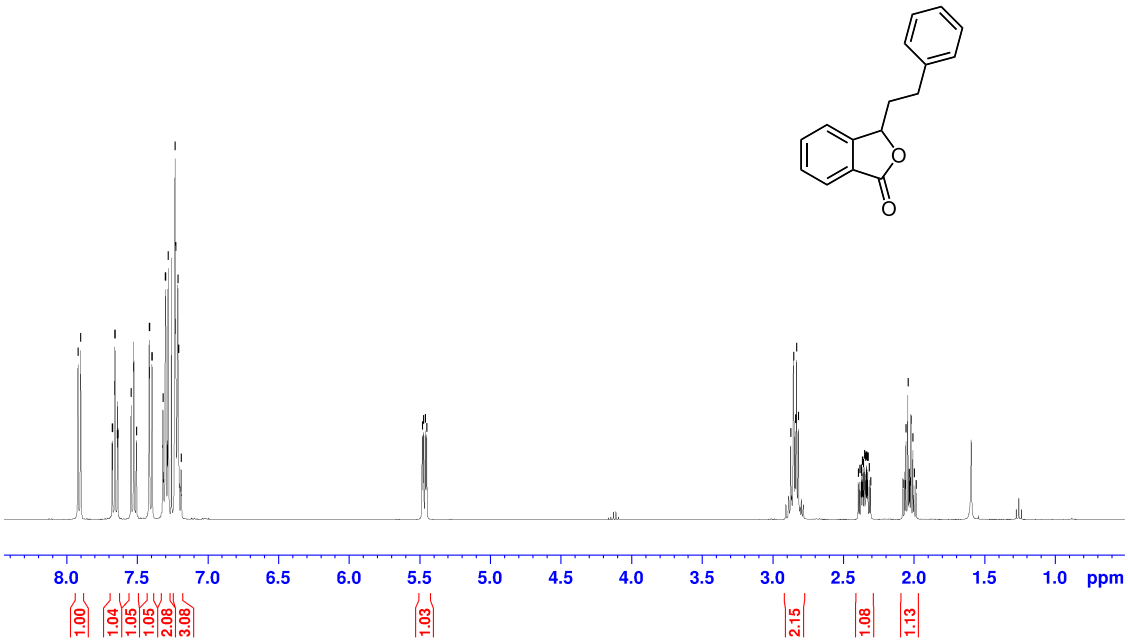
Table S2. DFT-calculated muon hfcs for **4Mu**, **5Mu**, and **6Mu** at UB3LYP/6-31G(d)

	4Mu	**5Mu**	**6Mu**
A_{μ}^{calc} (w/o isotope effect)	21.8	29.4	32.9
A_{μ}^{calc} (averaged, 0 K)	71.8	86.0	94.6
A_{μ}^{calc} (averaged, 298 K)	121.4	154.7	138.0

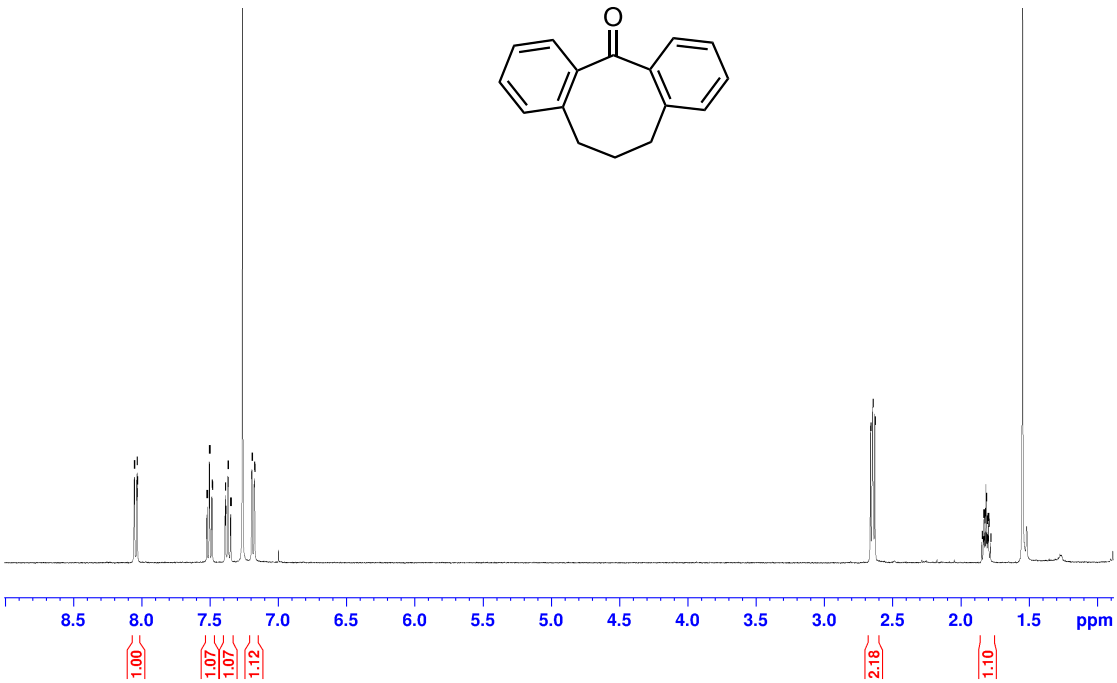
Copies of NMR charts



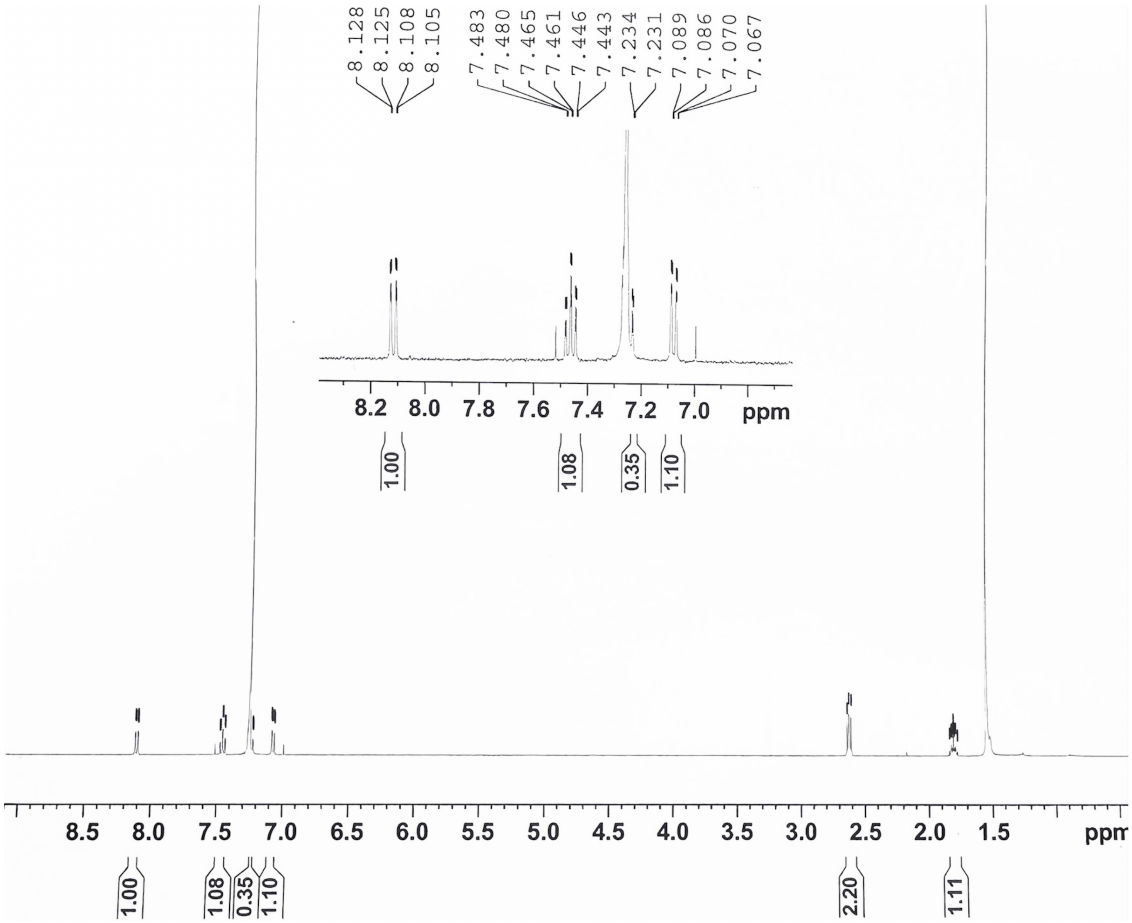
^{1}H NMR of **4** (400 MHz, $CDCl_3$)



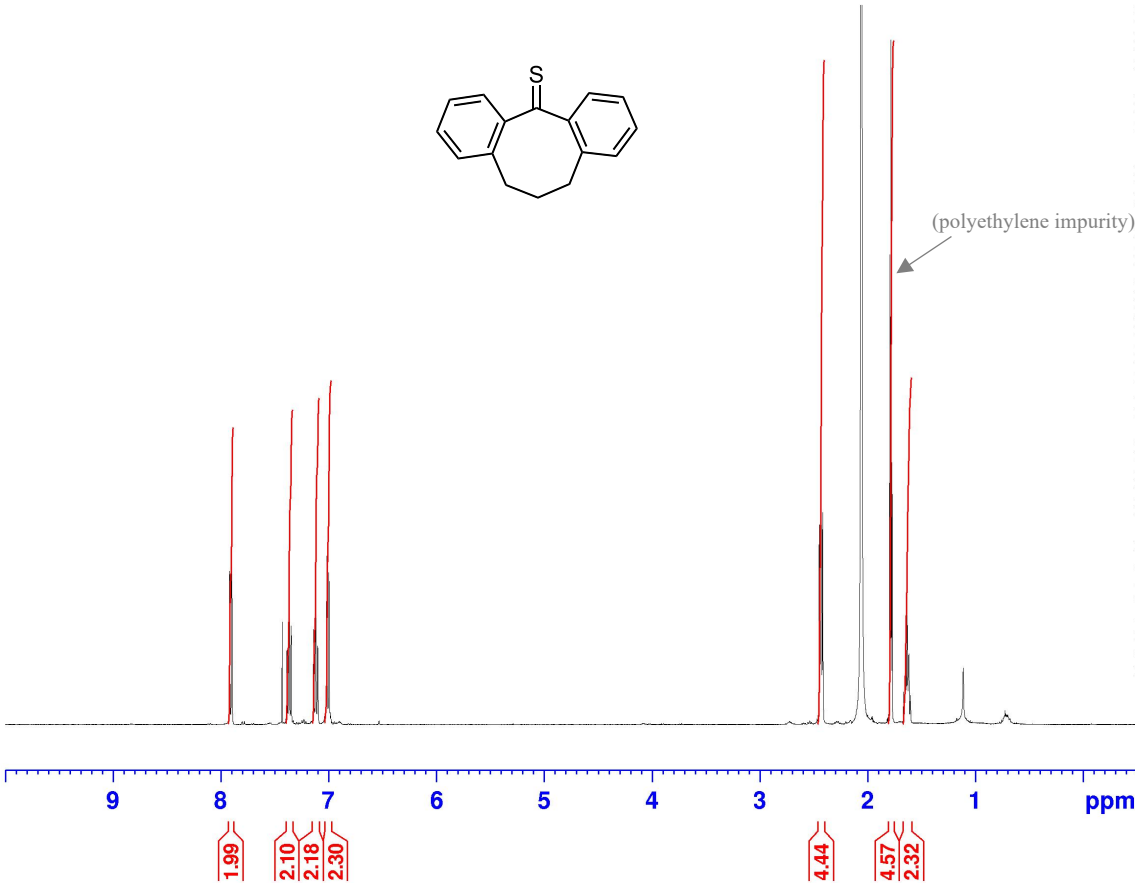
^{1}H NMR of **7** (400 MHz, $CDCl_3$)



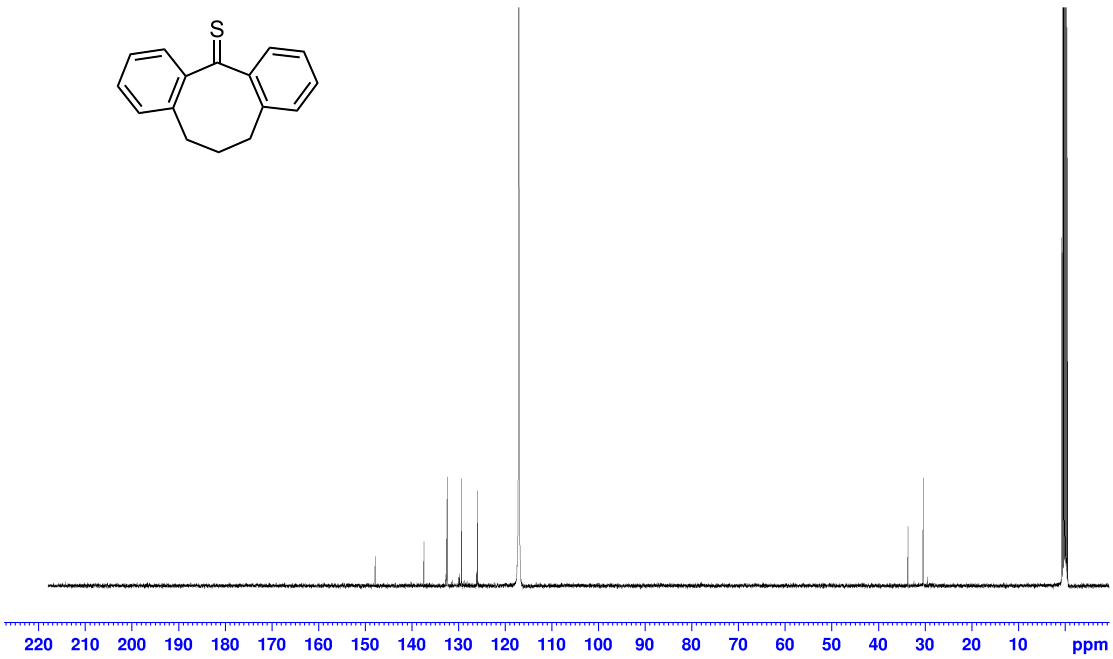
^{1}H NMR of **10** (400 MHz, $CDCl_3$)



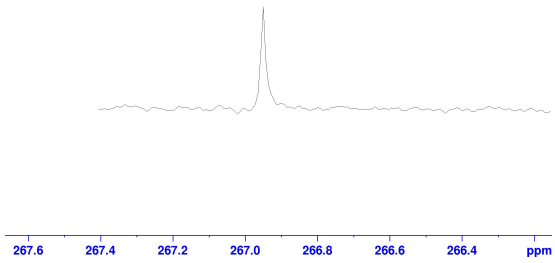
^{1}H NMR of **5** (400 MHz, $CDCl_3$)



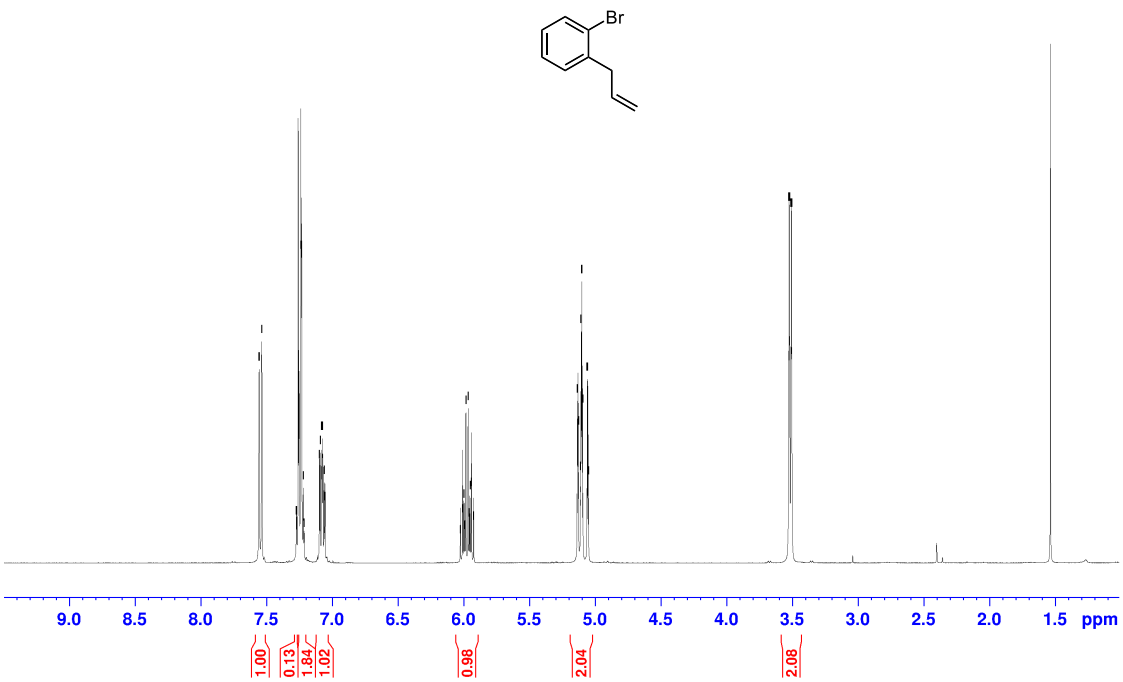
^{1}H NMR of **5** (400 MHz, acetonitrile-d_3)



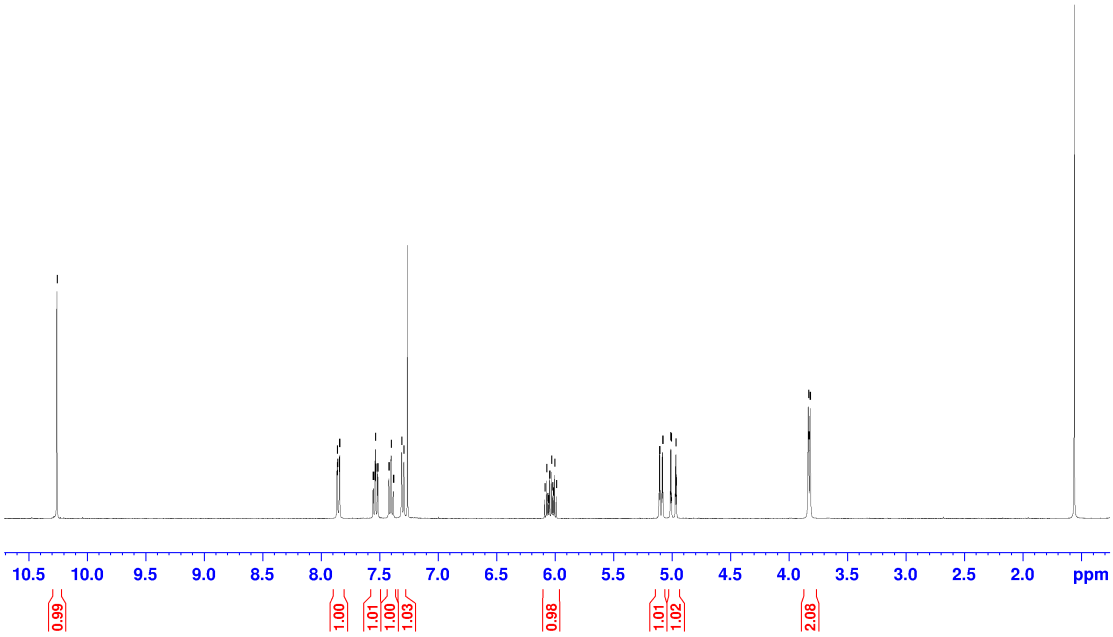
$^{13}C\{^{1}H\}$ NMR of **5** (101 MHz, acetonitrile-d_3)



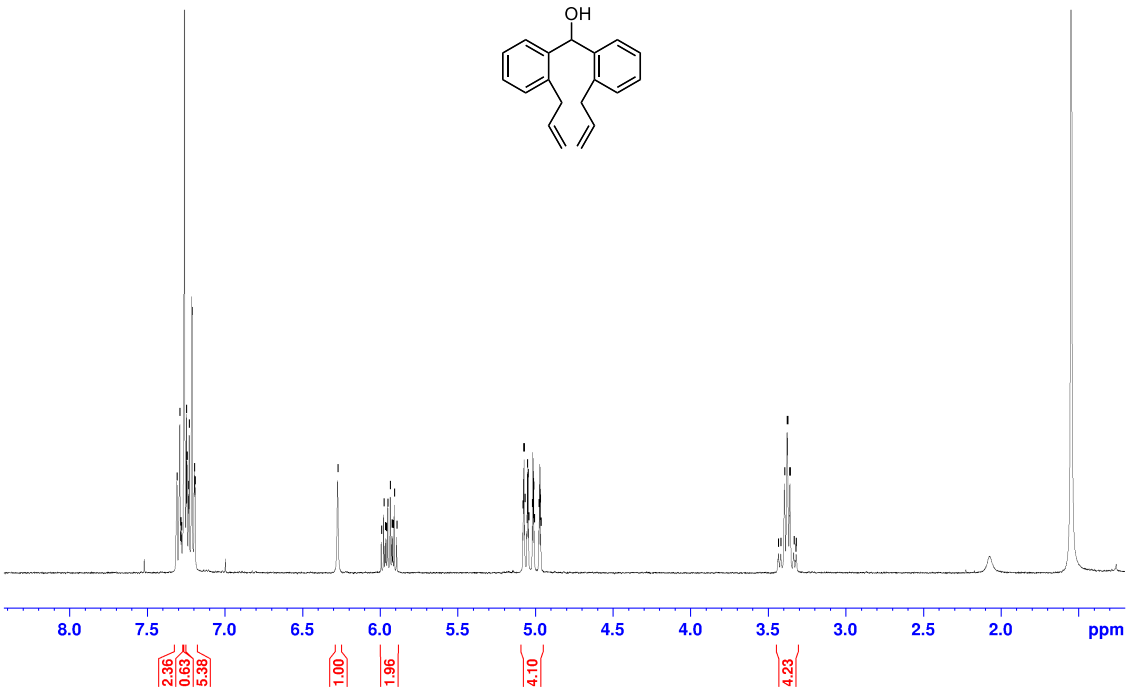
$^{13}C\{^{1}H\}$ NMR of **5** (C=S, 101 MHz, $CDCl_3$)



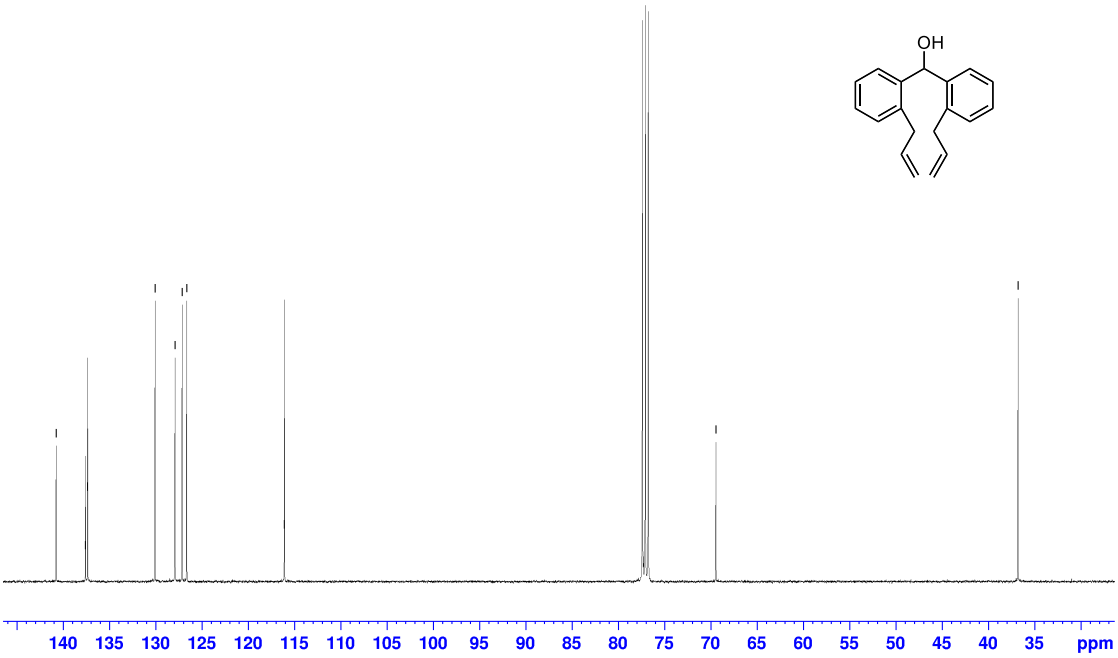
^{1}H NMR of **11** (400 MHz, $CDCl_3$)



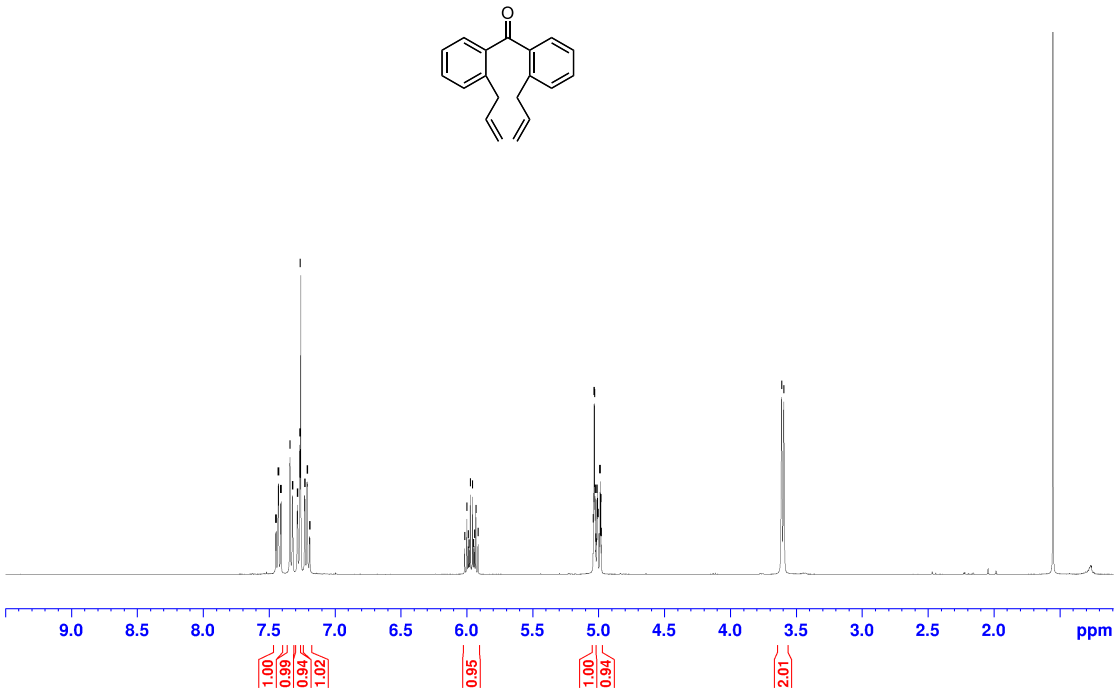
^{1}H NMR of **12** (400 MHz, $CDCl_3$)



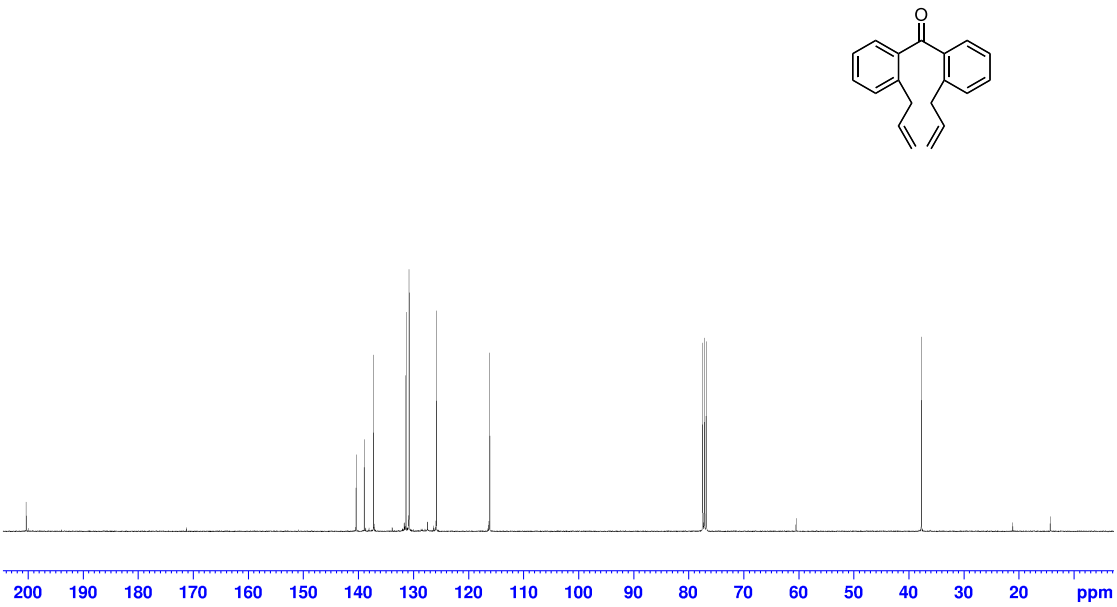
^{1}H NMR of **13** (400 MHz, $CDCl_3$)



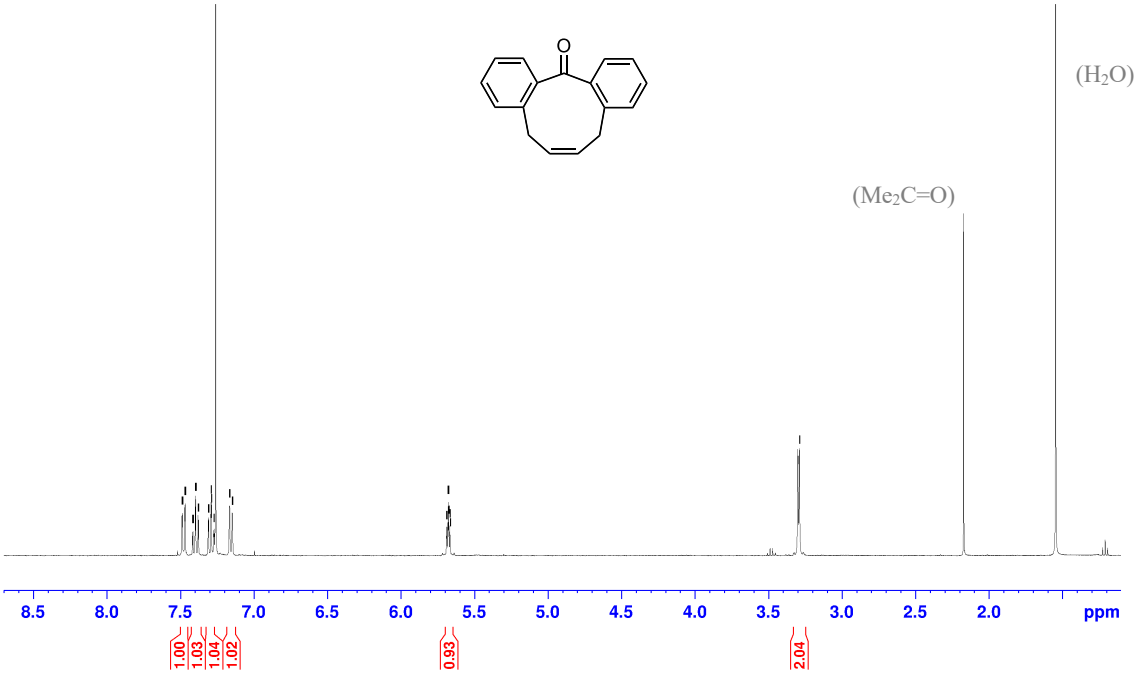
$^{13}C\{^{1}H\}$ NMR of **13** (101 MHz, $CDCl_3$)



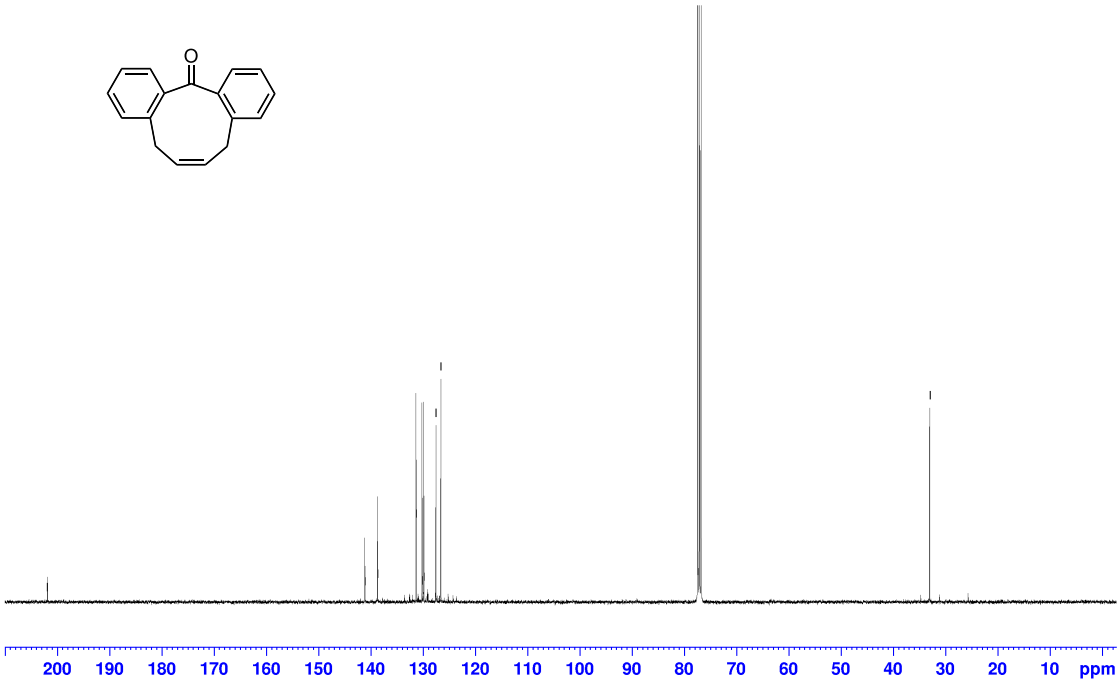
^{1}H NMR of **14** (400 MHz, $CDCl_3$)



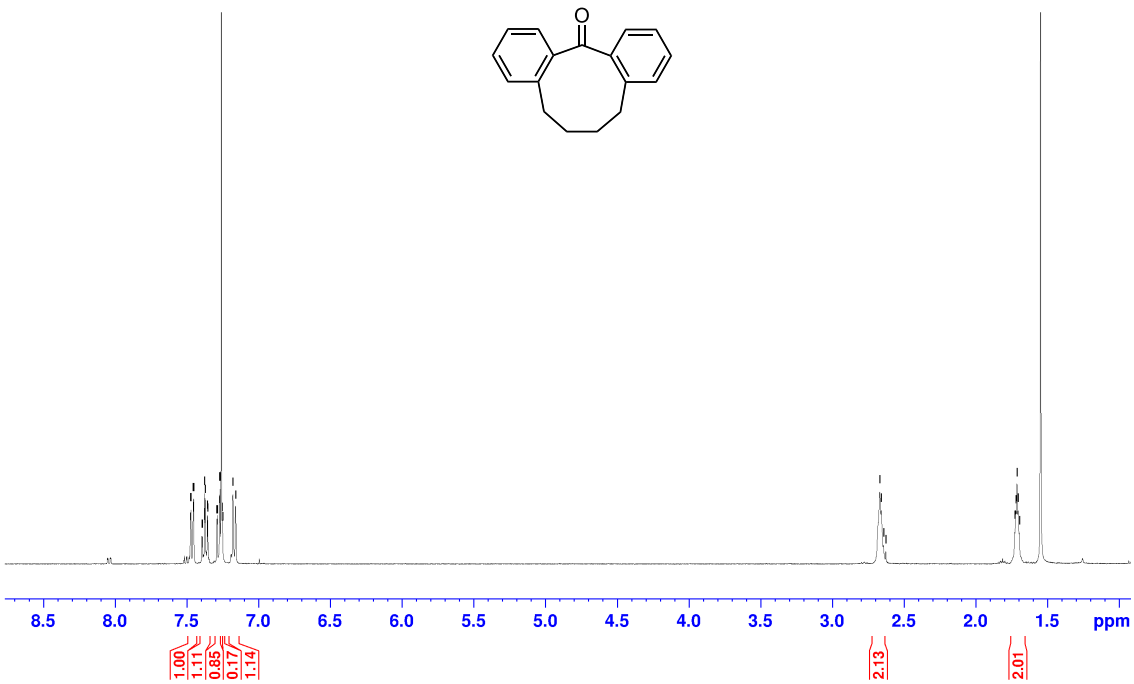
$^{13}C\{^{1}H\}$ NMR of **14** (101 MHz, $CDCl_3$)



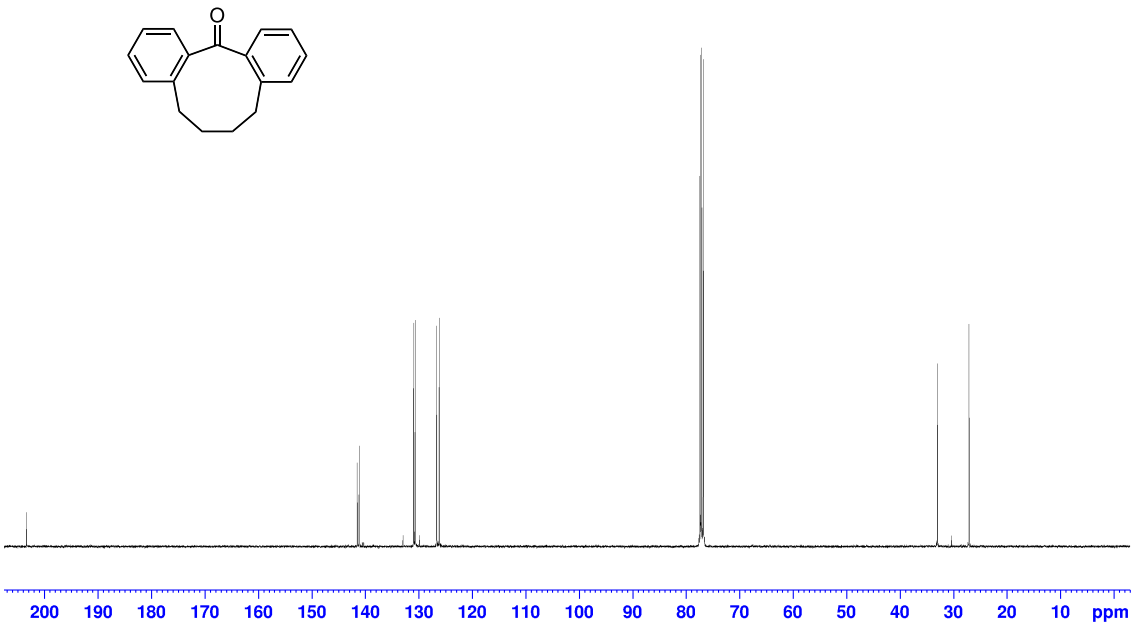
^{1}H NMR of **15** (400 MHz, $CDCl_3$)



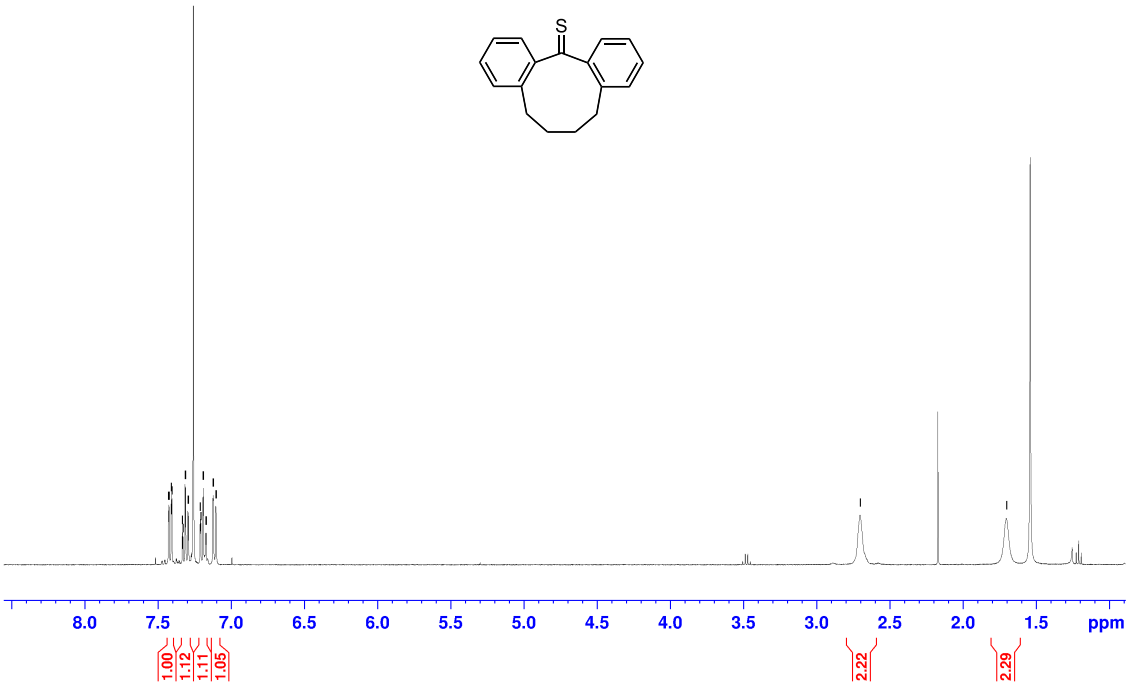
$^{13}C\{^{1}H\}$ NMR of **15** (101 MHz, $CDCl_3$)



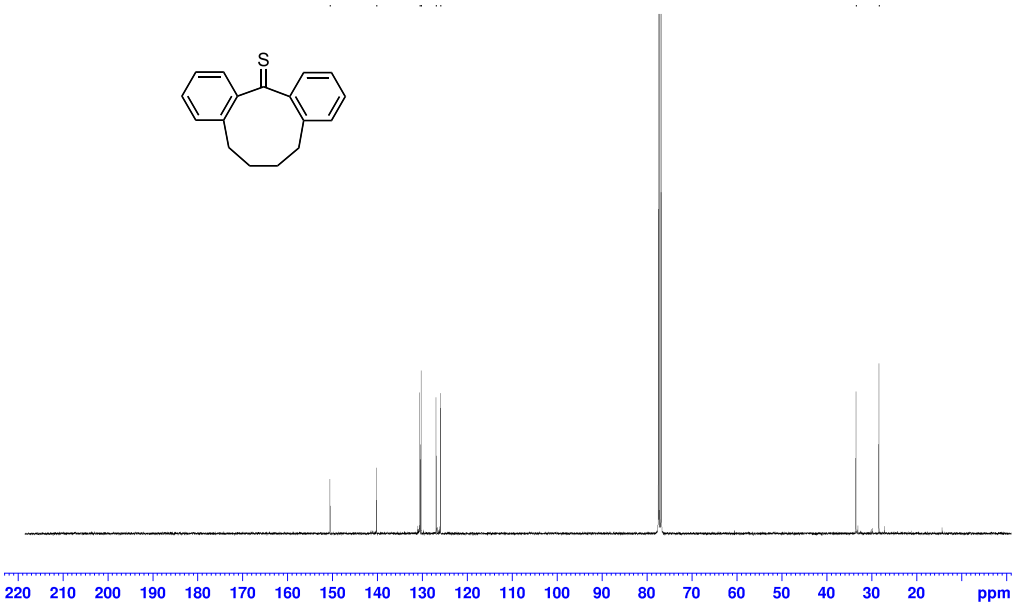
^{1}H NMR of **16** (400 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR of **16** (101 MHz, $CDCl_3$)



^{1}H NMR of **6** (400 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR of **16** (101 MHz, $CDCl_3$)