

•Supporting Information •

# NHC-Catalyzed Benzoin Condensation – Is It All Down to the Breslow Intermediate?

Julia Rehbein\*, Stephanie-M. Ruser, Jenny Phan

Universität Hamburg, Martin-Luther-King-Platz 6, 20255 Hamburg, Germany

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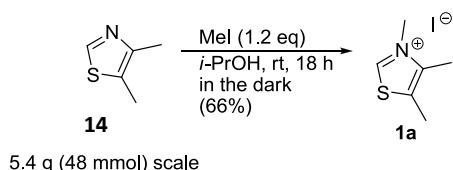
## A Experimental Section

### A.1. General Experimental Section

Chemicals were purchased from Acros and Aldrich and used as is, if not stated otherwise. All liquid aldehydes were freshly distilled and degassed before use. *i*-PrOH was dried over sodium and degassed, *i*-PrOD (= 2-propanol-d<sub>8</sub>, freshly opened ampoule) was dried statically over activated molecular sieves and then degassed before being used as a solvent in NMR kinetics. THF-d8 was distilled from Na/benzophenone. Et<sub>3</sub>N was dried over CaH and distilled prior to use. Other solvents were purchased as waterfree (Aldrich) or taken from the solvent purification system (MS Braun). Before application in the EPR-experiments all reaction mixtures were degassed by the freeze-pump-thaw method before initiation of the reaction by addition of the aldehyde. Two experimental samples were prepared in a glovebox (20.3 ppm O<sub>2</sub>) for matters of comparison. Synthesis of starting materials was conducted under inert atmosphere (N<sub>2</sub>) in dried glassware if no stated otherwise.

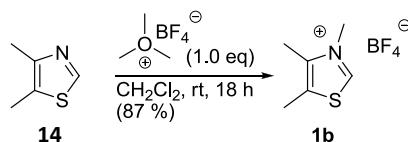
NMR spectra were run on a Fourier Bruker 300 MHz and Bruker Avance I 400 MHz spectrometer in *i*-propanol-d8, THF-d8 (both for kinetic measurements) and CDCl<sub>3</sub>, benzene-d6 and DMSO-d6 (for compound characterization). Chemical shifts are reported in ppm with the solvent resonance or TMS as internal standard (as specified): chloroform-d1: 7.26 (<sup>1</sup>H-NMR), 77.16 (13-C-NMR). Coupling constants *J* are given in Hertz (Hz). Multiplicities are classified as follows: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sept = septet and combinations thereof, or m = multiplet or br = broad signal. EPR spectra were recorded on a Bruker Elexsys E500 CW spectrometer.

### A.1.1 Synthesis of Pre-Catalysts

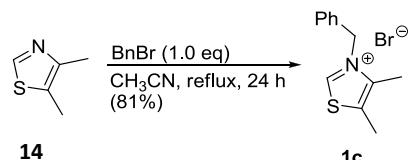


A solution of thiazole **14** (5.4 g, 48 mmol, 1 eq) in MeOH (30 mL, 0.6 mL/mmol **14**) was treated dropwise with MeI (3.5 mL, 57 mmol, 1.2 eq) and left stirring for 18 h at room temperature (flask

wrapped in tin foil). The solvent was evaporated under reduced pressure. The obtained yellow crystals were washed 4 × with 5 mL dry EtOAc (20 mL) and dried under vacuum to provide 5.3 g of pale peach crystals. Another 3 g were isolated after evaporation of the excess EtOAc and cooling to 0 °C, to afford a total yield of 8.3 g (66%). The analytical data of 3,4,5-trimethyl thiazolium iodide **1a** matches published data.<sup>1</sup> <sup>1</sup>**H-NMR** (300 MHz, CDCl<sub>3</sub>/DMSO 3/1). δ 2.13 (s, 3H), 2.19 (s, 3H), 3.86 (s, 3H), 10.03 (s, 1H). <sup>13</sup>**C-NMR** (125 MHz, CDCl<sub>3</sub>) δ 12.3, 12.9, 42.0, 132.7, 142.3, 156.4.



According to a procedure by Normand et al.<sup>2</sup> a solution of thiazole **14** (0.48 g, 4.3 mmol, 1.0 eq.) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL, 0.2 mL/ mmol **14**) was treated portionwise with trimethyloxonium tetrafluoroborate (0.60 g, 4.1 mmol, 1.0 eq.). The suspension was then stirred at room temperature for 18 h. Afterwards the solvent was evaporated under reduced pressure and the obtained residue was washed 3 x with 5 mL diethylether (15 mL). The with-yellow crystals were dried under vacuum. **1b** was obtained in 87% yield (0.76 g, 3.5 mmol). The analytical data of 3,4,5-trimethyl thiazolium tetrafluoroborate **1b** matches published data.<sup>2</sup> <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  2.46 (s, 3H), 2.52 (s, 3H), 4.13 (s, 3H), 9.69 (s, 1H). <sup>13</sup>C-NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  11.4, 12.5, 40.9, 99.9, 132.6, 154.9.



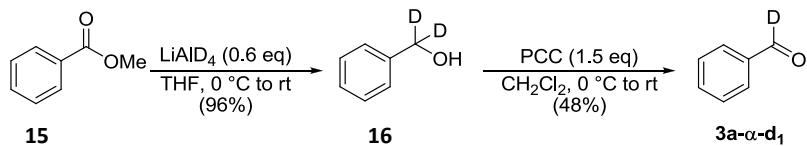
A solution of **14** (1.1 mL, 10 mmol, 1 eq) in CH<sub>3</sub>CN (5 mL, 0.5 mL/mmol **14**) was treated dropwise with benzyl bromide (1.19 mL, 10 mmol, 1.0 eq) at room temperature. After completed addition the reaction solution was heated to reflux for 4 h. After cooling to room temperature reaction mixture was kept at -30 °C (freezer) for 48 h. The obtained off-white crystals were recrystallized from EtOAc. The title compound **1c** was obtained in 81% yield (2.3 g, 8 mmol). <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>). δ 2.41 (s, 3H), 2.48 (s, 3H), 6.13 (s, 2H), 7.37 (m, 5H), 11.56 (s, 1H). <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) δ 12.2, 12.7, 57.3, 129.3, 129.4, 129.5, 131.8, 132.9, 142.1, 157.3.

### A.1.2 Synthesis of Substrates

### A.1.2.1 3- $\alpha$ -d<sub>1</sub>

<sup>1</sup> According to procedures by Y.-T. Chen and F. Jordan, *J. Org. Chem.*, 1991, **56**, 5029 and A. Kena Diba, C. Noll, M. Richter, M. T. Gieseler and M. Kalesse, *Angew. Chem.*, 2010, **122**, 8545; *Angew. Chem. Int. Ed.*, 2010, **49**, 8367.

<sup>2</sup> A. T. Normand, K. J. Hawkes, N. D. Clement, K. J. Cavell and B.F. Yates, *Organometallics*, 2007, **26**, 5352.

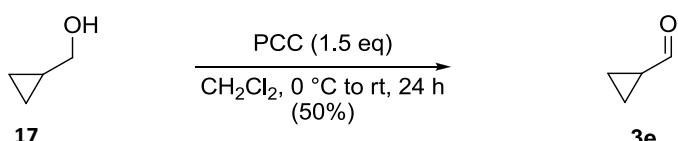


**3a- $\alpha$ -d<sub>1</sub>** was prepared in a two-step sequence of LiAlD<sub>4</sub> reduction of methyl benzoate (**21**) followed by a PCC oxidation of benzyl alcohol-1-d<sub>2</sub> (**15**), providing **3a- $\alpha$ -d<sub>1</sub>** in > 95 atom% D and 48% yield after twofold distillation (75 °C – 76 °C, 22 mbar).

LiAlD<sub>4</sub> (2 g, 48 mmol, 0.6 eq) was suspended in THF (90 mL, 2 mL/ mmol LiAlD<sub>4</sub>) and cooled to 0 °C in an ice bath. A solution of methyl benzoate **15** (19 mL, 80 mmol, 1 eq) in THF (10 mL, 0.15 mL/ mmol ester) was added dropwise via syringe. The reaction slurry was allowed to warm to room temperature over night and then quenched by the subsequent addition of 15 mL EtOAc and after 30 min of 3 x 5 mL of H<sub>2</sub>O over 60 min. The white suspension was filtered and the residue washed 6 x with 50 mL of CH<sub>2</sub>Cl<sub>2</sub>. The solution was dried over MgSO<sub>4</sub> and the solvent was removed under reduced pressure providing **16** in > 95 atom% D and 96% chemical yield (8.46 g). <sup>[3]</sup> **1H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 4.69 (0.0 H), 7.31 (m, 1 H), 7.37 (m, 4 H); <sup>13</sup>**C-NMR** (75 MHz, CDCl<sub>3</sub>): δ 64.93, 127.0, 127.7, 128.6, 140.7.

To a bright orange suspension of PCC (3 g, 12.1 mmol (98%), 1.5 eq) in CH<sub>2</sub>Cl<sub>2</sub> (15 mL, 1.2 mL/ mmol **16**) a solution of **16** (0.9 g, 8.1 mmol, 1 eq) in CH<sub>2</sub>Cl<sub>2</sub> (0.5 mL CH<sub>2</sub>Cl<sub>2</sub>/mmol **22**) was added via syringe. The reaction mixture turned dark brown immediately. The reaction was stopped after 5 h by filtration of the slurry through a pad of silica (CH<sub>2</sub>Cl<sub>2</sub> as eluent). The solvent was removed under reduced pressure and the crude product **3a- $\alpha$ -d1** distilled twice (75–76 °C, 22 mbar; 48% yield). Spectroscopic data as reported in literature. <sup>[4]</sup> **1H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 7.57 (m, 2 H), 7.66 (m, 1 H), 7.93 (m, 2 H). <sup>13</sup>**C-NMR** (75.5 MHz, CDCl<sub>3</sub>) δ 126.7, 128.9, 129.7, 136.1, 192.2 (COD).

#### A.1.2.2 **3e**



4.9 mL (58 mmol) scale

Pyridinium chlorochromate (PCC) (18.8 g, 87 mmol 1.5 eq) was suspended in CH<sub>2</sub>Cl<sub>2</sub> (120 mL, 1.4 mL/mmol PCC) and cooled to 0 °C. A solution of cyclopropyl methanol **17** (4.9 mL, 58 mmol, 1 eq) in CH<sub>2</sub>Cl<sub>2</sub> (15 mL CH<sub>2</sub>Cl<sub>2</sub>, 0.3 mL/mmol **17**) was added via syringe at 0 °C. The ice bath was removed after 30 min and the reaction mixture was allowed to warm to room temperature over the next 16 h. The brown slurry was filtered through a plug of silica (solvent CH<sub>2</sub>Cl<sub>2</sub>) and the aldehyde was purified by distillation (fraction boiling a 90 °C was collected). The product **3e** was obtained as a colorless liquid in 57 % yield (2.4 g, 34 mmol) with spectroscopic data corresponding to reported data. <sup>[5]</sup>

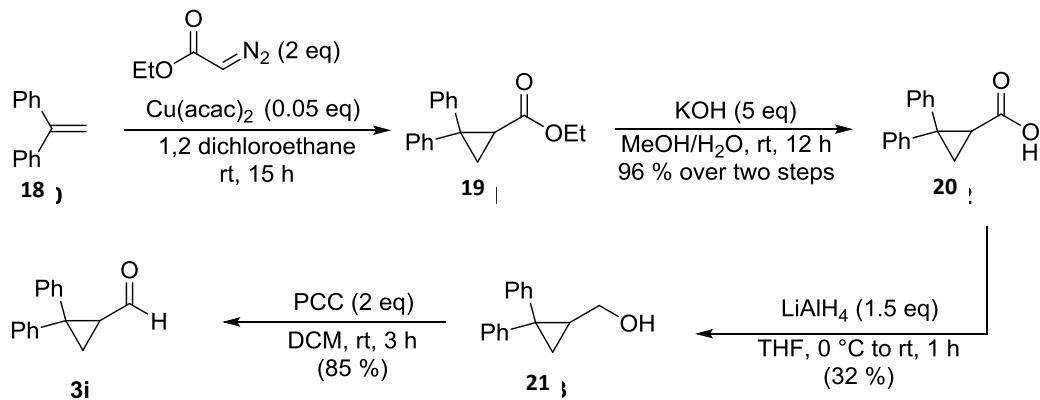
<sup>3</sup> S. R. Golisz, J. A. Labinger and J. E. Bercaw, *Organometallics*, 2010, **29**, 5026.

<sup>4</sup> A. Griesbeck, S. Bondock and P. Cygon, *J. Am. Chem. Soc.*, 2003, **125**, 901.

<sup>5</sup> NMR data from commercially available cyclopropane carboxaldehyde (CAS 1489-69-6, Aldrich). The NMR data provided by X. Wang et al. (X. Wang , R. Liu, Y. Jin, X. Liang, *Eur. J. Org. Chem.* 2008, **14**, 2679) reports six protons too many 0.88-0.93 (m, 6H) , but otherwise matches our data.

**<sup>1</sup>H-NMR** ( $\text{CDCl}_3$ , 300 MHz, 25 °C):  $\delta$  [ppm] = 8.90 (d,  $^3J$  = 5.8 Hz, 1 H), 1.89–1.79 (m, 1 H), 1.09–1.06 (m, 4 H). **<sup>13</sup>C-NMR** (125 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  [ppm] = 201.5, 22.7, 7.3.

### A.1.2.3 3i



A mixture of diphenylethylene **18** (3.0 g, 16.6 mmol) and copper acetoacetate (0.20 g, 0.76 mmol) in dry 1,2-dichloroethane (20 ml/ 1.2 mL/mmol **18**) was stirred at room temperature under nitrogen atmosphere. A yellow solution of ethyl diazoacetate (2.84 g, 24.9 mmol) in dry 1,2-dichloroethane (20 ml, 0.8 mL/mmol diazoacetate) was added dropwise with a syringe pump over 15 h (0.02 mL/min) at room temperature. After completing the addition, the reaction was stirred for another 12 h at room temperature. Subsequently the solvent was evaporated under reduced pressure and the crude product **25** was used directly in the next step.

2,2-diphenylcyclopropanecarboxylic acid ethyl ester **19** (5.5 g, 21 mmol) was dissolved in MeOH (200 mL, 10 mL/ mmol **19**) and treated with 50 mL KOH (aq) (5.5 g, 98 mmol). The reaction mixture was stirred at room temperature for 19 h. Work-up was accomplished by addition of conc. HCl (8 mL) and water (100 mL) until a pH of 4 of the reaction solution was reached and subsequent extraction with a total of 150 mL dichloromethane (3 x 50 mL). The combined organic phases were washed twice with water (200 mL in total) and dried over  $\text{MgSO}_4$ . Evaporation of the solvent afforded the free acid **20** as a yellow solid. **Yield:** 3.8 g (16 mmol), 96% over two steps from **18**; Analytic data as reported.<sup>[6]</sup> **<sup>1</sup>H NMR** (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.67 (dd,  $J$  = 8.1, 4.8 Hz, 1H), 2.12 (dd,  $J$  = 5.9, 4.9 Hz, 1H), 2.51 (dd,  $J$  = 8.0, 5.9 Hz, 1H), 7.13–7.38 (m, 10H), 10.9 (bs, 1H, -OH); **<sup>13</sup>C NMR** (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  20.9, 28.6, 41.2, 126.7, 127.1, 127.2, 127.5, 128.5, 128.6, 129.7, 129.8, 139.9, 144.7, 176.2 ppm.

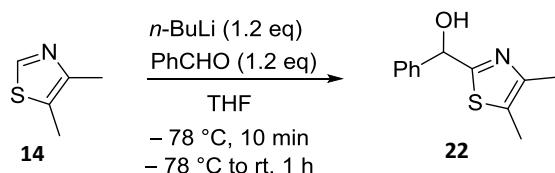
$\text{LiAlH}_4$  (0.11 g, 3.0 mmol, 1.4 eq) was suspended in THF (20 mL, 7 mL/ mmol  $\text{LiAlH}_4$ ) and cooled to 0 °C in an ice bath. A solution of **20** (0.50 g, 2.1 mmol, 1.0 eq) in THF (10 mL, 5 mL/ mmol **20**) was added dropwise at 0 °C. After the hydrogen evolution has ceased, the reaction was brought to room temperature by removing the ice bath and stirred for another 2 h. The gray-greenish slurry was treated with 50 mL of EtOAc and stirred for another 15 min. After addition of water (10 mL) the phases were separated and the aqueous phase was extracted 5 x with  $\text{Et}_2\text{O}$  (5 x 50 mL). The combined organic phases were washed 3 x with water (3 x 100 mL) and then dried over  $\text{MgSO}_4$ . Evaporation of the solvent under reduced pressure provided **21** as a yellow oil in 32 % yield (0.15 g,

<sup>6</sup> M. Schmittel, A. A. Mahajan, G. Bucher, J. W. Bats, *J. Org. Chem.*, 2007, **72**, 2166.

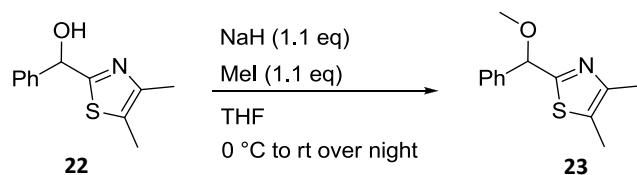
0.68 mmol,  $R_f$  = 0.04 (hexanes/Et<sub>2</sub>O = 9:1). Spectroscopic data as reported.<sup>[6]</sup> **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  [ppm] = 1.36–1.20 (m, 1 H), 1.41 (m, 1 H), 2.10–1.97 (m, 1 H), 3.39 (dd,  $J$  = 11.6, 7.9 Hz, 1 H), 3.52 (dd,  $J$  = 11.6, 6.3 Hz, 1 H), 7.46–7.13 (m, 10 H). **<sup>13</sup>C-NMR** (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  [ppm] = 18.0, 27.9, 35.8, 64.0, 126.1, 126.9, 128.0, 128.4, 128.7, 130.2.

**21** (0.15 g, 0.68 mmol, 1.0 eq) was dissolved in CH<sub>2</sub>Cl<sub>2</sub> (15 mL, 2 mL/mmol **27**). PCC (0.31 g, 1.5 mmol, 2.2 eq) was added and the reaction mixture was stirred for 3 h at room temperature. The brown suspension was filtrated through Celite and the residue was washed with CH<sub>2</sub>Cl<sub>2</sub> (200 mL). The brown solution was concentrated under reduced pressure and the crude product was purified by column chromatography (hexanes /Et<sub>2</sub>O 9:1;  $R_f$ -value: 0.2 in hexanes/ Et<sub>2</sub>O 9:1) providing **3i** in 62% yield (0.094 g (0.42 mmol, 62 %) as a colourless solid. Analytical data of **3i** as reported in literature.<sup>[6]</sup> **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  [ppm] 1.89 (dd,  $J$  = 8.4, 5.2 Hz, 1 H), 2.26 (t,  $J$  = 5.3 Hz, 1 H), 2.55 (ddd,  $J$  = 8.4, 6.8 Hz, 5.4 Hz, 1 H), 7.44–7.15 (m, 10 H), 8.68 (d,  $J$  = 6.8 Hz, 1 H). **<sup>13</sup>C-NMR** (100 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  [ppm] 20.4, 36.9, 41.0, 127.0, 127.5, 127.6, 128.8, 129.0, 130.2, 139.5, 144.0, 200.7. **MS (ESI)**:  $m/z$  (%) = 223.1 [M+H]<sup>+</sup>.

#### A.1.2.4 *O*-methylated Breslow-Intermediate *OMe*-**7b-a**

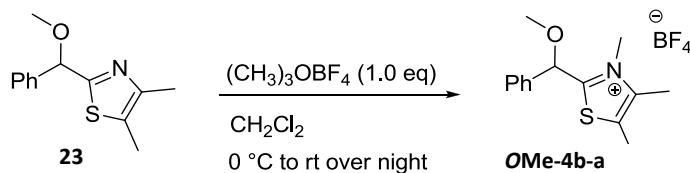


According to a procedure of Capriati et al.<sup>7</sup> Thiazole **14** (1.00 g, 0.94 mL, 8.84 mmol, 1.0 eq) was dissolved in dry THF (90 mL, 10 mL/mmol thiazole) and cooled to –78 °C. To this solution *n*-BuLi (0.68 g, 10.60 mmol, 1.2 eq) was added dropwise at –78 °C (the solution turned pale yellow). Then PhCHO, **3a**, (1.13 g, 10.6 mmol, 1.2 eq) in dry THF (5 mL, 0.5 mL/mmol **3a**) was added at –78 °C. After the complete addition of **3a** the reaction solution was stirred at –78 °C for 10 min. Afterwards the cooling bath was removed and the reaction solution was allowed to warm to rt for an hour. Then the solution was quenched with saturated aqueous NH<sub>4</sub>-solution. The phases were separated and the aqueous phase was extracted three times with 15 mL Et<sub>2</sub>O (45 mL). Subsequently the combined organic phases were dried with MgSO<sub>4</sub>, filtered and the solvent was removed under reduced pressure. The crude product was purified by recrystallization from PE/Et<sub>2</sub>O. Compound **22** was obtained as off-white crystals in a yield of 43% (0.84 g, 3.83 mmol). Spectra match published data.<sup>7</sup> **<sup>1</sup>H-NMR**: (CDCl<sub>3</sub>, 300 MHz)  $\delta$ [ppm]: 7.49–7.45 (m, 2H), 7.40–7.31 (m, 3H), 5.94 (s, 1H), 2.29 (s, 6H). **<sup>13</sup>C-NMR**: (CDCl<sub>3</sub>, 75 MHz)  $\delta$ [ppm]: 169.2, 147.5, 141.8, 128.8, 128.5, 127.4, 126.7, 73.7, 14.7, 11.5.  **$R_f$** : (Et<sub>2</sub>O/PE: 1/1) = 0.7.



<sup>7</sup> V. Capriati, F. Saverio, G. Ingrosso, C. Granito, L. Troisi, *Eur. J. Org. Chem.*, 2002, 478.

Carbinol **22** (1.00 g, 4.56 mmol, 1.0 eq) was dissolved in dry THF (10 mL, 2 mL/ mmol carbinol) and this solution was then added dropwise via syringe to a suspension of NaH (60% in mineral oil; 0.12 g, 5.02 mmol, 1.1 eq) in dry THF (25 mL, 5 mL/ mmol NaH) at 0 °C. The reaction mixture was stirred for 10 min at 0 °C until H<sub>2</sub>-evolution had ceased. Afterwards MeI (0.71 g, 5.02 mmol, 1.1 eq) was added via syringe at 0 °C. The reaction solution was allowed to warm up to rt overnight. Subsequently the reaction was quenched with saturated aqueous NH<sub>4</sub>Cl-solution and the aqueous phase was extracted three times with 15 mL CH<sub>2</sub>Cl<sub>2</sub> (45 mL). The combined organic phases were dried with MgSO<sub>4</sub>, filtered and the solvent was evaporated under reduced pressure. The clean crude product (orange oil) was used in the next step without further purification. Compound **23** was obtained in quantitative yield.  
**<sup>1</sup>H-NMR:** (CDCl<sub>3</sub>, 300 MHz) δ[ppm]: 7.48–7.44 (m, 2H), 7.38–7.28 (m, 3H), 5.48 (s, 1H), 3.45 (s, 3H), 2.29 (d, *J* = 1.9 Hz, 6H). **<sup>13</sup>C-NMR:** (CDCl<sub>3</sub>, 75 MHz) δ[ppm]: 11.3, 14.7, 57.4, 83.1, 126.7, 127.1, 128.2, 128.6, 139.9, 147.7, 167.4. **R<sub>f</sub>:** (Et<sub>2</sub>O/PE: 1/1) = 0.75.



According to a procedure of Barletta et al.<sup>8</sup> A solution of compound **23** (1.06 g, 4.56 mmol, 1.0 eq) in CH<sub>2</sub>Cl<sub>2</sub> (45 mL, 10 mL, mmol **23**) was treated with Meerwein salt (0.64 g, 4.56 mmol, 1.0 eq) at 0 °C. After the addition of the Meerwein salt the reaction was allowed to warm up to rt overnight in the thawing ice bath. The solvent was evaporated under reduced pressure and the resulting amorphous residue was washed three times with 10 mL Et<sub>2</sub>O (30 mL). Compound **OMe-4b-a** was obtained in quantitative yield. Spectroscopic data matches reported ones. **<sup>1</sup>H-NMR:** (CDCl<sub>3</sub>, 300 MHz) δ[ppm]: 7.45 (s, 5H), 5.91 (s, 1H), 3.84 (s, 3H), 3.47 (s, 3H), 2.45 (s, 3H), 2.39 (s, 3H). **<sup>13</sup>C-NMR:** (CDCl<sub>3</sub>, 75 MHz) δ[ppm]: 172.4, 144.1, 134.2, 130.8, 130.5, 129.7, 128.5, 127.3, 78.8, 57.8, 38.4, 12.3, 12.1.

The transformation of **OMe-4b-a** into **OMe-5b-a** was conducted according to a procedure of Mayr and coworkers.<sup>9</sup> Therefore, a solution of **OMe-4b-a** (349 mg, 0.5 mmol, 1 eq) in THF (distilled from sodium and degassed by several cycle of freeze-pump-thaw; 2.5 mL, 5 mL/ mmol **OMe-4b-a**) was cooled to –30 °C and added dropwise to a suspension of NaH (60% in mineral oil; 15 mg, 0.5 mmol, 1 eq) at –30 °C. The reaction mixture was kept at -20 °C over 16 h in the dark (reaction vessel wrapped up in tin foil). For analysis an aliquot was taken, transferred into a Schlenk tube under N<sub>2</sub>-atmosphere. Subsequently the solvent was evaporated under reduced pressure. The orange residue was taken up in benzene-d6 and analyzed by <sup>1</sup>H spectroscopy under inert atmosphere. The recorded data matches published spectra and indicates complete conversion to two double bond isomers (major and minor). **<sup>1</sup>H-NMR:** (C<sub>6</sub>D<sub>6</sub>, 300 MHz) δ[ppm]: 1.32 (s, 3H<sup>major</sup> + 3H<sup>minor</sup>), 1.58 (s, 3H<sup>minor</sup>), 1.67 (s, 3H<sup>major</sup>), 2.43 (s, 3 H<sup>major</sup>), 3.00 (s, 3 H<sup>minor</sup>), 3.35 (s, 3 H<sup>minor</sup>), 3.50 (s, 3 H<sup>major</sup>), 6.96 – 7.03 (m, 1

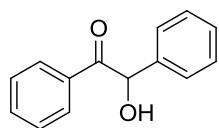
<sup>8</sup> G. Barletta, A. C. Chung, C. B. Rios, F. Jordan, and M. Schlege, *J. Am. Chem. Soc.*, 1990, **112**, 8144.

<sup>9</sup> B. Maji and H. Mayr, *Angew. Chem. Int. Ed.*, 2012, **51**, 10408.

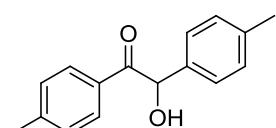
$\text{H}^{\text{major}} + \text{H}^{\text{minor}}$ ), 7.19–7.23 (m, 2H $^{\text{major}}$ ), 7.28 – 7.35 (m, 2H $^{\text{minor}}$ ), 7.40 – 7.45 (m, 2 H $^{\text{major}}$ ), 7.55 – 7.60 (m, 2 H $^{\text{minor}}$ ), 7.80 – 7.84 (m, 2 H $^{\text{minor}}$ ).

### A.1.3 Analytical data of isolated benzoin products

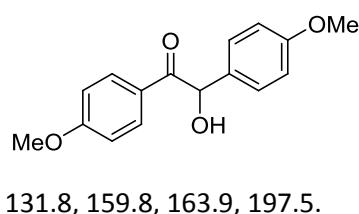
Benzoin products **9** were isolated from NHC-catalysed benzoin reactions with 0.4 M solutions of **3a,d,e,f,g** (2 mmol), 0.1 eq **1a** and 0.1 eq KOH in *i*-PrOH (5 mL). Purification of **9a,d,e,f,g** was achieved by recrystallization of the crude products from petrolether/ CH<sub>2</sub>Cl<sub>2</sub> 3/1 and by column chromatography in case of **9h** and **9i**.



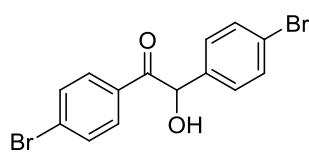
For **9a** spectroscopic data resembles reported data<sup>[10]</sup>: **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 4.59 (d, *J* = 6.2 Hz, 1H; OH), 5.97 (d, *J* = 6.2 Hz, 1H), 7.26 – 7.37 (m, 5H), 7.41 (m, 2H), 7.52 (m, 1H), 7.93 (m, 2H); **<sup>13</sup>C-NMR** (75 MHz, CDCl<sub>3</sub>): 76.2, 127.7, 128.6, 128.7, 129.1, 133.4, 133.9, 138.9, 198.9.



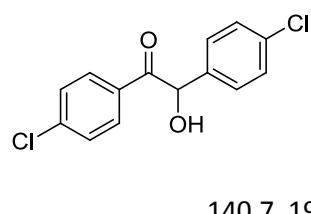
For **9d** spectroscopic data resembles reported data in literature<sup>[10]</sup>: **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 2.28 (s, 3H), 2.35 (s, 3H), 5.89 (s, 1H), 7.10–7.22 (m, 6H), 7.81 (d, *J* = 8.3 Hz, 2H); **<sup>13</sup>C-NMR** (75 MHz, CDCl<sub>3</sub>): δ 21.1, 21.7, 75.8, 127.6, 129.4, 129.8, 136.3, 138.3, 144.9, 198.5.



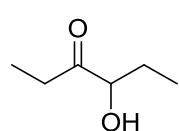
For **9e** spectroscopic data resembles reported data in literature<sup>[11]</sup>: **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 3.75 (s, 3H), 3.81 (s, 3H), 5.84 (s, 1H), 6.84 (dd, *J* = 8.9, 4.8 Hz, 4H), 7.23 (m, 1H), 7.25 (m, presumably 1H, overlay with CHCl<sub>3</sub>) 7.83–7.95 (m, 2H); **<sup>13</sup>C-NMR** (75 MHz, CDCl<sub>3</sub>): δ 55.2, 55.5, 75.2, 113.9, 114.5, 126.3, 129.0, 131.6, 131.8, 159.8, 163.9, 197.5.



For **9f** spectroscopic data resembles reported data<sup>[10]</sup>: **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 5.86 (s, 1H), 7.20–7.15 (m, 2H), 7.56–7.42 (m, 4H), 7.76–7.71 (m, 2H); **<sup>13</sup>C-NMR** (75 MHz, CDCl<sub>3</sub>): 75.3, 122.9, 129.3, 129.6, 130.4, 131.9, 132.2, 132.4, 137.6, 197.5.



For **9g** spectroscopic data resembles reported data<sup>[10]</sup>: **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 4.48 (d, *J* = 5.9 Hz, 1H; OH), 5.88 (d, *J* = 5.9 Hz, 1H), 7.28 m (4 H) overlaying with CHCl<sub>3</sub> signal, 7.39 (m, 2H), 7.83 (m, 2H). **<sup>13</sup>C-NMR** (75 MHz, CDCl<sub>3</sub>): 75.5, 129.1, 129.2, 129.5, 130.4, 131.5, 134.7, 137.1, 140.7, 197.4.

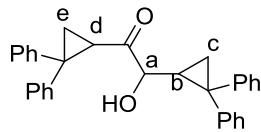


**9h** resembles reported data<sup>[12]</sup>: **<sup>1</sup>H-NMR** (300 MHz, CDCl<sub>3</sub>): δ 0.93 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>), 1.12 (t, *J* = 6.7 Hz, 3H, CH<sub>3</sub>), 1.54–1.73 (m, 2H), 2.37–2.50 (m, 2H), 3.50 (d, *J* = 4.8 Hz, 1H, OH), 4.14–4.20 (m, 1H).

<sup>10</sup> Y. Shimakawa, T. Morikawa, S. Sakaguchi *Tetrahedron Letters* **2010**, 51, 1786.

<sup>11</sup> A. B. Powell, Y. Suzuki, M. Ueda, C. W. Bielawski, A. H. Cowley *J. Am. Chem. Soc.* **2011**, 133, 5218.

<sup>12</sup> P. Boutoute, G. Mousset, H. Veschambre, *New J. Chem.*, 1998, 247.



**9i** was obtained as a mixture of three diastereomers, ratio not assigned. Protons were assigned based on COSY and HSQC spectra. <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>): δ 1.2–1.35 (m, 1H<sub>c</sub>), 1.42–1.70 (m, 3H; H<sub>b</sub>, H<sub>e</sub>, OH), 1.72–2.0 (m, 1H<sub>e</sub>), 2.3–3.02 (m, 1H<sub>d</sub>), 3.48–3.75 (m, 1H<sub>a</sub>), 6.95–7.54 (m, 20 H<sub>arom</sub>); <sup>13</sup>C-NMR (75 MHz, CDCl<sub>3</sub>): δ 15.6, 17.2, 19.2, 21.6/21.1; 28.3/28.9; 31.7/31.8, 35.0, 43.8, 75.0/77.8, 99.9, 107.2, 126.2, 127.1, 127.3/127.4, 127.6, 127.8, 128.4, 128.8/128.9, 129.6/129.7, 137.58/137.8, 139.6, 143.5, 144.5/144.7, 205.6/205.3/206.6. IR (neat) ν 3465, 1695 cm<sup>-1</sup>. HRMS (ESI) calcd for C<sub>32</sub>H<sub>28</sub>O<sub>2</sub> 444.2089, found 911.4071 which corresponds to the mass of the dimer with one sodium ion.

## A.2. EPR Experiments

### A.2.1 General Information

EPR experiments were conducted in septum sealed quartz tubes under inert atmosphere. Therefore oven-dried EPR tubes (100 °C, 24 h) were in turn evacuated (fine vacuum) and refilled with N<sub>2</sub> several times before being filled with 0.3 mL reaction solution. The reaction solutions were made up of precatalysts, KOH and solvent in a Schlenk tube. This solution and the freshly distilled aldehydes were degassed separately by at least 3 cycles of freeze-pump-thaw method. After rewarming of the samples to room temperature the reaction was started by the addition of a specified amount of aldehyde. Exclusion of light was achieved by wrapping the reaction vessels in tin foil prior to aldehyde addition and in between EPR measurements. For comparison certain samples were made up in a glove box (<23 ppm O<sub>2</sub>).

The first EPR spectrum was obtained 10–15 min after addition (as specified) due to necessary adjustments of the EPR-spectrometer; subsequently the EPR-signal was followed over time in 30 min intervals for 3–4 h. To obtain reliable quantitative data, for every aldehyde tested the EPR signal was checked for saturation effects by simply increasing the microwave power until the signal intensity stopped scaling with the square root of the microwave power. All data was then recorded under non-saturation conditions.

**Data analysis:** EPR spectra were obtained as a first order derivative plot. Raw data was read into EPRtoolbox<sup>13</sup> or csw2epr<sup>14</sup> and converted to csv-files that in turn were fed into Origin<sup>®15</sup>. Determination of the maximum peak in the signals led to the intensity values that were used in the progression curves (A.2.3.1). Under non-saturation conditions the EPR signal intensity scales with the square root of the microwave power. For matters of comparability all EPR signals were referenced to a microwave power of 2.63 mW (see columns ‘Corrected EPR Signal’ in Tables 1–7). *i*-PrOD := 2-propanol-d8.

**Fitting of EPR-spectra to structures:** A conformational analysis of **7a-a** has been conducted as described in the Computational Section B. Of the identified two conformers of the zwitterionic structure **7a-a** and the cationic form **7a-a-H** after protonation of the oxygen atom the isotropic Fermi contact couplings have been calculated (prop = EPR) and the derived data has been used for starting the fitting process of the experimental spectrum together with coupling constants that could

<sup>13</sup> EPRtoolbox v13.7 as downloaded from <http://morganbye.net/eprtoolbox/> in April 2013

<sup>14</sup> Csv2epr written by Harold Toms & Ray Burton Smith as downloaded from <http://epr.sbccs.qmul.ac.uk/node/8> in December 2014.

<sup>15</sup> OriginPro 9.0.0G, 64-bit

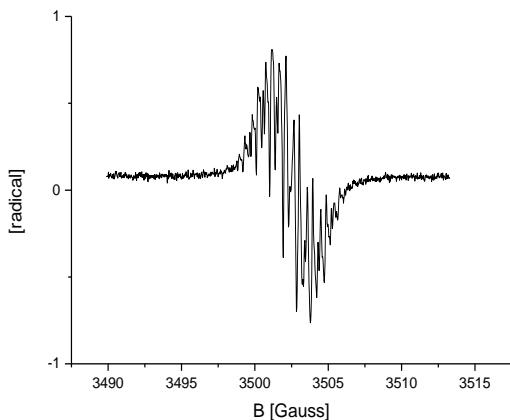
be directly read off the experimental spectra. The deviations of the coupling constants of the fitting process from the four calculated structures are summarized in Tables 1 and 4.

**Control samples:** Following combinations of reagents did not provide an EPR signal:

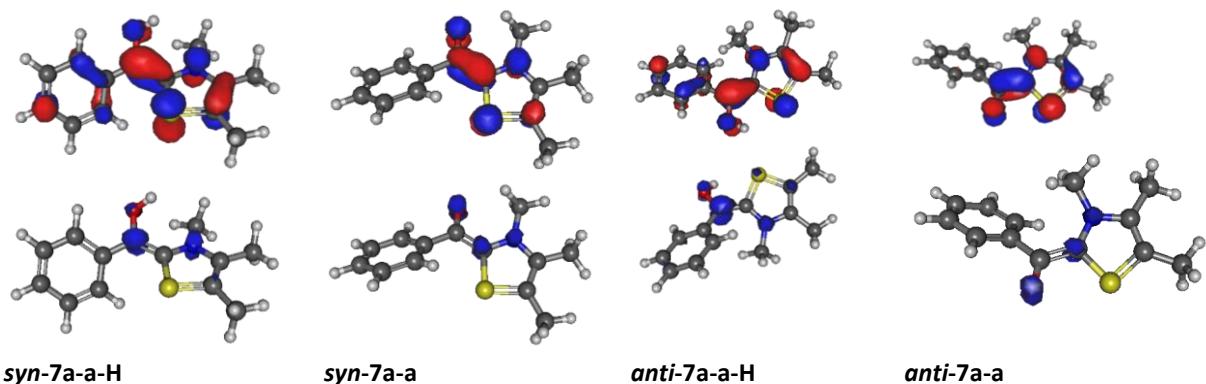
- **3a** and KOH in *i*-PrOH (Cannizarro reactions of electronricher aldehydes do need harsher conditions see citations under endnote [12] in the main text)
- **3a** and **1a** in *i*-PrOH
- **1a** and KOH in *i*-PrOH

**Trapping of 7:** Intermolecular trapping attempted with TEMPO (10eq) and DMPO (10 eq) was not successful, indicating a radical pair **[6·7]**. Trapping with O<sub>2</sub> did provide oxidations products as known from literature (see citations under endnote [8] in the main text). Also NO released from TritylSNO (10 fold excess) under typical reaction conditions (0.1 M in PhCHO, 1 eq **1a**, 1 eq KOH in *i*-PrOH) led to an immediate quench of the usual EPR signal as described in A.2.2, with the benzoin reaction being stopped also. The condition for a successful intermolecular trapping is a dissociation of the radical pair **[6·7]** to separated species. Presumably the dissociation rate is not high enough in the protic polar solvent and therefore the intramolecular reactions with molecules bigger than O<sub>2</sub> or NO cannot compete (for influence of O<sub>2</sub> on EPR spectra see Section A.2.2.5. Intramolecular trapping with the ultrafast radical clock **3i**, e.g. ring opening did not take place. This result does not prove that the radical is not formed in this position but rather provides evidence that indeed **7** is formed and not **7a-H**. This becomes apparent when one compares the spin densities there is much less spin densities of both structures. There is only very low spin density at the former carbonyl carbon atom in **7**.

An EPR-spectrum ((center field 3501,15G, μwave-power 10.50 mW, SweepTime= 41.94 s) of radical **6a** was obtained of a 0.4 M solution of **3a** in THF (5 mL) after the addition of Na (1 eq).



**Table 1** Detailed analysis of dependence of simulated Fermi-contact couplings on conformation and protonation (index H). For definition of *syn* and *anti* see section B.2. Rendered structures illustrating calculated SOMOs and spin densities (uB3LYP/6-31G\*).

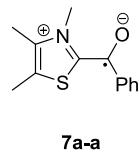


Fitted with $r^2=0.93$		<i>anti</i> -7a-a	<i>anti</i> -7a- a-H	<i>syn</i> -7a-a	<i>syn</i> -7a-a- H	Best fit	deviation to exp. fit in %
<b>4.918</b>	3-CH <sub>3</sub>	3.834	3.697	<b>4.950</b>	3.893	4.950	0.7
<b>0.353</b>	4-CH <sub>3</sub>	0.736	<b>0.309</b>	0.830	0.853	0.309	-12.5
<b>2.057</b>	5-CH <sub>3</sub>	<b>2.044</b>	3.893	2.530	3.288	2.044	-0.6
<b>2.317</b>	N	<b>3.000</b>	3.654	3.293	3.893	3.000	29.5
<b>0.450</b>	ortho-H (2x)	<b>0.407</b>	2.119	2.533	2.119	0.407	-9.6
<b>0.530</b>	para-H	<b>0.536</b>	2.552	0.474	2.552	0.536	1.1
<b>2.440</b>	S	2.196	3.288	<b>2.533</b>	3.578	2.533	3.8
<b>Population of conformers at 298 K based on <math>\Delta G</math> [%]</b>		<b>1</b>	<b>62</b>	<b>99</b>	<b>38</b>		

Based on the highest correlations the most likely structure are both zwitterionic forms of **7a** not the protonated ones.

## A.2.2 EPR-Spectra

### A.2.2.1 Spectra of 7a-a: Dilution Study, Solvent Isotope Effect



EPR spectra (Figure 1-5; Table 2) of radical **7a-a** were derived of the following reaction solutions: 3,4,5-trimethyl thiazolium iodide **1a** was suspended in *i*-PrOH or *i*-PrOD as specified in Table 1. After addition of KOH (equimolar amounts to **1a**) the reaction turned yellow after 5–10 min. Then the reaction mixture was degassed as described above and benzaldehyde **3a** was added via  $\mu$ L syringe under inert atmosphere.

The shape of the EPR-spectrum is independent concentration and ratio of **3a** to **1a**. The radical concentration increases with increasing catalyst loading (see main text also), in *i*-PrOD (Entry 1,3, Table 1), and decreases with overall lower concentrations (Entry 1, 5, 6 in Table 1). The inverse solvent isotope effect has been described for the benzoin condensation in MeOH and MeOD respectively by White and Leeper<sup>16</sup>. The fact that this is also observed for the radical formation

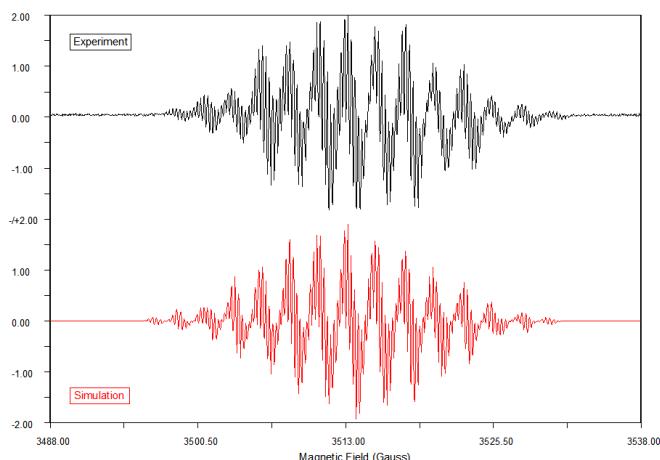
<sup>16</sup> White, M. J.; Leeper, F. J. *J. Org. Chem.* **2001**, *66*, 5124.

strengthens our conclusion, that the radical is involved in the catalytic cycle. On a molecular scale the inverse solvent isotope effect can be rationalized by the reversibility of the benzoin condensation and the tendency of deuterium to end up in the stronger bond. Formed benzoin will enrich in OD and the reverse reaction from benzoin to [6•7] will accumulate the radical pair [6•7] as the transfer of the deuterium atom back to the former carbonyl center is higher in energy than the similar hydrogen atom transfer.

**Table 2**

entry	<b>1a</b>	[PhCHO] M	solvent	[radical] max	EPR spectrum No
1	0.1 eq	0.4 M	<i>i</i> -PrOH	3.1	Figure 1
2	0.1 eq	0.4 M	<i>i</i> -PrOD	5.0	Figure 2
3	0.2 eq	0.2 M	<i>i</i> -PrOH	6.0	-
4	0.4 eq	0.1 M	<i>i</i> -PrOD	9.6	Figure 4
5	0.4 eq	0.1 M	<i>i</i> -PrOH	7.0	-
6	0.1 eq	0.1 M	<i>i</i> -PrOH	1.3	Figure 5
7	0.1 eq	0.04 M	<i>i</i> -PrOH	0.8	Figure 6
8	1 eq	0.1 M	<i>i</i> -PrOD	10.0	Figure 7

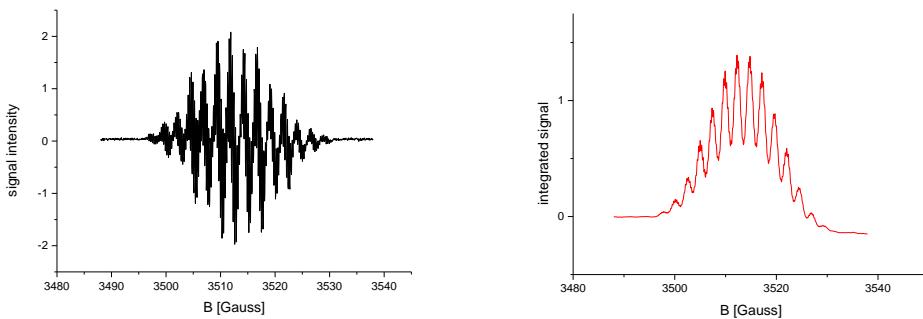
**Figure 1** Experimental and fitted EPR-spectrum ( $r^2 = 0.93$ ) of reaction solution of **3a** (0.4 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOH).



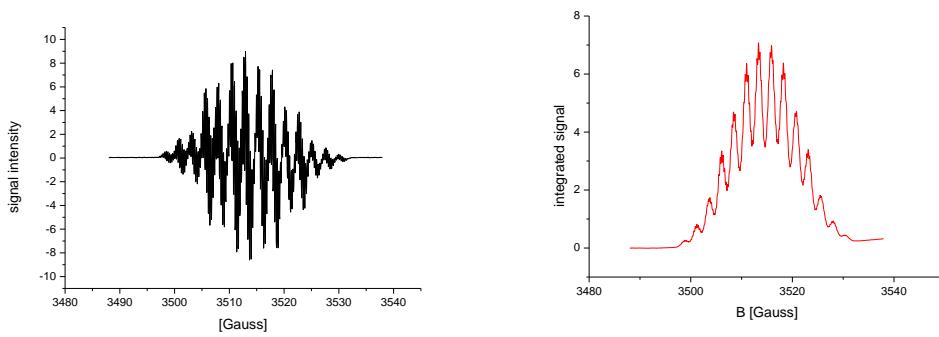
**Figure 2** Experimental EPR-spectrum and first integration of the EPR signal derived of reaction solution of **3a** (0.4 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOD; ;  $\mu$ -wave power 2.09 mW) after 23 min of PhCHO addition.



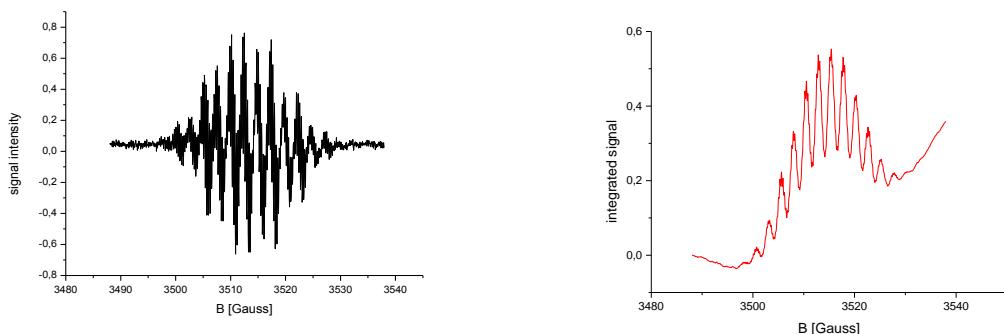
**Figure 3** Experimental EPR-spectrum and first integration of the EPR signal derived of reaction solution of **3a** (0.2 M, 0.2 eq **1a**, 0.2 eq KOH, *i*-PrOD;  $\mu$ -wave power 2.64 mW) after 7 min of PhCHO addition.



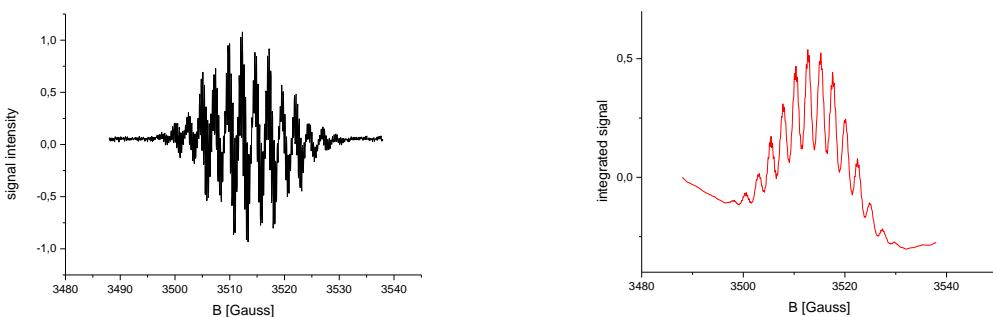
**Figure 4** Experimental EPR-spectrum and first integration of the EPR signal derived of reaction solution of **3a** (0.1 M, 0.4 eq **1a**, 0.4 eq KOH, *i*-PrOD;  $\mu$ -wave power 2.64 mW) after 5 min of PhCHO addition.



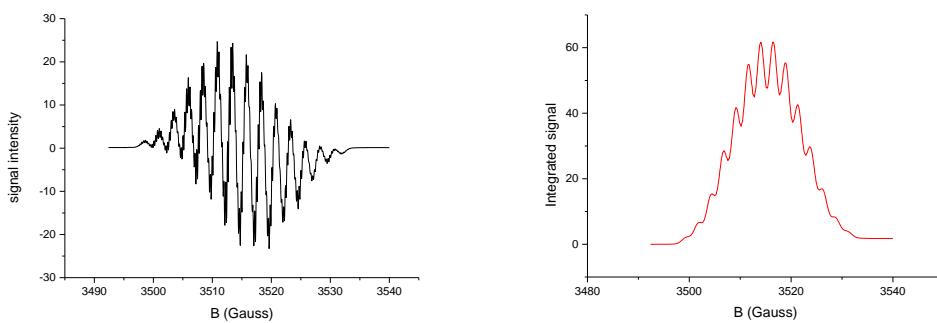
**Figure 5** Experimental EPR-spectrum and first integration of the EPR signal derived of reaction solution of **3a** (0.1 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOD;  $\mu$ -wave power 2.642 mW) after 10 min of PhCHO addition.



**Figure 6** Experimental EPR-spectrum and first integration of the EPR signal derived of reaction solution of **3a** (0.04 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOD;  $\mu$ -wave power 10 mW) after 10 min of PhCHO addition.

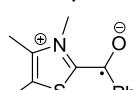


**Figure 7** Experimental EPR-spectrum and first integration of the EPR signal derived of reaction solution of **3a** (0.1 M, 1 eq **1a**, 1.0 eq KOH, *i*-PrOD;  $\mu$ -wave power 2.64 mW) after 9 min of PhCHO addition



#### A.2.2.2 Spectra of **7a-a** derived of **3a- $\alpha$ -d1**

EPR spectra (Figure 8, 9) of radical **7a-a** were also derived of the following reaction solutions: 3,4,5-trimethyl thiazolium iodide **1a** was suspended in *i*-PrOH or *i*-PrOD as specified in Table 3. After addition of KOH (equimolar amounts to **1a**) the reaction turned yellow within 5–10 min. Then the reaction mixture was degassed as described above and **3a- $\alpha$ -d<sub>1</sub>** was



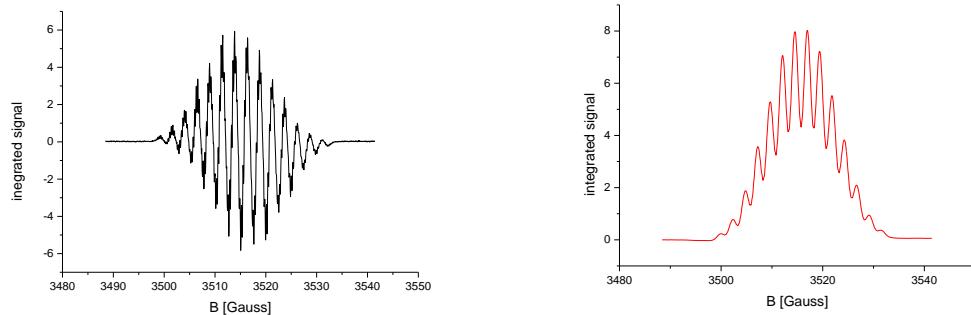
**7a-a**

added via  $\mu\text{L}$  syringe under inert atmosphere. The EPR-spectra are identical to the ones observed of reaction solutions of **3a** and **1a** (Figure 9).

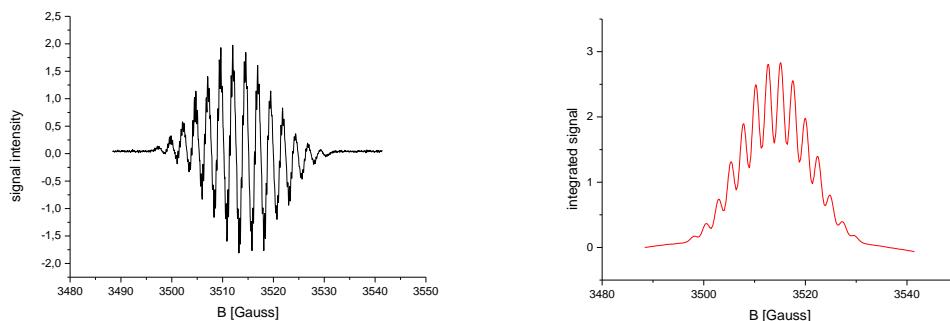
**Table 3**

entry	<b>1a</b> eq	[ <b>3a-<math>\alpha</math>-d<sub>1</sub></b> ] mol/L	solvent	EPR spectrum see
1	0.1	0.4	<i>i</i> -PrOD	See A.2.3
2	0.2	0.2	<i>i</i> -PrOD	Figure 8
3	0.2	0.2	<i>i</i> -PrOH	Figure 9
4	0.4	0.1	<i>i</i> -PrOD	See A.2.3
5	1	0.1	<i>i</i> -PrOD	See A.2.3

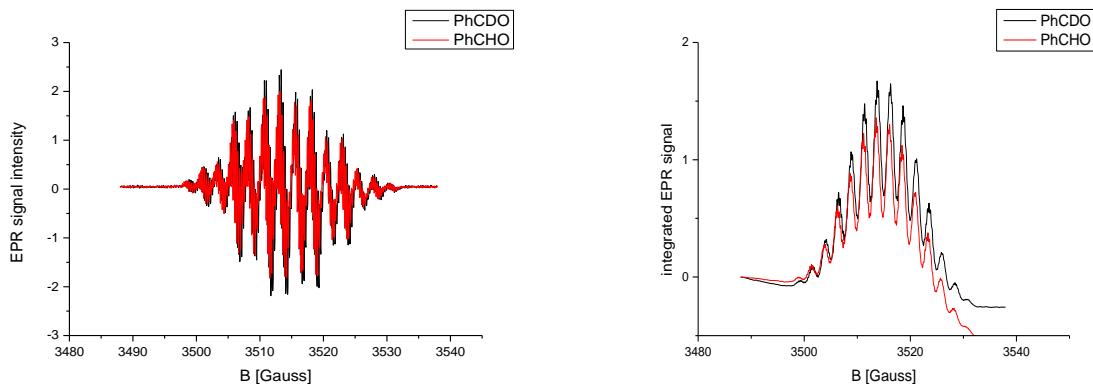
**Figure 8** Experimentally observed signal and first integration of the EPR signal derived of a reaction solution of **3a- $\alpha$ -d<sub>1</sub>** (0.2 M, 0.2 eq **1a**, 0.1 eq KOH, *i*-PrOD;  $\mu$ -wave power 5.2 mW).



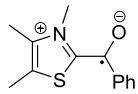
**Figure 9** Experimentally observed signal and first integration of the EPR signal derived of a reaction solution of **3a- $\alpha$ -d<sub>1</sub>** (0.2 M, 0.2 eq **1a**, 0.1 eq KOH, *i*-PrOH;  $\mu$ -wave power 5.2 mW).



**Figure 10** Overlayed spectra of experiments described in Table 1, Entry 3 (**2a** and **8a**) and Table 2, Entry 1 (**2a- $\alpha$ -d<sub>1</sub>** and **1a**).

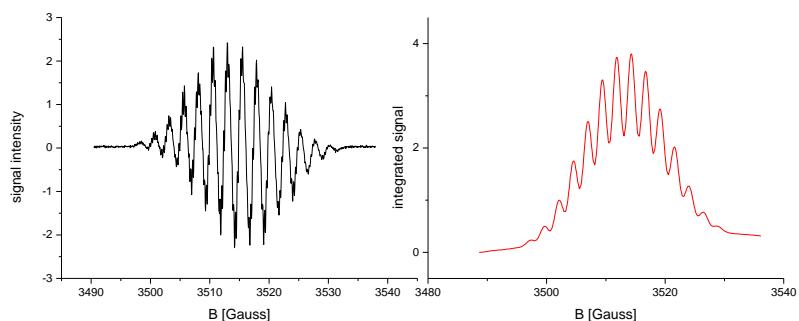


### A.2.2.3 Exclusion of a Counterion Effect (**7b-a**)

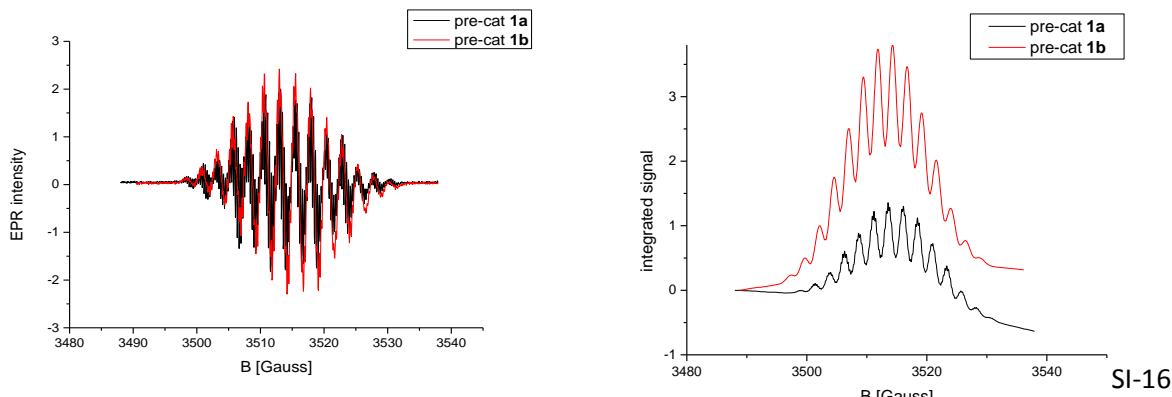


An identical EPR spectrum (Figure 11) of radical **7b-a** was derived of the following reaction solution: 3,4,5-trimethyl thiazolium tetrafluoroborate **8b** (25.8 mg, 0.12 mmol, 0.1 eq) and KOH (6.7 mg, 0.12 mmol, 0.1 eq) were suspended/dissolved in *i*-PrOH (3 mL). After degassing, **3a** (122  $\mu$ L, 1.2 mmol, 1.0 eq.) was added to the yellow reaction mixture. The identity of both spectra proves that radical formation is not due to redox processes of the iodide counterion.

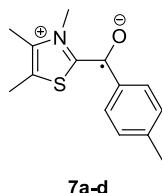
**Figure 11** **3a** (1.0 eq.), 3,4,5-trimethyl thiazolium tetrafluoroborate **1b** (0.1 eq) and KOH (0.1 eq) in *i*-PrOH (3 mL). After degassing, **3a** (122  $\mu$ L, 1.2 mmol, 1.0 eq.)



**Figure 12** Overlaid spectra of experiments described in Table 1, Entry 1 (**1a** and **3a**) and spectrum derived of **1b** and **3a**.

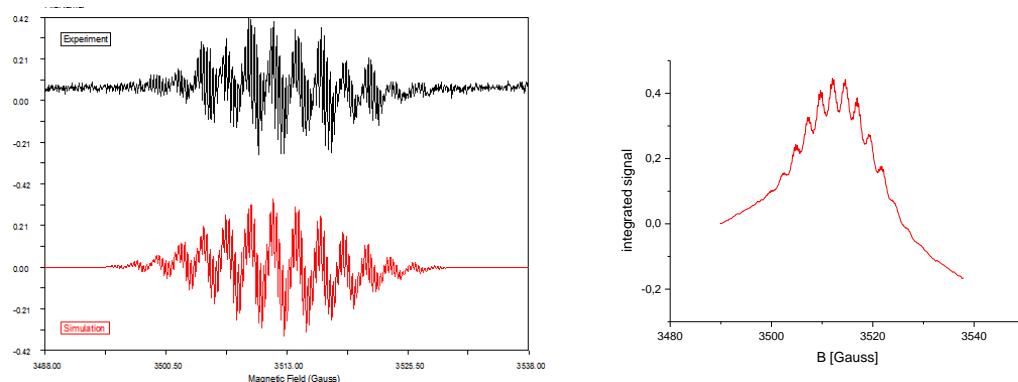


#### A.2.2.4 EPR spectra obtained from **1a**, KOH and Different Aromatic Aldehydes (**3d-g**)

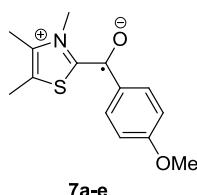


EPR spectra (Figure 12) of radical **7a-d** was derived of the following reaction solution: 3,4,5-trimethyl thiazolium iodide **1a** (5.61 mg, 0.02 mmol, 0.1 eq) and KOH (1 mg, 0.02 mmol, 0.1 eq) in *i*-PrOH (5 mL). Due to small amounts of **1a** and KOH a 10-fold higher concentrated solution was prepared and diluted accordingly. After degassing, **3d** (23.6 µL, 0.2 mmol, 1 eq) was added to the yellow reaction mixture by µL syringe.

**Figure 13** Experimental and fitted EPR-spectrum ( $r^2 = 0.90$ ) of reaction solution of **3d** (0.04 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOH).

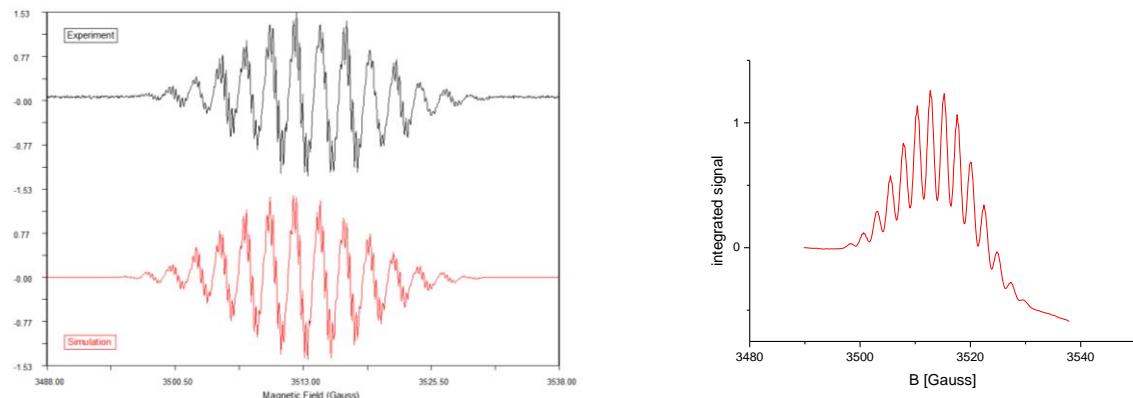


entry	experimental			predicted ( <b>7a-d</b> ) [Error! Bookmark not defined.]		
	hfcs [Gauss]	spin	number of equivalent nuclei	hfcs [Gauss]	spin	
1	4.894	0.5	3	3.8	N-CH <sub>3</sub>	0.5
2	0.297	0.5	3	0.79	4-CH <sub>3</sub>	0.5
3	1.973	0.5	3	2.11	3-CH <sub>3</sub>	0.5
4	2.132	0.5	1	3.02	N	0.5
5	2.593	1.5	1	2.19	S	1.5
6	0.652	0.5	2	0.42	2 H <sub>ar</sub>	0.5
7	-	0.5	-	0.27	2 H <sub>ar</sub>	0.5

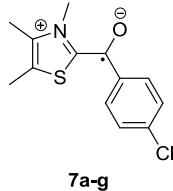


EPR spectra (Figure 13) of radical **7a-e** was derived of the following reaction solution: 3,4,5-trimethyl thiazolium iodide **1a** (5.61 mg, 0.02 mmol, 0.1 eq) and KOH (1 mg, 0.02 mmol, 0.1 eq) were in *i*-PrOH (5 mL). Due to small amounts of **1a** and KOH a 10-fold higher concentrated solution was prepared and an aliquot thereof diluted accordingly. After degassing, **3e** (24.3 µL, 0.2 mmol, 1 eq) was added to the yellow reaction mixture by µL syringe.

**Figure 14** Left: Experimental and fitted EPR-spectrum ( $r^2 = 0.96$ ) of reaction solution of **3e** (0.04 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOH) after 33 min. Right: Integrated EPR signal.

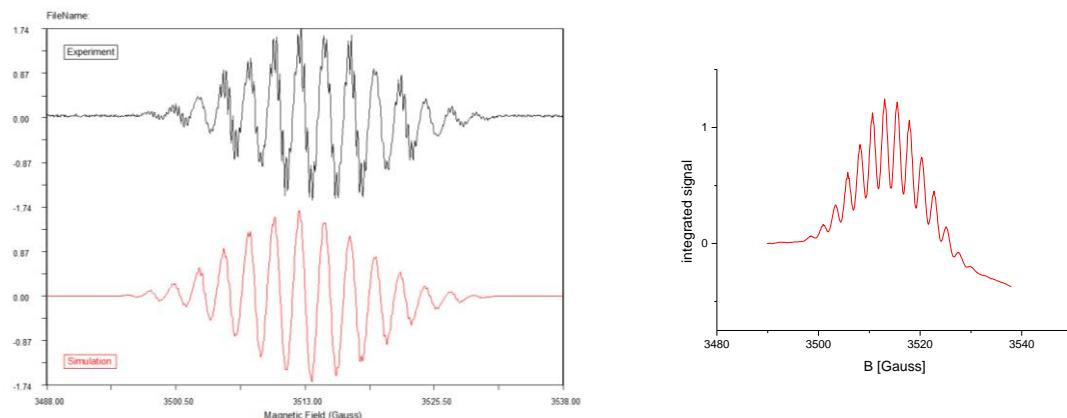


entry	experimental			predicted ( <b>7a-e</b> ) <sup>[Error! Bookmark not defined.]</sup>	
	hfcs [Gauss]	spin	number of equivalent nuclei	hfcs [Gauss]	spin
1	4.919	0.5	3	3.33	<i>N</i> -CH <sub>3</sub>
2	0.293	0.5	3	0.66	4-CH <sub>3</sub>
3	2.008	0.5	3	1.86	3-CH <sub>3</sub>
4	2.268	1	1	3.30	N
5	2.568	1.5	1	2.40	S
6	0.635	0.5	2	0.52	2 H <sub>ar</sub>

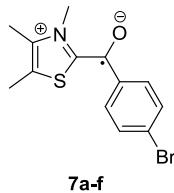


EPR spectra (Figure 5) of radical **7a-g** was derived of the following reaction solution: 3,4,5-trimethyl thiazolium iodide **1a** (5.61 mg, 0.02 mmol, 0.1 eq) and KOH (1 mg, 0.02 mmol, 0.1 eq) were in *i*-PrOH (5 mL). Due to small amounts of **1a** and KOH a 10-fold higher concentrated solution was prepared and an aliquot thereof diluted accordingly. After degassing, **3g** (28.1 mg, 0.2 mmol, 1 eq) was added to the yellow reaction mixture.

**Figure 15** Left: Experimental and fitted EPR-spectrum ( $r^2 = 0.95$ ) of reaction solution of **3g** (0.04 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOH) after 10 min. Right: Integrated EPR spectrum.

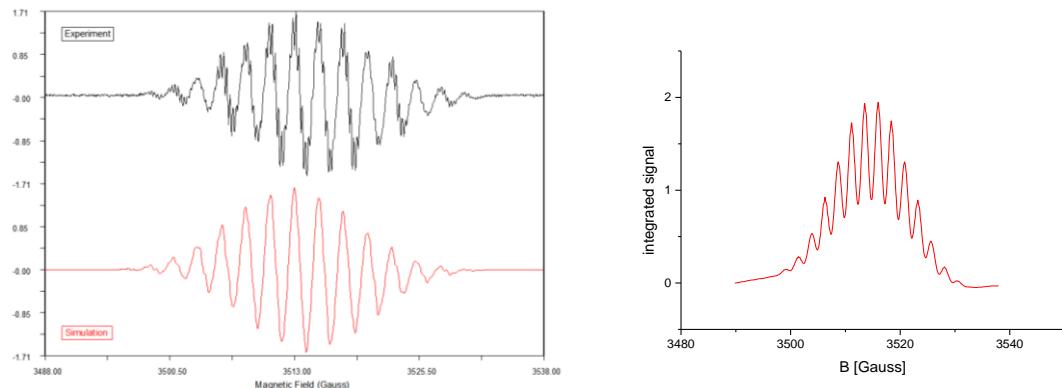


entry	experimental			predicted ( <b>7a-g</b> )		
	hfcs [Gauss]	spin	number of equivalent nuclei	hfcs [Gauss]	spin	
1	4.968	0.5	3	3.87	<i>N</i> -CH <sub>3</sub>	0.5
2	0.304	0.5	3	0.71	4-CH <sub>3</sub>	0.5
3	2.057	0.5	3	2.07	3-CH <sub>3</sub>	0.5
4	2.317	1	1	3.00	N	0.5
5	2.567	1.5	1	2.20	S	1.5
6	0.297	0.5	2	0.31	2 H <sub>ar</sub>	0.5



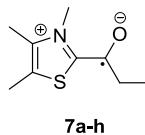
EPR spectra (Figure 5) of radical **7a-f** was derived of the following reaction solution: 3,4,5-trimethyl thiazolium iodide **1a** (5.61 mg, 0.02 mmol, 0.1 eq) and KOH (1 mg, 0.02 mmol, 0.1 eq) were suspended/dissolved in *i*-PrOH (5 mL). Due to small amounts of **1a** and KOH a 10-fold higher concentrated solution was prepared and an aliquot thereof diluted accordingly. After degassing, **3f** (37.0 mg, 0.2 mmol, 1 eq) was added to the yellow reaction mixture.

**Figure 16** Experimental and fitted EPR-spectrum ( $r^2 = 0.97$ ) of reaction solution of **3f** (0.04 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOH).



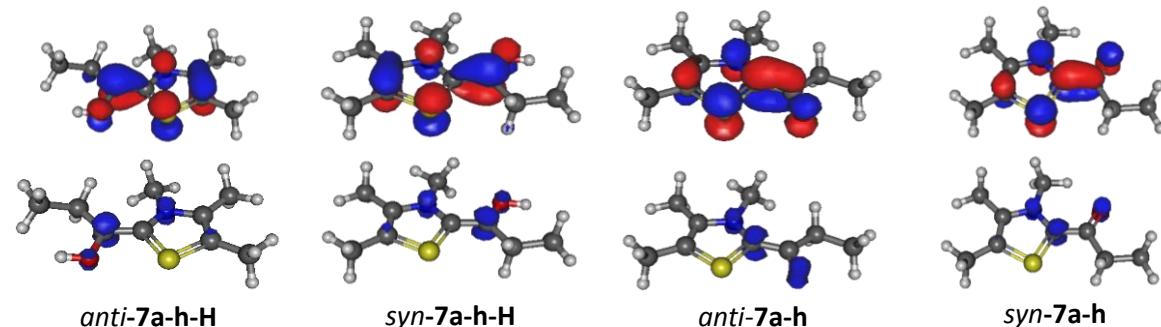
entry	experimental			predicted ( <b>7a-f</b> )		
	hfcs [Gauss]	Spin	Number of equivalent nuclei	hfcs [Gauss]	Spin	
1	4.919	0.5	3	3.73	<i>N</i> -CH <sub>3</sub>	0.5
2	0.548	0.5	3	0.71	4-CH <sub>3</sub>	0.5
3	2.273	0.5	3	2.08	3-CH <sub>3</sub>	0.5
4	2.268	1	1	2.99	N	0.5
5	2.508	1.5	1	2.20	S	1.5
6	0.049	0.5	2	0.33	2 H <sub>ar</sub>	0.5

### A.2.2.5 EPR spectra obtained of **1a**, KOH and aliphatic aldehydes



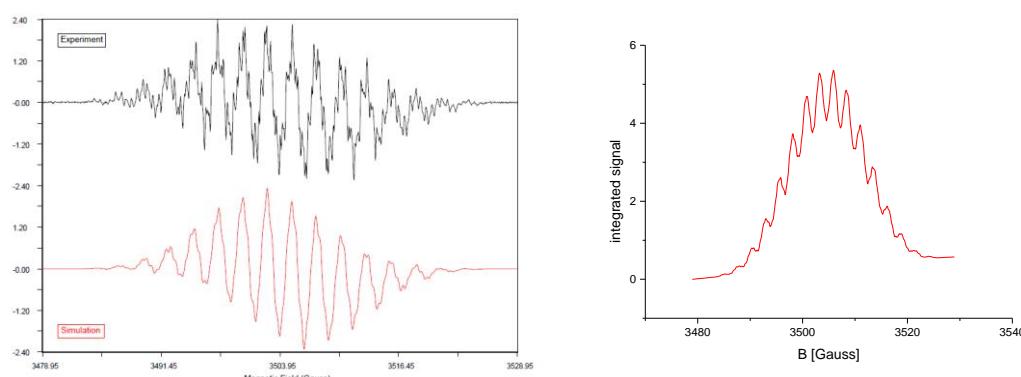
For the simplest aliphatic aldehyde **3h** a similar analysis for its possible conformers and protonation states of **7a-h** (Table 4) has been conducted as for **7a-a** (Table 2). Comparably to the study of **7a-a** the zwitterionic radicals **7a-h** show the best correlation with the experimental data.

**Table 4** Detailed analysis of dependence of simulated Fermi-contact couplings on conformation of **7a-h**.



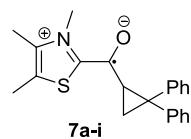
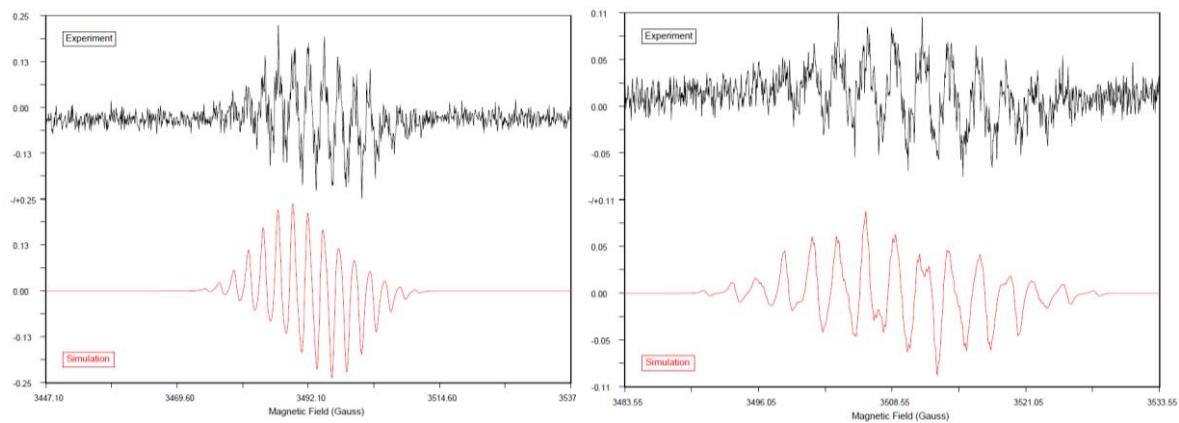
<b>7a-h</b>	<b>Fitted with <math>r^2=0.93</math></b>		<b>anti-7a-h</b>	<b>anti-7a-h-H</b>	<b>syn-7a-h</b>	<b>syn-7a-h-H</b>	<b>Best prediction</b>	<b>deviation to exp. fit in %</b>
	5.337	3-CH <sub>3</sub>	4.774	5.437	<b>5.431</b>	6.156	5.431	1.8
	0.808	4-CH <sub>3</sub>	0.909	<b>0.838</b>	1.051	0.850	0.838	3.7
	2.266	5-CH <sub>3</sub>	<b>2.249</b>	4.454	2.775	4.915	2.249	-0.7
	2.562	N	<b>3.386</b>	4.054	3.450	4.334	3.386	32.2
	2.340	CH <sub>2</sub>	<b>2.250</b>	12.416	5.093	6.106	2.250	-3.9
	2.515	S	<b>2.434</b>	3.194	2.600	3.851	2.434	-3.2
<b>Relative magnitude of conformers based on <math>\Delta G [\%]</math></b>			<b>0.02</b>	<b>1.1</b>	<b>99.98</b>	<b>98.9</b>		

**Figure 17 Top:** Experimental and fitted EPR-spectrum ( $r^2 = 0.91$ ) obtained of reaction solution of **3h** (0.4 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOH). **Below:** Calculated Spin densities (uB3LYP/6-31G\*).

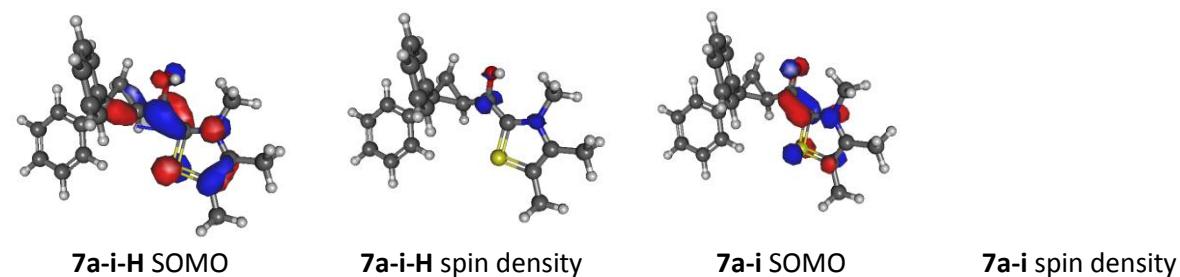


Influence of oxygen is easily spotted by a decrease of signal to noise in the EPR-spectra. The sample with oxygen contamination was prepared as follows: The reaction mixture of **1a** and KOH in *i*-PrOH was degassed as described in A.2.1. then freshly distilled, but not degassed propionaldehyde **3h** was added. The signal needs an unusually long time to build up (40-50 min) and is weak compared to the oxygen-free sample.

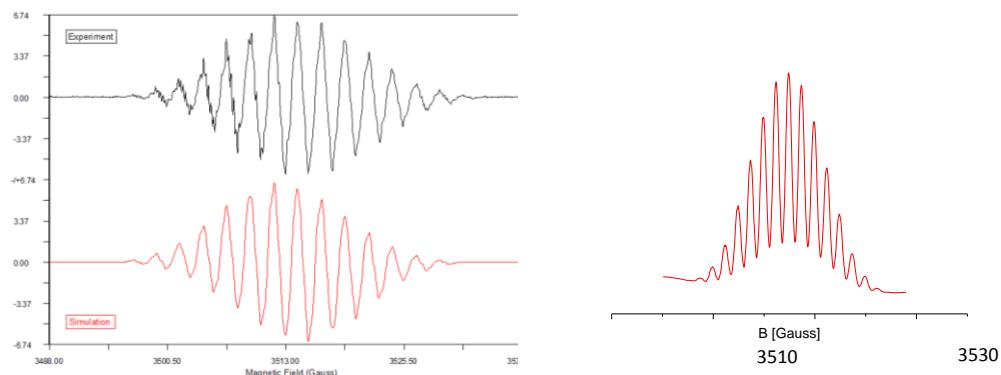
**Figure 18** EPR spectra recorded after 10 min after addition of degassed (left) and with not-degassed **3h** (right).



Radical clock **3i** was subjected to the standard reaction conditions (see Figure 19) in order to measure the radical lifetime. However as mentioned in A.2.1 the ring-opening did not take place. This observation may be explained by the spin density distribution within **7a-i**.

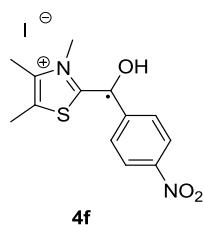


**Figure 19** Experimental and fitted EPR-spectra ( $r^2 = 0.98$ ) obtained of reaction solution of **3i** (0.4 M, 0.1 eq **1a**, 0.1 eq KOH, *i*-PrOH).



entry	experimental [Error! Bookmark not defined.]			predicted ( <b>7a-i</b> ) [Error! Bookmark not defined.]		
	hfcs [Gauss]	spin	number of equivalent nuclei	hfcs [Gauss]		spin
1	5.04	0.5	3	5.38	N-CH <sub>3</sub>	0.5
2	0.50	0.5	3	1.00	4-CH <sub>3</sub>	0.5
3	2.40	0.5	3	2.83	3-CH <sub>3</sub>	0.5
4	3.17	0.5	1	3.45	N	0.5
5	2.28	1.5	1	2.43	S	1.5
6	0.22	0.5	1	1.06	H <sub>cp</sub>	0.5

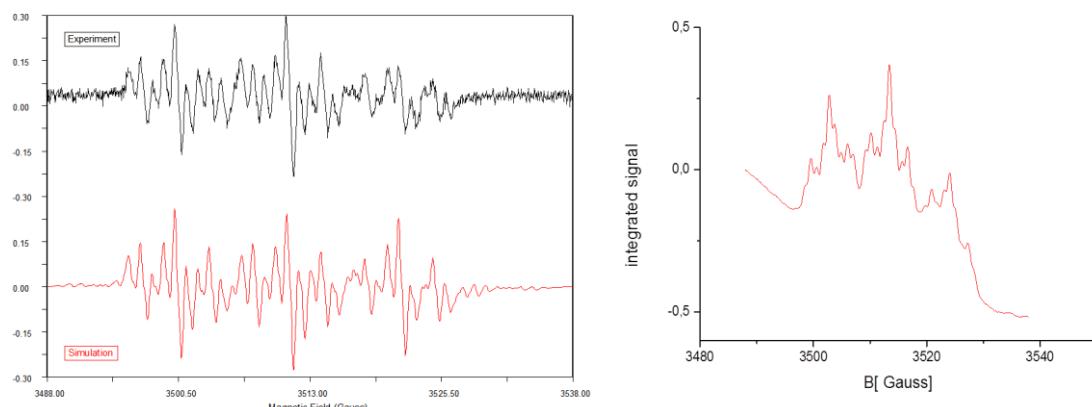
### A.2.2.6 EPR spectra obtained of **1a**, KOH and *p*-Nitrobenzaldehyde **3j** – Connection to Cannizarro-Reaction



EPR spectra of radical **7a-j** and presumably the radical anion of **3j** were derived of the following reaction mixture: 3,4,5-trimethyl thiazolium iodide **1a** (34 mg, 0.12 mmol, 0.1 eq) and KOH (7 mg, 0.12 mmol, 0.1 eq) in 3 mL *i*-PrOH, after degassing the deep yellow suspension **3j** (181 mg, 1.2 mmol, 1 eq) was added.

The reaction of **3j** with **1a** did not provide **9j**, but delivered a weak EPR-signal that could be fitted only by using the structures **7a-j** and the radical anion of **3j** in a 1:1 ratio. The similarity to the spectrum observed in the Cannizarro process (Figure-21) is remarkable.

**Figure 20** Experimental and fitted EPR-spectrum ( $r^2 = 0.92$ ) of reaction solution of **7j** (0.4 M, 0.1 eq **8a**, 0.1 eq KOH, *i*-PrOH). EPR set-up: centre field: 3513 G, SW 50.0G  $\mu$ -wave power: 10.5 mW, sweep time = 41.94 s.



species 1

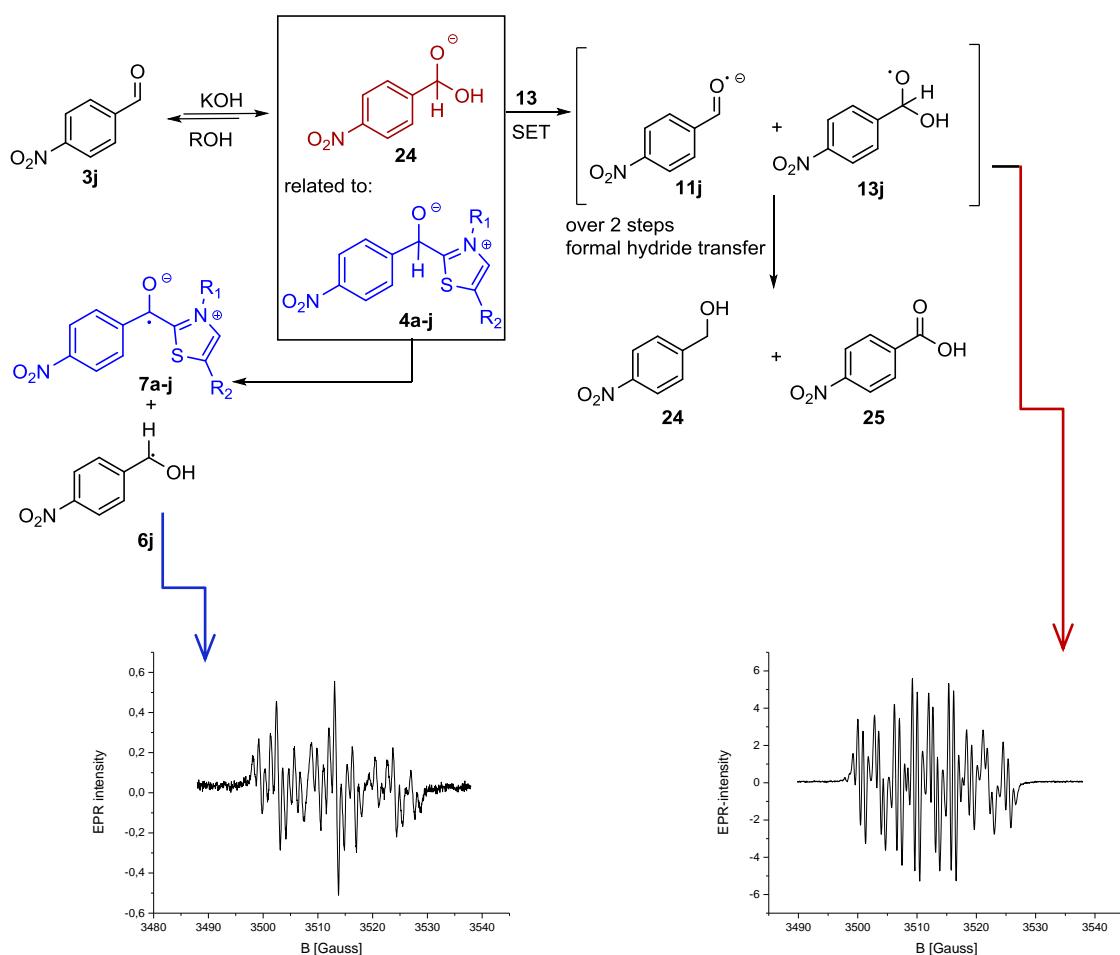
species 2

experimental [Error! Bookmark not defined.]

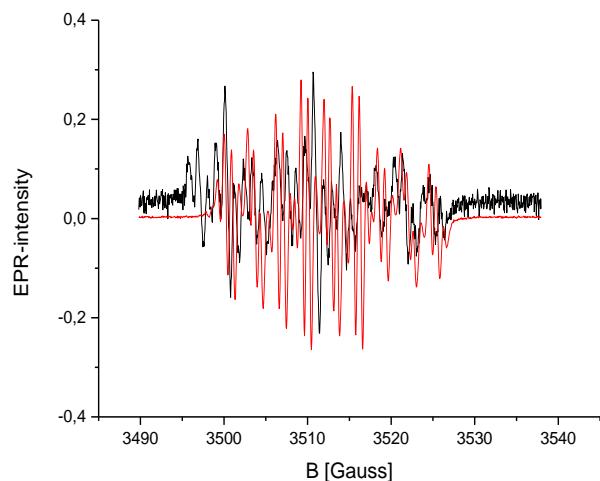
entry	hfcs [Gauss]	spin	number of equivalent nuclei
SPECIES 1 <sup>a, b</sup>			
1	10.630	1	1
2	0.353	0.5	1
3	1.059	0.5	2
4	3.258	0.5	2
SPECIES 2 <sup>b, c</sup>			
1	10.981	1	1
2	1.684	1	1
3	1.062	0.5	1
4	1.129	0.5	3
5	5.459	0.5	3

<sup>a</sup> g-shift: -1.923. <sup>b</sup> relative concentration: 50%. <sup>b</sup> g-shift: -0.688.

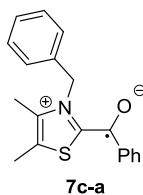
**Figure 21** The close relationship between the Cannizarro process and the Benzoin condensation is exemplified in the following reaction scheme and spectroscopically supported by the occurrence of related radical species.



**Figure 22** Comparison of EPR-Spectra derived of reaction solutions made up of **3j** (1 eq), KOH (0.1 eq) and without (black) and with (red) **1a** (0.1 eq) in *i*-PrOH. The spectra are not identical but closely related!

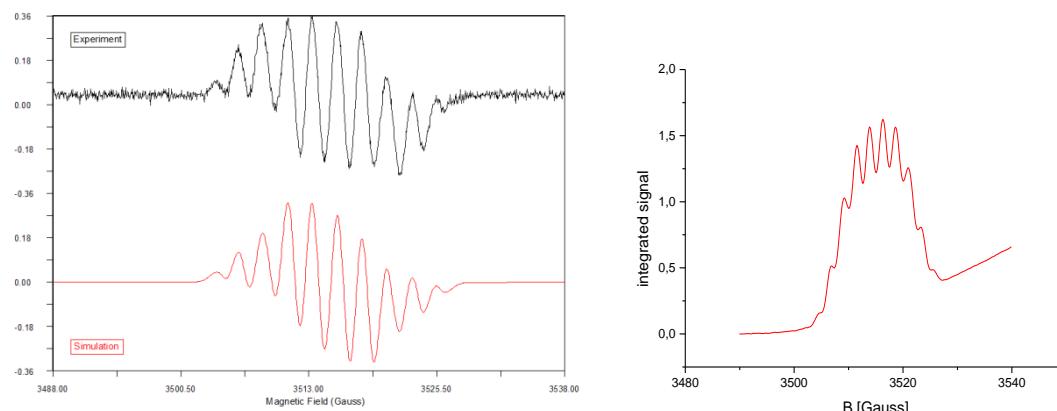


#### A.2.2.7 EPR spectra obtained of **1c-e**, KOH and benzaldehyde **3a**



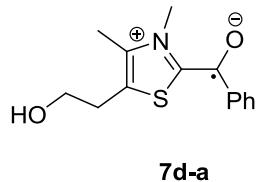
EPR spectra of radical **7c-a** were derived of the following reaction mixture: 3-benzyl-4,5-dimethyl thiazolium bromide **1c** (34 mg, 0.12 mmol, 0.1 eq) and KOH (7 mg, 0.12 mmol, 0.1 eq) in 3 mL *i*-PrOH, the deep yellow suspension was degassed and **3a** (122  $\mu$ L, 1.2 mmol, 1 eq) was added.

**Figure 23** Experimental and fitted EPR-spectrum ( $r^2 = 0.96$ ) of reaction solution of **3a** (0.4 M, 0.1 eq **1c**, 0.1 eq KOH, *i*-PrOH). EPR set-up: centre field: 3513 G, SW 50.0G  $\mu$ -wave power: 10.5 mW, sweep time = 41.94 s.



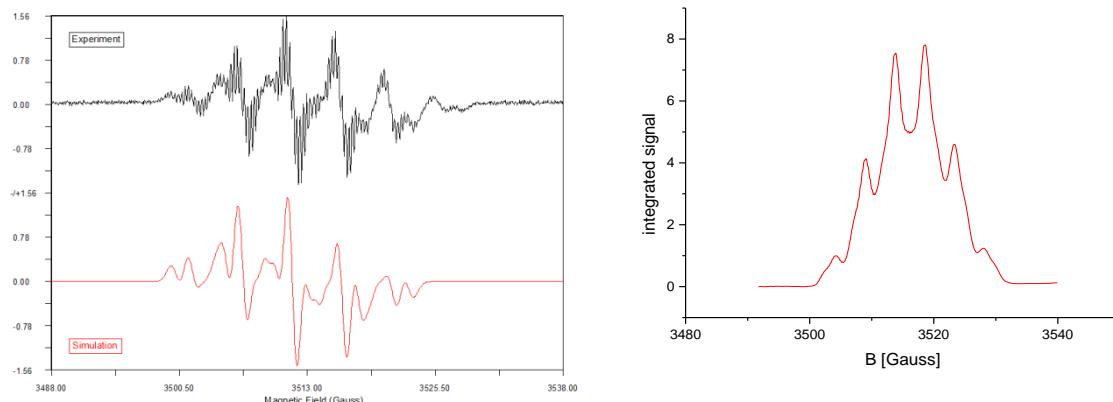
Cmpd	exp.	Calculated based on structure shown		Fitting of exp. data	$r^2$ of fitting
	$\alpha$ [Gauss]	coupling partner	$\alpha$ [Gauss] <sup>a</sup>	$\alpha$ [Gauss]	
<b>7c-a</b>	2.35 0.21	3-CH <sub>2</sub> Ph	2.085 (0.98)	1.917	0.97
		4-CH <sub>3</sub>	0.218 (0.61)	0.218	
		5-CH <sub>3</sub>	3.314 (1.791)	2.637	
		N	3.436 (3.641)	2.759	

		<i>ortho</i> -H (2x)	2.152 (0.399)	2.179	
		<i>para</i> -H	2.521 (0.467)	2.563	
		S	3.699 (2.316)	-	

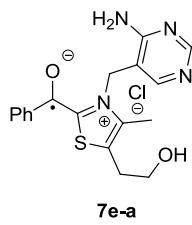


EPR spectra of radical **7d-a** were derived of the following reaction mixture: 3,4-dimethyl-5-(2-hydroxyethyl) thiazolium iodide **1d** (34 mg, 0.12 mmol, 0.1 eq) and KOH (7 mg, 0.12 mmol, 0.1 eq) were suspended in 3 mL *i*-PrOH, after degassing the colorless suspension **3a** (122 µL, 1.2 mmol, 1 eq) was added. Upon addition of aldehyde the reaction mixture turns immediately into a dark orange.

**Figure 24** Experimental and fitted EPR-spectrum ( $r^2 = 0.85$ ) of reaction solution of **3a** (0.4 M, 0.1 eq **1d**, 0.1 eq KOH, *i*-PrOH). EPR set-up: centre field: 3513 G, SW 50.0G µ-wave power: 2.635 mW, sweep time = 41.94 s.



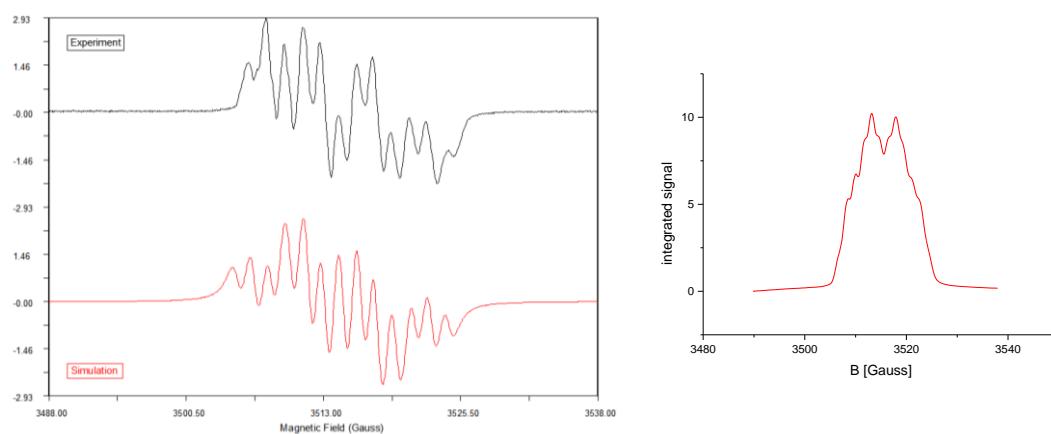
Cmpd	exp.	Calculated based on structure shown		Fitting of exp. data	$r^2$ of fitting
<b>7d-a</b>	<b>4.8</b> <b>1.6</b> <b>0.3</b>	<b>3-CH<sub>3</sub></b>	<b>3.926 (2.967)</b>	<b>4.794</b>	<b>0.85</b>
		4-CH <sub>3</sub>	0.766 (0.700)	0.578	
		5-CH <sub>2</sub> CH <sub>3</sub> OH	1.861 (1.200)	1.618	
		<i>N</i>	3.577 (2.967)	4.394	
		<i>ortho</i> -H (2x)	1.743 (0.351)	0.459	
		<i>para</i> -H	1.875 (0.470)	0.466	
		S	-	-	



EPR spectra of radical **7e-a** were derived of the following reaction mixture: Thiamine hydrochloride **1e** (40.5 mg, 0.12 mmol, 0.1 eq) and KOH (14 mg, 0.2 mmol, 0.2 eq) were suspended in 3 mL *i*-PrOH, after degassing the bright yellow suspension **3a** (122 µL, 1.2 mmol, 1 eq) was added.

**Figure 25** Experimental and fitted EPR-spectrum ( $r^2 = 0.80$ ) of reaction solution of **3a** (0.4 M, 0.1 eq **1e**, 0.2 eq KOH, *i*-PrOH). EPR set-up: centre field: 3514.95 G, SW 50.0G  $\mu$ -wave power: 2.663 mW, sweep time = 41.94 s.

Cmpd	exp.	Calculated based on structure shown		Fitting of exp. data	$r^2$ of fitting
<b>7e-a</b>	4.7 3.2 1.1	3-CH <sub>2</sub> Ar	1.947 (1.214)	1.511	0.99
		4-CH <sub>3</sub>	0.852 (0.589)	0.265	
		5-CH <sub>2</sub> CH <sub>3</sub> OH	1.947 (0.775)	1.511	
		<i>N</i>	3.529 (3.546)	3.763	
		<i>ortho</i> -H (2x)	1.503 (0.318)	0.179	
		<i>para</i> -H	1.560 (0.407)	0.395	
	<i>S</i>	-	-	-	-



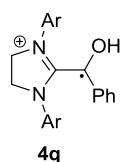
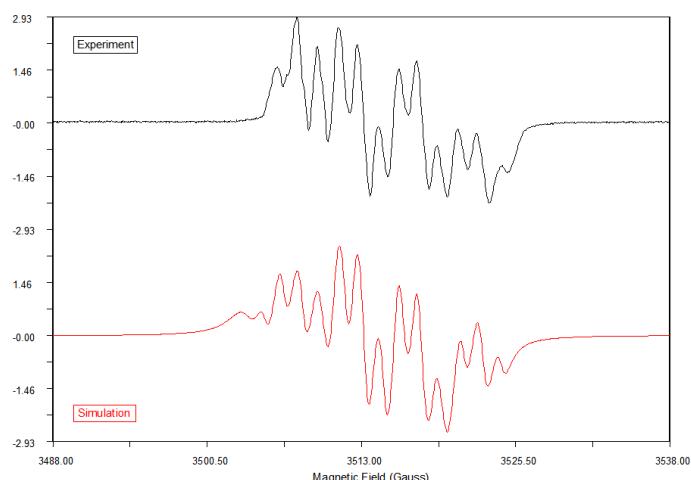
A significantly better fit was obtained ( $r^2 = 0.91$ ) by using a 1:1 ratio of **6a** : **7e-a** (Table 6, Figure 26).

**Table 5** Experimental and fitted EPR-spectrum ( $r^2 = 0.91$ ) of reaction solution of **3a** (0.4 M, 0.1 eq **1e**, 0.2 eq KOH, *i*-PrOH). EPR set-up: centre field: 3514.95 G, SW 50.0G  $\mu$ -wave power: 2.663 mW, sweep time = 41.94 s.

experimental			
SPECIES 1 = <b>7e-a</b> (50%) <sup>a</sup>			
entry	hfcs [Gauss]	spin	number of equivalent nuclei
1	5.010	0.5	2
2	1.517	0.5	2
3	3.032	1	1
SPECIES 2 = <b>6a</b> (50%) <sup>b</sup>			
1	5.346	0.5	2
2	4.075	0.5	2

<sup>a</sup> g-shift: 1.733. <sup>b</sup> g-shift: 0.342.

**Figure 26** Experimental and fitted EPR-spectrum ( $r^2 = 0.91$ ) of reaction solution of **3a** (0.4 M, 0.1 eq **1e**, 0.2 eq KOH, *i*-PrOH). EPR set-up: centre field: 3514.95 G, SW 50.0G  $\mu$ -wave power: 2.663 mW, sweep time = 41.94 s.

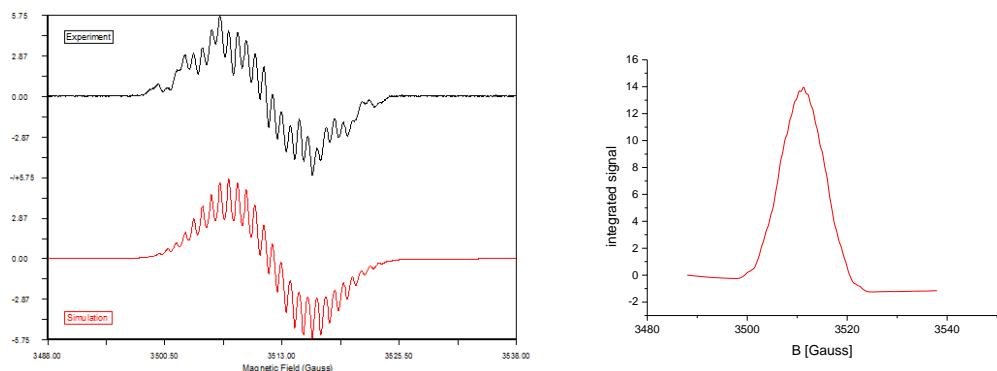


EPR spectra of radical **7f-a** were derived of the following reaction solution: In a glove box catalyst SiPr<sup>17</sup> **1f** (60 mg, 153  $\mu$ mol) was weighted into an oven-dried Schlenk tube. The catalyst was then dissolved in 2.1 mL THF-d<sub>8</sub> to prepare a stock solution before the Schlenk tube was taken out of the glove-box. The

Ar = 2,-bis(isopropyl)phenyl stock solution was stored under inert atmosphere (N<sub>2</sub>) at 4 °C. A 0.7 mL aliquot of this solution (20 mg/0.7 mL, 51  $\mu$ mol, 1 eq) was transferred via syringe into a rubber septum sealed oven dried NMR-tube that has been evacuated and flushed with N<sub>2</sub> several times. To that distilled benzaldehyde **2a** (5.2  $\mu$ L, 51  $\mu$ mol, 1 eq) was added by  $\mu$ L-syringe. The reaction was followed by <sup>1</sup>H NMR every 30 s for 1 hour. The first <sup>1</sup>H NMR after aldehyde addition was recorded after 2 min. For the EPR studies 0.3 mL aliquot of the stock solution (8.5 mg/ 0.3 mL, 22  $\mu$ mol, 1 eq) was transferred into an oven dried and N<sub>2</sub>-flushed EPR-tube (vide supra). **2a** (2.3  $\mu$ L, 22  $\mu$ mol, 1 equiv.) was then added by  $\mu$ L syringe to start the reaction. The first EPR spectrum was recorded 10 min after aldehyde addition.

**Figure 27** Experimental and fitted EPR-spectrum ( $r^2 = 0.98$ ) of reaction solution of **3a** (0.17 M, 1 eq **1f**, THF-d<sub>8</sub>). EPR set-up: centre field: 3513.00 G, SW 50.0G  $\mu$ -wave power: 0.66 mW, sweep time = 41.94 s.

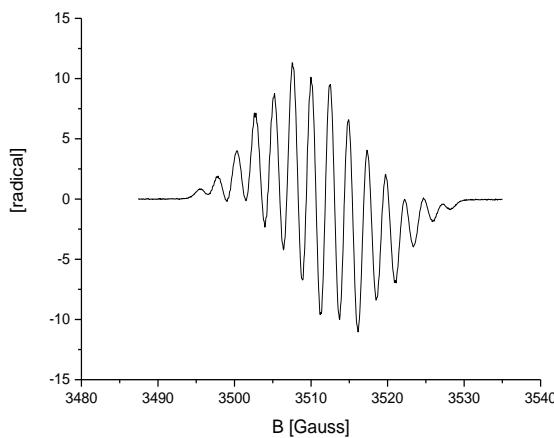
<sup>17</sup> SiPr: 1,3-bis[2,6-di(propan-2-yl)phenyl]-2-imidazolidinylidene used as purchased.



experimental [Error! Bookmark not defined.]			
entry	hfcs [Gauss]	spin	number of equivalent nuclei
1	2.649	1	1
2	2.833	0.5	3
3	2.819	0.5	1
4	1.841	0.5	1
5	1.324	0.5	1
6	0.921	0.5	3
7	0.856	0.5	3

#### A.2.2.8 EPR spectra obtained of

EPR-spectra of **OMe-5b-a** and of the reaction solution of **OMe-5b-a** with **3a**. A similar aliquot (0.1 mL of a 0.1 M THF solution of **OMe-5b-a** (preparation of that see A1.2.4) was taken and transferred into another Schlenk tube and diluted with 0.9 mL THF-d8 (distilled from Na, degassed by several cycles of freeze-pump-thaw-technique) so that the resulting concentration of **OMe-5b-a** was 0.01 M. An EPR-experiment was run on that sample and the original 0.1 M sample. Both did not return an EPR-signal ( $\mu$ w-power = 10.49 mW, centre-field 3510 G, sweep-time = 41.94 s). Then freshly distilled and degassed **3a** (10.2  $\mu$ L, 1 eq) was added to the 0.01 M sample of **OMe-5b-a** and a CW-EPR-experiment was run on that within 8 min after addition of **3a** ( $\mu$ w-power = 0.662 mW, centre-field 3510 G, sweep-time = 41.94 s). The signal shown in the main text was obtained. Considering the microwavepower and concentration of the starting material the signal is by a factor 20 bigger than any other one obtained of the normal catalysis solution of **3a** (0.04M, 0.4 eq **1a** and 0.4 eq KOH).



### A.2.3 Time-resolved EPR studies

#### A.2.3.1 Raw data of time-resolved EPR-studies

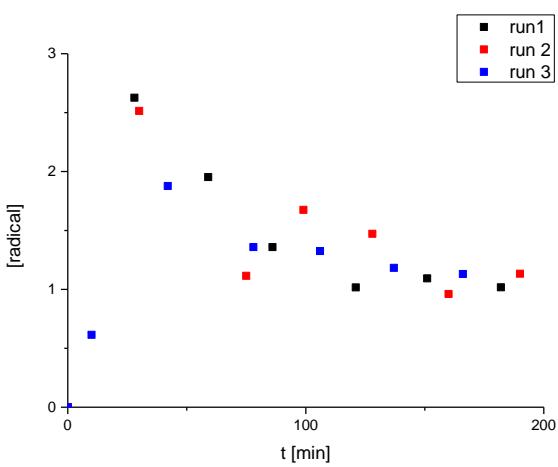
##### A.2.3.1 EPR data of **1a** and **3a**

**Table 7** EPR data of reaction with **3a** (0.4 M) and **1a** (0.1 eq) in *i*-PrOH with parameters set as: centre field 3515 G (run 1,3), 3512 G (run 2); sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweeptime 41.94 s ; microwave power 2.640 mW (run 1), 2.637 mW (run 2), 10.49 mW (run 3).

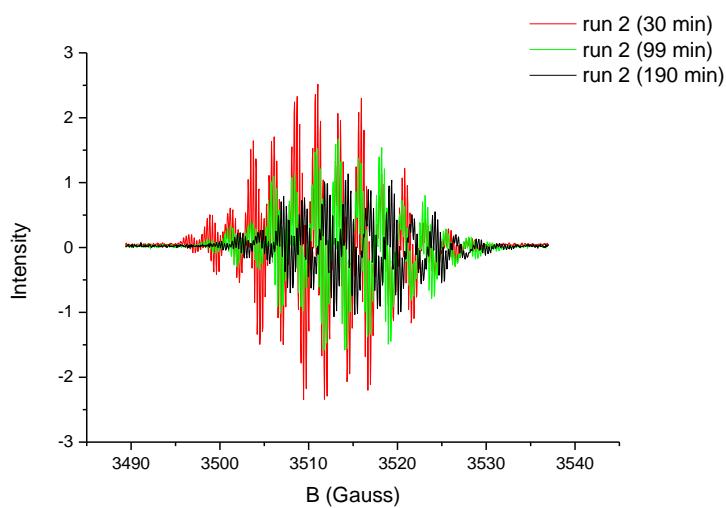
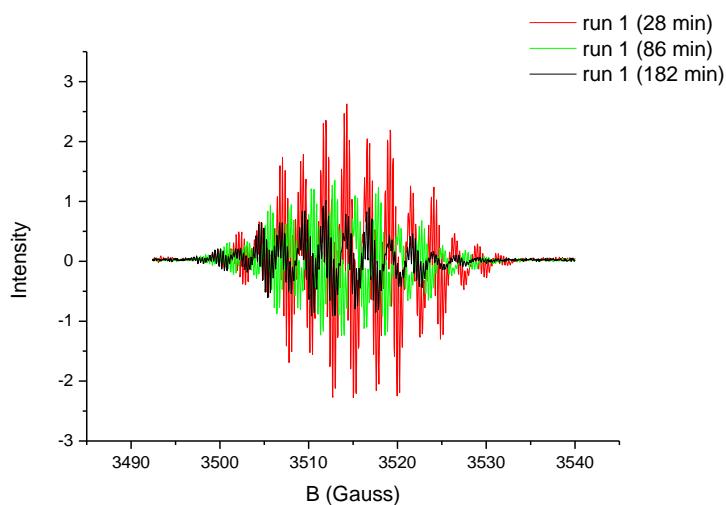
run 1			run 2			run 3		
t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>	t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>	t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>
0	0	0	0	0	0	0	0	0
28	2.6263	2.6213	30	2.5145	2.5111	10	1.2274	0.6146
59	1.9532	1.9495	75	1.1150	1.1135	42	3.7490	1.8772
86	1.3585	1.3559	99	1.6745	1.6723	78	2.7130	1.3585
121	1.0164	1.0145	128	1.4721	1.4702	106	2.6466	1.3252
151	1.0936	1.0915	160	0.9608	0.9596	137	2.3627	1.1830
182	1.0171	1.0152	190	1.1332	1.1317	166	2.2579	1.1306
						209	2.1576	1.0803

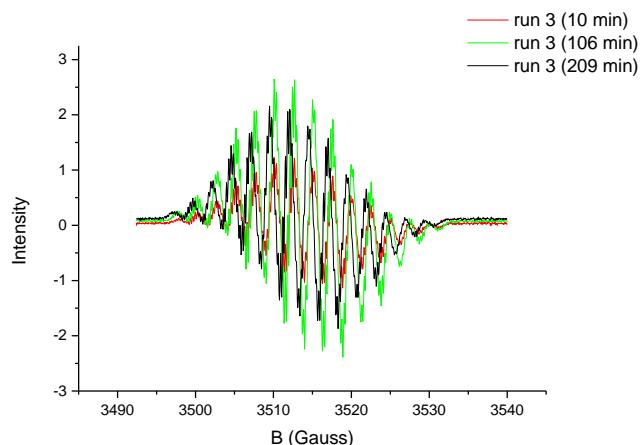
<sup>a</sup> referring to 2.63 mW

**Figure 28** Data of Table 7: PhCHO **2a** (0.4 M), 3,4,5-trimethylthiazolium iodide (0.1 eq) and KOH (0.1 eq) in *i*-PrOH.



**Figure 29:** EPR-spectra of the reaction solution of **3a** (0.4 M), 3,4,5-trimethylthiazolium iodide **1a** (0.1 eq) and KOH (0.1 eq) in *i*-PrOH (**Table 7**, run 1-3).



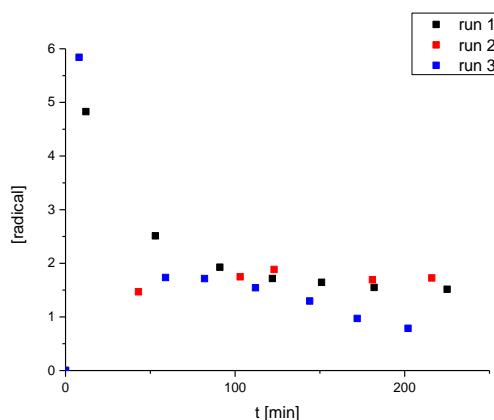


**Table 8** EPR data of reaction with PhCHO **3a** (0.2 M), 3,4,5-trimethylthiazolium iodide **1a** (0.2 eq) and KOH (0.2 eq) in *i*-PrOH. With parameters set as: run 1: centre field 3515 G; sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweeptime 41.94 s; microwave power 2.635 mW; run 2: centre field 3511 G; sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweeptime 41.94 s; microwave power 2.635 mW; run 3: centre field 3513 G; sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweeptime 41.94 s; microwave power 2.64 mW.

run 1			run 2			run 3		
t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>	t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>	t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>
0	0	0	0	0	–	0	0	–
12	4.8287	4.8241	43	1.469	–	8	5.841	–
53	2.5127	2.5104	103	1.748	–	59	1.734	–
91	1.9272	1.9254	123	1.884	–	82	1.714	–
122	1.7167	1.7151	181	1.693	–	112	1.544	–
151	1.6456	1.6440	216	1.727	–	144	1.297	–
182	1.5493	1.5478	–	–	–	172	0.971	–
225	1.5151	1.5137	–	–	–	202	0.788	–

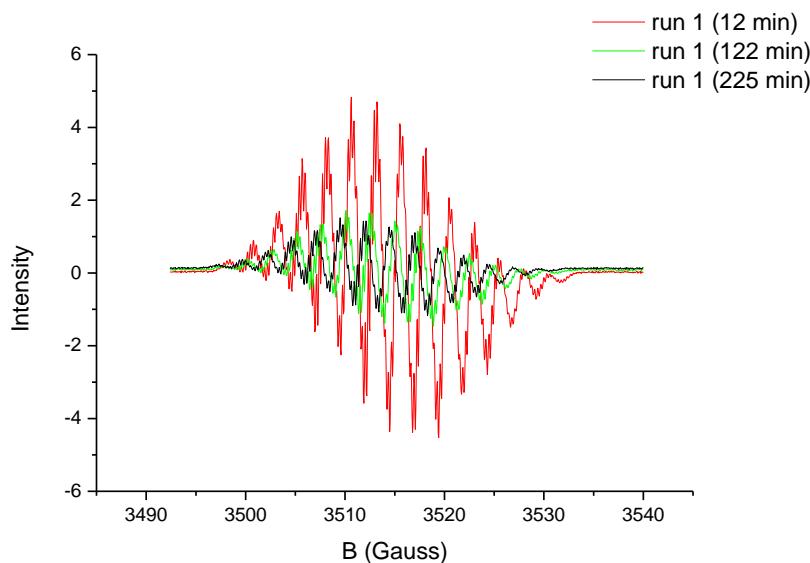
<sup>a</sup> referring to 2.63 mW

**Figure 30** Data of Table 8: PhCHO **3a** (0.2 M), 3,4,5-trimethylthiazolium iodide **1a** (0.2 eq) and



KOH (0.2 eq) in *i*-PrOH.

**Figure 31:** EPR-spectra of the reaction solution of PhCHO **3a** and 3,4,5-trimethylthiazolium iodide **1a** in *i*-PrOH (0.2 M PhCHO, 0.2 eq **1a**, 0.2 eq KOH) (run 1 see **Table 8**).

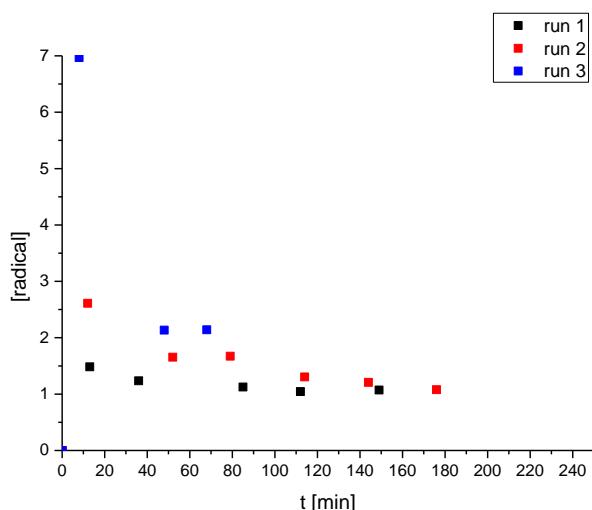


**Table 9** EPR data of reaction with **3a** (0.1 M), 3,4,5-trimethylthiazolium iodide **1a** (0.4 eq) and KOH (0.4 eq) in *i*-PrOH. With parameters set as: centre field 3509 G (run 1), 3512 G (run 2) 3513 (run 3); sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweeptime 41.94 s; microwave power 2.63 mW (run 1) 2.64mW (run 2, 3).

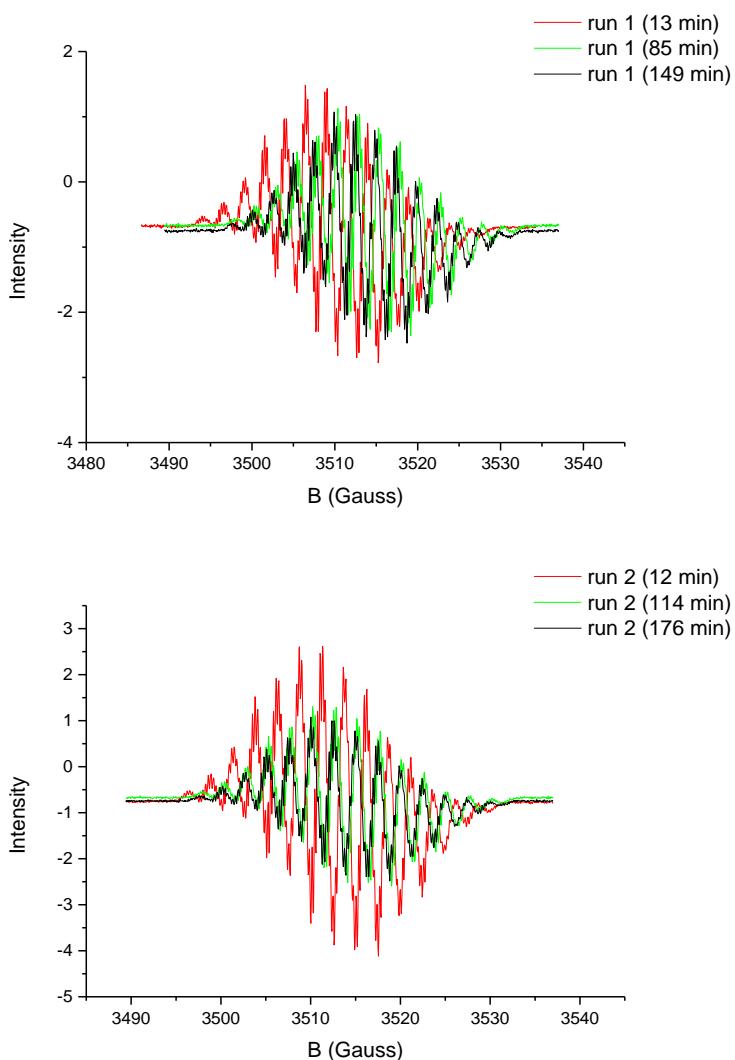
run 1		run 2 <sup>a</sup>		run 3 <sup>a</sup>	
t [min]	EPR-signal (maximum)	t [min]	EPR-signal (maximum)	t [min]	EPR-signal (maximum)
0	0	0	0	0	0
13	1.4839	12	2.6116	8	6.968
36	1.2352	52	1.6552	48	2.1339
85	1.1249	79	1.6726	68	2.1412
112	1.0439	114	1.3039	98	1.975
149	1.0724	144	1.2087	128	2.127
–	–	176	1.0773	158	1.493
–	–	–	–	188	1.333
–	–	–	–	218	1.019

<sup>a</sup> referring to 2.63 mW

**Figure 32** Data of Table 9: PhCHO **3a** (0.1 M), 3,4,5-trimethylthiazolium iodide **1a** (0.4 eq) and KOH (0.4 eq) in *i*-PrOH.



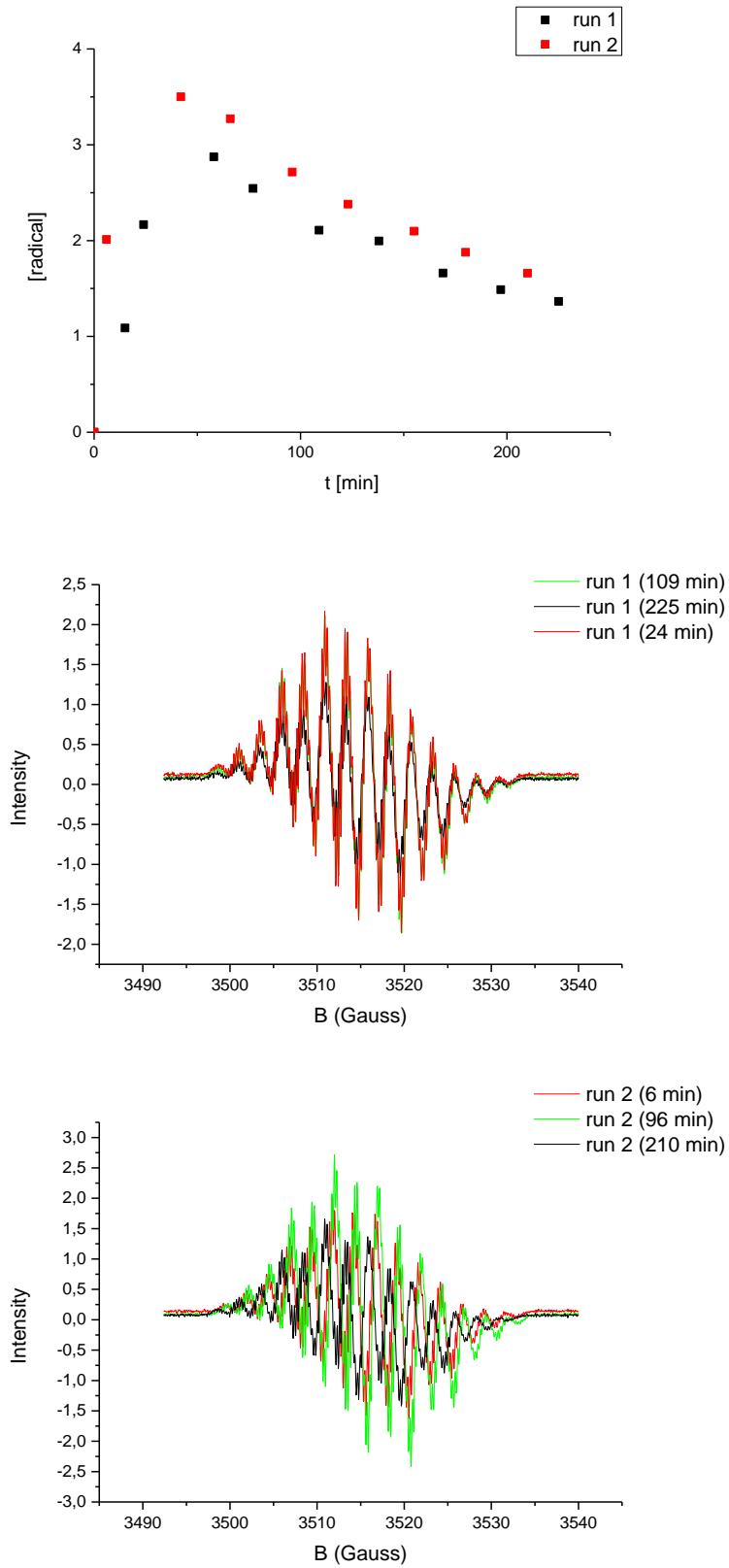
**Figure 33:** EPR-spectra of the reaction solution of PhCHO **3a** and 3,4,5-trimethylthiazolium iodide **1a** in *i*-PrOH (0.1 M PhCHO, 0.4 eq cat, 0.4 eq KOH) (run 1-2 see **Table 6**).



**Table 10** EPR data of reaction with **3a** (0.4 M), **1a** (0.1 eq) and KOH (0.1 eq) in *i*-PrOD. With parameters set as: centre field 3515 G (run 1, 2); sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweeptime 41.94 s); microwave power 2.633 mW (run 1) 2.631 mW (run 2).

run 1		run 2	
t [min]	EPR-signal (maximum)	t [min]	EPR-signal (maximum)
0	0	0	0
15	1.0876	6	2.0114
24	2.1669	42	3.5008
58	2.8733	66	3.2714
77	2.5444	96	2.7151
109	2.1082	123	2.3799
138	1.9960	155	2.0986
169	1.6607	180	1.8782
197	1.4882	210	1.6604
225	1.3656	–	–

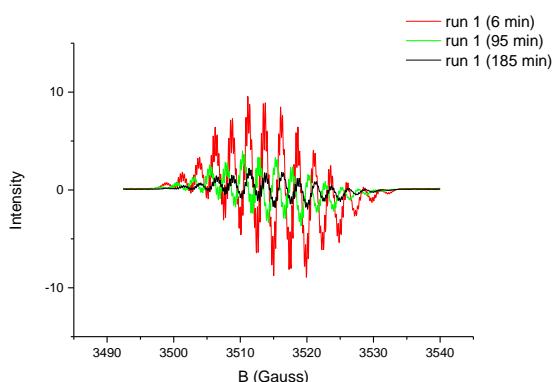
**Figure 34** Data of Table 10: **3a** (0.4 M), **1a** (0.1 eq) and KOH (0.1 eq) in *i*-PrOD.



**Table 8** EPR data of reaction with **3a** (0.1 M, 3,4,5-trimethylthiazolium iodide (0.4 eq) and KOH (0.4 eq) in *i*-PrOD. With parameters set as: centre field 3515 G (run 1, 2); sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweep time 41.94 s; microwave power 2.63 mW (run 1&2).

run 1 <sup>a</sup>			run 2 <sup>a</sup>	
t [min]	EPR-signal (maximum)	Corrected EPR-signal (ref. to 2.63 mW)	t [min]	EPR-signal (maximum)
0	0	0	0	0
6	9.5579	9.5542	5	7.9984
35	5.3700	5.3679	37	2.6520
64	4.5267	4.5249	66	2.0285
95	3.9874	3.9859	95	2.1802
127	3.0780	3.0769	126	1.5680
157	2.7295	2.7285	156	1.5339
185	2.2179	2.2171	-	-
-	-	-	-	-

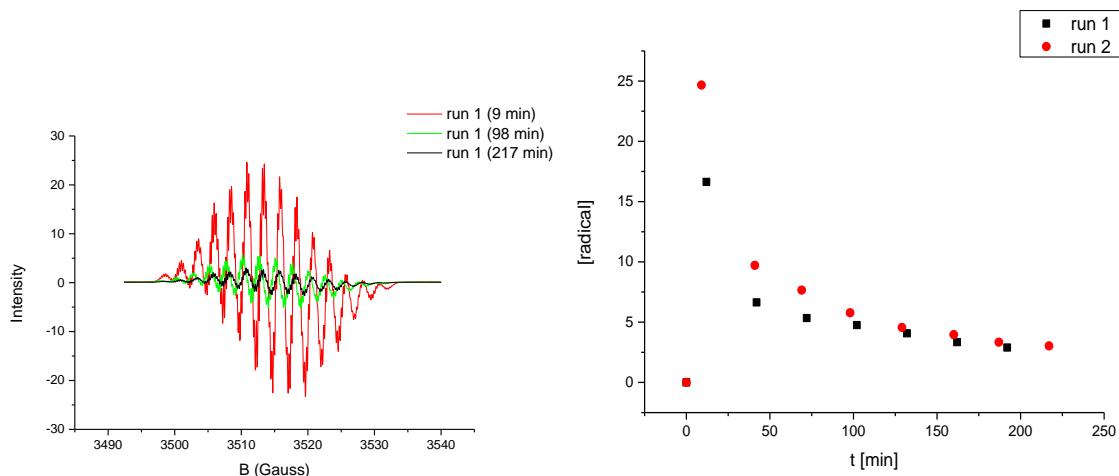
**Figure 35:** EPR-spectra of the reaction solution of **3a** and **1a** in *i*-PrOD (0.1 M PhCHO, 0.4 eq cat, 0.4 eq KOH) (run 1 see **Table 8**).



**Table 9** EPR data of reaction with **3a** (0.1 M), **1a** (1.0 eq) and KOH (1.0 eq) in *i*-PrOD. With parameters set as: centre field 3515 G (run 1, 2); sweep width 50 G;  $t_{\text{const}}$  10.24 ms; sweeptime 41.94 s); microwave power 2.635 mW (run 1); 0.66 mW (run 2).

run 1 <sup>a</sup>			run 2 <sup>a</sup>		
t [min]	EPR-signal (maximum)	Corrected EPR-signal (ref. to 2.63 mW)	t [min]	EPR-signal (maximum)	Corrected EPR-signal (ref. to 2.63 mW)
0	0	0	0	0	0
9	24.664	24.641	12	8.32	16.63
41	9.7147	9.7055	42	3.32	6.63
69	7.6577	7.6505	72	2.67	5.33
98	5.7773	5.7718	102	2.38	4.757
129	4.5651	4.5607	132	2.04	4.08
160	3.9662	3.9624	162	1.67	3.38
187	3.3444	3.3413	192	1.45	2.89
217	3.0272	3.0243	-	-	-

**Figure 36:** EPR-spectra of the reaction solution of PhCHO **2a** and 3,4,5-trimethylthiazolium iodide in *i*-PrOD (0.1 M PhCHO, 1.0 eq cat, 1.0 eq KOH) (run 1 see Table 9) and plotted data of Table 9.

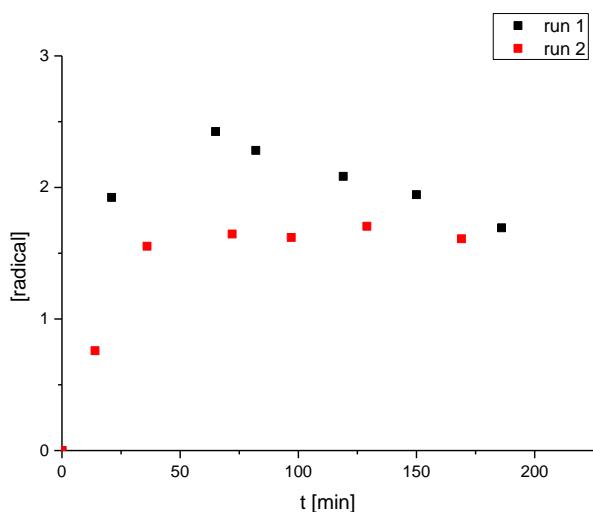


**Table 10** EPR data of reaction with **3a- $\alpha$ -d<sub>1</sub>** (0.4 M), **1a** (0.1 eq) and KOH (0.1 eq) in *i*-PrOD. With parameters set as follows: centre field 3511 G (run 1, 2), sweep width 50 G; t<sub>const</sub> 10.24 ms; sweeptime 41.94 s); microwave power 2.643 mW (run 1) and 10.50 mW (run 3).

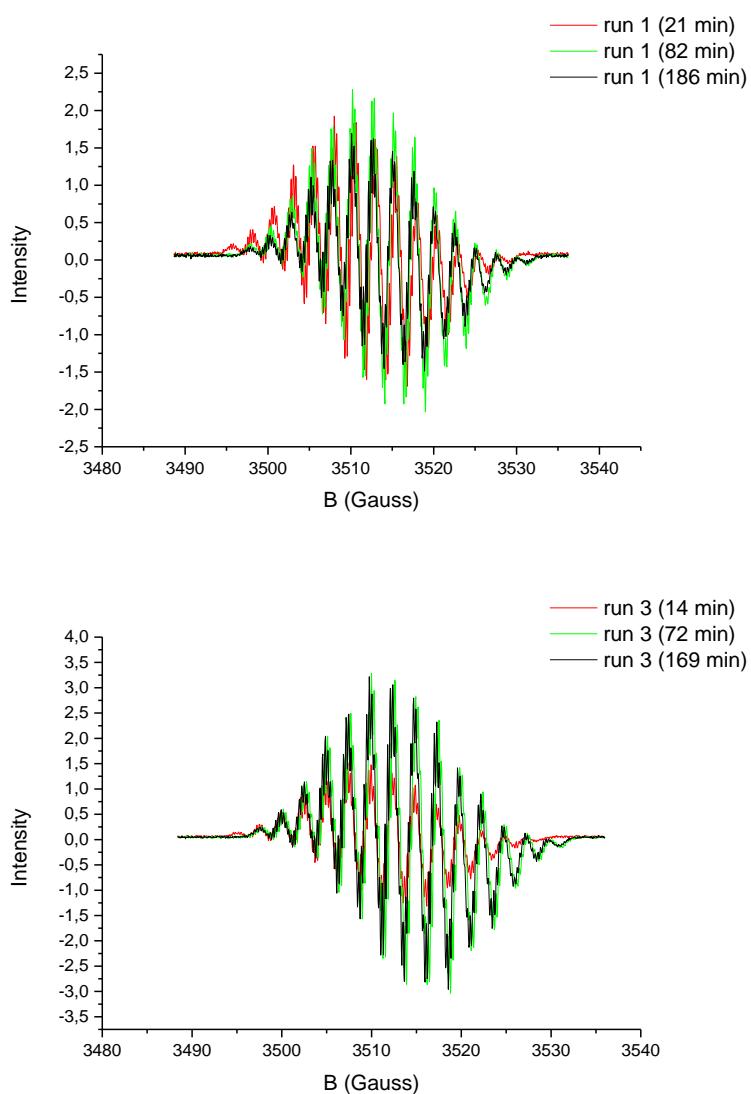
run 1 <sup>a</sup>			run 2 <sup>a</sup>		
t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>	t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>
0	0	0	0	0	0
21	1.9243	1.9196	14	1.5162	0.7588
65	2.4250	2.4190	36	3.1037	1.5533
82	2.2812	2.2755	72	3.2879	1.6455
119	2.0839	2.0788	97	3.2364	1.6197
150	1.9456	1.9408	129	3.4062	1.7047
186	1.6931	1.6889	169	3.2169	1.6100

<sup>a</sup> referring to 2.63 mW

**Figure 37** Data of Table 10: **3a- $\alpha$ -d<sub>1</sub>** (0.4 M), **1a** (0.1 eq) and KOH (0.1 eq) in *i*-PrOD.



**Figure 38:** EPR-spectra of the reaction solution of **3a- $\alpha$ -d<sub>1</sub>** and **1a** in *i*-PrOD (0.4 M **3a- $\alpha$ -d<sub>1</sub>**, 0.1 eq cat, 0.1 eq KOH) (**Table 10**).

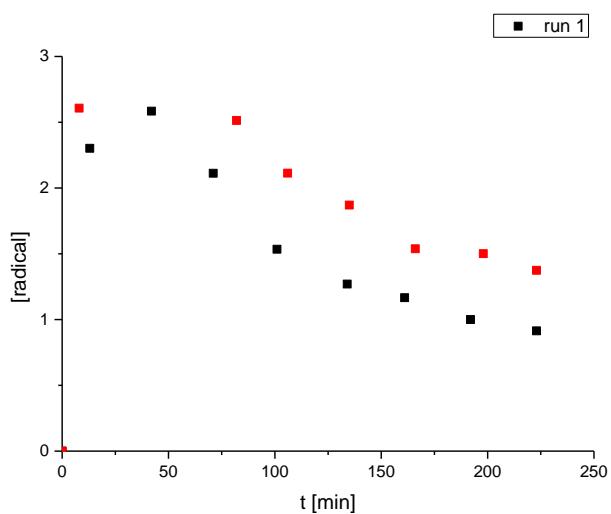


**Table 11** EPR data of reaction with **3a- $\alpha$ -d<sub>1</sub>** (0.2 M) and **1a** (0.2 eq) and KOH (0.2 eq) in *i*-PrOD. With parameters set as: centre field 3515 G (run 1, 2); sweep width 50 G; t<sub>const</sub> 10.24 ms; sweeptime 41.94 s); microwave power 2.63 mW (run 1) 2.64 mW (run 2).

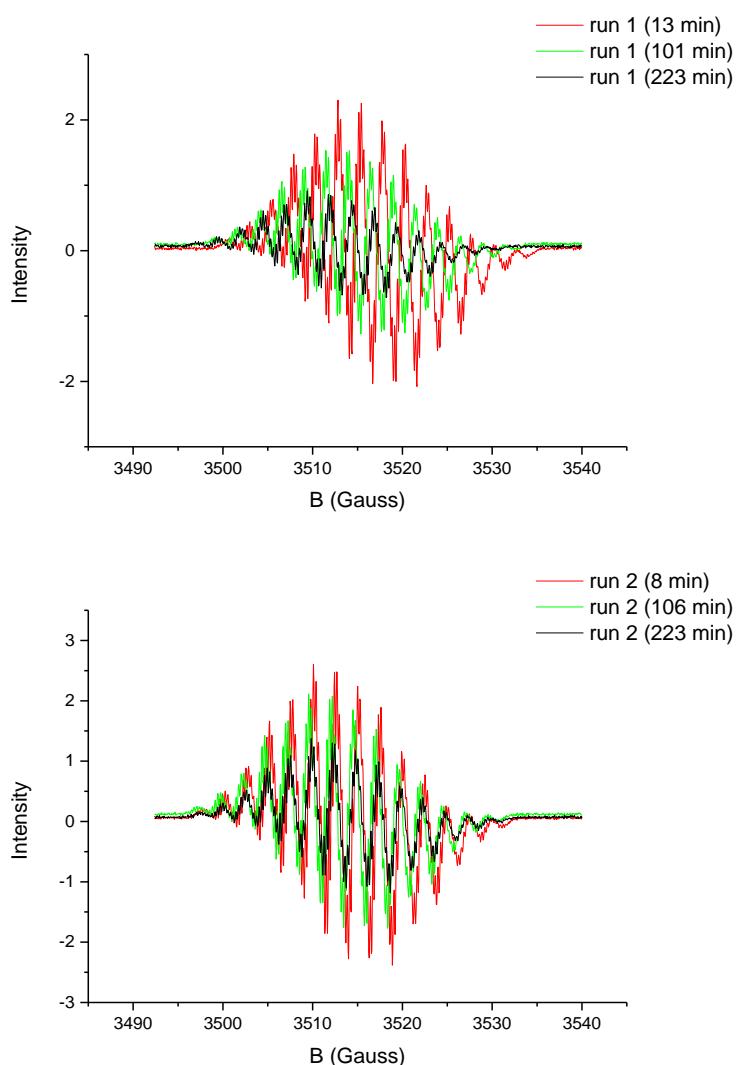
run 1			run 2		
t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>	t [min]	EPR-signal (maximum)	Corrected EPR-signal <sup>a</sup>
0	0	0	0	0	0
13	2.3018	2.3001	8	2.6068	2.6024
42	2.5846	2.5826	36	3.9467	3.9399
71	2.1121	2.1105	82	2.5132	2.5089
101	1.5344	1.5332	106	2.1134	2.1098
134	1.2699	1.2689	135	1.8701	1.8669
161	1.1660	1.1651	166	1.5379	1.5353
192	0.9997	0.9989	198	1.5009	1.4983
223	0.9140	0.9133	223	1.3741	1.3717

<sup>a</sup> 0.2 M [PhCDO **2a**]<sub>0</sub>, 0.2 eq 3,4,5-trimethylthiazolium iodide **8a** and 0.2 eq KOH

**Figure 39** Data of Table 11: **3a- $\alpha$ -d<sub>1</sub>** (0.4 M), **1a** (0.2 eq) and KOH (0.2 eq) in *i*-PrOD.



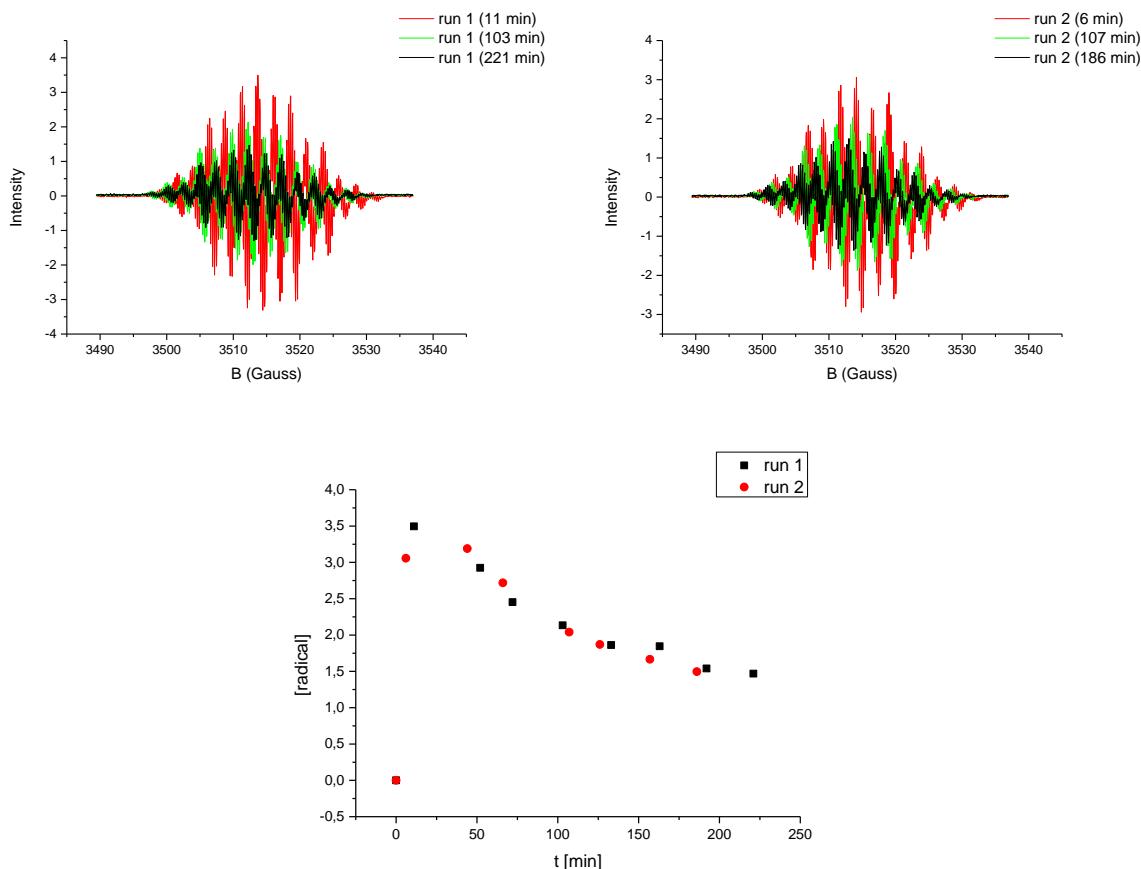
**Figure 40:** EPR-spectra of the reaction solution of **3a- $\alpha$ -d<sub>1</sub>** and **1a** in *i*-PrOD (0.2 M **3a- $\alpha$ -d<sub>1</sub>**, 0.2 eq **1a**, 0.2 eq KOH) (run 1-2 see Table 11).



**Table 12** EPR data of reaction with **3a- $\alpha$ -d<sub>1</sub>** (0.1 M), **1a** (0.4 eq) and KOH (0.4 eq) in *i*-PrOD. With parameters set as follows: centre field 3512 G (run 1, 2); sweep width 50 G; t<sub>const</sub> 10.24 ms; sweeptime 41.94 s); microwave power 2.627 mW (run 1), 2.638 mW (run 2).

run 1 <sup>a</sup>			run 2 <sup>a</sup>		
t [min]	EPR-signal (maximum)	Corrected EPR-signal (ref. to 2.63 mW)	t [min]	EPR-signal (maximum)	Corrected EPR-signal (ref. to 2.63 mW)
0	0	0	0	0	0
11	3.4958	3.4978	6	3.0574	3.0528
52	2.9248	2.9265	44	3.1896	3.1847
72	2.4529	2.4543	66	2.7184	2.7143
103	2.1333	2.1345	107	2.0410	2.0379
133	1.8627	1.8638	126	1.8704	1.8676
163	1.8460	1.8471	157	1.6660	1.6635
192	1.5401	1.5401	186	1.4959	1.4937
221	1.4683	1.4683			

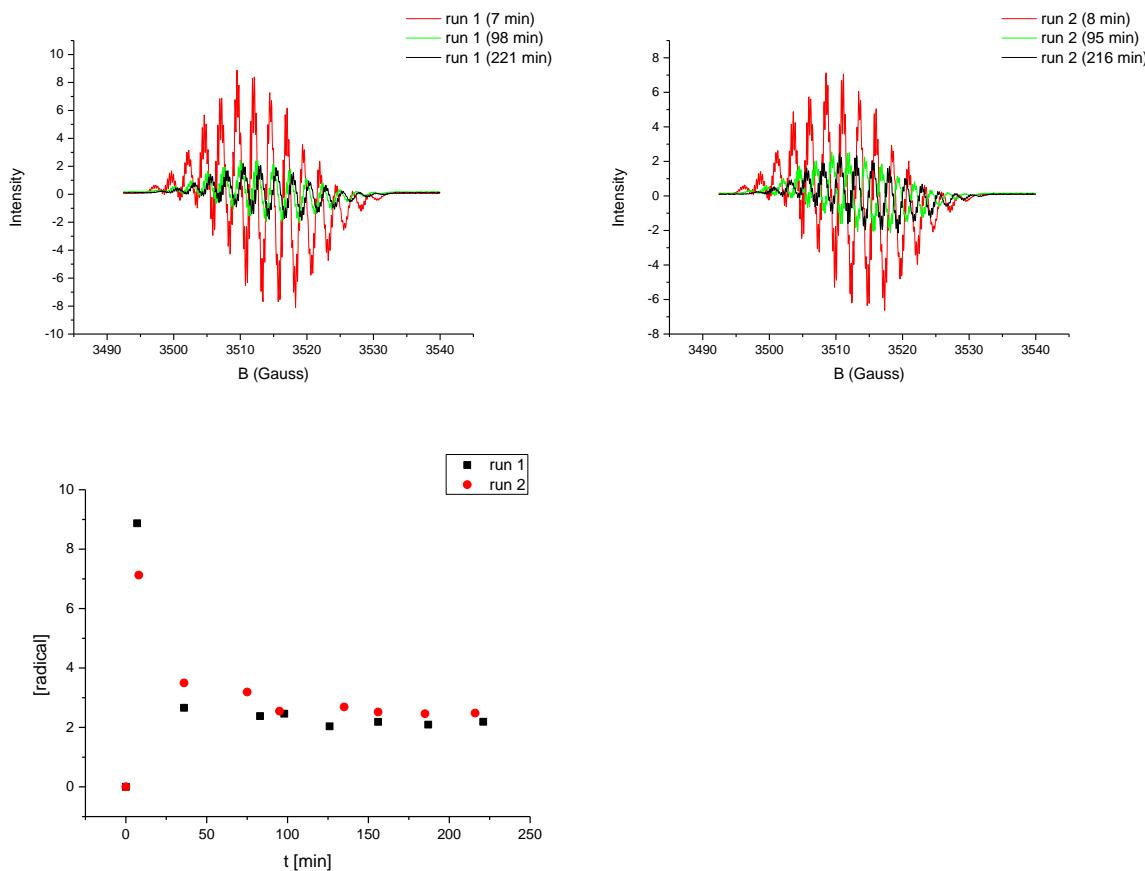
**Figure 41:** EPR-spectra of the reaction solution of **with** **3a- $\alpha$ -d<sub>1</sub>** (0.1 M), **1a** (0.4 eq) and KOH (0.4 eq) in *i*-PrOD (run 1-3 see Table 12).



**Table 13** EPR data of reaction with **3a- $\alpha$ -d<sub>1</sub>** (0.1 M), **1a** (1 eq) and KOH (1 eq) in *i*-PrOD. With parameters set as: centre field 3515 G (run 1, 2); sweep width 50 G; t<sub>const</sub> 10.24 ms; sweeptime 41.94 s; microwave power 2.634 mW (run 1) 2.633 mW (run 2).

run 1 <sup>a</sup>			run 2 <sup>a</sup>		
t [min]	EPR-signal (maximum)	Corrected EPR-signal (ref. to 2.63 mW)	t [min]	EPR-signal (maximum)	Corrected EPR-signal (ref. to 2.63 mW)
0	0	0	0	0	0
7	8.8713	8.8646	8	7.1278	7.1237
36	2.6602	2.6582	36	3.4995	3.4975
83	2.3816	2.3798	75	3.1940	3.1922
98	2.4604	2.4586	95	2.5481	2.5467
126	2.0379	2.0363	135	2.6903	2.6888
156	2.1865	2.1848	156	2.5188	2.5174
187	2.0961	2.0945	185	2.4619	2.4606
221	2.1925	2.1908	216	2.4833	2.4819

**Figure 42:** EPR-spectra of the reaction solution 3a- $\alpha$ -d<sub>1</sub> (0.1 M), **1a** (1 eq) and KOH (1 eq) in *i*-PrOD (0.1 M PhCDO, 1.0 eq cat, 1.0 eq KOH) (run 1-2 see Table 13).



#### A.2.3.2 Fitting of Time-Resolved EPR spectroscopy

The fits were conducted with the Program SimFit<sup>18</sup> and the quality of the fits evaluated by various statistical tests as implemented in the software's algorithm (Durbin-Watson test, Shapiro-Wilks, Akaike AIC (Schwarz SC) and mean-square deviations). First a 2-parameter, i.e. bi-exponential model (Eq. 1) and a 3-parameter model (Eq. 2) for describing a transient response from baseline to baseline (Model 6 in the fitting subunit of SimFit) were applied in fitting the progression curves obtained during the 2 to 3 independent runs of time-resolved EPR measurements under same conditions (raw data above). The same concentrations have been chosen for the EPR and NMR kinetics.

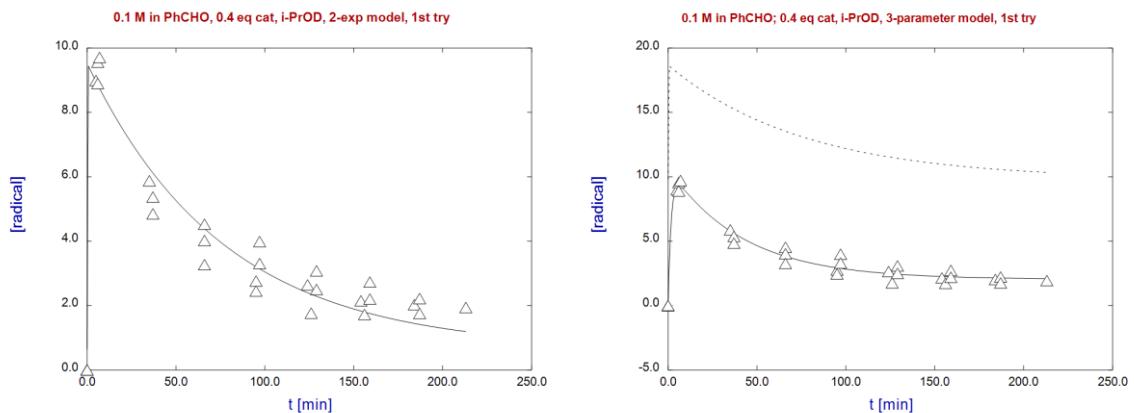
$$\text{Eq. 1} \quad f(t) = [\text{radical}](t) = A_1 \times \exp(-k_1 \times t) + A_2 \times \exp(-k_2 \times t) + C$$

with  $A_1 = -A_2$  and  $C := \text{constant}$ , i.e.  $[\text{radical}]_{\text{eq}}$

$$\text{Eq. 2} \quad f(t) = [\text{radical}](t) = A_1 \times \exp(-k_1 \times t) + A_2 \times \exp(-k_2 \times t) + A_3 \times \exp(-k_3 \times t) + C$$

with  $A_1 = -A_2$ ,  $A_2 = -A_3$  and  $C := \text{constant}$ , i.e.  $[\text{radical}]_{\text{eq}}$

<sup>18</sup> Simfit Windows 7.0.6 academic 32-bit version written by W. G. Bardsley, University of Manchester, U.K. as downloaded from www.simfit.org.uk in December 2014.



**Figure 43** Combined data of Table 8, 0.1 M in **3a**, 0.4 eq **1a** and 0.4 eq KOH in *i*-PrOD. Left: Solid line 1<sup>st</sup> fit with bi-exponential model ( $r^2=0.944$ ). Right: Dotted line shows rejected relaxed fit with the 2-parameter model and the solid line represents 1<sup>st</sup> fit with 3-parameter model ( $r^2=0.976$ ).

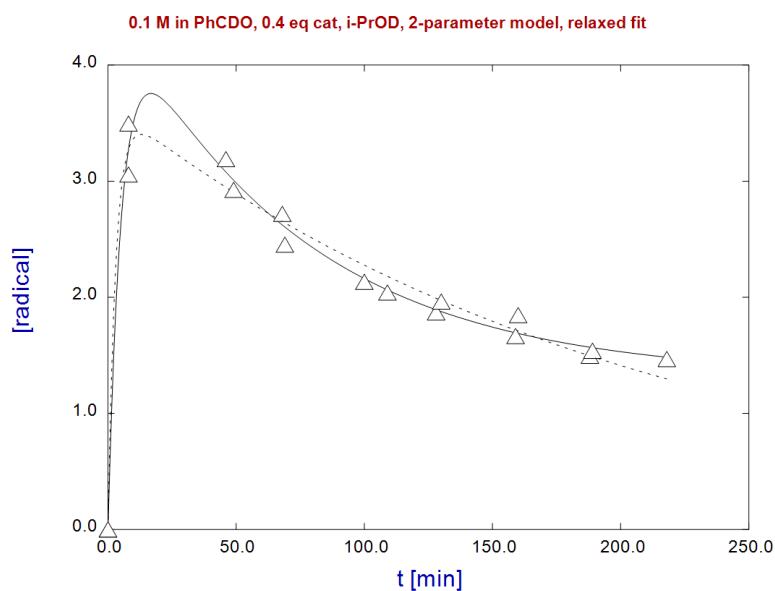
#### 1st fit, 2-exponential model rejected

$r^2$			
0.944			
$r$ max	$k$ form [ $\text{min}^{-1}$ ]	$k$ decline [ $\text{min}^{-1}$ ]	$C$
8.879 $\pm 0.425$	105.7 $\pm 0$	0.01308 $\pm 0.00146$	0.6448 $\pm 0.297$

#### 1st fit, 3-exponential model

$r^2$			
0.976			
$r$ max	$k$ form	$k$ decline	$C$
8.14 $\pm 0$	0.59 $\pm 0$	0.02403 $\pm 0$	2.042 $\pm 0.234$

Based on F-Test fit with 3-parameter model is satisfactory at a 5% significance level compared to the fit with the 2-parameter model.



**Figure 44** Combined data of Table 10, 0.1 M in PhCDO, 0.4 eq pre-cat **1a**, 0.4 eq KOH in *i*-PrOD: dotted line represents rejected 1<sup>st</sup> fit with 2-parameter model ( $r^2=0.980$ ). Solid line represents relaxed fit of 2-parameter model ( $r^2=0.988$ ).

<b>r<sup>2</sup></b>	Verdict		
0.988	quite good		
<b>r max</b>	<b>k form</b>	<b>k decline</b>	<b>C</b>
3.597	0.19	0.014	1.314
0.4	0.04	0.003	0.186

Based on F-Test relaxed fit with the 2-parameter model is satisfactory at a 5% significance level compared to 1<sup>st</sup> fit and following fits with the 3-parameter model.

KIE of radical formation for reaction with 0.1 M aldehyde and 0.4 eq 1a, 0.4 eq KOH in *i*-PrOD is  $k_H/k_D$  0.59/0.19 = **3.1**.

### A.3. NMR

#### A. 3.1 NMR studies- Conversion to Benzoin

NMR-experiments were conducted in similar manner to the EPR experiments. With TMS or *i*-PrOH as internal standard absolute concentrations of **2**, **3** and **7** could be determined. Indicative signals for **3a** to **3j**, **4a-a** and **9a** to **9i** that were used for integration and are summarized in Table 14. In case that the reaction took place in deuterated solvent, H/D-exchange was observed. In such cases the following signals have been integrated: **3a/3a- $\alpha$ -d1** 7.93 (2H) and **9a** 7.97 (2H).

**Table 14** Indicative signals for determination of conversion.

entry	substrate <b>3</b>		benzoin products <b>9</b>		adducts <b>4</b>	
	cmpd	$\delta$ [ppm]	cmpd	$\delta$ [ppm]	cmpd	$\delta$ [ppm]
1	<b>3a</b>	9.93	<b>9a</b>	5.97 (1H)/ 7.92(2H)	<b>4a</b>	6.58
2	<b>3b</b>	8.9	<b>9b</b>	3.93 (1H)	-	-
3	<b>3e</b>	9.89	<b>9d</b>	5.85 (1H)/ 7.81 (2H)	-	-
4	<b>3f</b>	9.88	<b>9e</b>	5.84 (1H)/7.85 (2H)	-	-
5	<b>3g</b>	10.20	<b>9f</b>	5.88 (1H)/7.83 (2H)	-	-
6	<b>3h</b>	9.74	<b>9h</b>	4.18 (1H)	-	-
7	<b>3i</b>	8.68	<b>9i</b>	3.48 (1H)	-	-
8	<b>3j</b>	10.16	<b>9j</b>	-	-	-

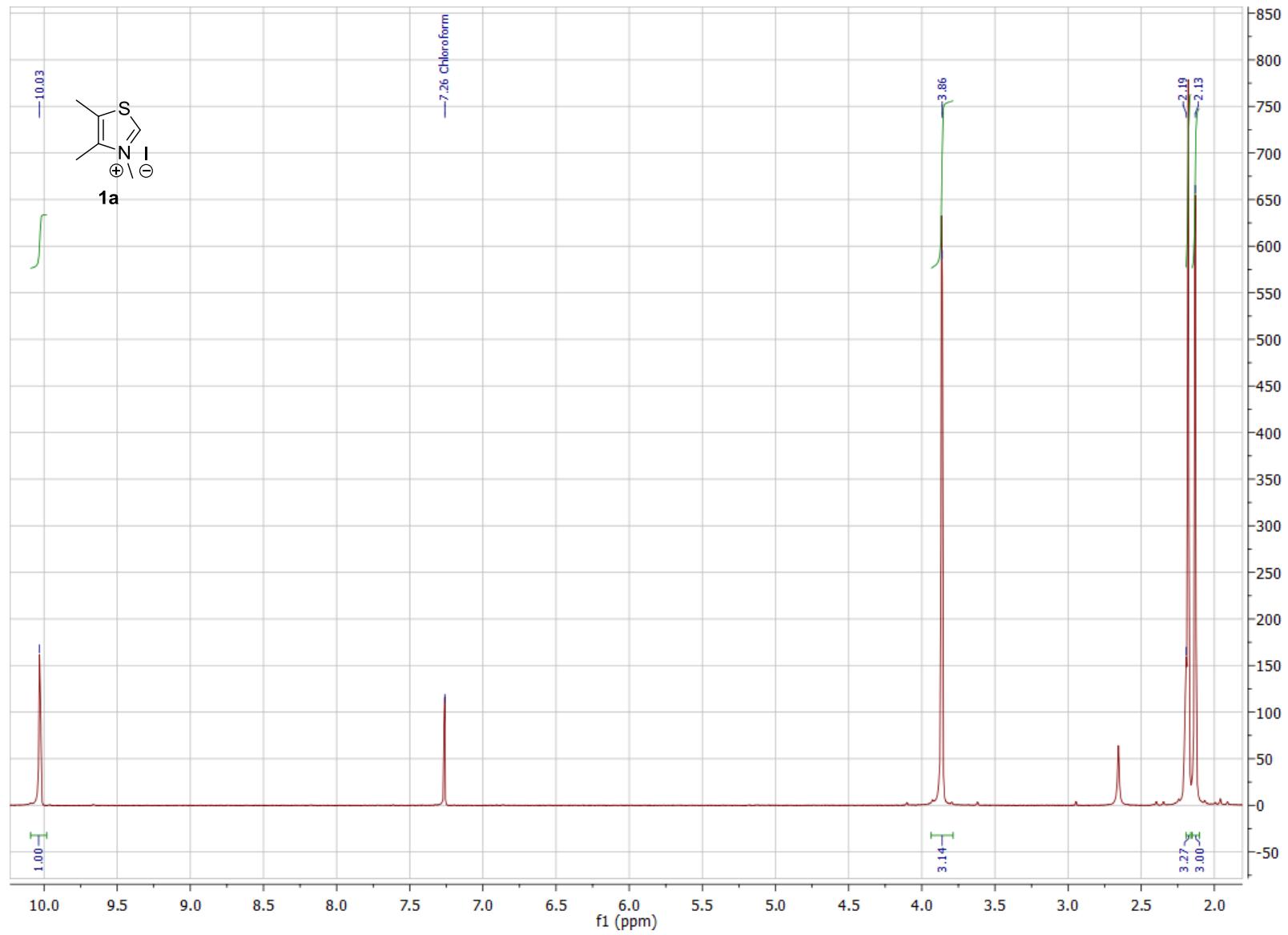
#### A.3.1.1 Overview of Tested Catalysts and Aldehydes – Correlation with Benzoin Formation

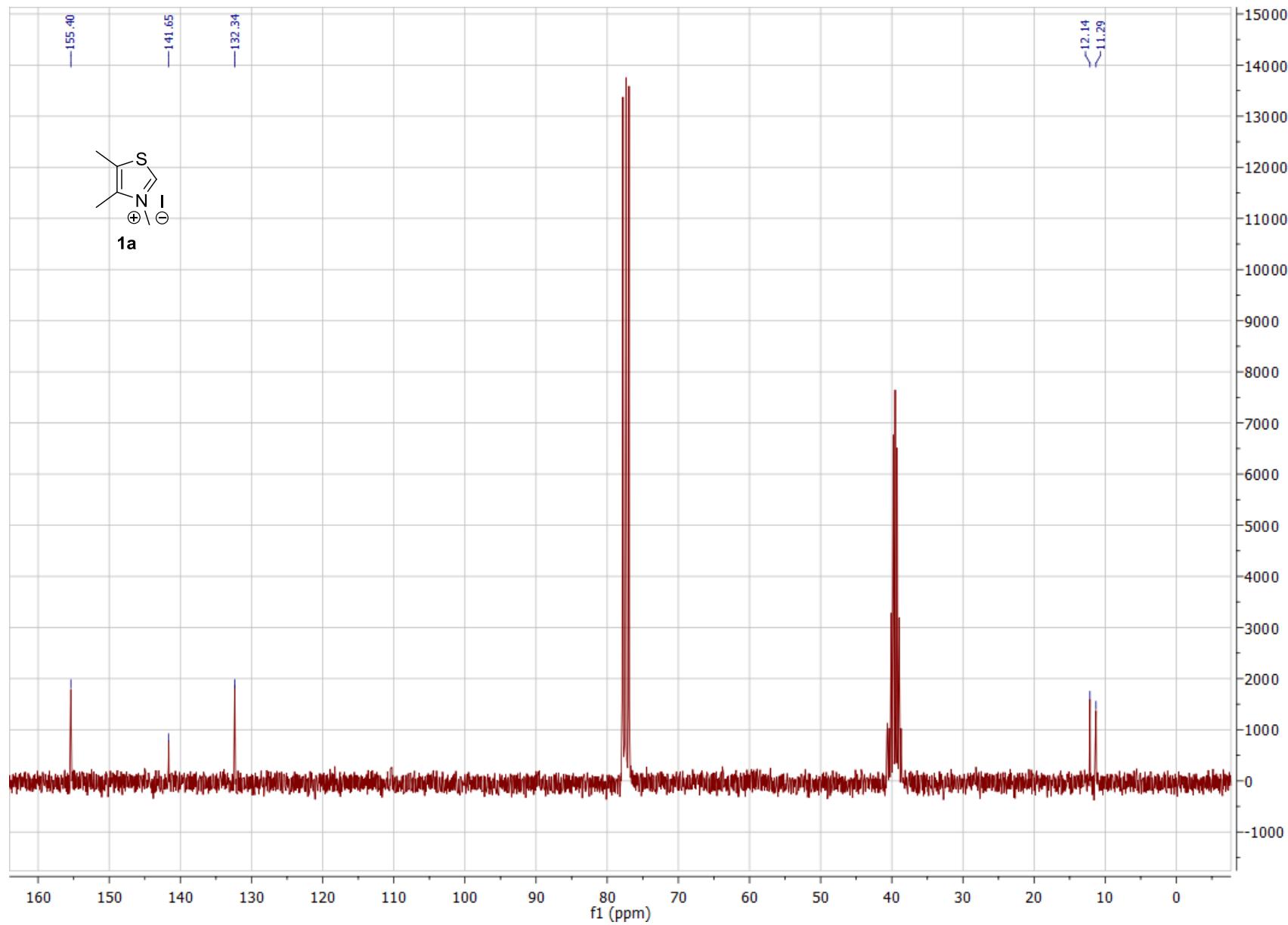
**Table 15** 0.4 M in **3a**, 0.1 eq pre-cat in *i*-PrOH if not stated otherwise. Determined after evaporation of solvent under reduced pressure and re-solvation in CDCl<sub>3</sub>. Pre-catalysts: 3,4-Dimethyl-5-(2-hydroxyethyl)thiamine chloride (**1d**), Thiamine hydrochloride (**1e**)

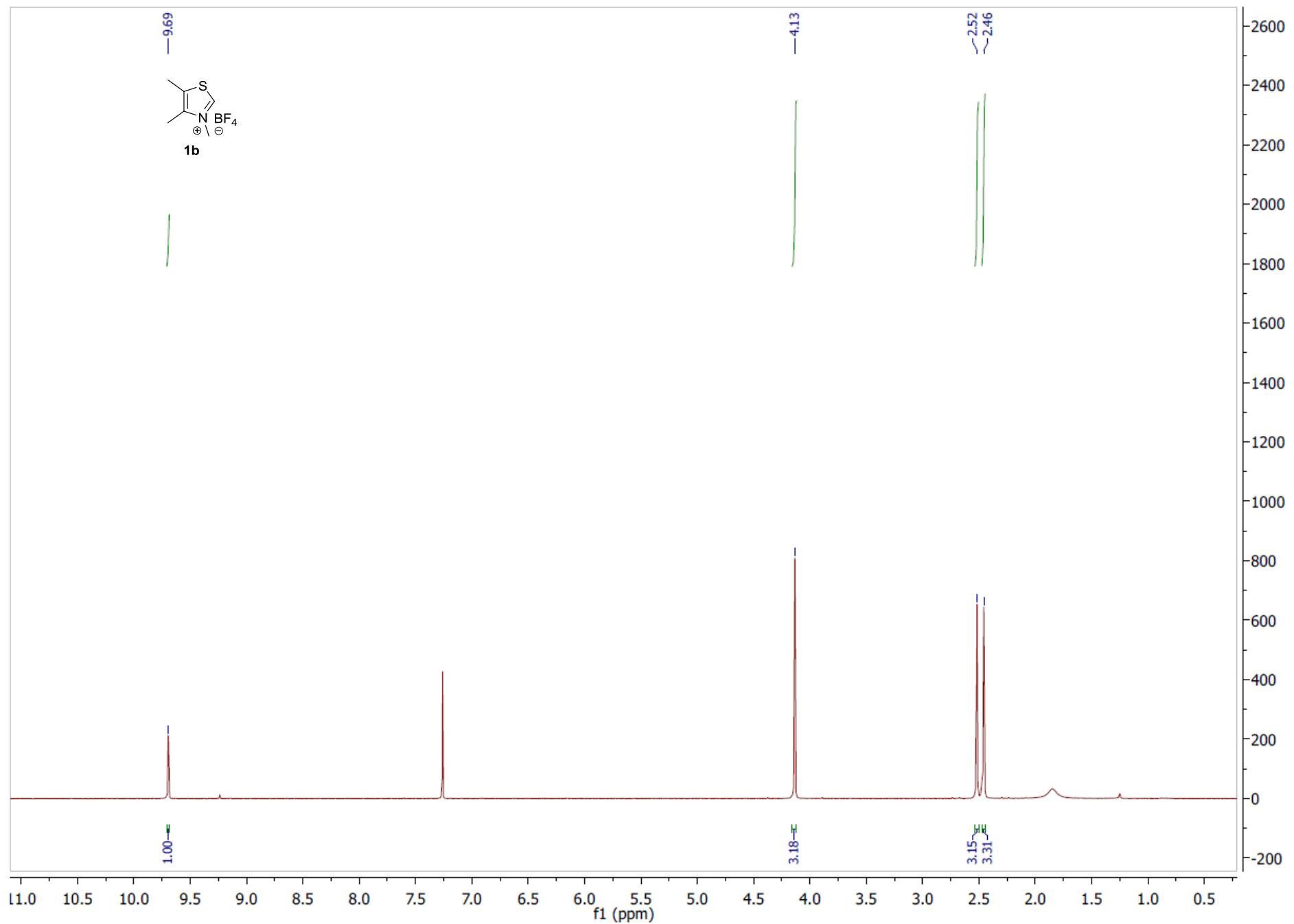
entry	(Pre)-catalyst	RCHO	EPR signal?	benzoin formed?	conversion to benzoin after 3h [%]
1	<b>1a</b>		Yes	Yes	56
2	<b>1b</b>		Yes	Yes	98
3	<b>1c</b>	<b>3a</b>	Yes	Yes	99
4	<b>1d</b>		Yes	Yes	58
5	<b>1e</b>		Yes	Yes	80
6		<b>3a</b>	Yes	Yes <sup>a</sup>	56 <sup>a</sup>
7		<b>3b</b>	No	Yes	>95
8		<b>3d</b>	Yes	Yes	44 <sup>a</sup>
9		<b>3e</b>	Yes	Yes	5 <sup>a</sup>
10	<b>1a</b>	<b>3f</b>	Yes	Yes	80 <sup>a</sup>
11		<b>3g</b>	Yes	Yes	16 <sup>a</sup>
12		<b>3h</b>	Yes	Yes	30
13		<b>3i</b>	Yes	Yes	>95
17		<b>3j</b>	Yes	No	-

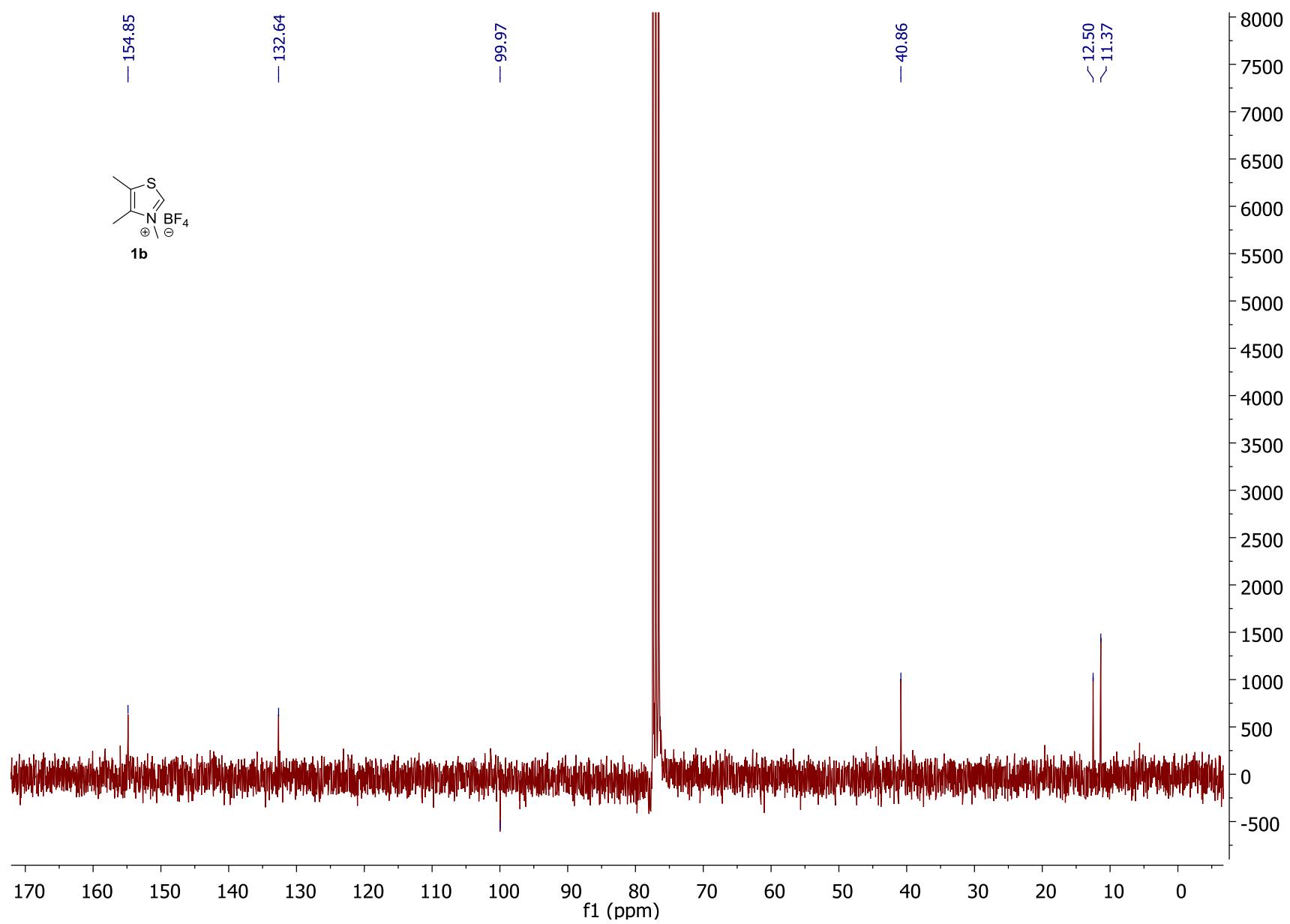
<sup>a</sup> Reaction conditions as follows in *i*-PrOH after 2h ([**3a**]<sub>0</sub> = 0.04M, 0.1 eq **1a** and 0.1 eq KOH)

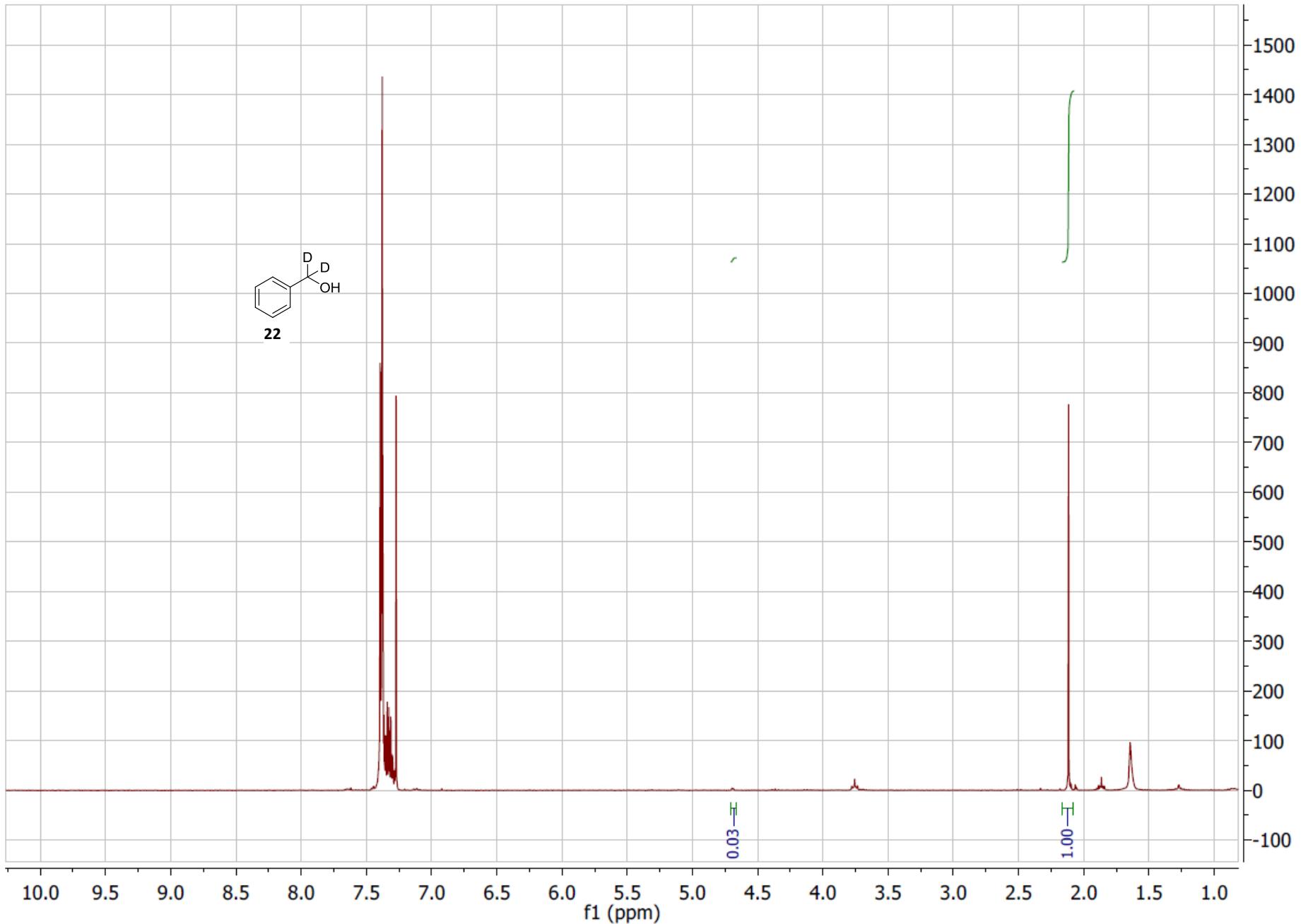
### A.3.2 NMR spectra

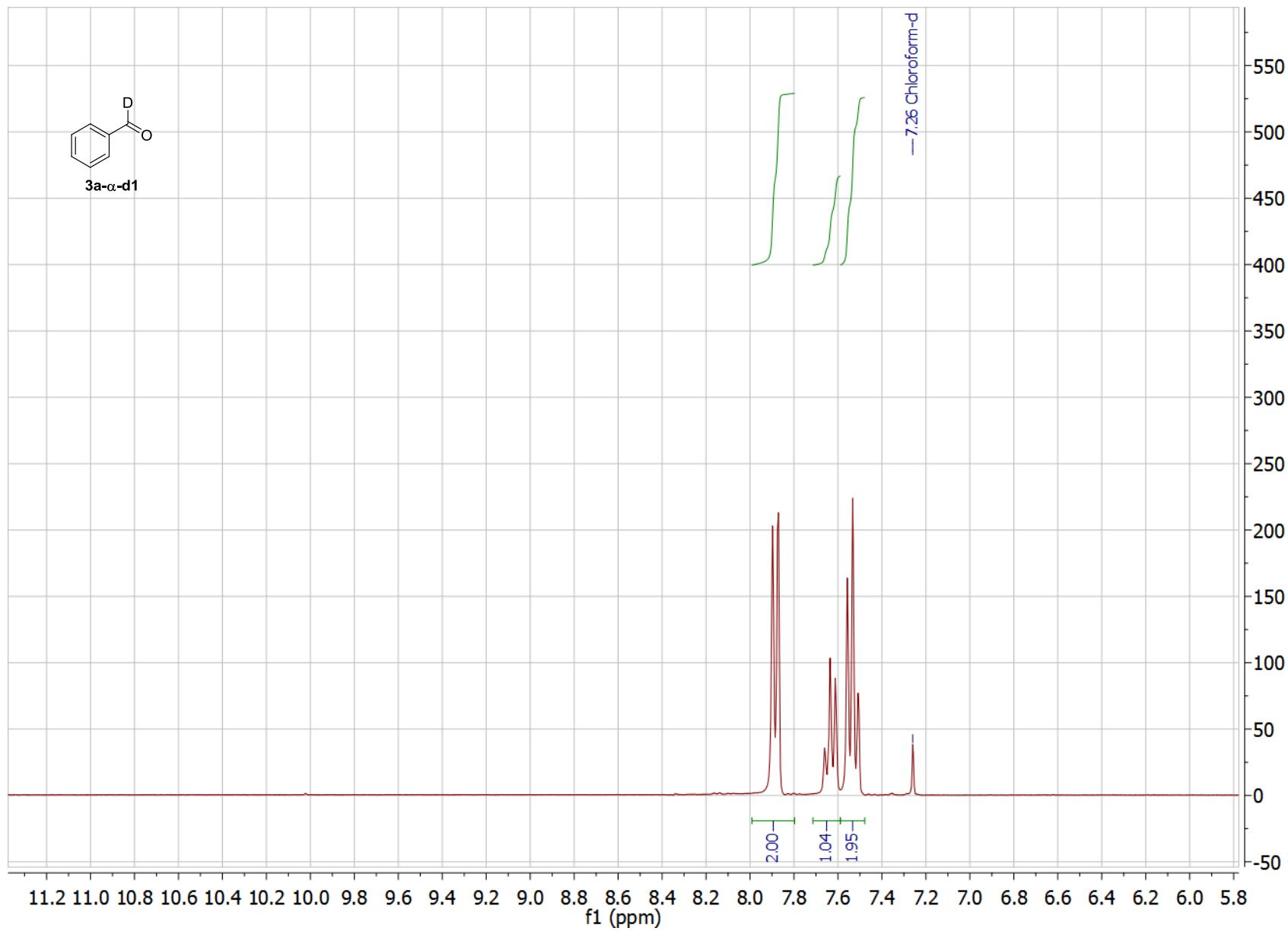


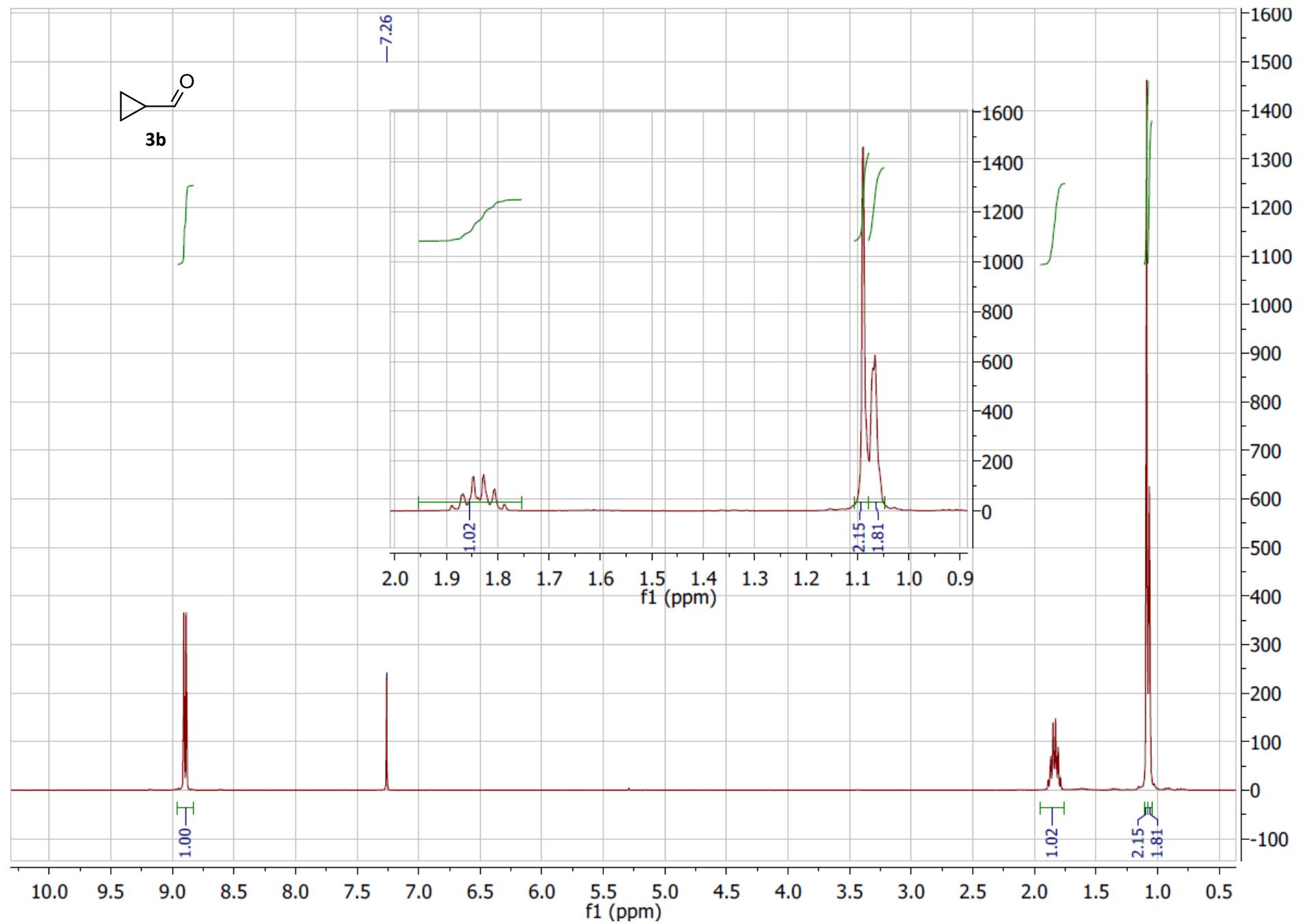


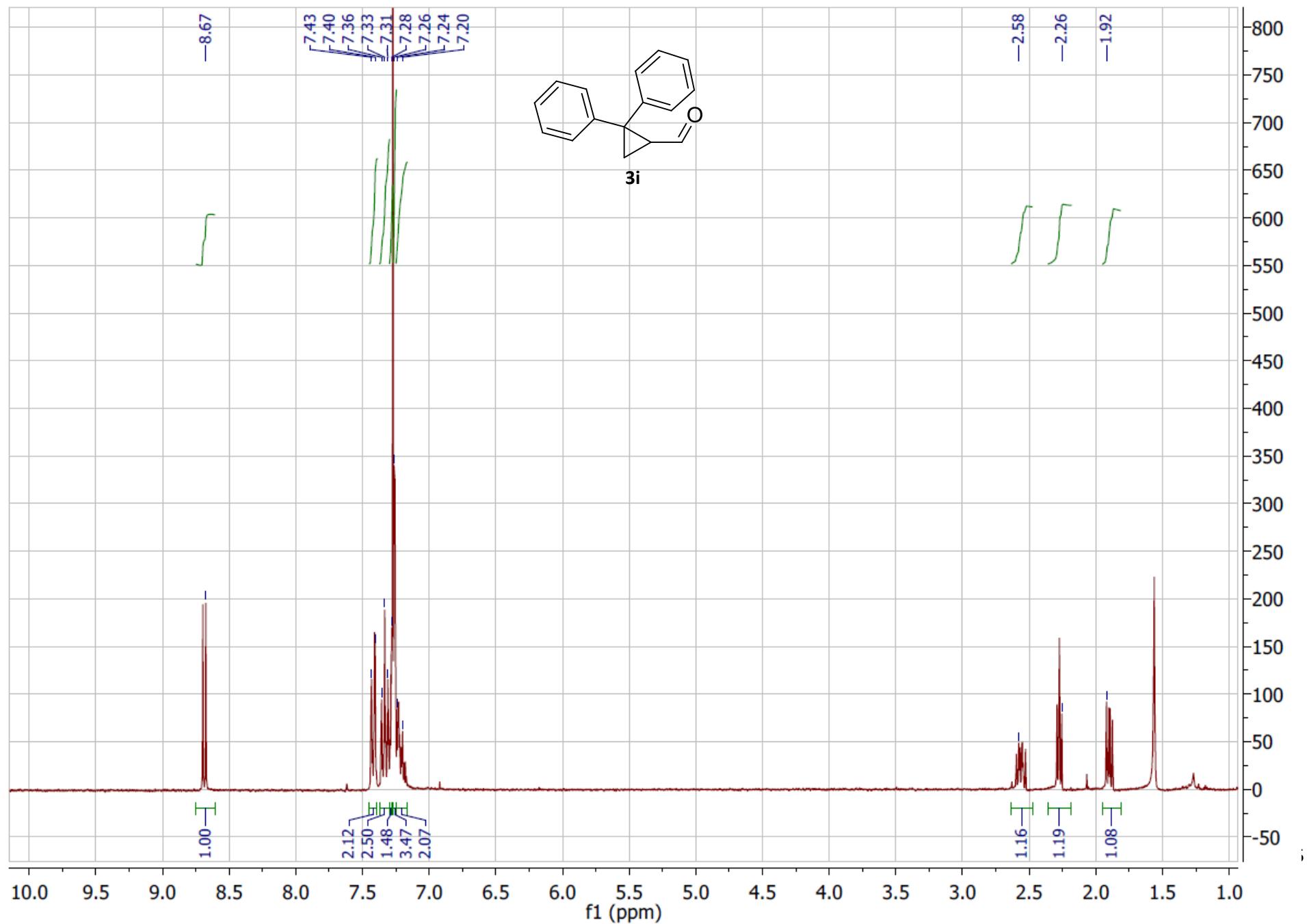


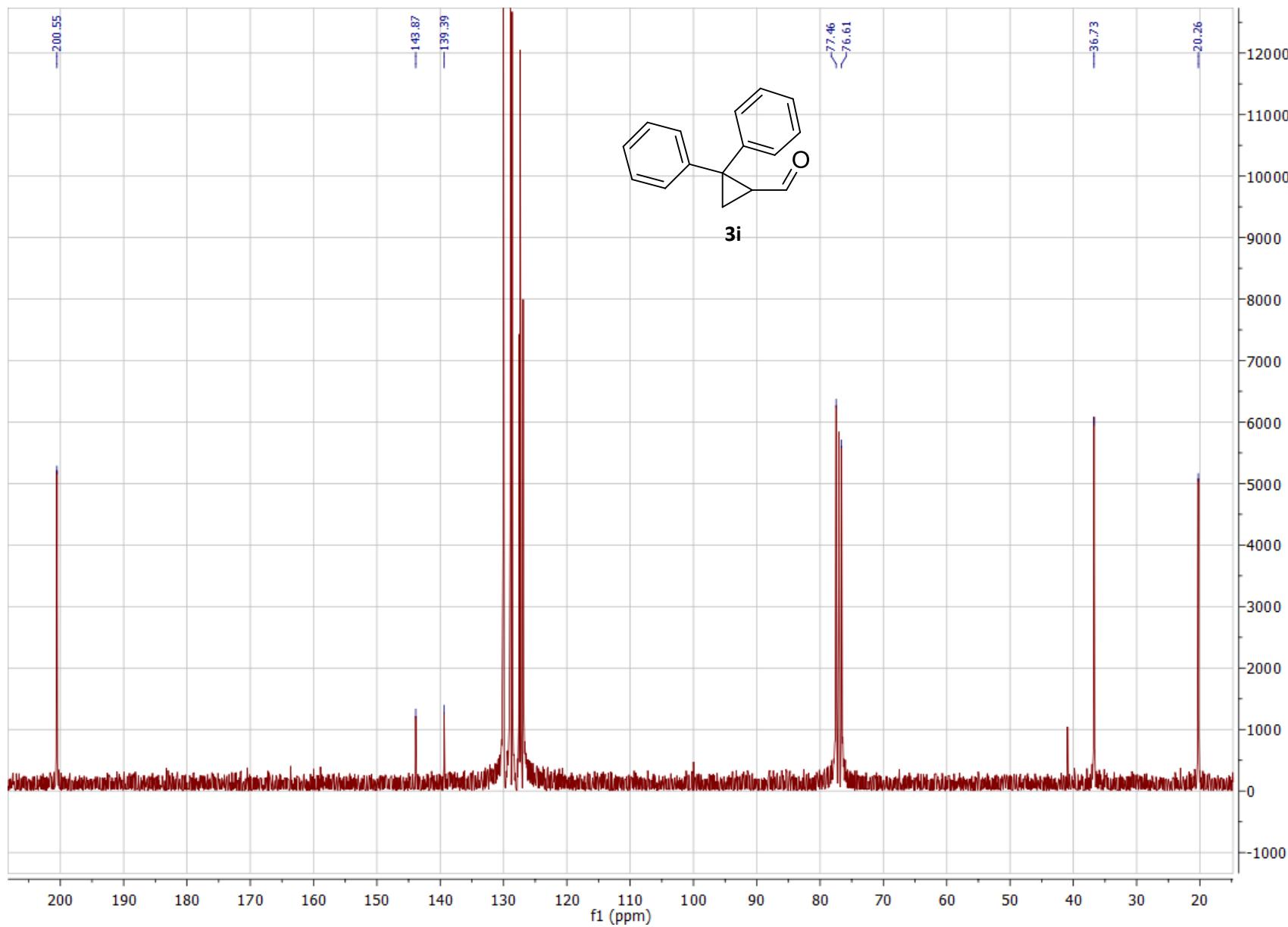


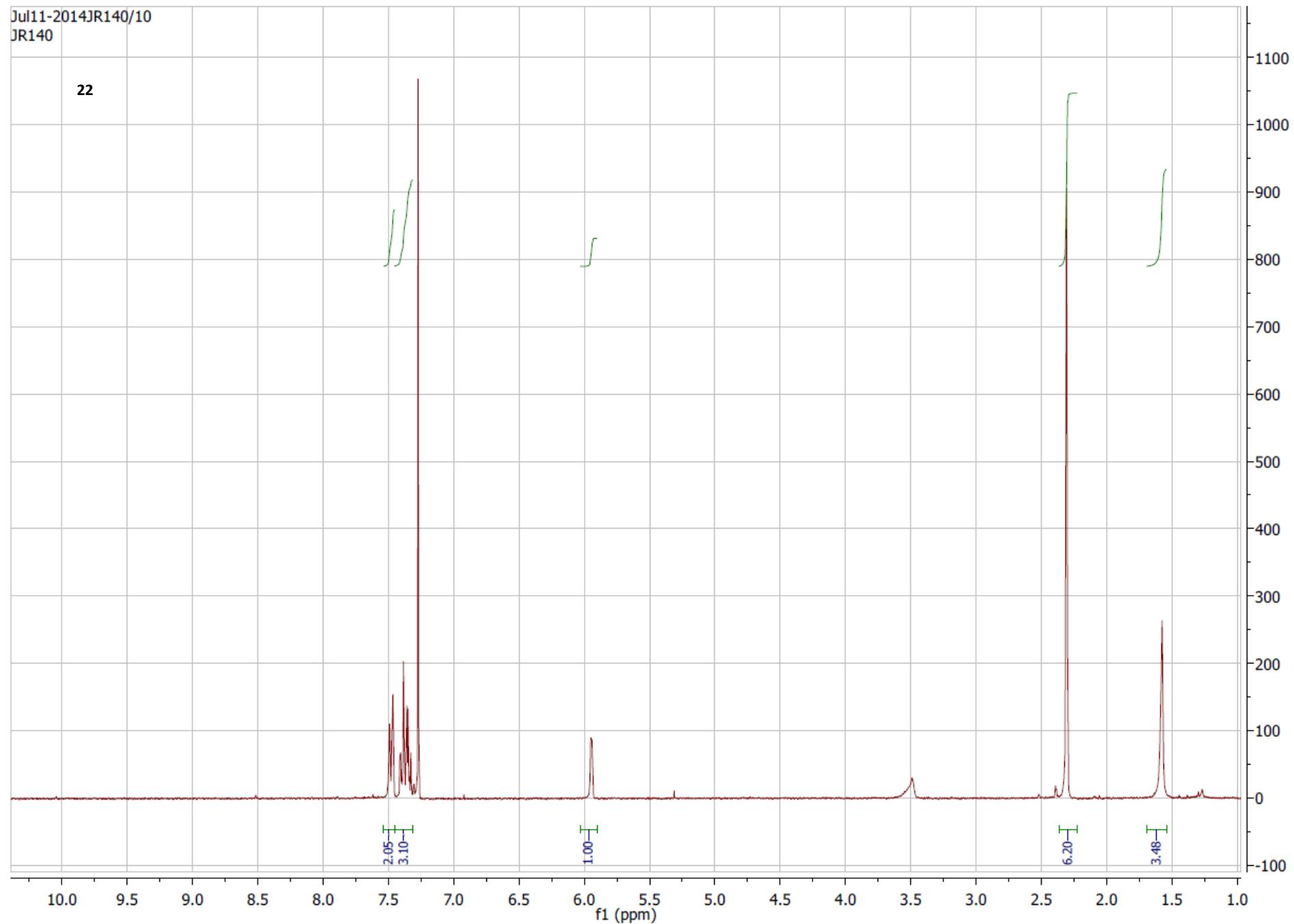


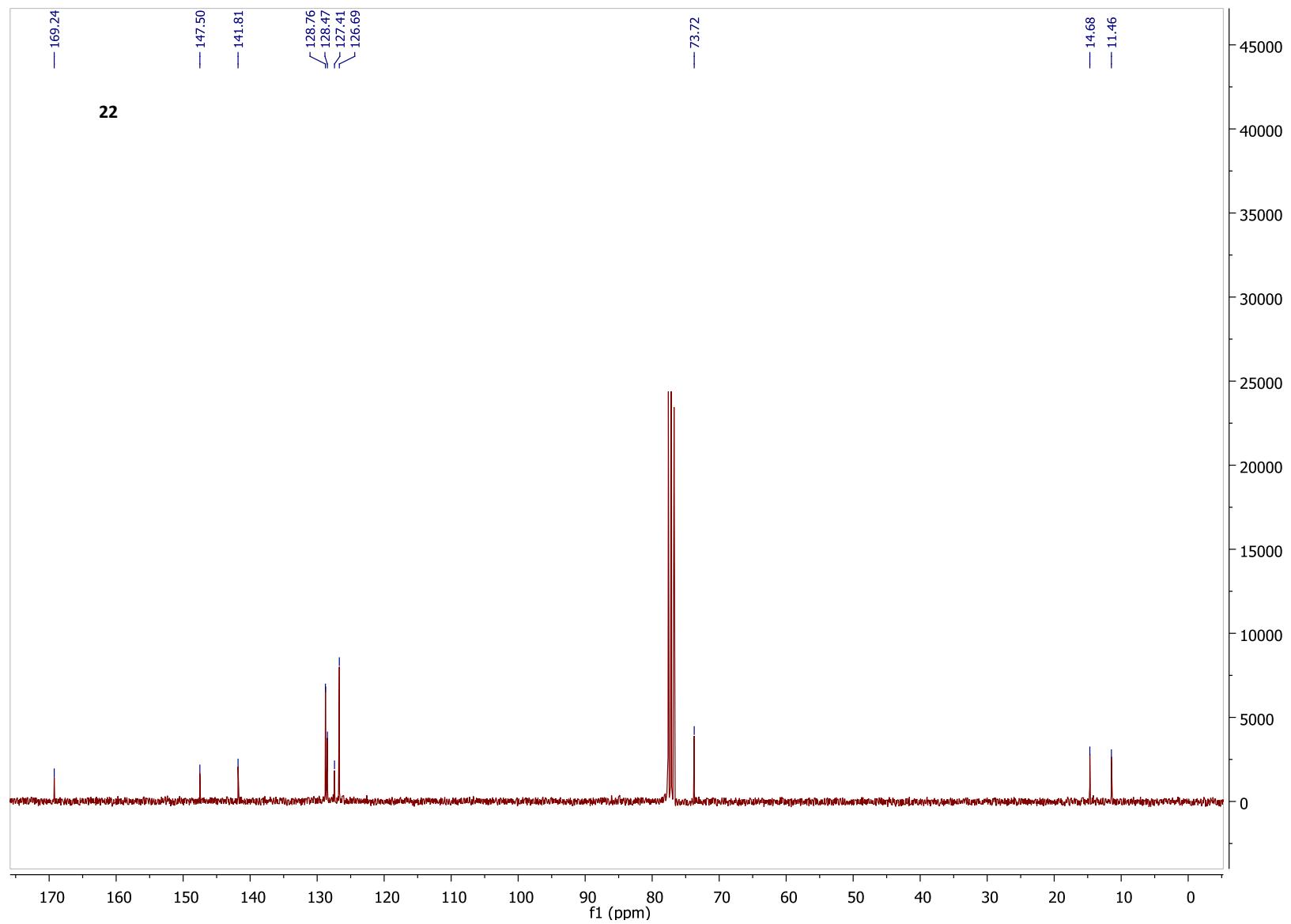




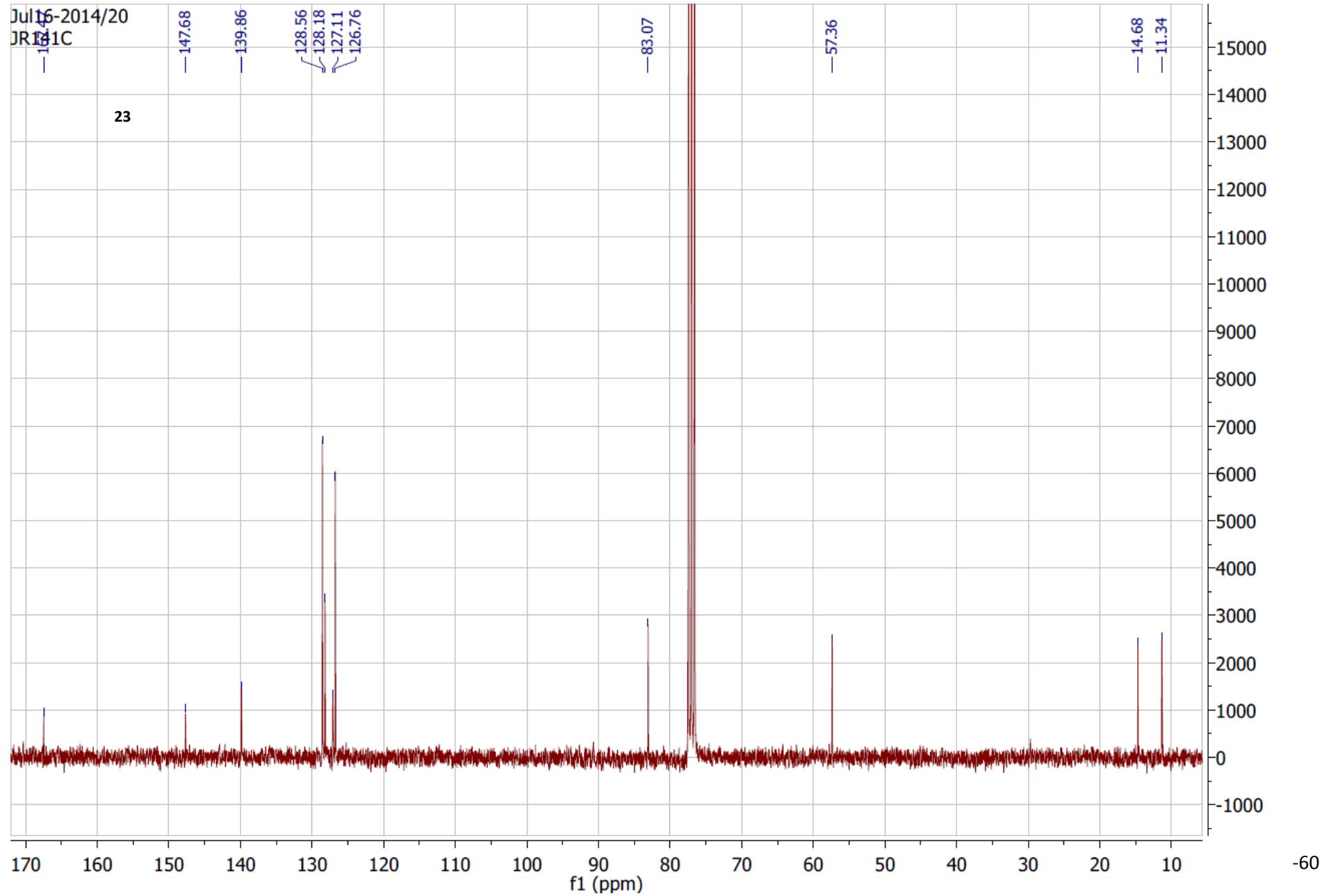


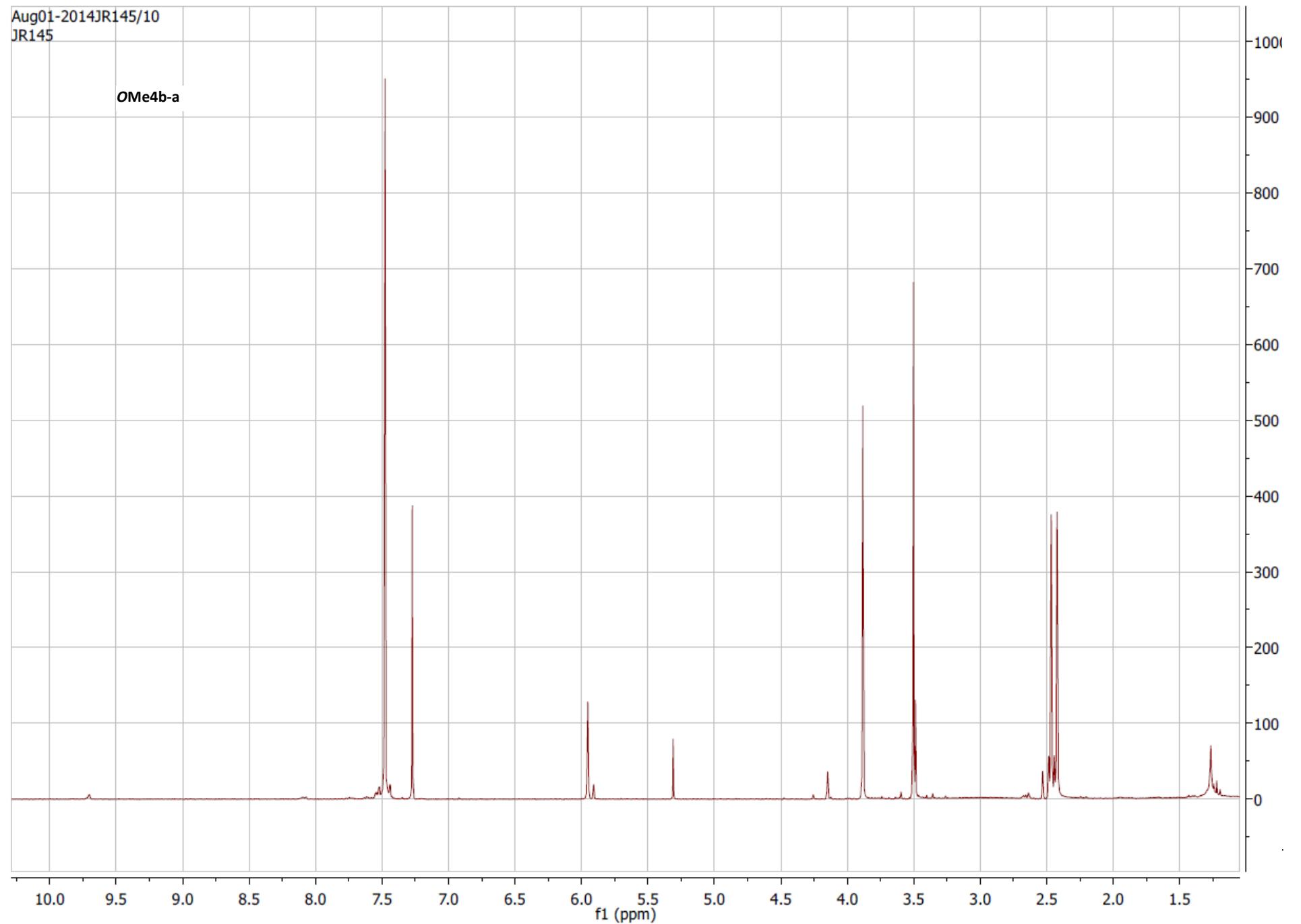


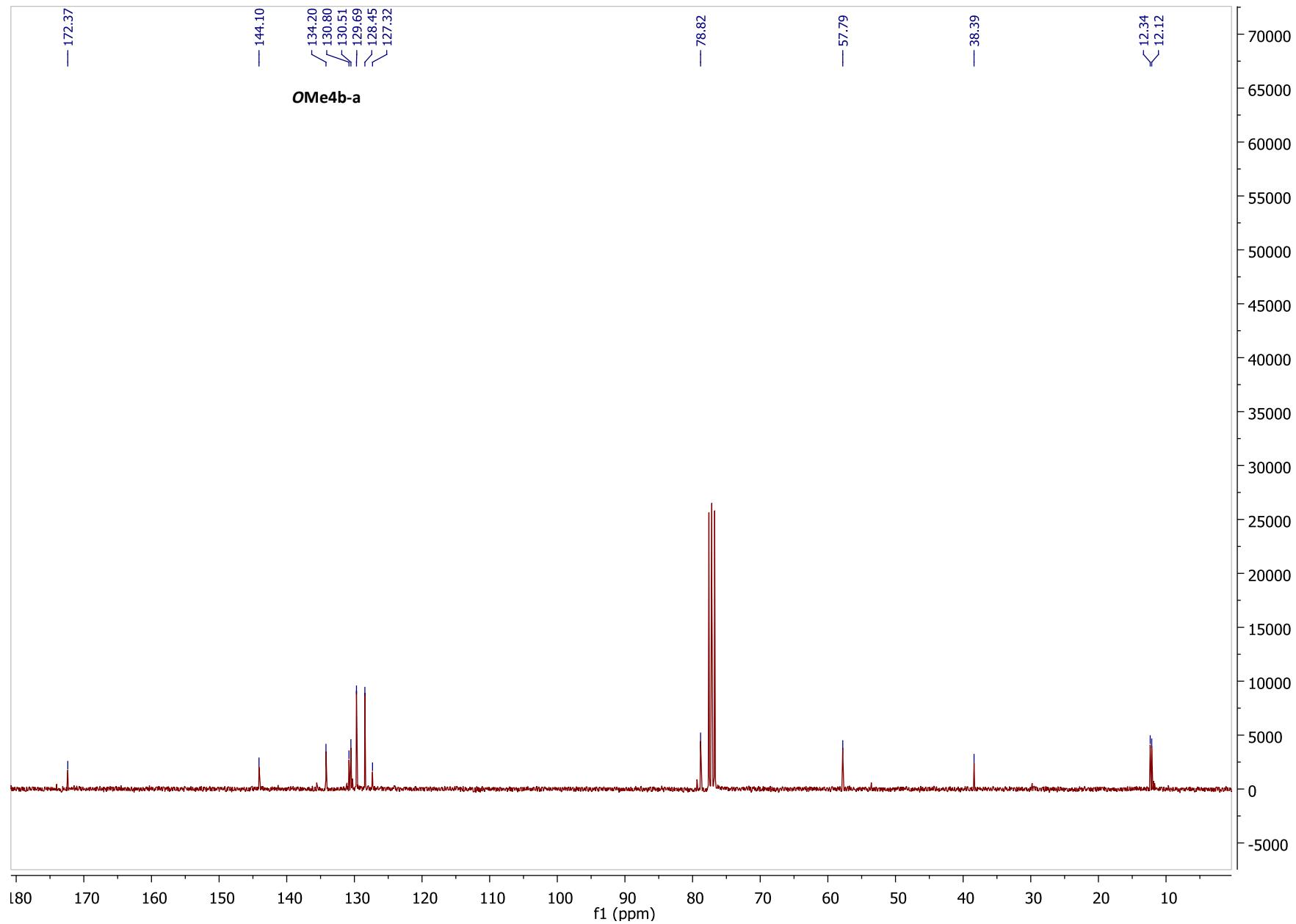


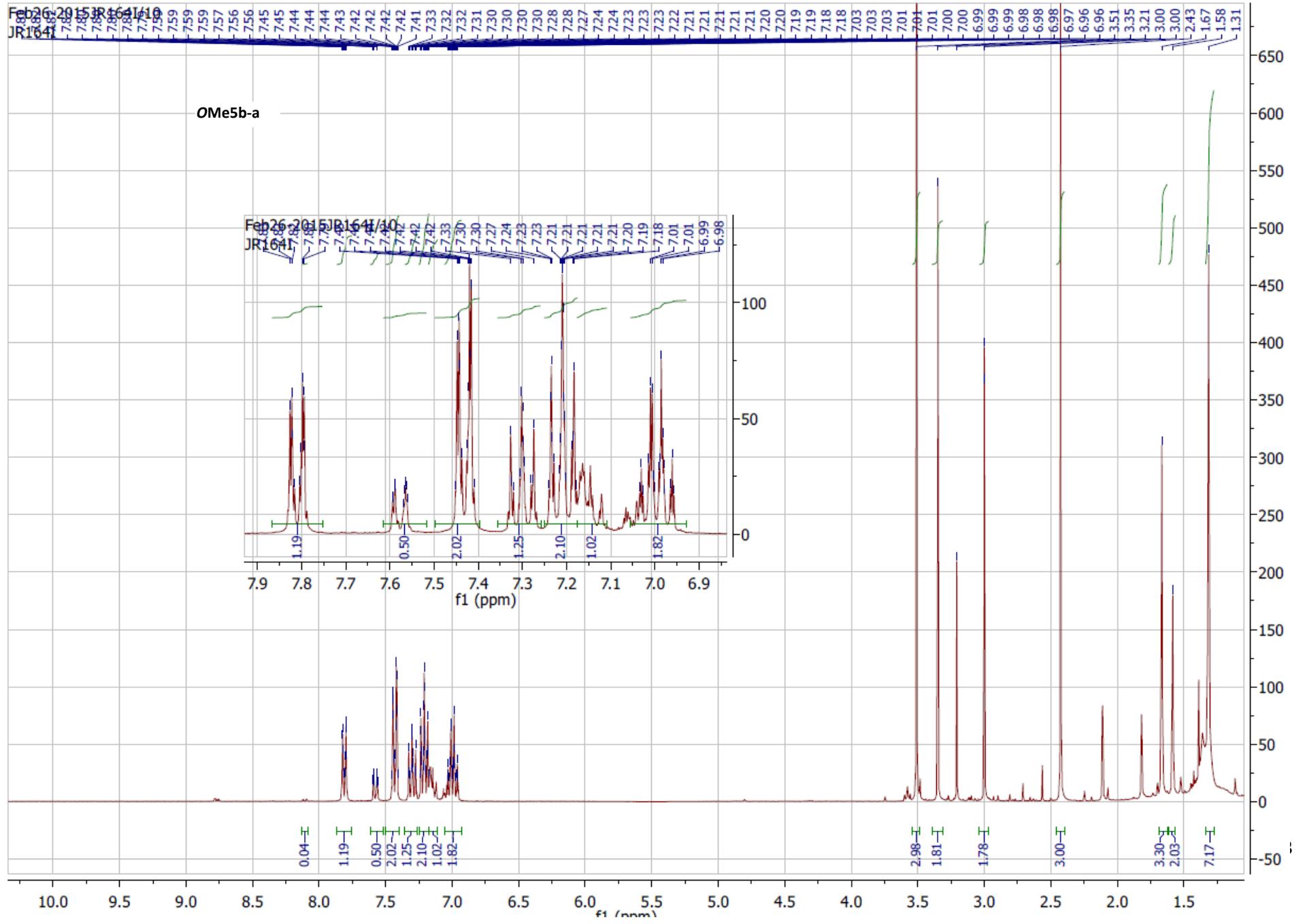


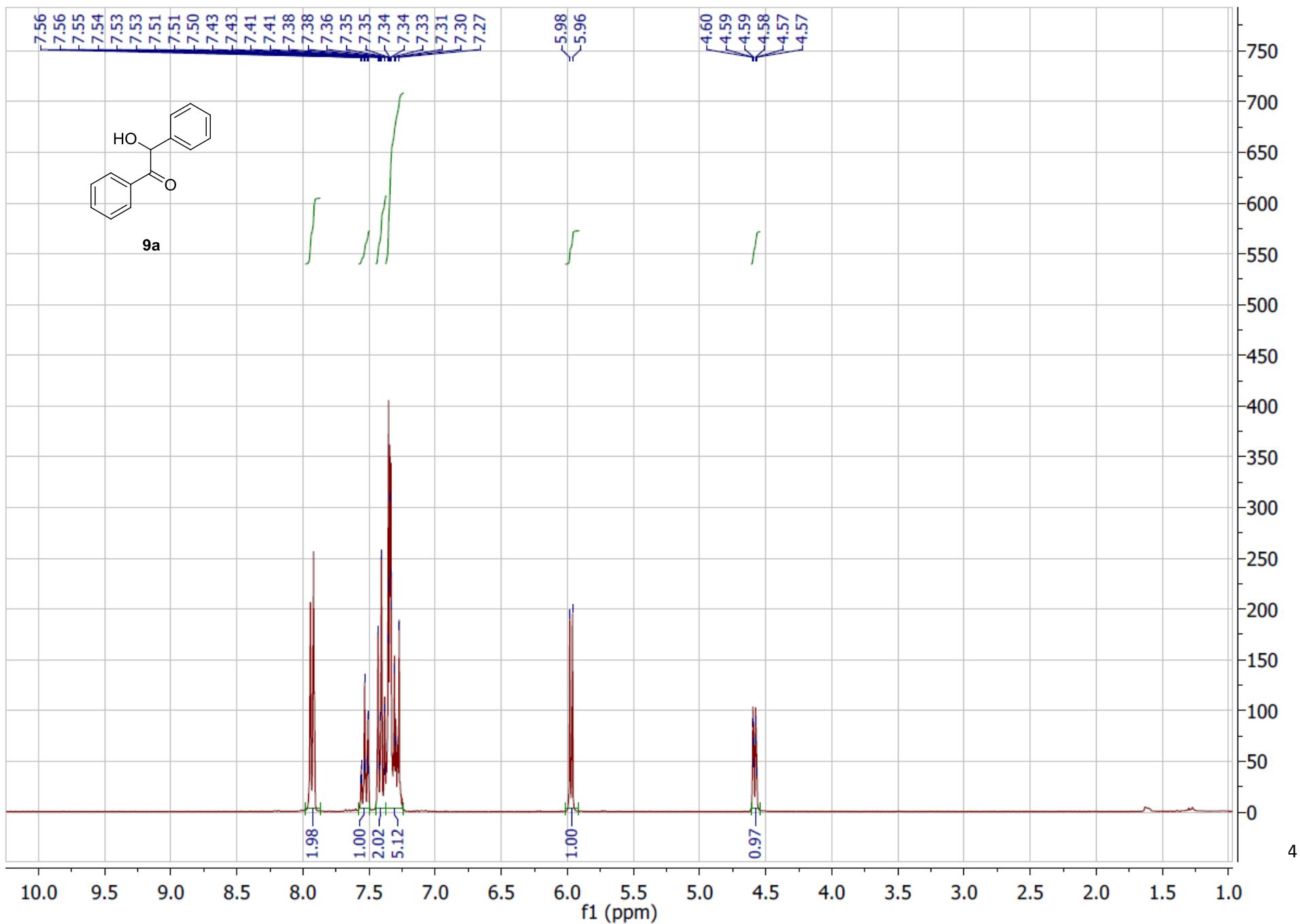


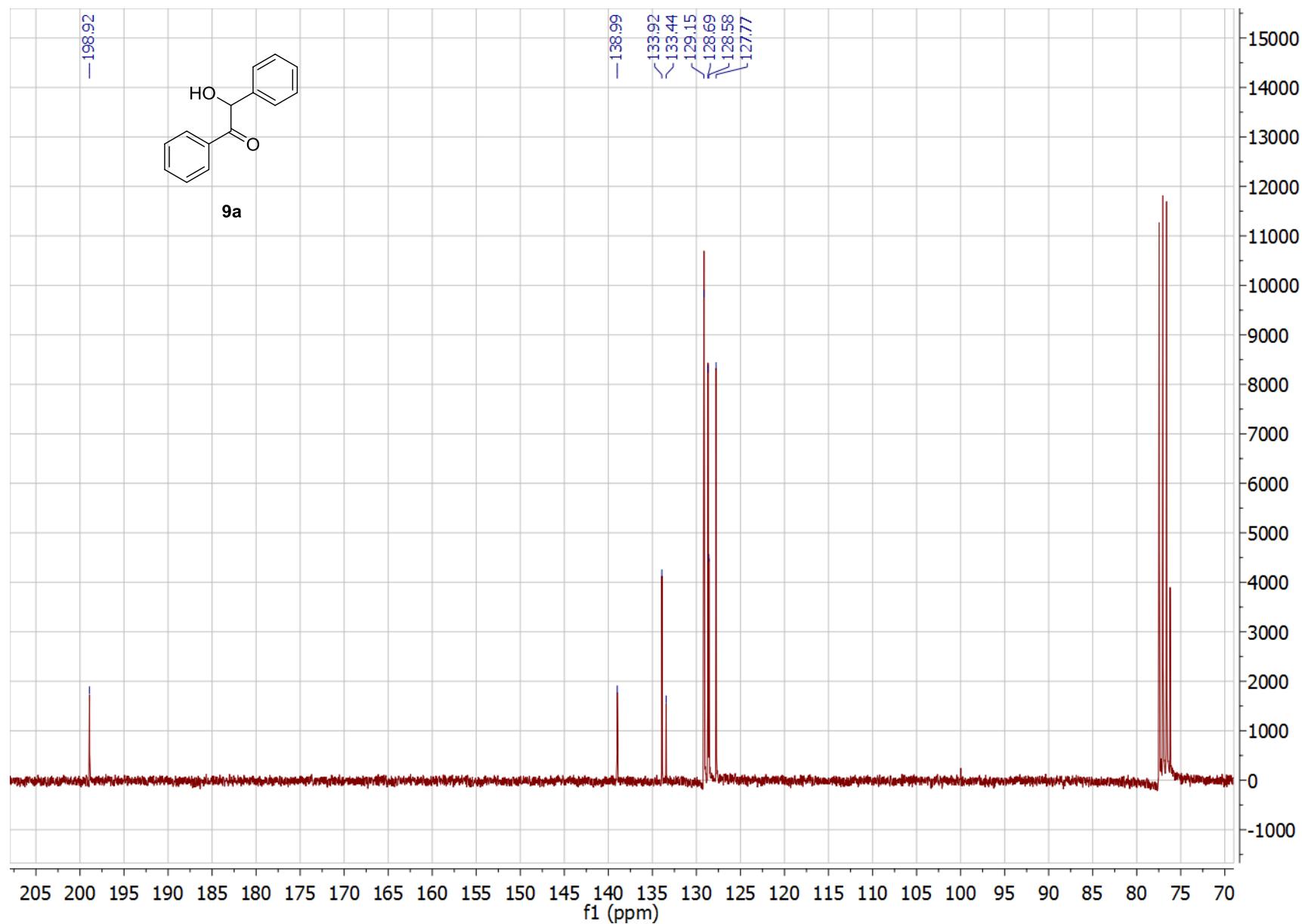


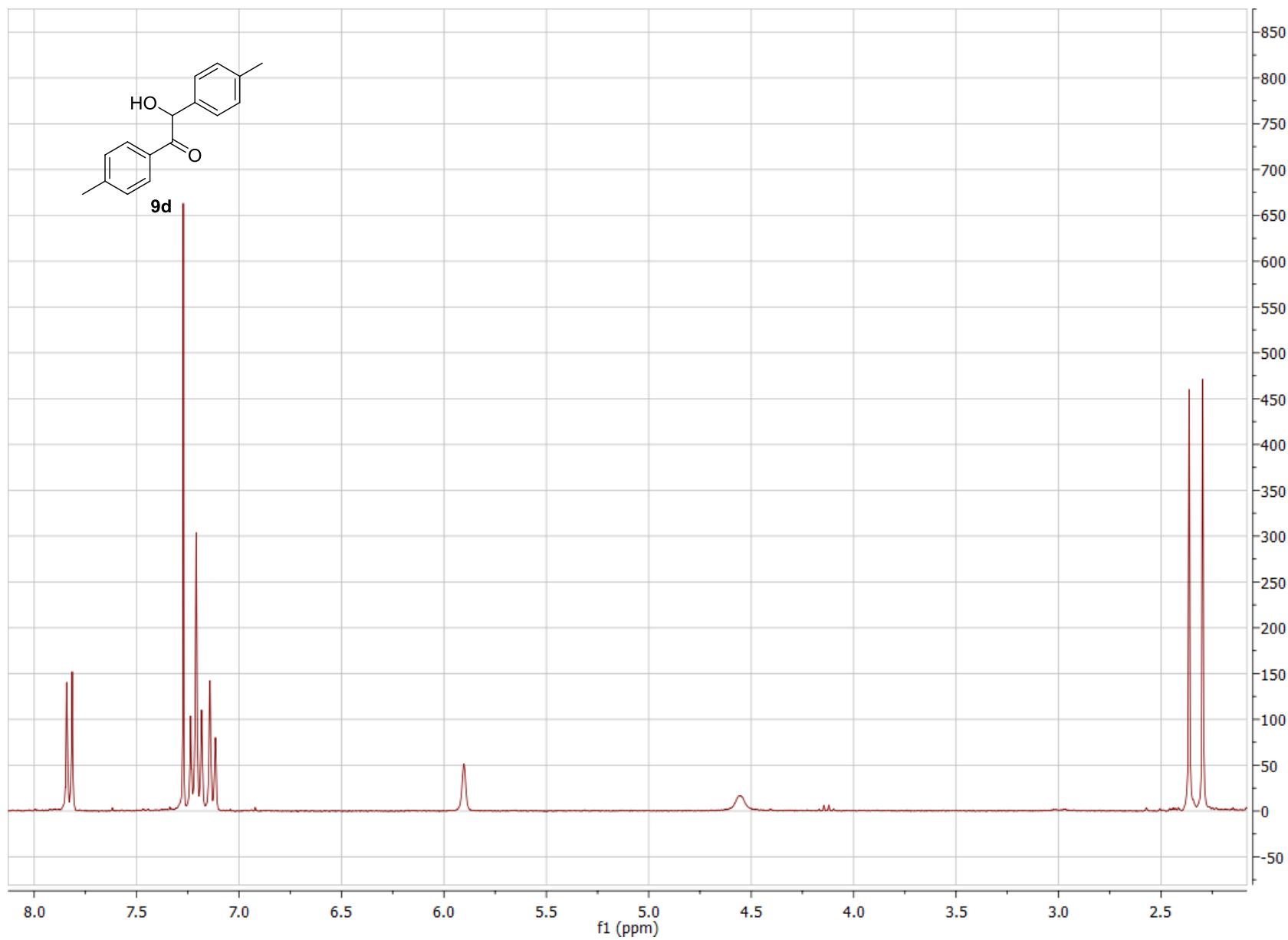


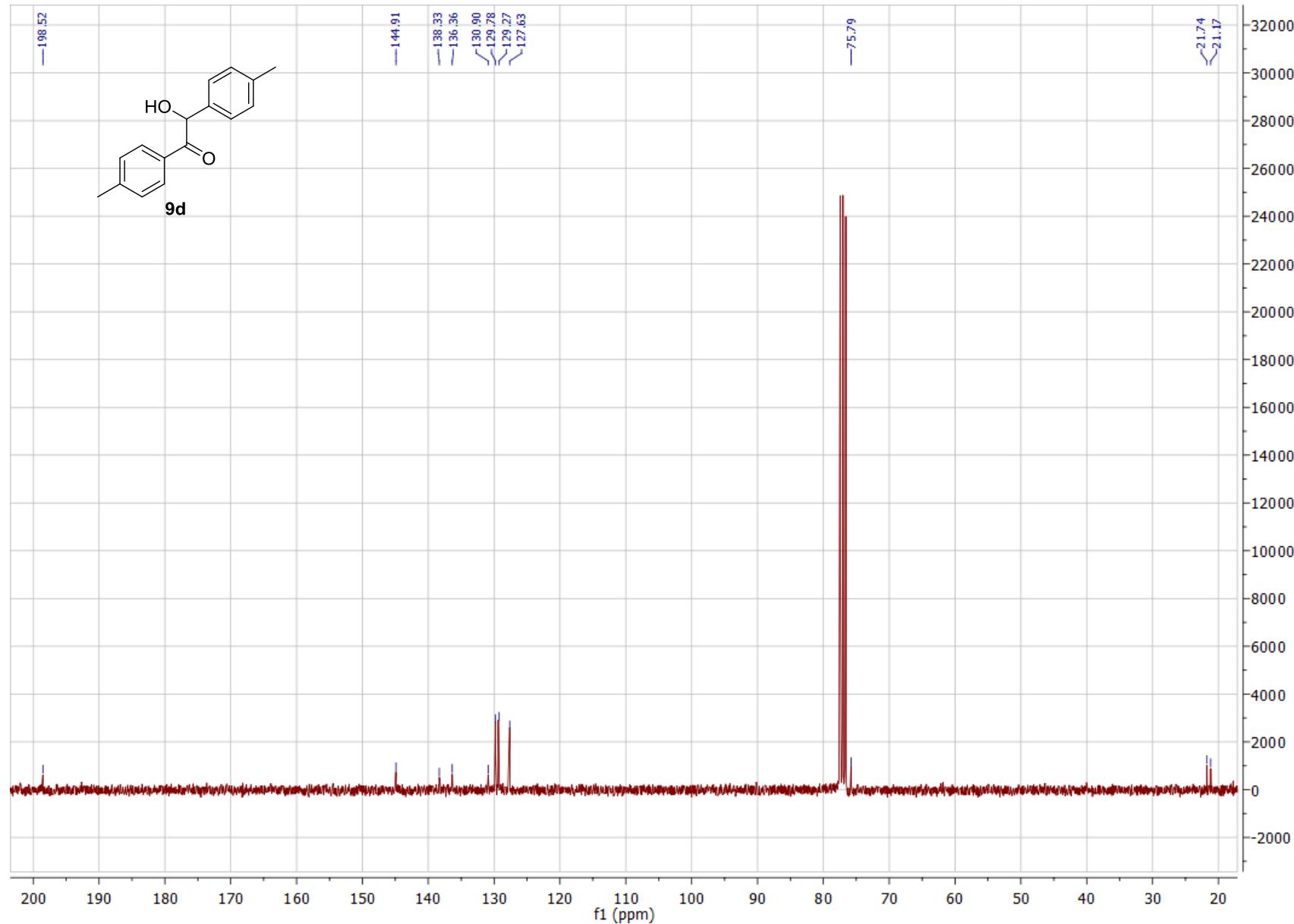


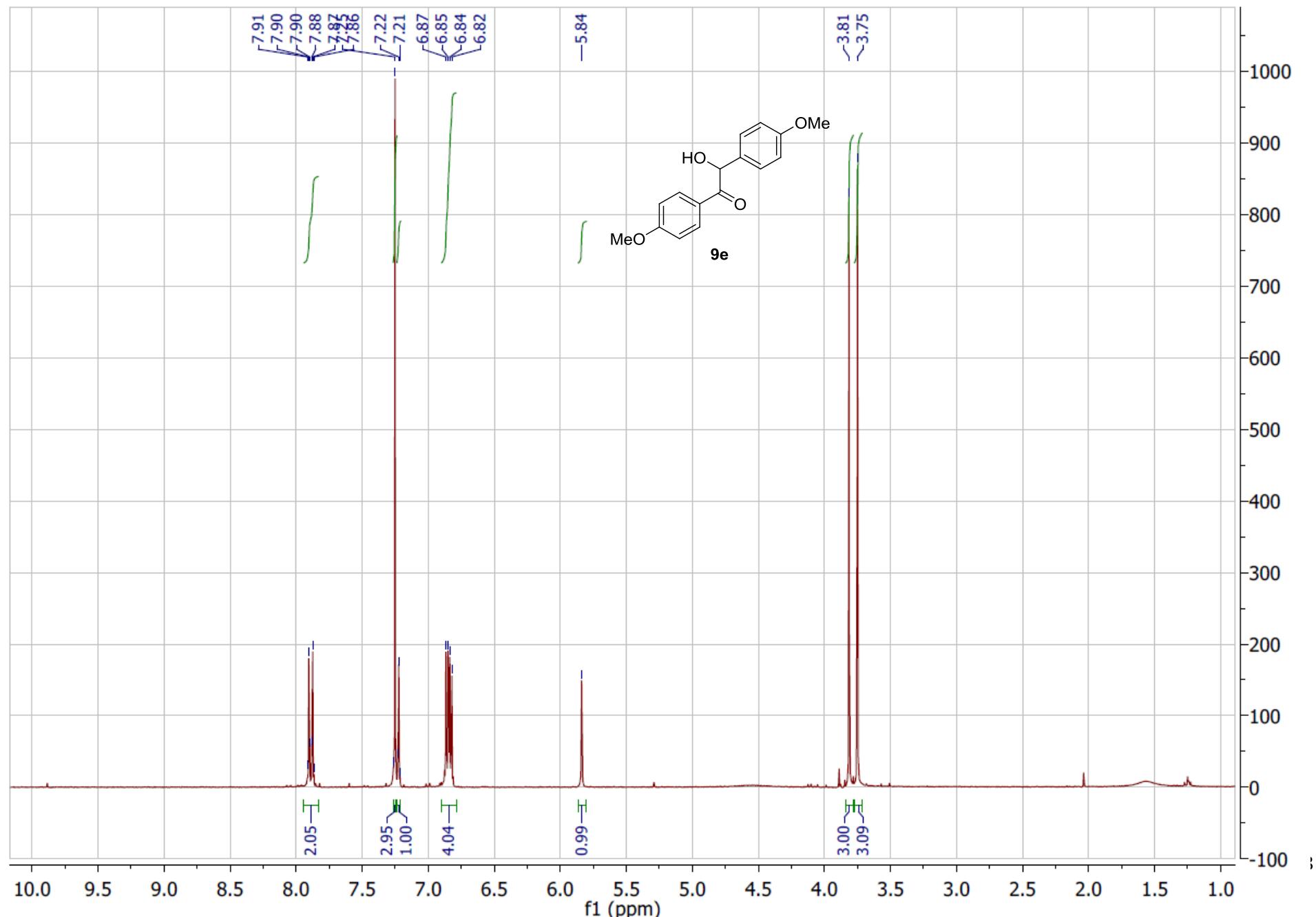


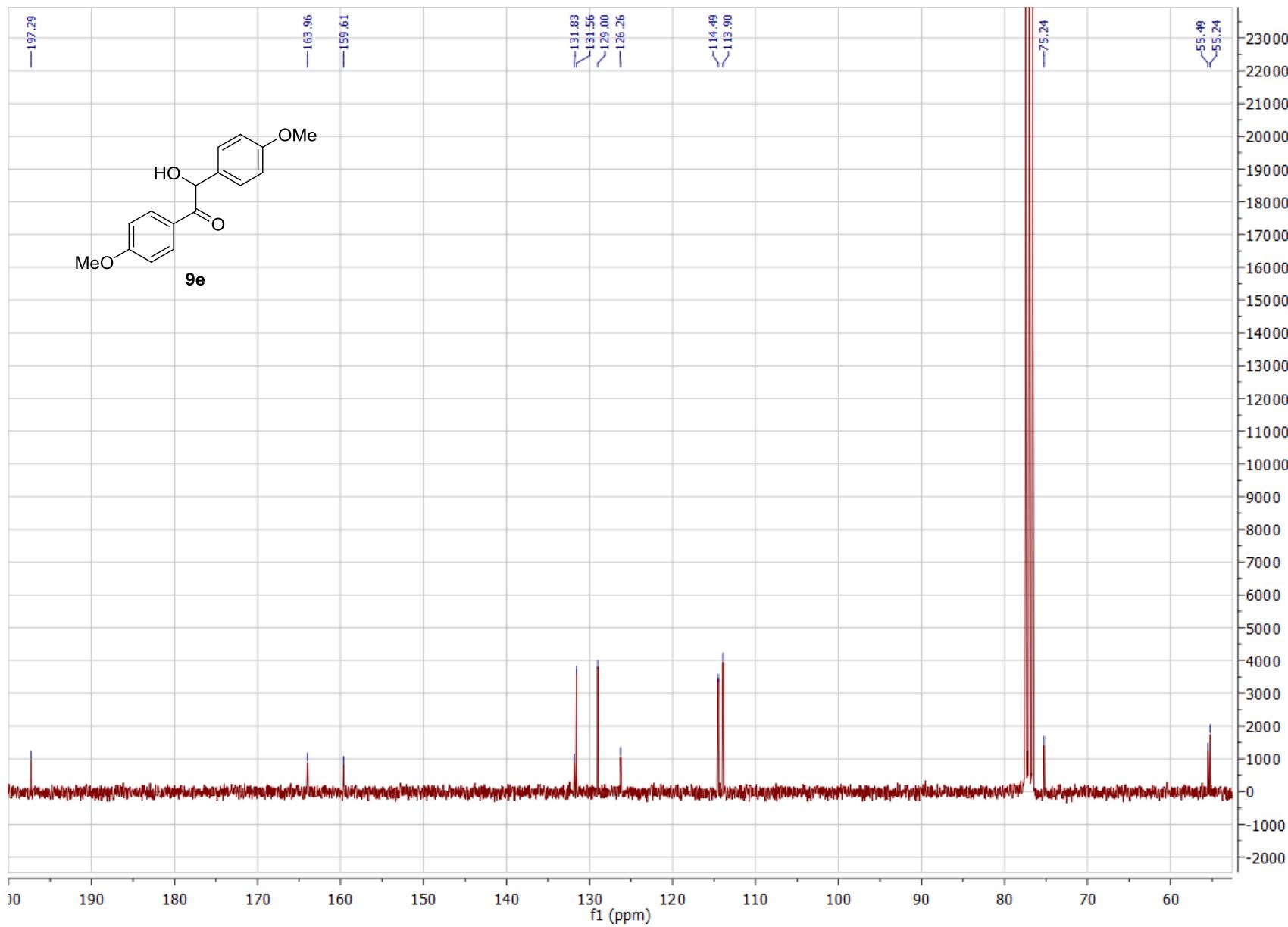


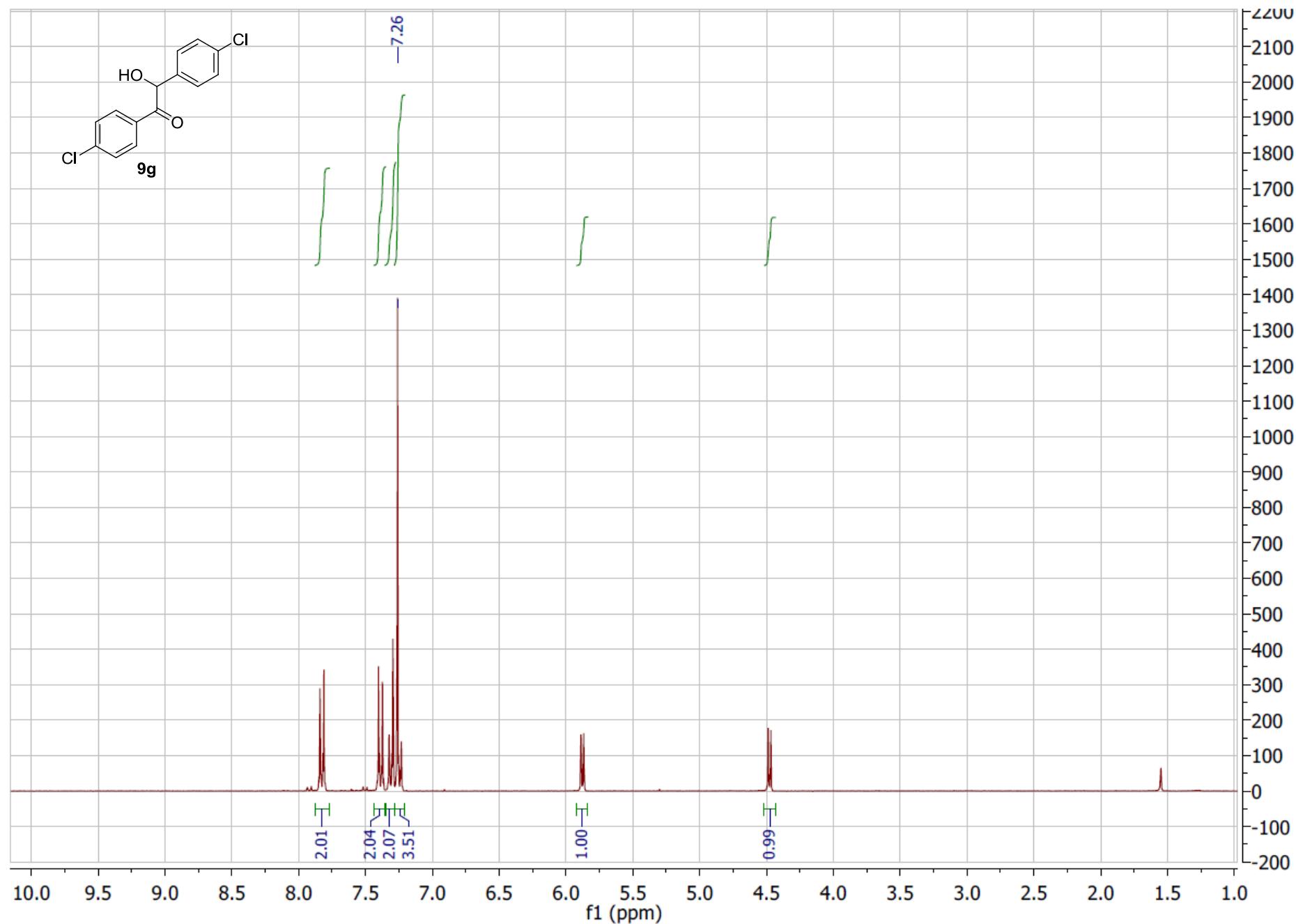


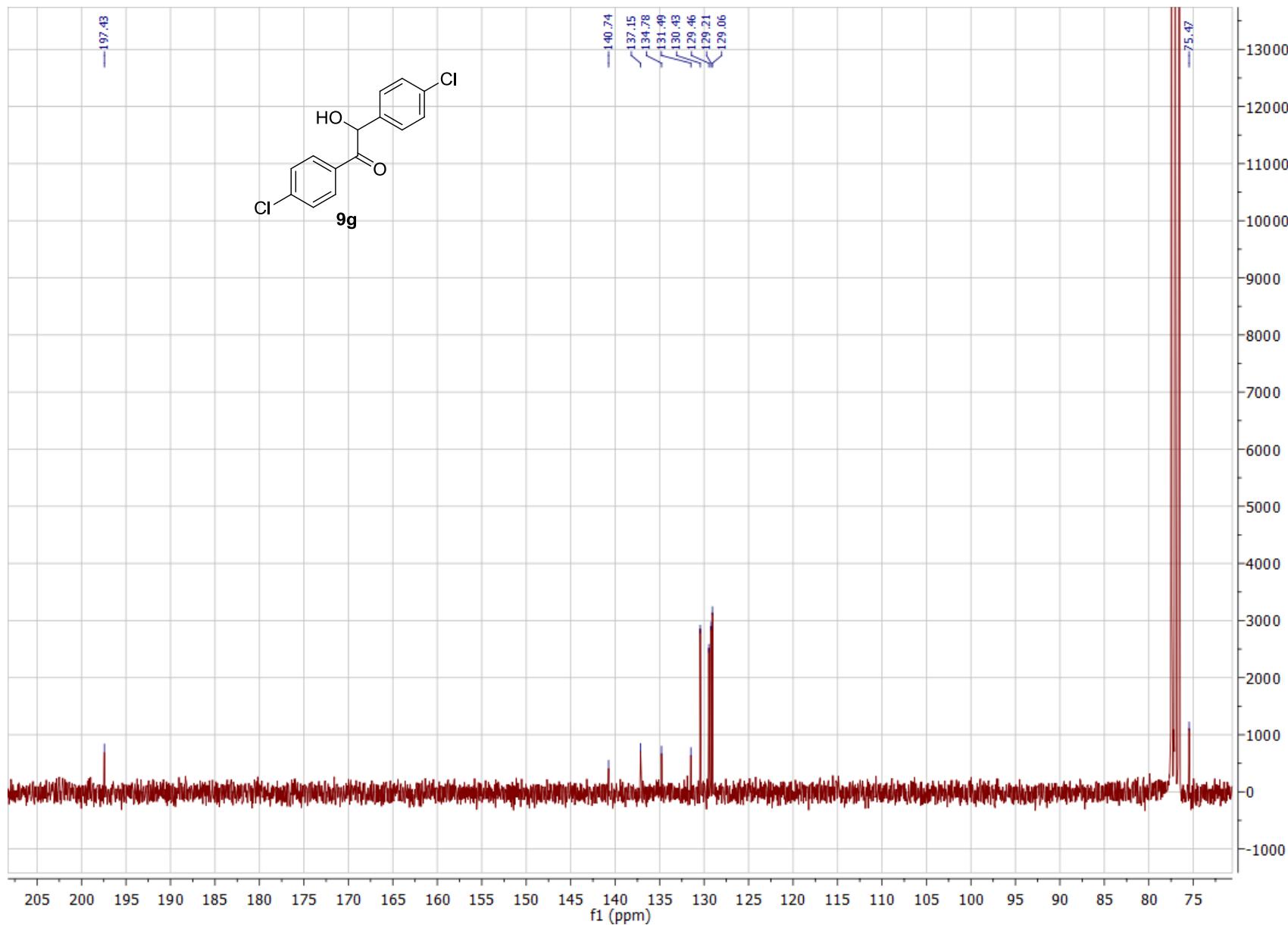


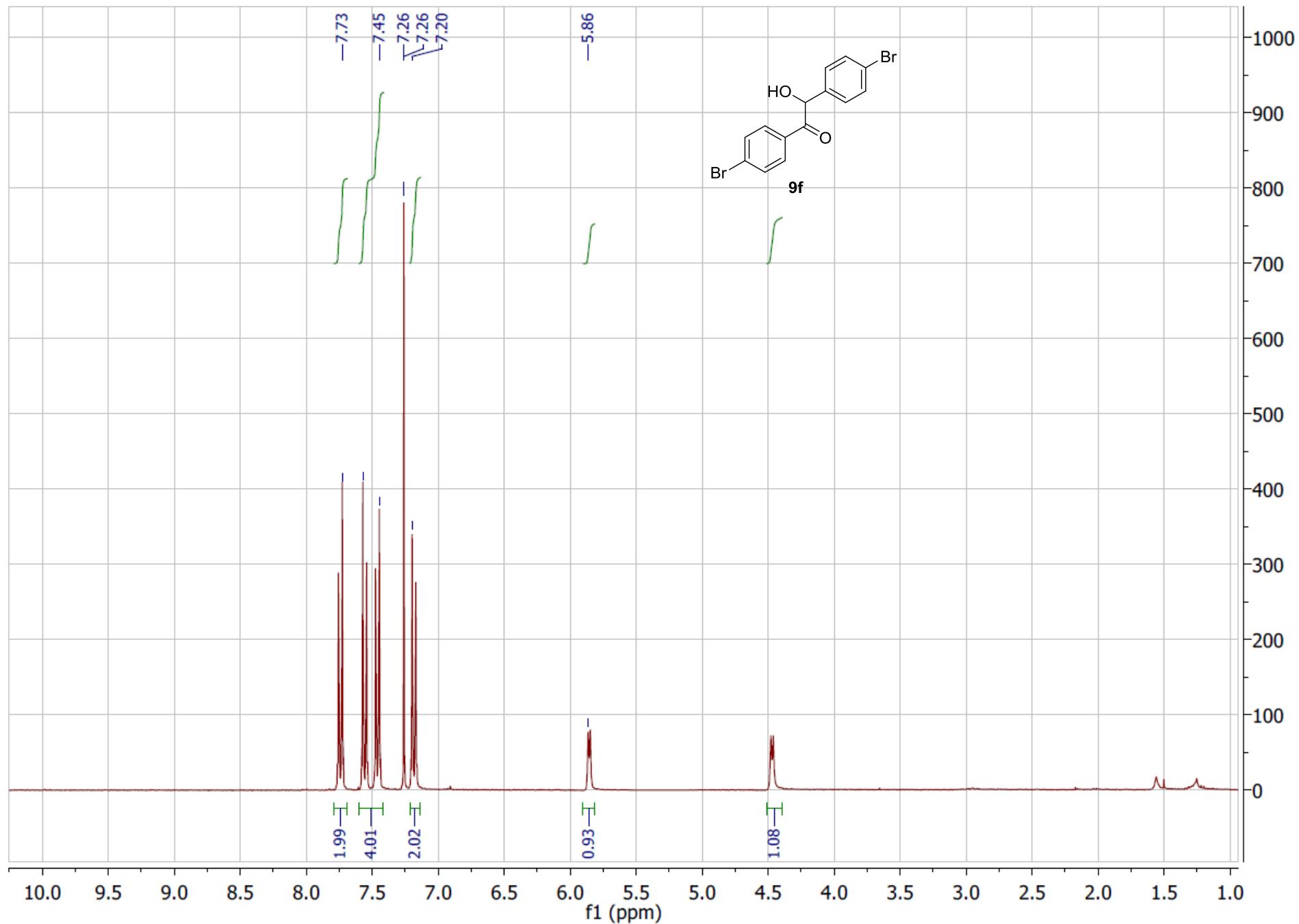


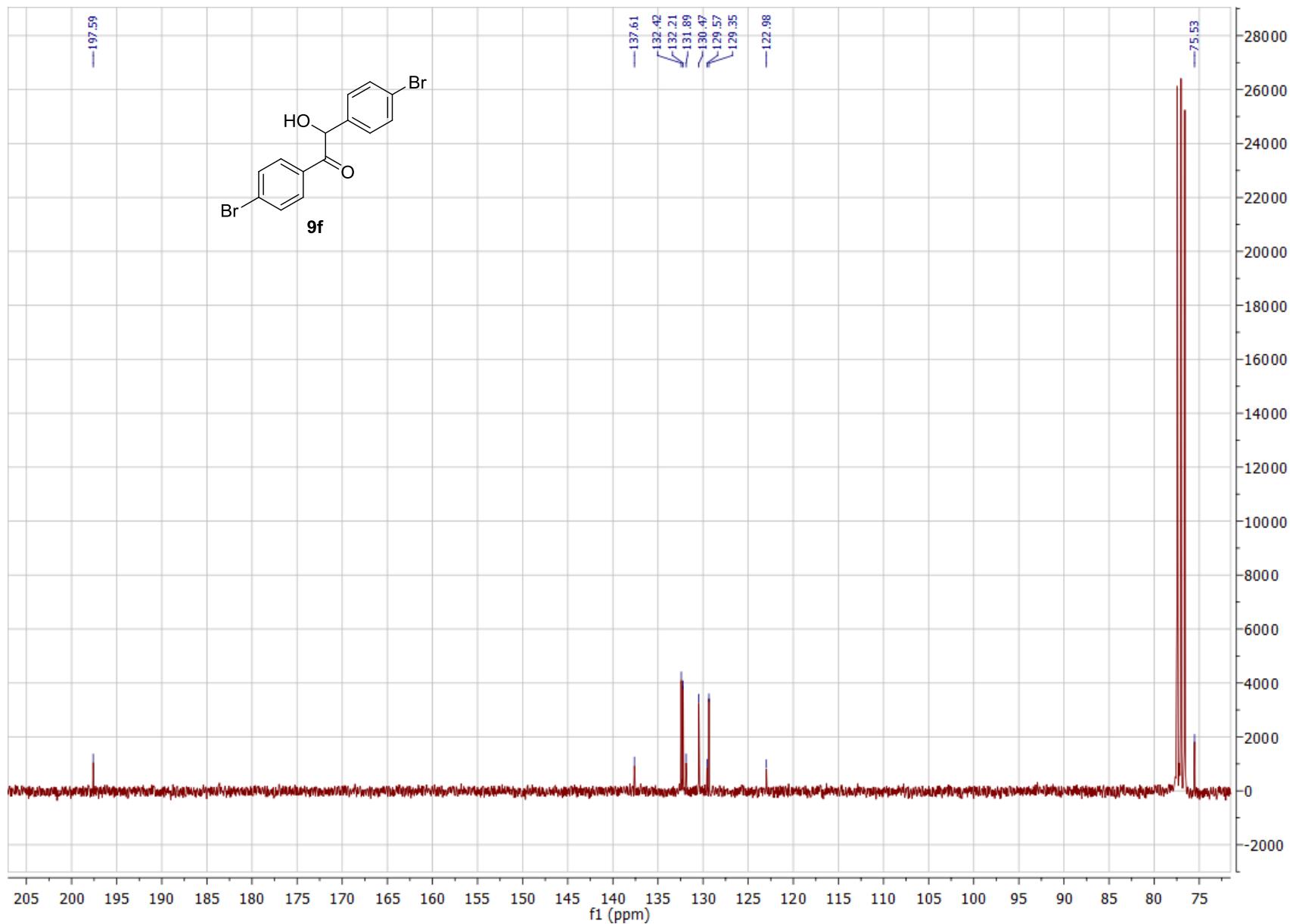


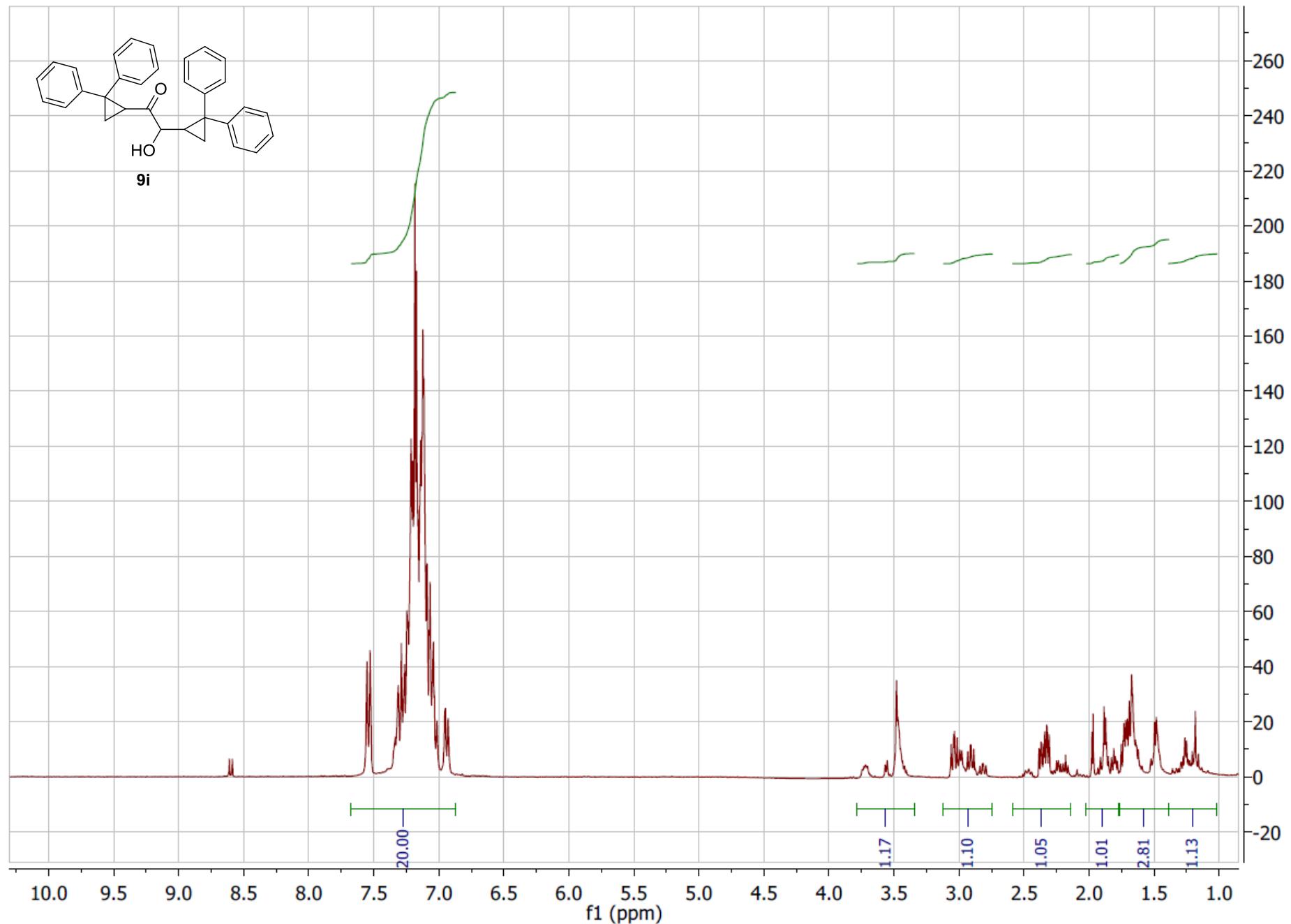


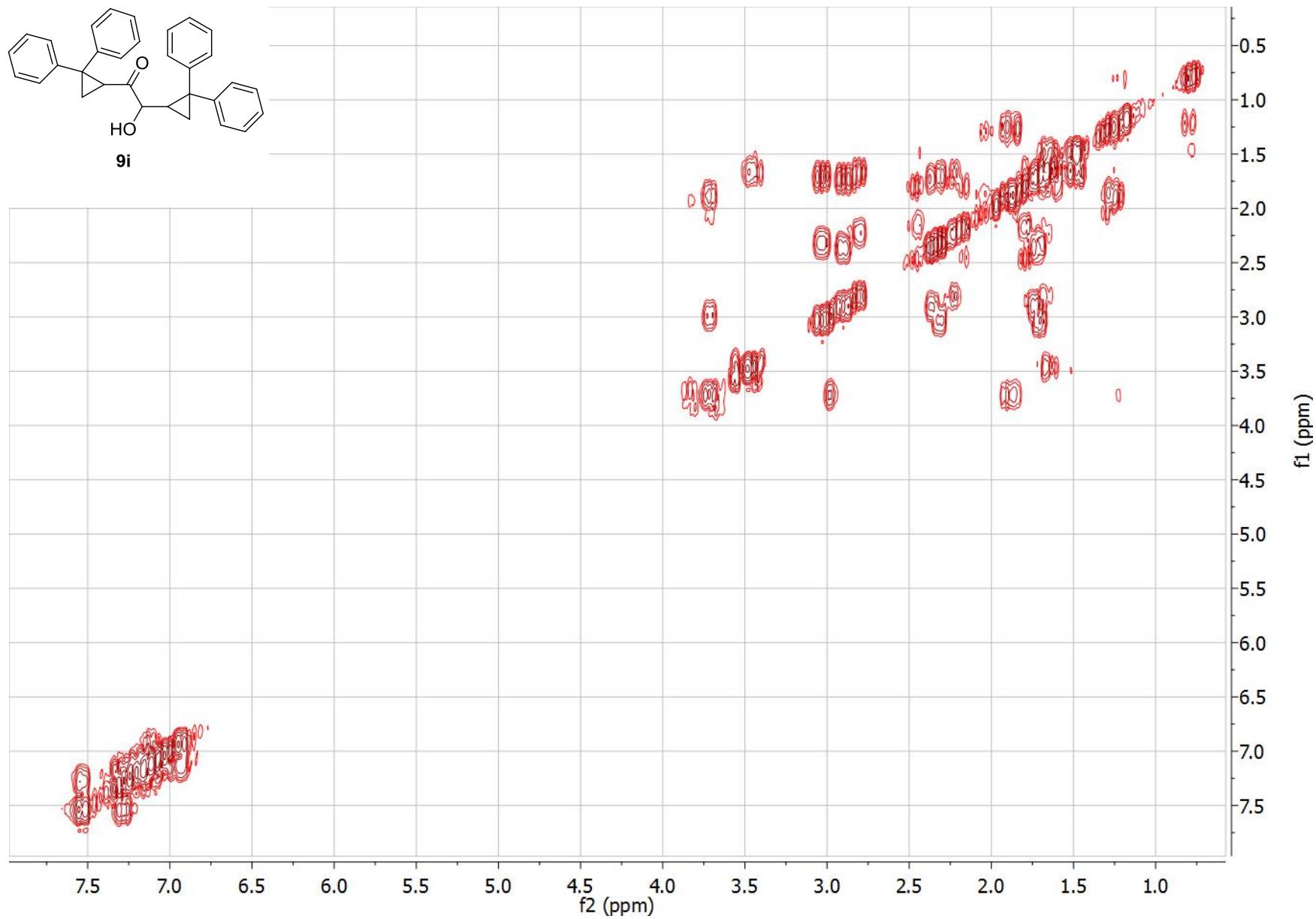
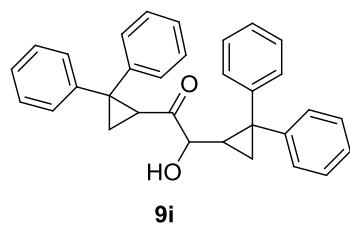


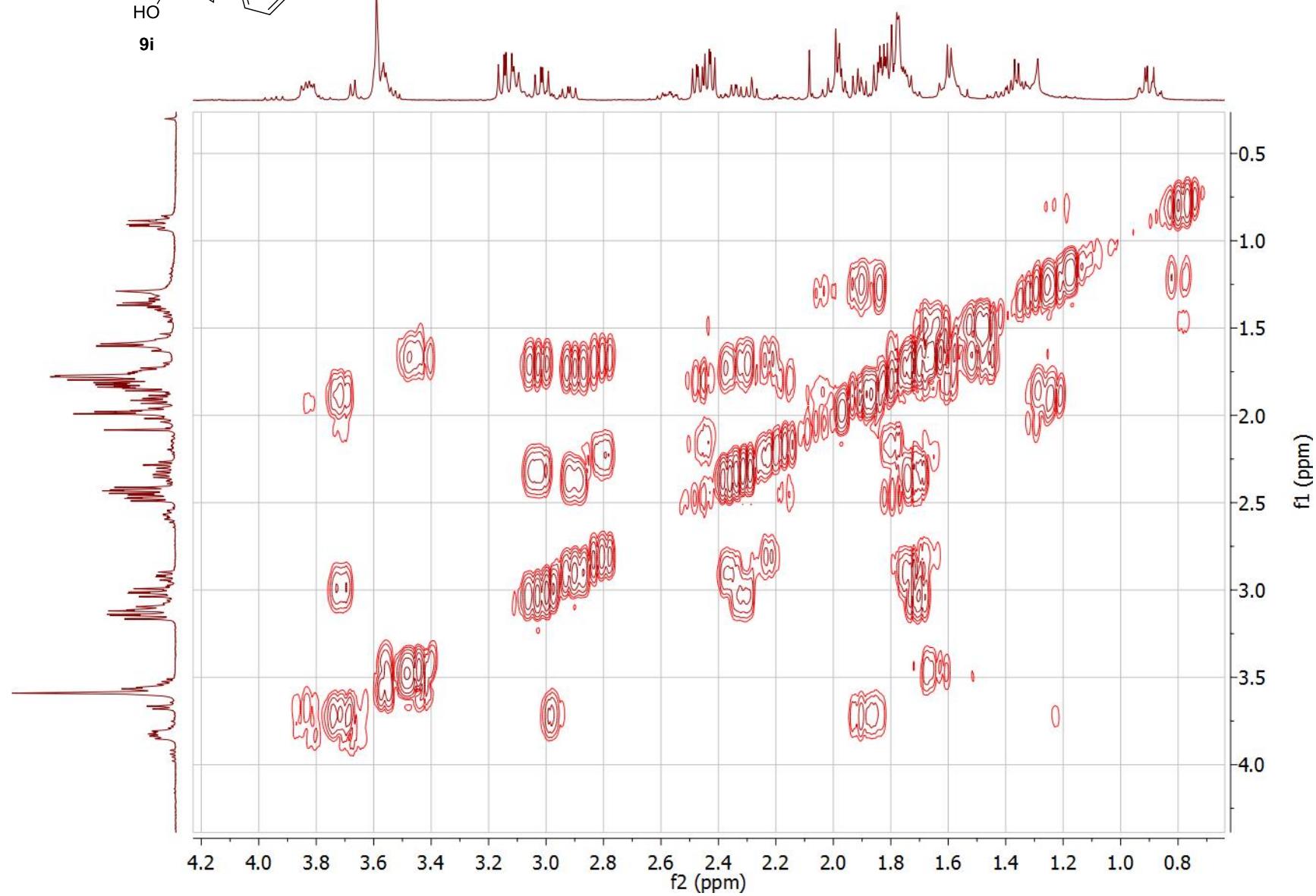
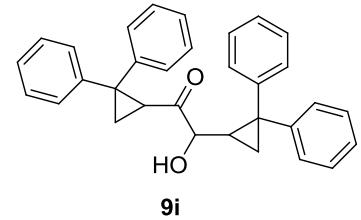


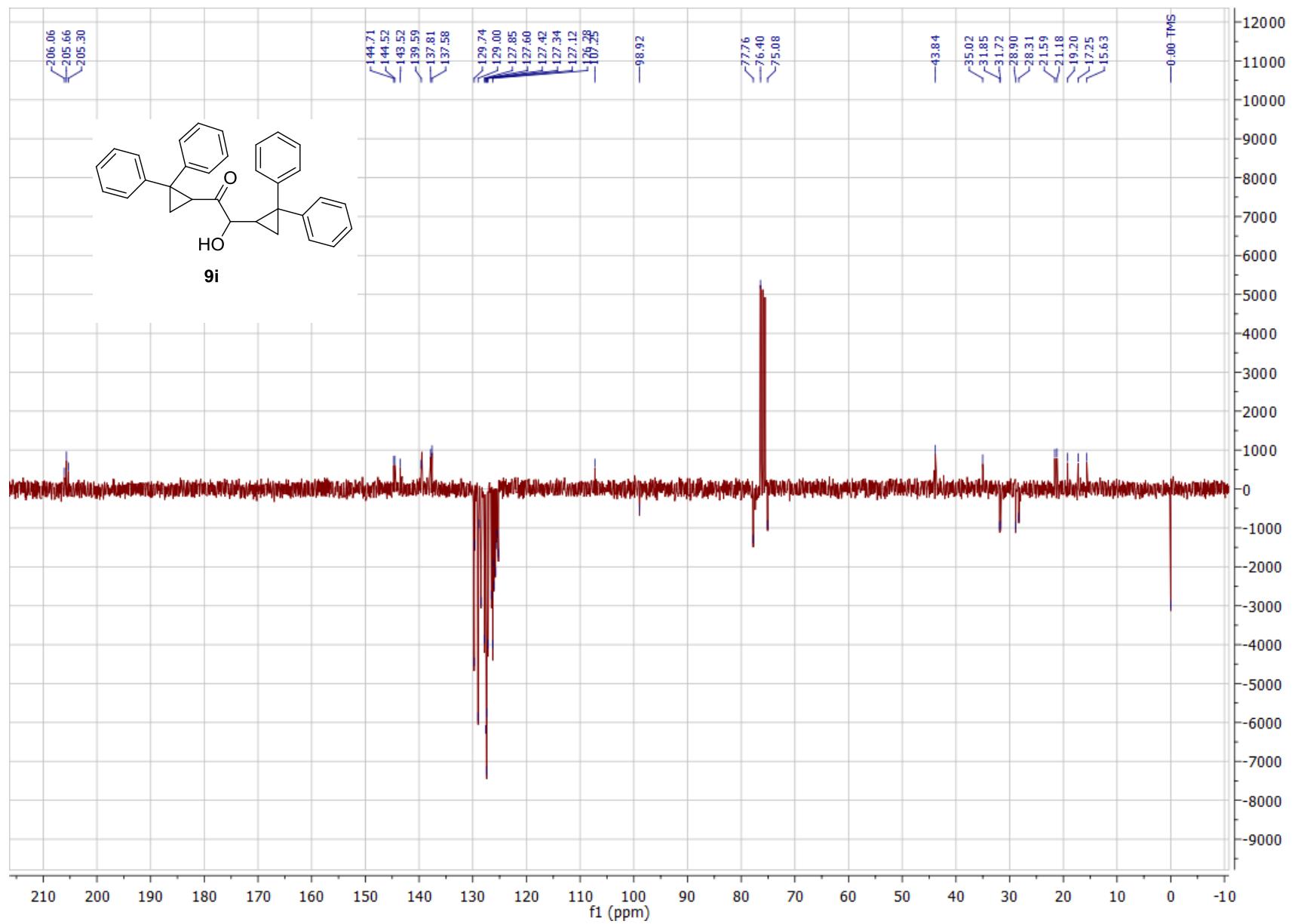


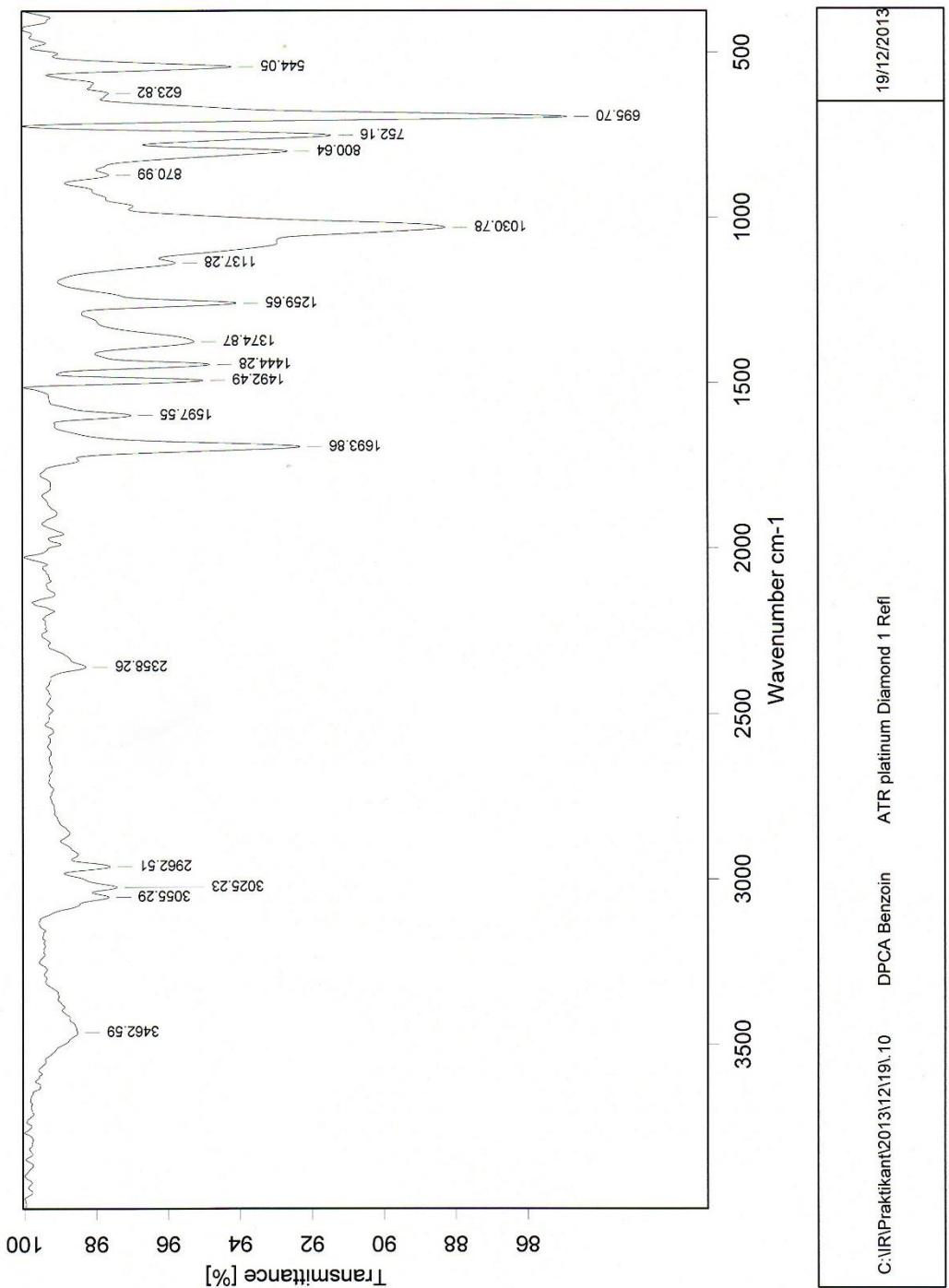
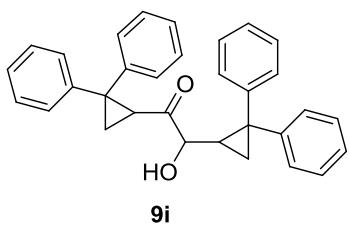




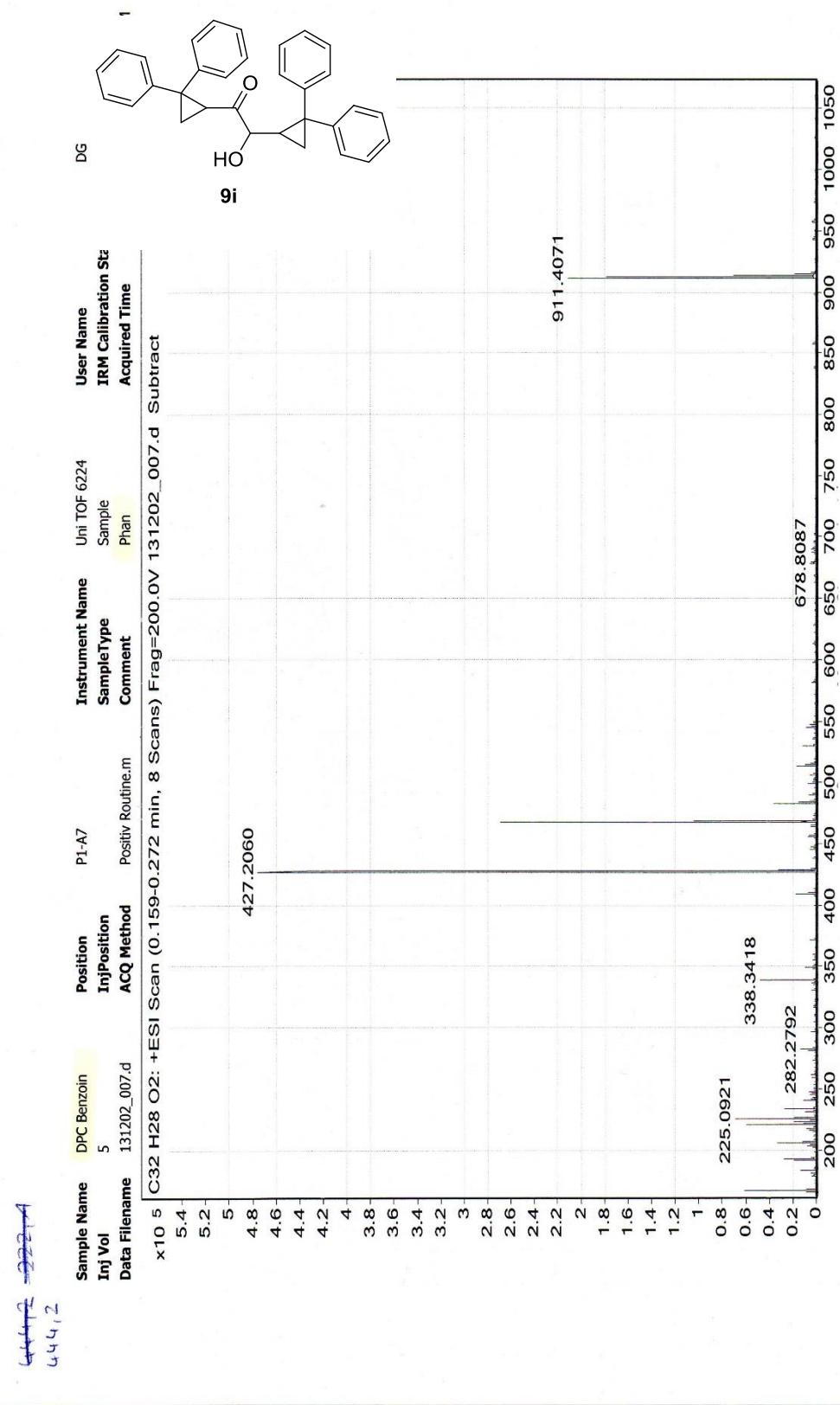








Seite 1 von 1



## B. Computational Chemistry

### B.1. General Computational Section

All calculations have been conducted using the Gaussian09 suite of programs.<sup>[19]</sup> Density functional theory calculations were initially carried out at the B3LYP/6-31G\* level of theory,<sup>[20]</sup> as this level of theory usually provides most efficiently suitable geometric accuracy. For better results of energy values the M06-2X functional with a higher basis set was employed (vide infra). Stationary points were confirmed as ground states by calculated harmonic vibrational frequencies.<sup>[21]</sup> Approximate free energies were obtained through thermochemical analysis of the frequency calculations, using the thermal correction to the Gibbs free energy as reported in Gaussian09. This takes into account zero-point effects, thermal enthalpy corrections, and entropy. All energies reported in this paper are enthalpies in kcal mol<sup>-1</sup> at 298 K if not stated otherwise. Frequencies remained unscaled.

BDE and RSE-values were calculated using three different levels of theory for the three test systems of **2a** and aldehydes **3a,b,c**: uB3LYP/6-31G\* as a so-called spectroscopy method<sup>22</sup> for subsequent calculations of Fermi contact couplings. In the area of *ab initio* methods ROMP2/6-311+G\*\* //B3LYP/6-31G\*<sup>23</sup> has been used previously to provide good absolute BDE values<sup>24</sup> and therefore was chosen to complement the B3LYP data. To complete the analysis a hybrid-meta functional, uM06-2X, (with 6-31++G\*\* basis)<sup>25</sup> has been selected to allow for inclusion of dispersion interactions.<sup>26</sup> M06-2X was also shown to provide good energy values of radicals without the potential problem of spin contamination as it is often seen with Møller-Plesset derived methods.<sup>27</sup> To include solvent effects implicitly PCM has been used (solvent= 2-propanol). For predicting Fermi contact couplings of the postulated radicals **7** a composite basis set was generated of EPR-II basis set<sup>28</sup> on C, H, O, N and 6-31\* on Cl, Br, S and combined with the hybrid functional B3LYP.

<sup>19</sup> Frisch, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian, Inc., Wallingford CT, **2009**.

<sup>20</sup> a) Lee, C. T.; Yang, W. T.; Parr, R. G. *Physical Review B* **1988**, *37*, 785–789; c) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648–5652; d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623–11627; e) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098–3100. f) Hehre, W. J.; Ditchfie, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257–2261; g) Harihara, P.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213–222.

<sup>21</sup> McIver, J. W.; Komornic, A. *J. Am. Chem. Soc.* **1972**, *94*, 2625–2633.

<sup>22</sup> Koch, W.; Holthausen, M. C. A: *Chemist's Guide to Density Functional Theory* Wiley VCH: Weinheim **2002**.

<sup>23</sup> Head-Gordon, M.; Pople, J. A.; Frisch, M. J. *J. Chem. Phys. Lett.* **1988**, *153*, 503–506.

<sup>24</sup> (a) Zavitsas, A. A. *J. Phys. Chem. A* **2003**, *10*, 897. (b) Hemelsoet, K.; Van Speybroeck, V.; Waroquier, M. *J. Phys. Chem. A* **2008**, *112*, 13566–13573.

<sup>25</sup> Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215–241.

<sup>26</sup> Zakrzewski, V. G.; Ortiz, J. V.; Nichols, J. A.; Heryadi, D.; Yeager, D. L.; Golab, J. T. *Int. J. Quant. Chem.*, **1996**, *60*, 29–36.

<sup>27</sup> Zao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2008**, *112*, 1095–1099.

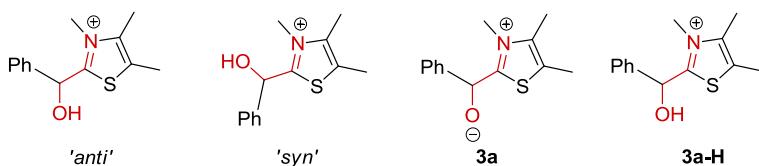
<sup>28</sup> Barone, V. in *Recent Advances in Density Functional Methods, Part I*, Ed. D. P. Chong in World Scientific Publ. Co.: Singapore, **1996**.

Since the same trends were predicted with B3LYP as with M06-2X and MP2 the larger catalyst systems **1b-f** were calculated using B3LYP.

Visualization of geometries, molecular orbitals and spin densities was achieved with Gabedit.<sup>29</sup>

## B. 2. Optimized xyz-Matrices and Thermodynamic Data

Two different conformers for adducts **3a** and **4a** have been used as starting points for the geometry optimization. These conformers were specified by the dihedral angle as depicted in **Figure SI-21** and annotated arbitrarily with 'syn' and 'anti'. Three different energy values were then calculated for BDE and RSE values: Minimal energy, maximal energy (lowest energy conformer of **3** and the highest of **4**) and most likely energy value utilizing the most stable conformers of each compound (reported in the main text).



**Figure-SI 7** Definition of conformers of adducts **3** and **4** exemplified by **4a**. Protonation state of the compound is indicated in the name by an H, e.g. **3a-H** and **4a-H** for the structures with a protonated oxygen atom.

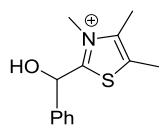
### B.2.1 B3LYP/6-31G\*

#### B.2.1.1 B3LYP/6-31G\* RSE and BDES for 4a-a, 4a-b, 4a-c

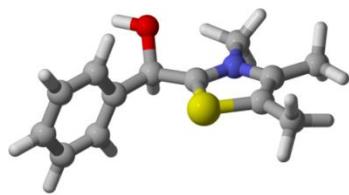
entry	cmpd	$\Delta H_{(I-II)}$ [kcal/mol]	BDE [kcal/mol]	RSE [kcal/mol]
1	<b>4a-a</b>	—	36.8 (min) <sup>a</sup>	—
2	—		39.7 (max) <sup>b</sup>	
3	<i>syn</i> - <b>4a-a-H</b>		36.8 (prob) <sup>c</sup>	
4	<i>anti</i> - <b>4a-a-H</b>	-0.3	71.9 (min) <sup>a</sup>	—
5	<i>syn</i> - <b>7a-a</b>		72.2 (max) <sup>b</sup>	
6	<i>anti</i> - <b>7a-a</b>		72.0 (prob) <sup>c</sup>	
7	<i>syn</i> - <b>7a-a-H</b>	-2.9	—	-65.1 (min) <sup>b</sup>
8	<i>anti</i> - <b>7a-a-H</b>		—	-68.0 (max) <sup>a</sup>
			—	-68.0 (prob) <sup>c</sup>
			—	-32.6 (min) <sup>b</sup>
			—	-32.9 (max) <sup>a</sup>
			—	-32.9 (prob) <sup>c</sup>

<sup>a</sup> determined from least stable conformer of closed shell species **4** and most stable radical species **7**. <sup>b</sup> determined from most stable conformer of closed shell species **4** and least stable radical species **7**. <sup>c</sup> determined from most stable conformer of closed shell species **4** and most stable radical species **7**.

<sup>29</sup> Allouche, A. R. *J. Comput. Chem.* **2011**, 32, 174–182.



*syn*-4a-a-H



### xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

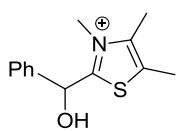
C	3.8237950000	-0.5035770000	1.2664500000
C	4.3278890000	-0.9546580000	0.0445620000
C	3.6497580000	-0.6664410000	-1.1422530000
C	2.4646340000	0.0682580000	-1.1103560000
C	1.9536500000	0.5197780000	0.1160170000
C	2.6413940000	0.2352890000	1.3025760000
C	0.6697680000	1.3289800000	0.1548320000
C	-0.5729660000	0.4557320000	0.0767100000
O	0.5488540000	2.2531410000	-0.9235560000
N	-1.8324100000	0.8954050000	0.1332380000
S	-0.5178010000	-1.2430830000	-0.0564150000
C	-2.2591370000	-1.3547830000	-0.0308920000
C	-2.8117660000	-0.1085880000	0.0744970000
C	-2.1921800000	2.3219940000	0.2783910000
C	-4.2642830000	0.2535250000	0.1213980000
C	-2.9318980000	-2.6905860000	-0.1399230000
H	4.3556360000	-0.7166600000	2.1887270000
H	5.2524930000	-1.5234520000	0.0164210000
H	4.0461910000	-1.0085110000	-2.0935410000
H	1.9442930000	0.3085880000	-2.0333240000
H	2.2592910000	0.5981940000	2.2543260000
H	0.6188180000	1.8553550000	1.1231330000
H	1.3786540000	2.7588180000	-0.9711580000
H	-2.9918920000	2.5560040000	-0.4250180000
H	-1.3239140000	2.9295310000	0.0371240000
H	-2.5350730000	2.5067580000	1.2997550000
H	-4.8752080000	-0.6489650000	0.1639530000
H	-4.5692620000	0.8147040000	-0.7698850000
H	-4.5036590000	0.8593880000	1.0019410000
H	-3.9866080000	-2.6187380000	0.1342840000
H	-2.4649940000	-3.4257280000	0.5231730000
H	-2.8758780000	-3.0784510000	-1.1635440000

### thermodynamic data

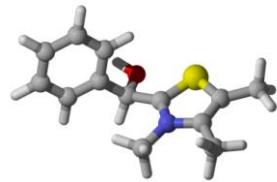
Zero-point correction=	0.266602 (Hartree/Particle)
Thermal correction to Energy=	0.282883
Thermal correction to Enthalpy=	0.283827
Thermal correction to Gibbs Free Energy=	0.221188

Sum of electronic and zero-point Energies= -1032.695279  
 Sum of electronic and thermal Energies= -1032.678998  
 Sum of electronic and thermal Enthalpies= -1032.678054  
 Sum of electronic and thermal Free Energies= -1032.740693

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.512	60.618	131.835



*anti*-4a-a-H



### xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

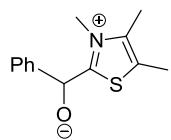
C	4.0874630000	0.8577790000	-0.1337060000
C	4.1670920000	0.4973000000	1.2119010000
C	3.1359580000	-0.2402230000	1.8018270000
C	2.0229620000	-0.6120020000	1.0503760000
C	1.9343050000	-0.2454510000	-0.3011770000
C	2.9745790000	0.4851650000	-0.8902260000
C	0.7581510000	-0.7012550000	-1.1537250000
C	-0.5906090000	-0.3235690000	-0.5743170000
O	0.6810990000	-2.1136460000	-1.2859250000
N	-1.1081700000	0.8989160000	-0.4498590000
S	-1.6685740000	-1.5221820000	-0.0169260000
C	-2.8566300000	-0.3138020000	0.4135410000
C	-2.3995930000	0.9365290000	0.1088710000
C	-0.4144640000	2.1239070000	-0.8905040000
C	-3.0937870000	2.2495760000	0.3013760000
C	-4.1596630000	-0.7297730000	1.0283010000
H	4.8918520000	1.4200680000	-0.5980780000
H	5.0331730000	0.7846530000	1.8004390000
H	3.2015500000	-0.5276580000	2.8469050000
H	1.2299580000	-1.1951170000	1.5118630000
H	2.9233930000	0.7511970000	-1.9441200000
H	0.8392020000	-0.2315720000	-2.1473690000
H	1.5816890000	-2.4754470000	-1.2585460000
H	-0.8342430000	2.4615740000	-1.8418750000
H	0.6482550000	1.9191610000	-0.9985650000
H	-0.5453640000	2.8995580000	-0.1357770000
H	-4.1090560000	2.0866170000	0.6647280000
H	-3.1648710000	2.8132030000	-0.6354970000

H	-2.5789920000	2.8778630000	1.0379740000
H	-4.8368250000	0.1216810000	1.1222750000
H	-4.0083320000	-1.1499490000	2.0289810000
H	-4.6603990000	-1.4892340000	0.4186640000

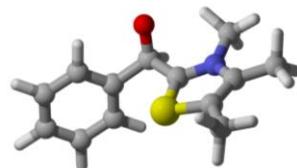
### thermodynamic data

Zero-point correction= 0.266292 (Hartree/Particle)  
 Thermal correction to Energy= 0.282729  
 Thermal correction to Enthalpy= 0.283673  
 Thermal correction to Gibbs Free Energy= 0.221278  
 Sum of electronic and zero-point Energies= -1032.695545  
 Sum of electronic and thermal Energies= -1032.679108  
 Sum of electronic and thermal Enthalpies= -1032.678164  
 Sum of electronic and thermal Free Energies= -1032.740559

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.415	60.911	131.322



**4a-a**



### xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

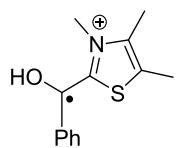
C	-3.9233690000	0.4211920000	-1.0246770000
C	-4.4086540000	0.8523120000	0.2116590000
C	-3.6863660000	0.5753160000	1.3762260000
C	-2.4853420000	-0.1304100000	1.2990600000
C	-1.9914940000	-0.5565850000	0.0603260000
C	-2.7178260000	-0.2797480000	-1.0994970000
C	-0.6802080000	-1.3485920000	-0.0674710000
C	0.5367770000	-0.4487650000	0.1548500000
O	-0.3699520000	-1.8071920000	-1.2883560000
N	1.7936330000	-0.9113040000	0.3069870000
S	0.5572150000	1.2529900000	-0.1200370000
C	2.3184790000	1.2900750000	-0.0997380000
C	2.8098420000	0.0476730000	0.1476970000
C	2.0214390000	-2.3621200000	0.3754420000
C	4.2478230000	-0.3584130000	0.2665450000
C	3.0445050000	2.5802590000	-0.3313650000

H	-4.4871910000	0.6287830000	-1.9312040000
H	-5.3479440000	1.3967410000	0.2709680000
H	-4.0633980000	0.9029350000	2.3422100000
H	-1.9304500000	-0.3580330000	2.2087120000
H	-2.3117680000	-0.6410350000	-2.0392910000
H	-0.6895330000	-2.1035160000	0.7626130000
H	1.3471770000	-2.7999160000	-0.3702720000
H	1.7976260000	-2.7407040000	1.3764750000
H	3.0595570000	-2.5800190000	0.1310400000
H	4.8929420000	0.5214420000	0.2365900000
H	4.5560130000	-1.0203780000	-0.5521150000
H	4.4421770000	-0.8811190000	1.2103630000
H	4.1255390000	2.4480890000	-0.2362660000
H	2.7390230000	3.3480730000	0.3896380000
H	2.8453240000	2.9743140000	-1.3352700000

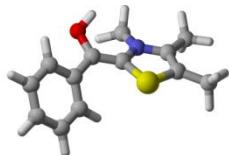
### thermodynamic data

Zero-point correction= 0.252597 (Hartree/Particle)  
 Thermal correction to Energy= 0.268448  
 Thermal correction to Enthalpy= 0.269393  
 Thermal correction to Gibbs Free Energy= 0.208623  
 Sum of electronic and zero-point Energies= -1032.263124  
 Sum of electronic and thermal Energies= -1032.247272  
 Sum of electronic and thermal Enthalpies= -1032.246328  
 Sum of electronic and thermal Free Energies= -1032.307098

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	168.454	59.326	127.900



*syn*-7a-a-H



### xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3778560000	0.2319050000	-0.5554040000
C	4.5303830000	-0.8985290000	0.2551970000
C	3.4320000000	-1.4173500000	0.9488780000
C	2.1837790000	-0.8200430000	0.8272300000
C	2.0107330000	0.3087450000	-0.0076270000
C	3.1350220000	0.8369070000	-0.6851550000
C	0.7274880000	0.9623510000	-0.1643880000
C	-0.5275380000	0.3334340000	-0.0350190000

O	0.7995710000	2.2859460000	-0.4712430000
N	-1.7369750000	0.9511550000	0.1875580000
S	-0.7841680000	-1.3653630000	-0.3595820000
C	-2.5178010000	-1.1792130000	-0.2280160000
C	-2.8500670000	0.1160480000	0.0584790000
C	-1.8694380000	2.3121970000	0.7437210000
C	-4.2273920000	0.6728460000	0.2565750000
C	-3.4015090000	-2.3749930000	-0.4113090000
H	5.2315540000	0.6377990000	-1.0891040000
H	5.5047040000	-1.3673620000	0.3546030000
H	3.5556740000	-2.2765220000	1.6006700000
H	1.3546390000	-1.1975250000	1.4164080000
H	3.0138300000	1.7086310000	-1.3177530000
H	0.0323370000	2.5705710000	-0.9958250000
H	-2.2279880000	3.0121980000	-0.0180080000
H	-0.9087680000	2.6452040000	1.1296150000
H	-2.5873190000	2.2907760000	1.5643860000
H	-4.9784360000	-0.0573040000	-0.0464840000
H	-4.3844220000	1.5774170000	-0.3405850000
H	-4.4194310000	0.9238940000	1.3068340000
H	-4.4551360000	-2.1011040000	-0.3293160000
H	-3.1943000000	-3.1364210000	0.3494950000
H	-3.2490930000	-2.8359350000	-1.3935600000

#### thermodynamic data

Zero-point correction= 0.254288 (Hartree/Particle)

Thermal correction to Energy= 0.270308

Thermal correction to Enthalpy= 0.271252

Thermal correction to Gibbs Free Energy= 0.209833

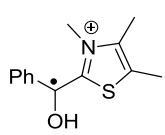
Sum of electronic and zero-point Energies= -1032.082080

Sum of electronic and thermal Energies= -1032.066061

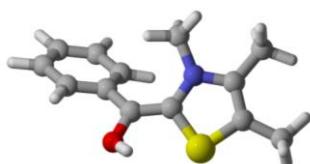
Sum of electronic and thermal Enthalpies= -1032.065117

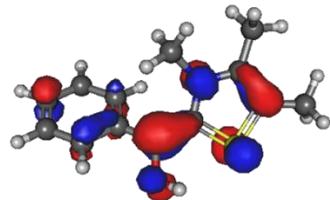
Sum of electronic and thermal Free Energies= -1032.126535

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.621	60.256	129.266

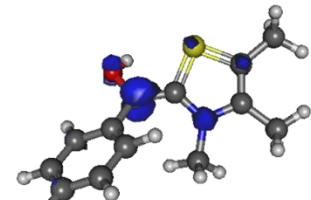


*anti*-7a-a-H





SOMO



spin-density

### **xyz-matrix**

31

XYZ file generated by gabedit : coordinates in Angstrom

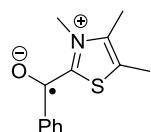
C	4.3598510000	-0.2221150000	-0.3792980000
C	4.4298950000	0.8671270000	0.4956690000
C	3.2739380000	1.3317310000	1.1338610000
C	2.0501280000	0.7221410000	0.8887260000
C	1.9639130000	-0.3667250000	-0.0083820000
C	3.1420220000	-0.8436800000	-0.6265400000
C	0.7098460000	-1.0591190000	-0.2377180000
C	-0.5931880000	-0.5274170000	-0.1335280000
O	0.8375690000	-2.3938810000	-0.4336240000
N	-1.0296060000	0.7454130000	-0.3932220000
S	-1.9351280000	-1.5274770000	0.3749490000
C	-3.0456490000	-0.1810850000	0.2503430000
C	-2.3909050000	0.9506650000	-0.1520090000
C	-0.2060240000	1.7661850000	-1.0634290000
C	-2.9904480000	2.3080790000	-0.3648510000
C	-4.4924720000	-0.3865530000	0.5792700000
H	5.2585130000	-0.5870780000	-0.8667030000
H	5.3849110000	1.3455920000	0.6904730000
H	3.3352250000	2.1556390000	1.8381970000
H	1.1665400000	1.0500460000	1.4286360000
H	3.0849420000	-1.6912100000	-1.3005450000
H	0.0626620000	-2.7721240000	-0.8863730000
H	-0.8252160000	2.2973860000	-1.7861070000
H	0.6135380000	1.2769670000	-1.5859000000
H	0.2044710000	2.4752960000	-0.3406320000
H	-4.0033240000	2.3419040000	0.0375610000
H	-3.0516850000	2.5647120000	-1.4294240000
H	-2.4068790000	3.0864250000	0.1377850000

H	-5.0491490000	0.5490730000	0.4983450000
H	-4.6190250000	-0.7661950000	1.5992570000
H	-4.9522200000	-1.1090610000	-0.1048840000

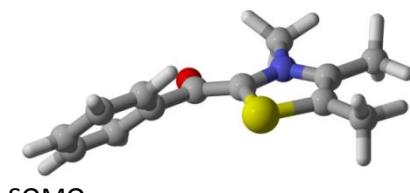
### thermodynamic data

Zero-point correction= 0.254382 (Hartree/Particle)  
 Thermal correction to Energy= 0.270298  
 Thermal correction to Enthalpy= 0.271242  
 Thermal correction to Gibbs Free Energy= 0.210292  
 Sum of electronic and zero-point Energies= -1032.082441  
 Sum of electronic and thermal Energies= -1032.066525  
 Sum of electronic and thermal Enthalpies= -1032.065581  
 Sum of electronic and thermal Free Energies= -1032.126532

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	169.615	60.157	128.281



*syn*-7a-a



spin-density

### xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

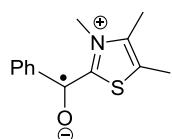
C	-4.3290160000	0.2846010000	-0.7082340000
C	-4.5503350000	-0.8656860000	0.0554310000
C	-3.5109670000	-1.3952900000	0.8204440000
C	-2.2522770000	-0.7912240000	0.8102450000
C	-2.0142790000	0.3521060000	0.0318060000
C	-3.0772340000	0.8926570000	-0.7111340000
C	-0.7084910000	1.0902810000	-0.0046370000
C	0.5267780000	0.3680090000	0.0851210000
O	-0.7177770000	2.3381950000	-0.1545360000
N	1.7781290000	0.9653720000	0.1745250000
S	0.7311970000	-1.3685880000	-0.1579130000
C	2.4881300000	-1.2004890000	-0.1960200000
C	2.8545540000	0.0941430000	-0.0046080000
C	1.9486330000	2.3885640000	0.4853080000
C	4.2603280000	0.6191780000	0.0292670000

C	3.3287010000	-2.4221970000	-0.4033570000
H	-5.1371820000	0.7091770000	-1.2985000000
H	-5.5290400000	-1.3384550000	0.0612010000
H	-3.6802050000	-2.2742960000	1.4371570000
H	-1.4659950000	-1.1949440000	1.4408920000
H	-2.8965760000	1.7981840000	-1.2811220000
H	2.9579870000	2.5466770000	0.8656750000
H	1.2233710000	2.6848950000	1.2408120000
H	1.7783980000	3.0079060000	-0.3981810000
H	4.9660460000	-0.1736530000	-0.2234270000
H	4.5348490000	0.9990300000	1.0212720000
H	4.4044520000	1.4339490000	-0.6897300000
H	4.3946870000	-2.1803280000	-0.3906260000
H	3.1084680000	-2.9042370000	-1.3644220000
H	3.1497510000	-3.1675680000	0.3824340000

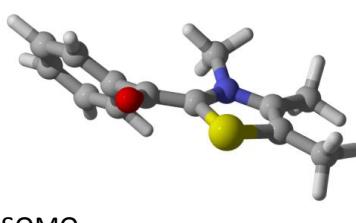
### thermodynamic data

Zero-point correction= 0.241757 (Hartree/Particle)  
 Thermal correction to Energy= 0.257536  
 Thermal correction to Enthalpy= 0.258480  
 Thermal correction to Gibbs Free Energy= 0.197229  
 Sum of electronic and zero-point Energies= -1031.706529  
 Sum of electronic and thermal Energies= -1031.690750  
 Sum of electronic and thermal Enthalpies= -1031.689806  
 Sum of electronic and thermal Free Energies= -1031.751056

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	161.606	58.709	128.913



*anti*-7a-a



SOMO

spin-density

### xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

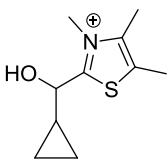
C	4.3356330000	-0.2571440000	-0.5046820000
C	4.4660570000	0.8323610000	0.3621250000

C	3.3551390000	1.2834390000	1.0771740000
C	2.1160780000	0.6632530000	0.9104850000
C	1.9704660000	-0.4173400000	0.0261680000
C	3.1026100000	-0.8851430000	-0.6604220000
C	0.6885580000	-1.1795070000	-0.1160740000
C	-0.5955930000	-0.5462940000	-0.0915820000
O	0.7222870000	-2.4324790000	-0.1990830000
N	-0.9962960000	0.7636290000	-0.3052620000
S	-1.9872350000	-1.5716820000	0.2127030000
C	-3.0564560000	-0.1657380000	0.1778350000
C	-2.3729050000	0.9707730000	-0.1138800000
C	-0.1509110000	1.7455110000	-0.9853870000
C	-2.9348250000	2.3564600000	-0.2438180000
C	-4.5180550000	-0.3526760000	0.4471150000
H	5.2005710000	-0.6217280000	-1.0529620000
H	5.4305650000	1.3168700000	0.4894050000
H	3.4558040000	2.1102510000	1.7758950000
H	1.2624950000	0.9962250000	1.4956910000
H	2.9940710000	-1.7510680000	-1.3059730000
H	-0.7701630000	2.3816220000	-1.6199390000
H	0.5701480000	1.2208820000	-1.6136160000
H	0.4031280000	2.3722270000	-0.2797270000
H	-3.9657240000	2.3827860000	0.1136270000
H	-2.9418200000	2.7089930000	-1.2833950000
H	-2.3595320000	3.0796990000	0.3460170000
H	-5.0659390000	0.5898000000	0.3640800000
H	-4.6936470000	-0.7548530000	1.4528370000
H	-4.9631920000	-1.0581040000	-0.2660210000

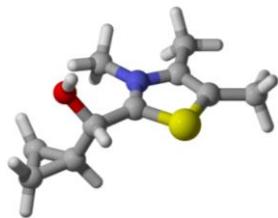
#### thermodynamic data

Zero-point correction= 0.241676 (Hartree/Particle)  
 Thermal correction to Energy= 0.257371  
 Thermal correction to Enthalpy= 0.258315  
 Thermal correction to Gibbs Free Energy= 0.197682  
 Sum of electronic and zero-point Energies= -1031.701772  
 Sum of electronic and thermal Energies= -1031.686078  
 Sum of electronic and thermal Enthalpies= -1031.685134  
 Sum of electronic and thermal Free Energies= -1031.745766

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	161.503	58.712	127.612



*syn*-3a-b-H



### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.5558620000	-0.6849260000	0.5441450000
C	-0.0706510000	-0.3919400000	0.3209670000
O	-2.0911250000	0.1145130000	1.5834570000
N	0.5219970000	0.7960570000	0.1915500000
S	1.0591860000	-1.6596170000	0.1216370000
C	2.3670540000	-0.5367730000	-0.1595860000
C	1.9015640000	0.7454160000	-0.0822070000
C	-0.1908180000	2.0881530000	0.3048030000
C	2.6799030000	2.0144060000	-0.2497420000
C	3.7538420000	-1.0429680000	-0.4197880000
C	-2.3589120000	-0.4775240000	-0.7369180000
C	-3.8642320000	-0.5626690000	-0.6875620000
C	-3.1992890000	0.7572540000	-0.9782770000
H	-1.6112490000	-1.7496460000	0.8125290000
H	-1.9304880000	-0.3133380000	2.4394840000
H	0.4159930000	2.7697590000	0.9013070000
H	-1.1423810000	1.9177690000	0.7988250000
H	-0.3431800000	2.5051650000	-0.6932590000
H	3.7016780000	1.7906560000	-0.5581280000
H	2.7355600000	2.5830270000	0.6859780000
H	2.2370580000	2.6615950000	-1.0142870000
H	4.4351650000	-0.2164400000	-0.6309260000
H	3.7735900000	-1.7216010000	-1.2791250000
H	4.1456420000	-1.5865280000	0.4470960000
H	-1.8817760000	-0.9217860000	-1.6082270000
H	-4.3297350000	-0.6694640000	0.2875780000
H	-4.3646520000	-1.0923640000	-1.4921570000
H	-3.2327130000	1.1508590000	-1.9899040000
H	-3.2560470000	1.5071310000	-0.1964860000

### thermodynamic data

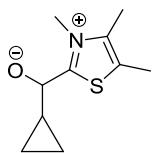
Zero-point correction=	0.248607 (Hartree/Particle)
Thermal correction to Energy=	0.263191
Thermal correction to Enthalpy=	0.264135
Thermal correction to Gibbs Free Energy=	0.206929
Sum of electronic and zero-point Energies=	-918.355635
Sum of electronic and thermal Energies=	-918.341051
Sum of electronic and thermal Enthalpies=	-918.340107
Sum of electronic and thermal Free Energies=	-918.397313

E (Thermal)

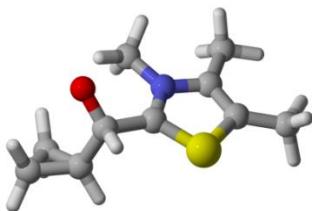
CV

S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	165.155	53.812	120.400



*syn*-3a-b



### xyz-matrix

**28**

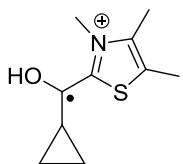
**XYZ file generated by gabedit : coordinates in Angstrom**

H	-1.6094020000	-1.5264550000	1.2110830000
O	-2.0220210000	0.4691160000	1.5386720000
H	4.0757980000	-1.6640910000	0.5369370000
S	0.9834940000	-1.6538090000	0.1843400000
C	-1.6349140000	-0.5031350000	0.7390680000
H	-4.2969730000	-0.1981450000	0.5329020000
C	-0.1237560000	-0.3341570000	0.3106710000
C	3.7137060000	-1.1341940000	-0.3521160000
C	2.3374240000	-0.5822890000	-0.1338920000
C	-3.9433360000	-0.5065200000	-0.4467640000
H	3.7322030000	-1.8421290000	-1.1887670000
C	-2.4547310000	-0.6915860000	-0.5688950000
N	0.5313100000	0.8174940000	0.1449180000
H	-1.0897670000	1.8964190000	0.8037970000
H	4.4263550000	-0.3361590000	-0.5758520000
H	-4.5998140000	-1.1726270000	-1.0009520000
C	1.9114980000	0.7094440000	-0.1142150000
H	-2.1106300000	-1.4819860000	-1.2382550000
H	0.4735200000	2.8302490000	0.7507310000
C	-0.1691250000	2.1155690000	0.2337510000
H	-2.9773530000	1.4628180000	-0.7094120000
H	2.7921210000	2.5548570000	0.5837600000
C	-3.1182560000	0.5057210000	-1.2026340000
C	2.7252340000	1.9494080000	-0.3281280000
H	3.7419040000	1.6893400000	-0.6282020000
H	-0.3951210000	2.4775830000	-0.7726560000
H	-3.1982400000	0.5456080000	-2.2863790000
H	2.2940460000	2.5807010000	-1.1130510000

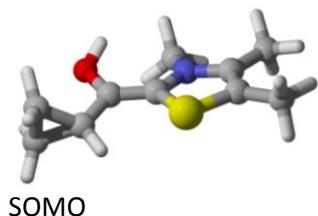
### thermodynamic data

Zero-point correction=	0.233866 (Hartree/Particle)
Thermal correction to Energy=	0.247941
Thermal correction to Enthalpy=	0.248885
Thermal correction to Gibbs Free Energy=	0.192697
Sum of electronic and zero-point Energies=	-917.925990
Sum of electronic and thermal Energies=	-917.911915
Sum of electronic and thermal Enthalpies=	-917.910971
Sum of electronic and thermal Free Energies=	-917.967159

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	155.585	52.243	118.258



*syn*-7a-b - H



spin-density

### xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.5245740000	0.3561940000	0.0450320000
C	-0.1502910000	0.1008890000	-0.0215570000
O	-2.0380300000	1.5656320000	0.3688140000
N	0.8956040000	1.0040360000	-0.0218110000
S	0.4798400000	-1.5322850000	-0.0280730000
C	2.1270620000	-0.9481410000	0.0144520000
C	2.1627260000	0.4201130000	0.0198360000
C	0.7151980000	2.4500850000	-0.2322710000
C	3.3883000000	1.2829190000	0.0480360000
C	3.2533460000	-1.9353480000	0.0352520000
C	-2.5284960000	-0.6620790000	-0.2437130000
C	-3.7579310000	-0.8092180000	0.6725300000
C	-3.9375730000	-0.2444990000	-0.6875980000
H	-1.4225800000	2.1015700000	0.8930150000
H	0.6400510000	2.9843270000	0.7224830000
H	-0.1735820000	2.6241090000	-0.8382430000
H	1.5745340000	2.8433390000	-0.7730240000
H	4.2714700000	0.6769170000	0.2522260000
H	3.3247600000	2.0476120000	0.8295310000
H	3.5545800000	1.7883090000	-0.9112640000
H	4.2203920000	-1.4293930000	0.0564470000
H	3.2312140000	-2.5749140000	-0.8545750000
H	3.1942760000	-2.5866650000	0.9146770000
H	-2.1476360000	-1.5752240000	-0.6888630000
H	-3.8148970000	-0.1316950000	1.5185390000
H	-4.0746340000	-1.8278410000	0.8741770000
H	-4.3801320000	-0.8620370000	-1.4628710000
H	-4.1268540000	0.8193370000	-0.7809200000

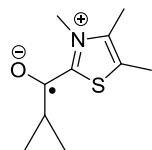
### thermodynamic data

Zero-point correction= 0.235923 (Hartree/Particle)

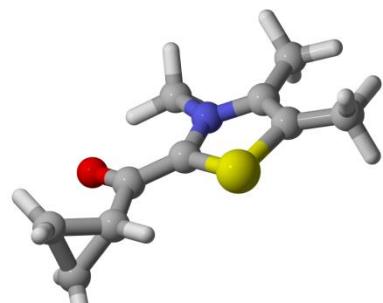
Thermal correction to Energy= 0.250439

Thermal correction to Enthalpy= 0.251383  
 Thermal correction to Gibbs Free Energy= 0.193618  
 Sum of electronic and zero-point Energies= -917.745458  
 Sum of electronic and thermal Energies= -917.730942  
 Sum of electronic and thermal Enthalpies= -917.729997  
 Sum of electronic and thermal Free Energies= -917.787763

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	157.153	53.556	121.578



*syn*-7a-b



SOMO

spin-density

### xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

H	1.2197570000	2.9017330000	-0.8893700000
H	-0.3186670000	2.6950540000	-0.0008420000
H	3.4188130000	1.9168770000	-0.8848620000
C	0.7465700000	2.4726790000	0.0008090000
H	1.2164880000	2.9002680000	0.8934670000
H	-3.9680580000	0.4887290000	-1.2447800000
C	3.3794010000	1.2695880000	-0.0005770000
H	3.4176930000	1.9193770000	0.8818950000
O	-2.0071560000	1.6318680000	-0.0006790000
N	0.8957270000	1.0146600000	-0.0002350000
H	-4.2815600000	-1.3225440000	-1.2756330000
H	4.2803100000	0.6540020000	0.0008590000
C	-3.8608190000	-0.4707320000	-0.7483560000
C	2.1514370000	0.4076520000	-0.0001510000
C	-1.5719230000	0.4531750000	-0.0000410000
C	-0.1781010000	0.1291770000	0.0000630000
C	-2.5558300000	-0.6819860000	0.0005160000
H	-2.1611080000	-1.6944260000	0.0015580000
C	2.1132600000	-0.9505200000	0.0000990000

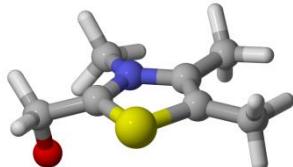
H	4.2036520000	-1.4532810000	0.0002160000
S	0.4431060000	-1.5253450000	0.0003070000
C	-3.8614680000	-0.4694460000	0.7478280000
H	3.1869850000	-2.5979970000	-0.8837910000
H	-3.9691060000	0.4908860000	1.2424810000
C	3.2288400000	-1.9482600000	0.0000110000
H	-4.2827180000	-1.3203150000	1.2762220000
H	3.1867780000	-2.5983630000	0.8835320000

### thermodynamic data

Zero-point correction= 0.223067 (Hartree/Particle)  
 Thermal correction to Energy= 0.237508  
 Thermal correction to Enthalpy= 0.238452  
 Thermal correction to Gibbs Free Energy= 0.179606  
 Sum of electronic and zero-point Energies= -917.376478  
 Sum of electronic and thermal Energies= -917.362036  
 Sum of electronic and thermal Enthalpies= -917.361092  
 Sum of electronic and thermal Free Energies= -917.419939

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	149.039	51.937	123.854

4a-c



### xyz-matrix

21

XYZ file generated by gabedit : coordinates in Angstrom

S	0.1918350000	-1.6555230000	0.2146470000
C	-0.9858810000	-0.4012770000	0.3492850000
N	-0.3858850000	0.8065510000	0.2757090000
C	0.9987530000	0.7745380000	0.0365370000
C	1.4924000000	-0.4891620000	-0.0315180000
C	-1.2224330000	2.0109320000	0.1896560000
C	1.7613540000	2.0573830000	-0.1029730000
C	2.8930250000	-0.9636130000	-0.2698080000
C	-2.4764780000	-0.6260830000	0.2442650000
O	-2.6050010000	-0.3058310000	-1.0552680000
H	-1.5963420000	2.2934190000	1.1776440000
H	-2.0475150000	1.7446410000	-0.4820590000
H	-0.6403910000	2.8330270000	-0.2235110000

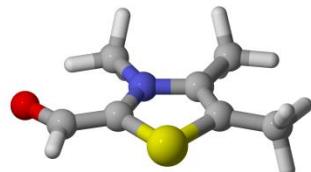
H	2.8329580000	1.8580750000	-0.1590220000
H	1.5906940000	2.7208930000	0.7527720000
H	1.4796880000	2.6041690000	-1.0113410000
H	3.5840080000	-0.1212610000	-0.3601670000
H	2.9633770000	-1.5508190000	-1.1935740000
H	3.2488870000	-1.5981100000	0.5511000000
H	-3.0097390000	0.0088520000	0.9963480000
H	-2.6982260000	-1.6800260000	0.5369740000

### thermodynamic data

Zero-point correction= 0.171607 (Hartree/Particle)  
 Thermal correction to Energy= 0.182901  
 Thermal correction to Enthalpy= 0.183845  
 Thermal correction to Gibbs Free Energy= 0.134642  
 Sum of electronic and zero-point Energies= -801.283603  
 Sum of electronic and thermal Energies= -801.272309  
 Sum of electronic and thermal Enthalpies= -801.271365  
 Sum of electronic and thermal Free Energies= -801.320568

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.772	40.359	103.556

7a-c



### xyz-matrix

20

XYZ file generated by gabedit : coordinates in Angstrom

S	0.3226560000	-1.7082570000	-0.0000500000
C	-0.9724770000	-0.5120020000	-0.0000540000
N	-0.4284440000	0.7620290000	-0.0000520000
C	0.9660120000	0.7959910000	-0.0000120000
C	1.5487110000	-0.4326030000	0.0000140000
C	-1.2518960000	1.9738160000	0.0000430000
C	1.6620090000	2.1244520000	-0.0000470000
C	2.9967510000	-0.8114280000	0.0000940000
C	-2.3409570000	-0.8897900000	0.0000410000
O	-3.3290790000	-0.1250280000	0.0000310000
H	-1.0436710000	2.5750120000	0.8918550000
H	-2.2953050000	1.6612390000	0.0000930000
H	-1.0437110000	2.5751090000	-0.8917120000
H	2.7449570000	1.9915980000	0.0001250000
H	1.3982660000	2.7182730000	0.8834520000
H	1.3984950000	2.7180870000	-0.8837440000

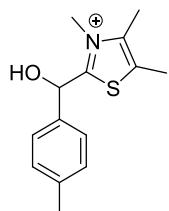
H	3.6378400000	0.0741780000	-0.0002610000
H	3.2556160000	-1.4089350000	-0.8834490000
H	3.2557170000	-1.4083240000	0.8840210000
H	-2.4878790000	-1.9887200000	0.0000740000

### thermodynamic data

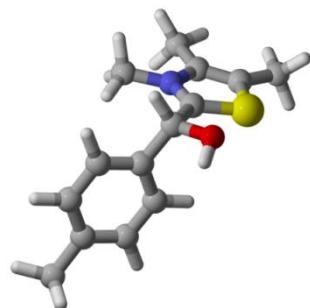
Zero-point correction=	0.160323 (Hartree/Particle)
Thermal correction to Energy=	0.171506
Thermal correction to Enthalpy=	0.172451
Thermal correction to Gibbs Free Energy=	0.122783
Sum of electronic and zero-point Energies=	-800.731745
Sum of electronic and thermal Energies=	-800.720562
Sum of electronic and thermal Enthalpies=	-800.719617
Sum of electronic and thermal Free Energies=	-800.769285

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	107.622	39.788	104.533

### B.2.2.2 B3LYP/6-31G\* RSE and BDES for 4a-d to 4a-g



*anti*-4a-d-H



### xyz-matrix

35

XYZ file generated by gabedit : coordinates in Angstrom

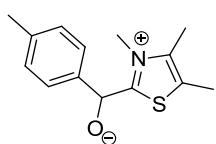
C	3.7391910000	0.5462430000	-0.6952160000
C	3.9593620000	0.3581630000	0.6752940000
C	2.9391450000	-0.2426870000	1.4320850000
C	1.7434070000	-0.6421500000	0.8442360000
C	1.5325050000	-0.4467570000	-0.5296150000
C	2.5445830000	0.1460770000	-1.2943330000
C	0.2607780000	-0.9367360000	-1.2034820000
C	-1.0066690000	-0.4112330000	-0.5592300000
O	0.1047790000	-2.3486330000	-1.1455100000
S	-2.0783930000	-1.4642590000	0.2480860000
C	-3.1653010000	-0.1445900000	0.6158700000
C	-2.6851870000	1.0272960000	0.1052160000
N	-1.4546810000	0.8445220000	-0.5543690000
C	-0.7486830000	1.9588690000	-1.2143150000

C	-3.3010880000	2.3907100000	0.1760460000
C	-4.4201880000	-0.4031760000	1.3949820000
C	5.2621830000	0.7616600000	1.3199540000
H	4.5139100000	1.0036700000	-1.3045730000
H	3.0878370000	-0.4000370000	2.4972630000
H	0.9768070000	-1.1129860000	1.4549100000
H	2.4071650000	0.2866310000	-2.3647380000
H	0.2656690000	-0.6007380000	-2.2530270000
H	0.9871790000	-2.7529260000	-1.1209220000
H	-1.2110210000	2.1655900000	-2.1834240000
H	0.2991020000	1.6958630000	-1.3434690000
H	-0.8114320000	2.8443140000	-0.5820570000
H	-2.7001660000	3.0783260000	0.7830820000
H	-4.2899520000	2.3321290000	0.6323340000
H	-3.4223140000	2.8327330000	-0.8189600000
H	-5.0425390000	0.4928060000	1.4434660000
H	-4.1914020000	-0.7077260000	2.4224450000
H	-5.0151880000	-1.1990770000	0.9347800000
H	5.9198810000	-0.1082800000	1.4431360000
H	5.1011300000	1.1881530000	2.3154140000
H	5.7999370000	1.4969760000	0.7146910000

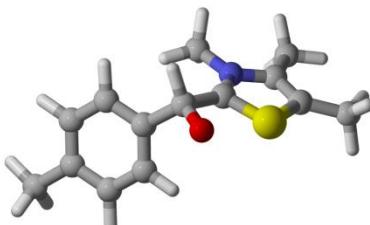
#### thermodynamic data

Zero-point correction= 0.294015 (Hartree/Particle)  
 Thermal correction to Energy= 0.312217  
 Thermal correction to Enthalpy= 0.313161  
 Thermal correction to Gibbs Free Energy= 0.246455  
 Sum of electronic and zero-point Energies= -1071.987886  
 Sum of electronic and thermal Energies= -1071.969684  
 Sum of electronic and thermal Enthalpies= -1071.968740  
 Sum of electronic and thermal Free Energies= -1072.035446

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	195.919	66.875	140.394



*anti*-4a-d



#### xyz-matrix

34

XYZ file generated by gabedit : coordinates in Angstrom

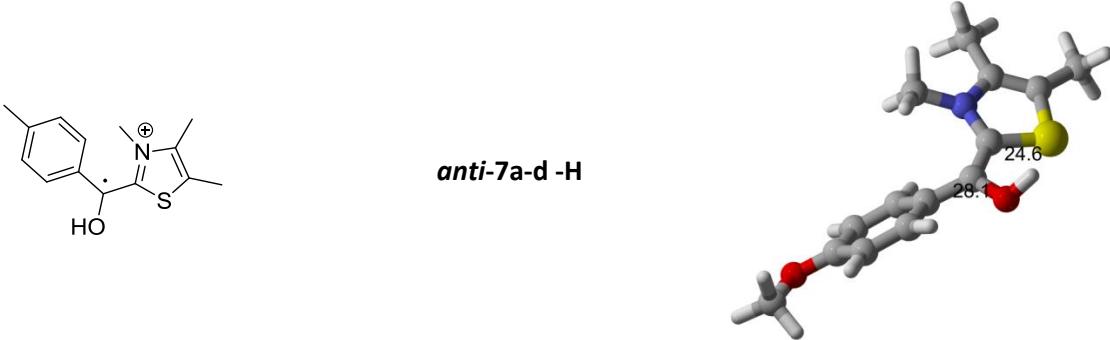
H	2.1541940000	0.6459080000	-2.2659690000
H	4.2667290000	1.4106900000	-1.2303720000
C	2.4079610000	0.3186940000	-1.2577290000

C	3.6082150000	0.7436440000	-0.6770960000
H	0.2381500000	-0.7468730000	-2.2698860000
H	-1.1460960000	2.4977150000	-1.8419880000
H	5.7843560000	1.5120640000	0.6224440000
H	0.3442940000	1.8014460000	-1.1413130000
C	-0.6799530000	2.1057560000	-0.9325370000
C	0.2316430000	-1.0684730000	-1.1904420000
C	1.5506680000	-0.5479380000	-0.5769320000
C	3.9841320000	0.3070970000	0.5962000000
C	5.2852020000	0.7476550000	1.2269230000
H	5.9822030000	-0.0930980000	1.3379690000
H	-0.6675350000	2.8850970000	-0.1680020000
O	-0.0393990000	-2.3487420000	-0.9552390000
N	-1.4257250000	0.9445520000	-0.4402640000
C	-0.9826440000	-0.3086570000	-0.5763440000
H	-3.3955000000	2.9608050000	-0.5321730000
H	5.1260670000	1.1644110000	2.2293450000
C	1.9364660000	-1.0109180000	0.6872730000
C	3.1257680000	-0.5818330000	1.2663230000
C	-2.6824370000	1.0502400000	0.1940590000
C	-3.2900760000	2.4049090000	0.4076460000
H	-2.6942170000	3.0221170000	1.0922380000
H	1.2988400000	-1.7384200000	1.1812970000
H	3.4068640000	-0.9506730000	2.2514780000
S	-2.0595780000	-1.4746230000	0.0480550000
H	-4.2861370000	2.3040750000	0.8428260000
C	-3.1680470000	-0.1764350000	0.5351180000
H	-5.0431720000	-1.2263830000	0.6533690000
C	-4.4557270000	-0.5029080000	1.2306970000
H	-5.0756600000	0.3859640000	1.3784400000
H	-4.2718870000	-0.9478080000	2.2162330000

#### thermodynamic data

Zero-point correction= 0.279626 (Hartree/Particle)  
 Thermal correction to Energy= 0.297471  
 Thermal correction to Enthalpy= 0.298415  
 Thermal correction to Gibbs Free Energy= 0.232488  
 Sum of electronic and zero-point Energies= -1071.548754  
 Sum of electronic and thermal Energies= -1071.530909  
 Sum of electronic and thermal Enthalpies= -1071.529965  
 Sum of electronic and thermal Free Energies= -1071.595892

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	186.666	65.472	138.755



### xyz-matrix

34

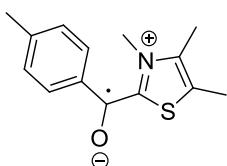
XYZ file generated by gabedit : coordinates in Angstrom

C	3.9486350000	0.6493460000	0.5145090000
C	4.1520880000	-0.4805660000	-0.2979480000
C	3.0316430000	-1.0591040000	-0.9212520000
C	1.7590540000	-0.5400470000	-0.7378360000
C	1.5570320000	0.5863960000	0.0921570000
C	2.6838780000	1.1847450000	0.7024810000
C	0.2511020000	1.1863510000	0.2570840000
C	-1.0047830000	0.5550870000	0.1322660000
O	0.2683440000	2.5348390000	0.4073600000
S	-2.3982080000	1.4334750000	-0.4581180000
C	-3.4106840000	0.0121280000	-0.3182040000
C	-2.6896520000	-1.0515460000	0.1488990000
N	-1.3560990000	-0.7366030000	0.4272370000
C	-0.4891530000	-1.6643660000	1.1728220000
C	-3.1939910000	-2.4417410000	0.3944050000
C	-4.8559400000	0.0978270000	-0.7021690000
C	5.5352760000	-1.0302510000	-0.5242500000
H	4.8003190000	1.1128110000	1.0048100000
H	3.1696650000	-1.9158410000	-1.5752100000
H	0.9212910000	-0.9740360000	-1.2760420000
H	2.5488910000	2.0588960000	1.3299140000
H	-0.5431480000	2.8624060000	0.8344690000
H	-1.0914340000	-2.1894620000	1.9144740000
H	0.2877450000	-1.0963910000	1.6800630000
H	-0.0208910000	-2.3885170000	0.5018140000
H	-3.2728980000	-2.6643330000	1.4654240000
H	-2.5366240000	-3.1912240000	-0.0587190000
H	-4.1869060000	-2.5668770000	-0.0387270000
H	-5.3475660000	-0.8715270000	-0.5986980000
H	-4.9736050000	0.4252240000	-1.7412130000
H	-5.3897590000	0.8125810000	-0.0652460000
H	5.5099550000	-2.0894400000	-0.7965620000
H	6.1626910000	-0.9148580000	0.3650130000
H	6.0325390000	-0.4930450000	-1.3430040000

**thermodynamic data**

Zero-point correction= 0.281849 (Hartree/Particle)  
Thermal correction to Energy= 0.299676  
Thermal correction to Enthalpy= 0.300620  
Thermal correction to Gibbs Free Energy= 0.234780  
Sum of electronic and zero-point Energies= -1071.376146  
Sum of electronic and thermal Energies= -1071.358319  
Sum of electronic and thermal Enthalpies= -1071.357375  
Sum of electronic and thermal Free Energies= -1071.423215

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	188.050	66.228	138.573

*anti-7a-d***xyz-matrix**

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XYZ file generated by gabedit : coordinates in Angstrom

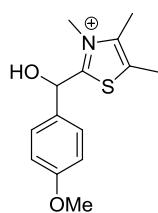
C	3.9195770000	0.6725850000	0.5889200000
C	4.1676930000	-0.4350750000	-0.2372060000
C	3.0893800000	-0.9780620000	-0.9461400000
C	1.8034380000	-0.4528940000	-0.8168800000
C	1.5559690000	0.6384560000	0.0285690000
C	2.6425370000	1.2091140000	0.7110290000
C	0.2193540000	1.3055660000	0.1275860000
C	-1.0126780000	0.5758700000	0.0951000000
O	0.1560320000	2.5589440000	0.1806350000
S	-2.4717740000	1.4828020000	-0.2660100000
C	-3.4297680000	-0.0013550000	-0.2211560000
C	-2.6677680000	-1.0740410000	0.1144410000
N	-1.3166510000	-0.7561720000	0.3324300000
C	-0.4174480000	-1.6541780000	1.0577270000
C	-3.1232280000	-2.4960960000	0.2660770000
C	-4.8939710000	0.0649810000	-0.5295440000
C	5.5544020000	-1.0236690000	-0.3498120000
H	4.7447180000	1.1249900000	1.1353810000
H	3.2607940000	-1.8143970000	-1.6207790000
H	0.9917730000	-0.8711850000	-1.4070010000
H	2.4646200000	2.0857360000	1.3261630000
H	0.1779780000	-2.2758140000	0.3816580000
H	-1.0002140000	-2.2993850000	1.7178280000
H	0.2663090000	-1.0596400000	1.6642980000
H	-2.4789960000	-3.1850510000	-0.2927550000

H	-4.1402130000	-2.6119930000	-0.1129650000
H	-3.1270860000	-2.8242200000	1.3135940000
H	-5.3706380000	-0.9140510000	-0.4309780000
H	-5.0744900000	0.4240840000	-1.5506560000
H	-5.4093280000	0.7539860000	0.1516850000
H	5.7839230000	-1.6732610000	0.5059020000
H	6.3216500000	-0.2415870000	-0.3732730000
H	5.6609620000	-1.6285970000	-1.2562930000

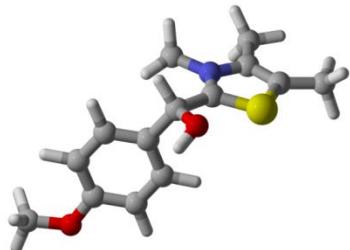
### thermodynamic data

Zero-point correction= 0.269145 (Hartree/Particle)  
 Thermal correction to Energy= 0.286766  
 Thermal correction to Enthalpy= 0.287710  
 Thermal correction to Gibbs Free Energy= 0.222148  
 Sum of electronic and zero-point Energies= -1070.992464  
 Sum of electronic and thermal Energies= -1070.974843  
 Sum of electronic and thermal Enthalpies= -1070.973899  
 Sum of electronic and thermal Free Energies= -1071.039461

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.948	64.770	137.986



*anti*-4a-e -H



### xyz-matrix

**36**

XYZ file generated by gabedit : coordinates in Angstrom

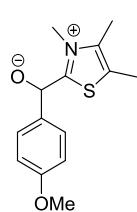
C	-3.4317520000	-0.2066590000	-0.8054480000
C	-3.6248170000	-0.1304760000	0.5821690000
C	-2.5720650000	0.3164170000	1.4060270000
C	-1.3561070000	0.6775420000	0.8527390000
C	-1.1490980000	0.6007640000	-0.5383710000
C	-2.2007680000	0.1609710000	-1.3499610000
C	0.1508420000	1.0663550000	-1.1660570000
C	1.3830210000	0.4431110000	-0.5403810000
O	0.3769070000	2.4652780000	-1.0293870000
S	2.4924580000	1.3939490000	0.3393600000
C	3.5071140000	0.0025350000	0.6453590000
C	2.9778280000	-1.1131450000	0.0625990000
N	1.7689190000	-0.8317230000	-0.6017570000

C	1.0175870000	-1.8683700000	-1.3337250000
C	3.5233430000	-2.5080510000	0.0651020000
C	4.7602890000	0.1522490000	1.4551850000
O	-4.7652460000	-0.4548380000	1.2222830000
C	-5.8911370000	-0.8934120000	0.4602230000
H	-4.2272440000	-0.5369260000	-1.4624790000
H	-2.7445570000	0.3739330000	2.4756950000
H	-0.5622540000	1.0312960000	1.5059720000
H	-2.0692230000	0.1140290000	-2.4292210000
H	0.1449260000	0.7922050000	-2.2333770000
H	-0.4853230000	2.9038430000	-0.9465670000
H	1.4859970000	-2.0458620000	-2.3057240000
H	-0.0118670000	-1.5405990000	-1.4635680000
H	1.0211960000	-2.7897050000	-0.7515030000
H	2.8752810000	-3.1977210000	0.6189950000
H	4.5029920000	-2.5260900000	0.5440550000
H	3.6448130000	-2.8981260000	-0.9514580000
H	5.3496500000	-0.7668680000	1.4374010000
H	4.5296460000	0.3822760000	2.5015320000
H	5.3892600000	0.9597530000	1.0660420000
H	-6.6812840000	-1.0807350000	1.1871850000
H	-5.6657280000	-1.8191470000	-0.0822870000
H	-6.2170210000	-0.1191860000	-0.2440960000

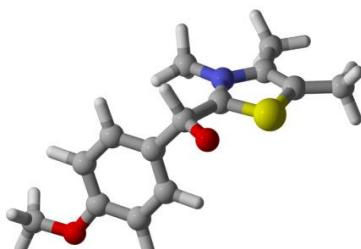
### thermodynamic data

Zero-point correction= 0.299187 (Hartree/Particle)  
 Thermal correction to Energy= 0.318161  
 Thermal correction to Enthalpy= 0.319105  
 Thermal correction to Gibbs Free Energy= 0.250950  
 Sum of electronic and zero-point Energies= -1147.189171  
 Sum of electronic and thermal Energies= -1147.170197  
 Sum of electronic and thermal Enthalpies= -1147.169253  
 Sum of electronic and thermal Free Energies= -1147.237408

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	199.649	70.057	143.444



*anti*-4a-e



### xyz-matrix

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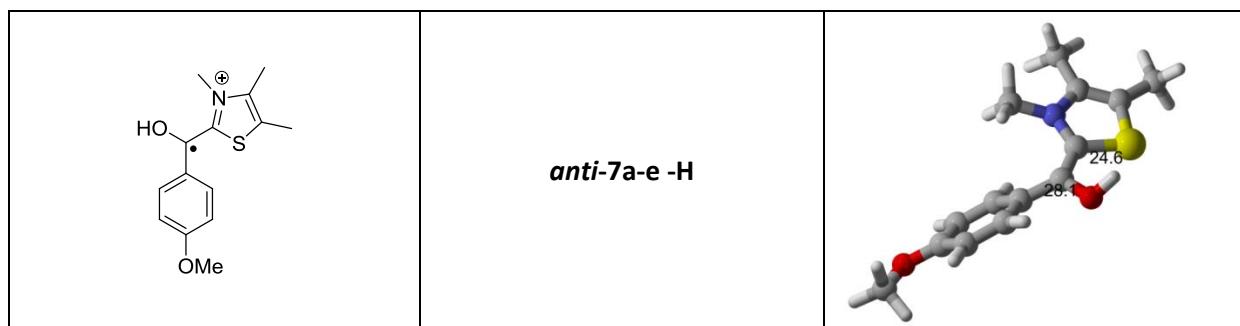
XYZ file generated by gabedit : coordinates in Angstrom

H	1.3617170000	2.4549980000	1.9137500000
H	0.1852210000	-0.9162780000	2.2587570000
H	3.5384690000	3.0877580000	0.6226240000
O	0.5472960000	-2.4449940000	0.8775460000
H	-1.8417400000	0.2960150000	2.3489800000
C	0.1976750000	-1.1949630000	1.1669870000
C	0.8912230000	2.0367660000	1.0185070000
H	5.4617280000	-0.9040190000	-0.7227310000
C	1.3533550000	-0.3359390000	0.5715180000
N	1.7090850000	0.9483400000	0.4773440000
H	-0.0937110000	1.6440380000	1.2652660000
S	2.4957980000	-1.4024670000	-0.1105620000
C	2.9459070000	1.1626860000	-0.1686290000
C	3.4564970000	2.5628490000	-0.3370810000
C	3.5079420000	-0.0148890000	-0.5615510000
H	4.4501190000	2.5476470000	-0.7888260000
H	0.7790400000	2.8224150000	0.2681040000
H	5.3455310000	0.7094510000	-1.4374120000
C	4.8047110000	-0.2286790000	-1.2833870000
C	-2.0753430000	0.0155850000	1.3220790000
C	-1.1582370000	-0.7355560000	0.5893390000
H	2.8088470000	3.1632730000	-0.9886140000
H	-4.0089190000	0.9643980000	1.3893970000
H	4.6389740000	-0.6819980000	-2.2681910000
C	-3.3140100000	0.3928610000	0.7838900000
C	-1.5179810000	-1.1453130000	-0.7037610000
H	-0.8327830000	-1.7911730000	-1.2451310000
C	-3.6405610000	0.0032960000	-0.5175360000
H	-6.1202480000	0.5266870000	0.4604110000
C	-2.7335690000	-0.7743540000	-1.2579490000
H	-5.4024360000	2.0463050000	-0.1506170000
C	-5.7828720000	1.0569010000	-0.4405240000
O	-4.8132330000	0.3110080000	-1.1538210000
H	-3.0197610000	-1.0867200000	-2.2581350000
H	-6.6273420000	1.1826640000	-1.1212520000

### thermodynamic data

Zero-point correction=	0.284920 (Hartree/Particle)
Thermal correction to Energy=	0.303435
Thermal correction to Enthalpy=	0.304379
Thermal correction to Gibbs Free Energy=	0.237383
Sum of electronic and zero-point Energies=	-1146.747817
Sum of electronic and thermal Energies=	-1146.729302
Sum of electronic and thermal Enthalpies=	-1146.728358
Sum of electronic and thermal Free Energies=	-1146.795354

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	190.408	68.561	141.006



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

```

C   -3.5903470000    0.7471370000   -0.4675180000
C   -3.7795300000   -0.4043560000    0.3219980000
C   -2.6627130000   -1.0320440000    0.9196610000
C   -1.3953210000   -0.5312490000    0.7201240000
C   -1.1819640000    0.6147600000   -0.0910190000
C   -2.3131060000    1.2478950000   -0.6589630000
C    0.1242120000    1.1950970000   -0.2647070000
C    1.3738000000    0.5534170000   -0.1378780000
O    0.1270860000    2.5466980000   -0.4244930000
S    2.7759420000    1.4240800000    0.4470190000
C    3.7758070000   -0.0092500000    0.3168500000
C    3.0465080000   -1.0681810000   -0.1444280000
N    1.7149200000   -0.7435930000   -0.4265810000
C    0.8471030000   -1.6605780000   -1.1827400000
C    3.5374510000   -2.4647750000   -0.3813140000
C    5.2209150000    0.0656680000    0.7036770000
O   -4.9649960000   -0.9737510000    0.5768140000
C   -6.1610050000   -0.3921230000    0.0434230000
H   -4.4330330000    1.2482290000   -0.9283550000
H   -2.8372820000   -1.8930520000    1.5560690000
H   -0.5577920000   -0.9914830000    1.2355630000
H   -2.1730500000    2.1367790000   -1.2639680000
H    0.9303060000    2.8504700000   -0.8830890000
H    1.4476710000   -2.1792780000   -1.9305670000
H    0.0722910000   -1.0841580000   -1.6839440000
H    0.3757800000   -2.3923370000   -0.5219570000
H    2.8730300000   -3.2049220000    0.0770500000
H    4.5293150000   -2.5968540000    0.0522360000
H    3.6134930000   -2.6958000000   -1.4507550000
H    5.7089690000   -0.9041960000    0.5881520000
H    5.3388840000    0.3793220000    1.7470310000

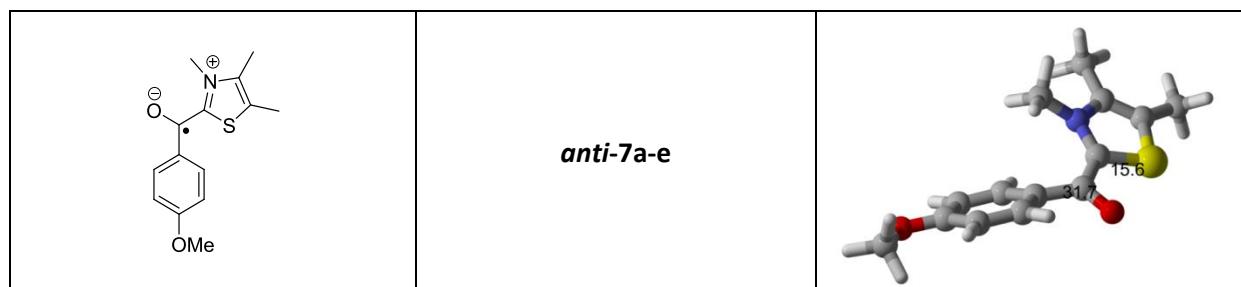
```

H	5.7586040000	0.7863530000	0.0767910000
H	-6.9738220000	-1.0243950000	0.3992010000
H	-6.1427970000	-0.3961110000	-1.0518660000
H	-6.2976620000	0.6292210000	0.4146110000

### thermodynamic data

Zero-point correction= 0.287302 (Hartree/Particle)  
 Thermal correction to Energy= 0.305848  
 Thermal correction to Enthalpy= 0.306792  
 Thermal correction to Gibbs Free Energy= 0.239834  
 Sum of electronic and zero-point Energies= -1146.579809  
 Sum of electronic and thermal Energies= -1146.561263  
 Sum of electronic and thermal Enthalpies= -1146.560319  
 Sum of electronic and thermal Free Energies= -1146.627277

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.922	69.382	140.924



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

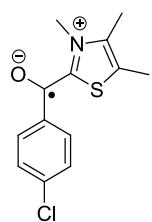
C	-3.5735170000	-0.7677870000	0.4824150000
C	-3.7849640000	0.3796300000	-0.2941060000
C	-2.6965270000	0.9935090000	-0.9322170000
C	-1.4169840000	0.4773220000	-0.7780670000
C	-1.1819740000	-0.6617620000	0.0137930000
C	-2.2844960000	-1.2813080000	0.6165250000
C	0.1561620000	-1.3197790000	0.1329610000
C	1.3844410000	-0.5823590000	0.1163530000
O	0.2287570000	-2.5721800000	0.1927260000
S	2.8525120000	-1.4782050000	-0.2409840000
C	3.7938070000	0.0187000000	-0.2200790000
C	3.0216890000	1.0859650000	0.1071440000
N	1.6746770000	0.7570660000	0.3378070000
C	0.8070810000	1.6365120000	1.1249200000
C	3.4536020000	2.5174410000	0.2355780000
C	5.2555720000	-0.0334580000	-0.5419610000
O	-4.9996760000	0.9676990000	-0.4984730000

C	-6.1419230000	0.3745420000	0.0986170000
H	-4.3998890000	-1.2684210000	0.9744290000
H	-2.8840390000	1.8630400000	-1.5548500000
H	-0.5904200000	0.9467250000	-1.3048770000
H	-2.1160060000	-2.1874200000	1.1899170000
H	0.3494010000	2.4159310000	0.5071260000
H	1.3850110000	2.1084100000	1.9247380000
H	0.0126250000	1.0430380000	1.5729310000
H	2.8154350000	3.1815350000	-0.3597170000
H	4.4797320000	2.6402270000	-0.1155520000
H	3.4185320000	2.8723790000	1.2734030000
H	5.7235720000	0.9501510000	-0.4469800000
H	5.4306200000	-0.3902580000	-1.5648600000
H	5.7831120000	-0.7181660000	0.1342570000
H	-6.9902280000	0.9945420000	-0.1973500000
H	-6.0657850000	0.3638320000	1.1940550000
H	-6.2990620000	-0.6508820000	-0.2608530000

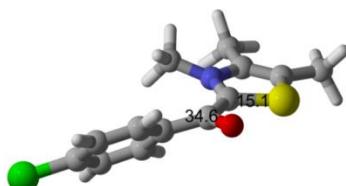
#### thermodynamic data

Zero-point correction= 0.274247 (Hartree/Particle)  
 Thermal correction to Energy= 0.292729  
 Thermal correction to Enthalpy= 0.293674  
 Thermal correction to Gibbs Free Energy= 0.225912  
 Sum of electronic and zero-point Energies= -1146.192399  
 Sum of electronic and thermal Energies= -1146.173918  
 Sum of electronic and thermal Enthalpies= -1146.172973  
 Sum of electronic and thermal Free Energies= -1146.240735

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	183.690	67.945	142.616



*anti*-7a-g



#### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

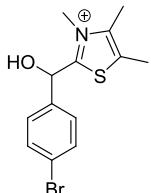
C	-3.5514040000	-0.9062580000	0.6426780000
C	-3.8131960000	0.2063780000	-0.1591710000
C	-2.7938470000	0.8360030000	-0.8715830000

C	-1.4899860000	0.3546780000	-0.7567880000
C	-1.1929950000	-0.7464700000	0.0612290000
C	-2.2474510000	-1.3828700000	0.7357330000
C	0.1704470000	-1.3603610000	0.1381330000
C	1.3727300000	-0.5841590000	0.0954400000
O	0.2782350000	-2.6115150000	0.1766880000
S	2.8570130000	-1.4288160000	-0.3057750000
C	3.7602050000	0.0881390000	-0.2505670000
C	2.9647780000	1.1261590000	0.1152350000
N	1.6301710000	0.7533150000	0.3499350000
C	0.7118420000	1.6055610000	1.1065170000
C	3.3680860000	2.5617970000	0.2839680000
C	5.2207500000	0.0816640000	-0.5829780000
Cl	-5.4598840000	0.8144660000	-0.2864260000
H	-4.3604860000	-1.3922650000	1.1778530000
H	-3.0205970000	1.6790000000	-1.5159660000
H	-0.7006150000	0.8226500000	-1.3387760000
H	-2.0262230000	-2.2646230000	1.3284340000
H	0.0975700000	2.2326850000	0.4525580000
H	1.2808890000	2.2457680000	1.7832460000
H	0.0480750000	0.9753360000	1.6987710000
H	2.6875440000	3.2347570000	-0.2506770000
H	4.3723580000	2.7233010000	-0.1117520000
H	3.3793450000	2.8714840000	1.3369390000
H	5.6632180000	1.0745420000	-0.4667190000
H	5.3971250000	-0.2453880000	-1.6154080000
H	5.7707920000	-0.6047640000	0.0730150000

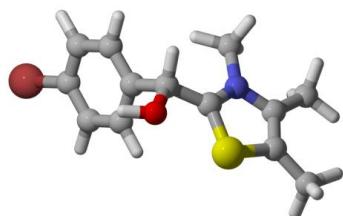
#### thermodynamic data

Zero-point correction= 0.231929 (Hartree/Particle)  
 Thermal correction to Energy= 0.248897  
 Thermal correction to Enthalpy= 0.249841  
 Thermal correction to Gibbs Free Energy= 0.185629  
 Sum of electronic and zero-point Energies= -1491.308072  
 Sum of electronic and thermal Energies= -1491.291104  
 Sum of electronic and thermal Enthalpies= -1491.290160  
 Sum of electronic and thermal Free Energies= -1491.354372

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	156.185	62.620	135.146
Electronic	0.000	0.000	1.377



*anti*-4a-f-H



### xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

C	2.7205860000	0.1460280000	1.2781010000
C	3.0451600000	0.0096090000	-0.0718570000
C	2.1042020000	0.2911240000	-1.0671750000
C	0.8258620000	0.7041030000	-0.7039460000
C	0.4777030000	0.8364790000	0.6490410000
C	1.4371630000	0.5619620000	1.6322430000
C	-0.8973000000	1.3470280000	1.0542670000
C	-2.0391890000	0.5505120000	0.4539790000
O	-1.1514680000	2.6729510000	0.6129220000
S	-3.0857540000	1.2525700000	-0.6956200000
C	-4.0203040000	-0.2200320000	-0.8076140000
C	-3.5156120000	-1.1722670000	0.0314370000
N	-2.3887570000	-0.7056230000	0.7338160000
C	-1.6895710000	-1.5443460000	1.7257720000
C	-4.0134400000	-2.5670220000	0.2549230000
C	-5.1902310000	-0.2970790000	-1.7427430000
Br	4.7858620000	-0.5584840000	-0.5657040000
H	3.4625210000	-0.0619860000	2.0410230000
H	2.3743350000	0.1898230000	-2.1124930000
H	0.1026470000	0.9330930000	-1.4822860000
H	1.1916250000	0.6842510000	2.6851000000
H	-0.9868690000	1.2866170000	2.1510540000
H	-0.3193900000	3.1729450000	0.6369490000
H	-2.2763680000	-1.5895520000	2.6471580000
H	-0.7058450000	-1.1261050000	1.9261700000
H	-1.5659710000	-2.5486460000	1.3200900000
H	-3.2915120000	-3.3168460000	-0.0900080000
H	-4.9388680000	-2.7272790000	-0.2994210000
H	-4.2241340000	-2.7592470000	1.3127160000
H	-5.7839460000	-1.1936150000	-1.5522950000
H	-4.8597880000	-0.3281250000	-2.7872640000
H	-5.8486750000	0.5696740000	-1.6255990000

### thermodynamic data

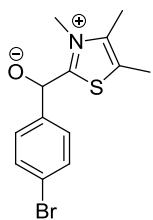
Zero-point correction= 0.256136 (Hartree/Particle)

Thermal correction to Energy= 0.273971

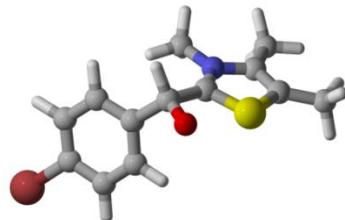
Thermal correction to Enthalpy= 0.274915

Thermal correction to Gibbs Free Energy= 0.207927  
 Sum of electronic and zero-point Energies= -3603.806196  
 Sum of electronic and thermal Energies= -3603.788361  
 Sum of electronic and thermal Enthalpies= -3603.787417  
 Sum of electronic and thermal Free Energies= -3603.854405

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	171.919	65.041	140.988



*anti-4a-f*



### xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

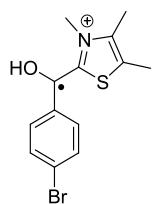
H	-2.6070730000	-1.0682290000	-1.8960400000
Br	-4.7938930000	0.4682200000	-0.5972360000
C	-2.2356290000	-0.8005400000	-0.9122330000
H	-0.3345530000	-1.8069430000	-1.1314300000
C	-3.0412020000	-0.0692280000	-0.0367750000
C	-0.9652180000	-1.1909570000	-0.4971520000
H	5.0019040000	-0.3586650000	-2.6264690000
C	-2.6030360000	0.2605170000	1.2416740000
C	-0.4825870000	-0.8405500000	0.7689830000
S	3.0918690000	-1.3695760000	-0.3350140000
C	5.2687190000	-0.0587280000	-1.6057850000
O	1.2519600000	-2.5352480000	0.7434400000
H	5.9536410000	-0.8189460000	-1.2128370000
H	-3.2541910000	0.8000150000	1.9213780000
C	4.0495180000	0.0662060000	-0.7418600000
C	-1.3198580000	-0.1326920000	1.6356090000
H	5.8198180000	0.8837050000	-1.6703930000
C	0.9278600000	-1.3234700000	1.1779720000
C	2.0149360000	-0.3916490000	0.5553700000
C	3.5250590000	1.1922480000	-0.1811390000
N	2.3575570000	0.8997390000	0.5564150000
H	3.3055050000	3.2602810000	-0.7873000000
H	-0.9841150000	0.0929260000	2.6472360000
H	1.0132560000	-1.1448990000	2.2865480000
H	4.9598980000	2.6482500000	-0.8019450000
C	4.0133070000	2.6082030000	-0.2598060000
H	0.6441070000	1.5026720000	1.5874370000
H	1.4183660000	2.7791650000	0.6320030000

C	1.6010330000	1.9224300000	1.2839720000
H	4.1833830000	3.0393390000	0.7342960000
H	2.1604340000	2.2499200000	2.1655770000

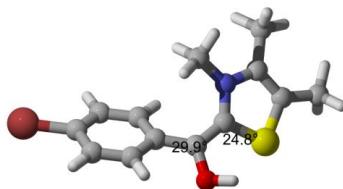
### thermodynamic data

Zero-point correction= 0.242139 (Hartree/Particle)  
 Thermal correction to Energy= 0.259528  
 Thermal correction to Enthalpy= 0.260472  
 Thermal correction to Gibbs Free Energy= 0.194805  
 Sum of electronic and zero-point Energies= -3603.374488  
 Sum of electronic and thermal Energies= -3603.357099  
 Sum of electronic and thermal Enthalpies= -3603.356155  
 Sum of electronic and thermal Free Energies= -3603.421822

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	162.856	63.605	138.208



*anti-7a-f-H*



### xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

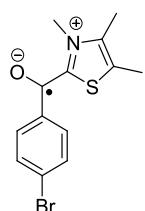
C	2.8647950000	1.1647190000	0.6614830000
C	3.1650870000	0.0208610000	-0.0877870000
C	2.1515940000	-0.7043460000	-0.7275980000
C	0.8337370000	-0.2931170000	-0.6002990000
C	0.5024210000	0.8453690000	0.1706440000
C	1.5465580000	1.5781400000	0.7819350000
C	-0.8587720000	1.3268950000	0.2690860000
C	-2.0459600000	0.5760480000	0.1269380000
O	-0.9689680000	2.6758130000	0.3625960000
S	-3.4873740000	1.2944370000	-0.5545620000
C	-4.3701900000	-0.2073260000	-0.3876270000
C	-3.5747130000	-1.1786940000	0.1550530000
N	-2.2891210000	-0.7279690000	0.4694400000
C	-1.3713550000	-1.5361910000	1.2904160000
C	-3.9585340000	-2.5987850000	0.4429730000
C	-5.7986300000	-0.2763280000	-0.8333810000
Br	4.9599650000	-0.5447750000	-0.2532250000
H	3.6608800000	1.7211820000	1.1432220000
H	2.4041080000	-1.5666950000	-1.3342980000

H	0.0592940000	-0.8260720000	-1.1437720000
H	1.3106800000	2.4656280000	1.3583310000
H	-1.8206550000	2.9450830000	0.7504120000
H	-1.9531730000	-2.0909480000	2.0266310000
H	-0.6799460000	-0.8740800000	1.8076190000
H	-0.8025810000	-2.2345860000	0.6717950000
H	-4.0666060000	-2.7828380000	1.5187280000
H	-3.2142610000	-3.3008160000	0.0527490000
H	-4.9139150000	-2.8354610000	-0.0263170000
H	-6.2161580000	-1.2692660000	-0.6561120000
H	-5.8935010000	-0.0562090000	-1.9027260000
H	-6.4155760000	0.4470260000	-0.2882530000

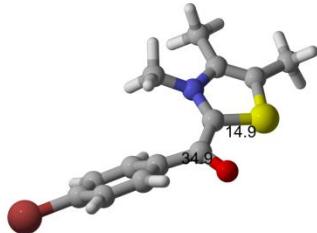
### thermodynamic data

Zero-point correction= 0.244068 (Hartree/Particle)  
 Thermal correction to Energy= 0.261520  
 Thermal correction to Enthalpy= 0.262464  
 Thermal correction to Gibbs Free Energy= 0.196375  
 Sum of electronic and zero-point Energies= -3603.194140  
 Sum of electronic and thermal Energies= -3603.176688  
 Sum of electronic and thermal Enthalpies= -3603.175744  
 Sum of electronic and thermal Free Energies= -3603.241833

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	164.106	64.346	139.096



*anti*-7a-f



### xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

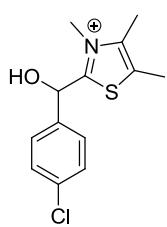
C	2.8300720000	-1.1562990000	-0.7065050000
C	3.1591270000	-0.0505560000	0.0786890000
C	2.1852020000	0.6353160000	0.8013370000
C	0.8570910000	0.2181330000	0.7137670000
C	0.4927270000	-0.8752630000	-0.0874810000
C	1.5028660000	-1.5695420000	-0.7727990000
C	-0.8999040000	-1.4229610000	-0.1355640000
C	-2.0630360000	-0.5896950000	-0.0887130000
O	-1.0682100000	-2.6680140000	-0.1538540000
S	-3.5805690000	-1.3589430000	0.3390680000

C	-4.4129780000	0.1974390000	0.2719060000
C	-3.5740110000	1.1924920000	-0.1153040000
N	-2.2607230000	0.7550270000	-0.3580250000
C	-1.3117300000	1.5540190000	-1.1347310000
C	-3.9116020000	2.6431570000	-0.2989570000
C	-5.8689840000	0.2638750000	0.6176900000
Br	4.9813310000	0.5233530000	0.1788280000
H	3.6038940000	-1.6872360000	-1.2504940000
H	2.4628600000	1.4726050000	1.4327030000
H	0.1022210000	0.7306440000	1.3041140000
H	1.2287040000	-2.4452170000	-1.3523170000
H	-0.6669330000	2.1653270000	-0.4952780000
H	-1.8572280000	2.2063340000	-1.8192830000
H	-0.6794700000	0.8857020000	-1.7193960000
H	-3.1948020000	3.2901870000	0.2200640000
H	-4.9029290000	2.8563250000	0.1047690000
H	-3.9194750000	2.9397420000	-1.3557160000
H	-6.2650360000	1.2750400000	0.4923130000
H	-6.0505780000	-0.0415130000	1.6558070000
H	-6.4570090000	-0.4039880000	-0.0243800000

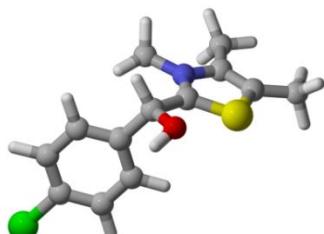
### thermodynamic data

Zero-point correction= 0.231587 (Hartree/Particle)  
 Thermal correction to Energy= 0.248737  
 Thermal correction to Enthalpy= 0.249681  
 Thermal correction to Gibbs Free Energy= 0.184388  
 Sum of electronic and zero-point Energies= -3602.817151  
 Sum of electronic and thermal Energies= -3602.800000  
 Sum of electronic and thermal Enthalpies= -3602.799056  
 Sum of electronic and thermal Free Energies= -3602.864350

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	156.085	62.897	137.422



*anti*-4a-g -H



### xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

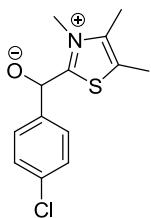
C	3.3981010000	-0.2976730000	0.9940800000
---	--------------	---------------	--------------

C	3.6495880000	-0.2116250000	-0.3761000000
C	2.6807820000	0.2864750000	-1.2538890000
C	1.4480500000	0.6925140000	-0.7524440000
C	1.1728000000	0.6040950000	0.6206340000
C	2.1597930000	0.1144570000	1.4857390000
C	-0.1490460000	1.1051110000	1.1846290000
C	-1.3619910000	0.4711120000	0.5321580000
O	-0.3515460000	2.4953430000	0.9775370000
S	-2.4151700000	1.3942900000	-0.4412790000
C	-3.4366370000	0.0048270000	-0.7285780000
C	-2.9518520000	-1.0897470000	-0.0709810000
N	-1.7703880000	-0.7939420000	0.6349720000
C	-1.0787190000	-1.8091650000	1.4517070000
C	-3.5180370000	-2.4758820000	-0.0343290000
C	-4.6499080000	0.1345210000	-1.6001170000
Cl	5.1920740000	-0.7260120000	-1.0031130000
H	4.1628460000	-0.6728070000	1.6653580000
H	2.8962540000	0.3555280000	-2.3146150000
H	0.7035460000	1.0897250000	-1.4373220000
H	1.9720810000	0.0646480000	2.5562470000
H	-0.1849110000	0.8696740000	2.2605790000
H	0.5058040000	2.9470130000	1.0403730000
H	-1.6241480000	-1.9613020000	2.3869360000
H	-0.0631070000	-1.4791830000	1.6576140000
H	-1.0354630000	-2.7456920000	0.8955410000
H	-2.8535530000	-3.1997340000	-0.5210300000
H	-4.4727550000	-2.5045790000	-0.5606860000
H	-3.6961720000	-2.8145830000	0.9922360000
H	-5.2441880000	-0.7813020000	-1.5809930000
H	-4.3695160000	0.3304360000	-2.6411540000
H	-5.2917050000	0.9564400000	-1.2658790000

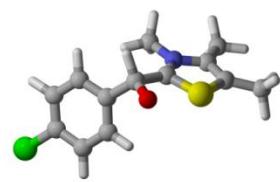
### thermodynamic data

Zero-point correction= 0.256705 (Hartree/Particle)  
 Thermal correction to Energy= 0.274274  
 Thermal correction to Enthalpy= 0.275218  
 Thermal correction to Gibbs Free Energy= 0.209598  
 Sum of electronic and zero-point Energies= -1492.296661  
 Sum of electronic and thermal Energies= -1492.279092  
 Sum of electronic and thermal Enthalpies= -1492.278148  
 Sum of electronic and thermal Free Energies= -1492.343768

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	172.109	64.651	138.110



*anti*-4a-g



### xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

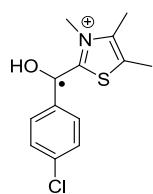
H	-3.1786680000	-1.0250000000	-2.0719800000
Cl	-5.2216720000	0.6565720000	-0.9677830000
C	-2.8457980000	-0.6934780000	-1.0935430000
H	-0.9846770000	-1.7926750000	-1.1257540000
C	-3.6622350000	0.1402940000	-0.3252610000
C	-1.6182850000	-1.1009760000	-0.5785730000
H	4.5038490000	-0.7523920000	-2.3946660000
C	-3.2753930000	0.5550060000	0.9458360000
C	-1.1861510000	-0.6686710000	0.6804740000
H	-3.9366060000	1.1748550000	1.5427770000
S	2.4170620000	-1.4358540000	-0.1692510000
C	4.7219290000	-0.3287530000	-1.4069590000
O	0.4688930000	-2.4298790000	0.8893920000
C	-2.0341360000	0.1418660000	1.4399780000
C	3.4608390000	-0.0800600000	-0.6346980000
H	5.3701080000	-1.0418080000	-0.8842100000
H	5.2939830000	0.5907260000	-1.5593780000
C	1.3384100000	-0.3428970000	0.5729480000
C	0.1775170000	-1.1738810000	1.2052770000
H	2.8657890000	3.1291290000	-0.9784640000
C	2.9581220000	1.1098360000	-0.2001280000
N	1.7390200000	0.9288800000	0.4881080000
H	-1.7412590000	0.4353530000	2.4474090000
H	4.4888600000	2.4490970000	-0.8543260000
H	0.8692790000	2.8382080000	0.3451890000
C	3.5148260000	2.4927770000	-0.3636160000
H	0.0036390000	1.6819700000	1.3723710000
H	0.2126850000	-0.9071090000	2.2988720000
C	0.9889560000	2.0396540000	1.0805500000
H	3.6542670000	2.9956470000	0.6011740000
H	1.5182950000	2.4285140000	1.9557020000

### thermodynamic data

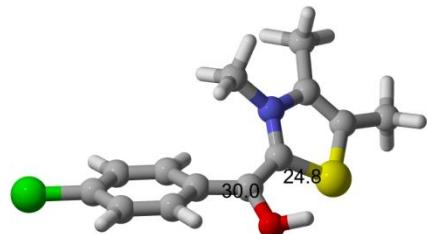
Zero-point correction=	0.242414 (Hartree/Particle)
Thermal correction to Energy=	0.259638
Thermal correction to Enthalpy=	0.260583
Thermal correction to Gibbs Free Energy=	0.195899

Sum of electronic and zero-point Energies= -1491.865395  
 Sum of electronic and thermal Energies= -1491.848170  
 Sum of electronic and thermal Enthalpies= -1491.847226  
 Sum of electronic and thermal Free Energies= -1491.911909

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	162.926	63.351	136.138



*anti-7a-g-H*



### xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

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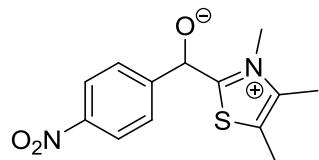
C      3.5824180000     0.8957320000     0.5821290000
C      3.8100250000    -0.2428080000    -0.2010480000
C      2.7495280000    -0.9009390000    -0.8383570000
C      1.4572090000    -0.4266970000    -0.6748040000
C      1.1983270000     0.7071060000     0.1295490000
C      2.2889880000     1.3707140000     0.7380780000
C     -0.1352630000     1.2536240000     0.2661730000
C     -1.3614650000     0.5666080000     0.1321570000
O     -0.1750370000     2.6035440000     0.3918670000
S     -2.7774990000     1.3722980000    -0.5031210000
C     -3.7323350000    -0.0862550000    -0.3514440000
C     -2.9767810000    -1.1090780000     0.1525940000
N     -1.6636380000    -0.7314680000     0.4490220000
C     -0.7730700000    -1.6064660000     1.2307070000
C     -3.4268710000    -2.5137680000     0.4189980000
C     -5.1715480000    -0.0706530000    -0.7662300000
Cl     5.4283860000    -0.8396790000    -0.3993270000
H      4.4156160000     1.3982450000     1.0609150000
H      2.9484090000    -1.7590390000    -1.4708650000
H      0.6465740000    -0.9063550000    -1.2150110000
H      2.1087440000     2.2541110000     1.3402250000
H     -1.0051220000     2.9068630000     0.8008920000
H     -1.3652930000    -2.1327890000     1.9796240000
H     -0.0243720000    -0.9969530000     1.7319830000
H     -0.2714230000    -2.3317550000     0.5855120000
H     -3.5179260000    -2.7164660000     1.4929810000
H     -2.7298180000    -3.2441840000    -0.0049460000
H     -4.4046280000    -2.6901550000    -0.0303570000
H     -5.6289180000    -1.0527380000    -0.6314590000
H     -5.2794480000     0.2092760000    -1.8201480000
H     -5.7441860000     0.6489250000    -0.1699490000

```

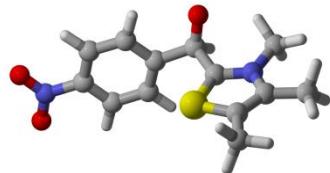
### thermodynamic data

Zero-point correction= 0.244611 (Hartree/Particle)  
 Thermal correction to Energy= 0.261782  
 Thermal correction to Enthalpy= 0.262726  
 Thermal correction to Gibbs Free Energy= 0.198120  
 Sum of electronic and zero-point Energies= -1491.684481  
 Sum of electronic and thermal Energies= -1491.667310  
 Sum of electronic and thermal Enthalpies= -1491.666366  
 Sum of electronic and thermal Free Energies= -1491.730972

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	164.270	63.975	135.975



*syn-4a-j*



### Xyz-matrix

33

XYZ file generated by gabedit : coordinates in Angstrom

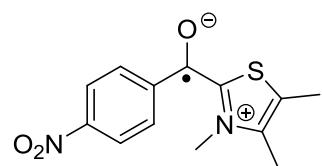
	C	O	N	S
C	-2.9902740000	-0.4462760000	-1.1169640000	
C	-3.5231290000	0.0378130000	0.0774730000	
C	-2.8000110000	0.0194500000	1.2718560000	
C	-1.5088960000	-0.4977830000	1.2570920000	
C	-0.9449210000	-0.9793270000	0.0676540000	
C	-1.6938290000	-0.9549190000	-1.1120720000	
C	0.4733850000	-1.5754140000	0.0112940000	
C	1.5335160000	-0.4719020000	0.1836320000	
O	0.8470570000	-2.1021950000	-1.1544070000	
N	2.8417850000	-0.7311670000	0.3560390000	
S	1.3027100000	1.1906320000	-0.1995670000	
C	3.0351420000	1.4977750000	-0.1737210000	
C	3.7050450000	0.3592330000	0.1478670000	
C	3.2873960000	-2.1236120000	0.5256390000	
C	5.1859310000	0.1812810000	0.2946690000	
C	3.5605820000	2.8677210000	-0.4784530000	
H	-3.5909740000	-0.4187060000	-2.0180340000	
H	-3.2565100000	0.3994250000	2.1775140000	
H	-0.9355880000	-0.5323240000	2.1816690000	
H	-1.2252800000	-1.3547860000	-2.0055650000	
H	0.5551750000	-2.2390900000	0.9146010000	
H	2.6898050000	-2.7109820000	-0.1816930000	
H	3.1194910000	-2.4568670000	1.5531900000	

H	4.3473890000	-2.1973970000	0.2901410000
H	5.6918660000	1.1452750000	0.2187830000
H	5.5988180000	-0.4696790000	-0.4855800000
H	5.4447840000	-0.2542130000	1.2665810000
H	4.6471550000	2.9067890000	-0.3665310000
H	3.1297160000	3.6207710000	0.1918740000
H	3.3214640000	3.1658310000	-1.5062460000
N	-4.8877570000	0.5811840000	0.0836810000
O	-5.3330810000	1.0063120000	1.1515960000
O	-5.5112850000	0.5848170000	-0.9786230000

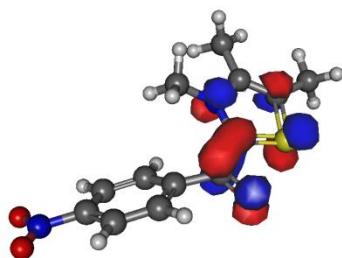
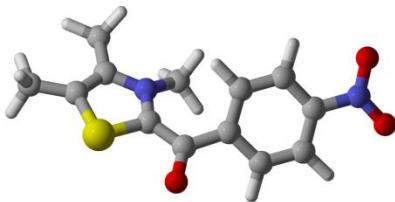
### Thermodynamic data

Zero-point correction= 0.255281 (Hartree/Particle)  
 Thermal correction to Energy= 0.273623  
 Thermal correction to Enthalpy= 0.274567  
 Thermal correction to Gibbs Free Energy= 0.207262  
 Sum of electronic and zero-point Energies= -1236.765288  
 Sum of electronic and thermal Energies= -1236.746946  
 Sum of electronic and thermal Enthalpies= -1236.746002  
 Sum of electronic and thermal Free Energies= -1236.813307

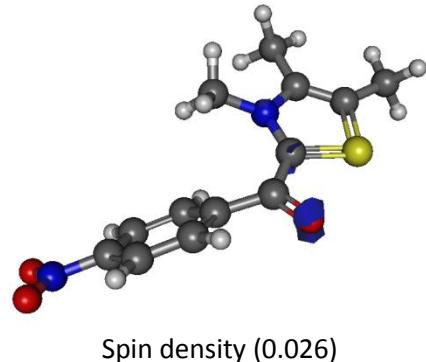
	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	171.701	67.764	141.656



*anti*- 7a-j



SOMO (0.058)



### Xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

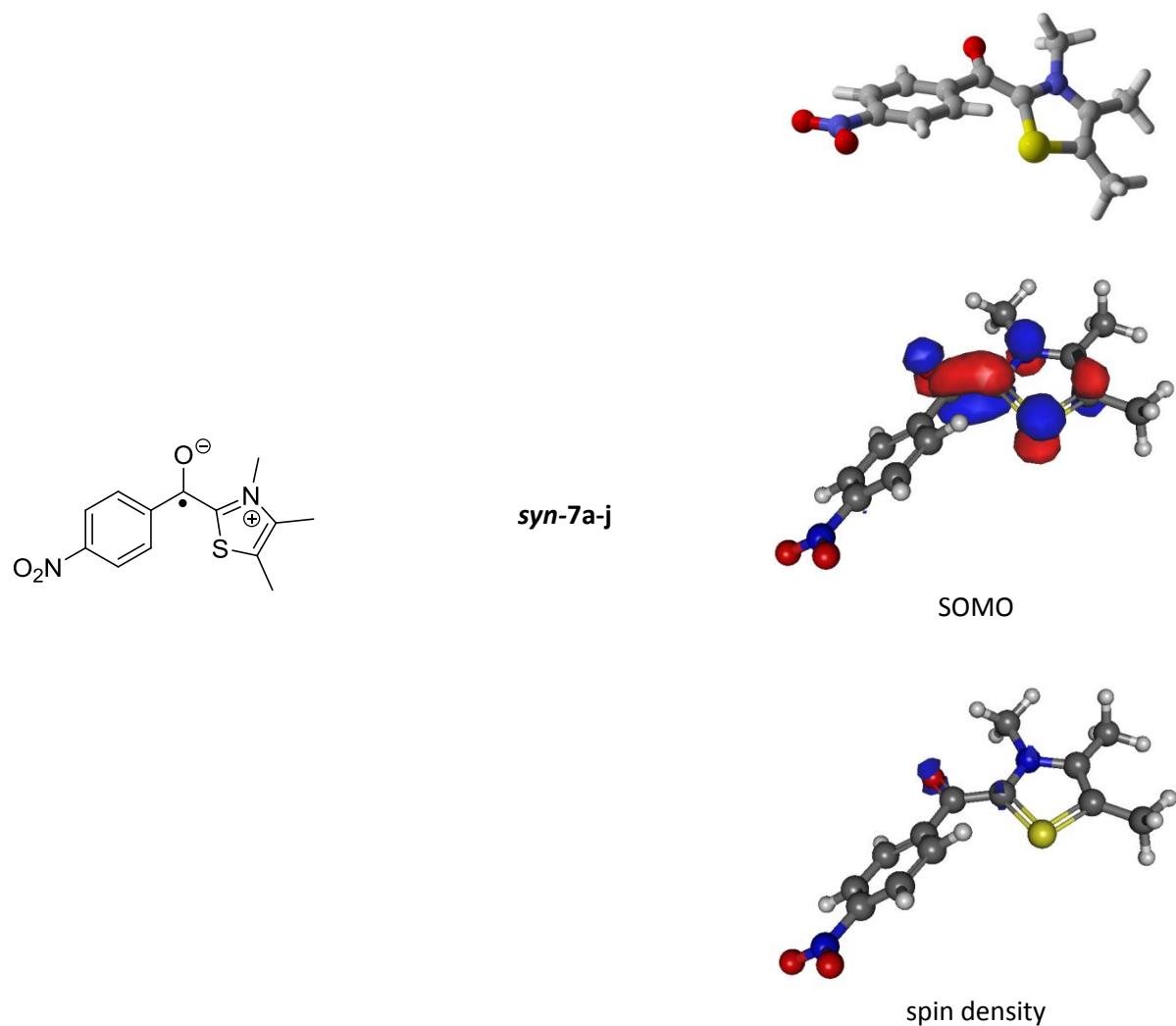
	C	-3.2982880000	-1.0657390000	0.5911710000
C	-3.5702930000	0.1007370000	-0.1284430000	
C	-2.5625250000	0.8102320000	-0.7822030000	
C	-1.2531200000	0.3533660000	-0.6875150000	
C	-0.9409440000	-0.8012750000	0.0544720000	
C	-1.9880440000	-1.5169350000	0.6654560000	
C	0.4309720000	-1.3866220000	0.1068370000	
C	1.6218620000	-0.5868420000	0.0752840000	
O	0.5667420000	-2.6368310000	0.1038790000	
N	1.8664190000	0.7338610000	0.3953590000	
S	3.1056680000	-1.3901700000	-0.3889790000	
C	3.9956200000	0.1273810000	-0.2626040000	
C	3.1937980000	1.1369220000	0.1655860000	
C	0.9424140000	1.5413790000	1.1945630000	
C	3.5825270000	2.5659880000	0.4065210000	
C	5.4537470000	0.1530710000	-0.6055330000	
H	-4.1112590000	-1.5955470000	1.0723380000	
H	-2.8196870000	1.6899050000	-1.3593730000	
H	-0.4683390000	0.8757590000	-1.2266660000	
H	-1.7474480000	-2.4340010000	1.1922690000	
H	1.5093580000	2.1515740000	1.8996540000	
H	0.2864520000	0.8764880000	1.7569320000	
H	0.3224050000	2.1947040000	0.5729730000	
H	4.5778670000	2.7608860000	0.0036030000	
H	3.6085250000	2.8169370000	1.4746360000	
H	2.8858130000	3.2585780000	-0.0796460000	
H	5.8838320000	1.1457410000	-0.4497960000	
H	5.6251820000	-0.1268660000	-1.6522280000	
H	6.0169110000	-0.5534770000	0.0167330000	
N	-4.9498170000	0.5858780000	-0.2113950000	
O	-5.1580960000	1.6209890000	-0.8492860000	
O	-5.8240050000	-0.0649220000	0.3645250000	

### Thermodynamic data

Zero-point correction= 0.244140 (Hartree/Particle)

Thermal correction to Energy= 0.262382  
 Thermal correction to Enthalpy= 0.263326  
 Thermal correction to Gibbs Free Energy= 0.195966  
 Sum of electronic and zero-point Energies= -1236.202726  
 Sum of electronic and thermal Energies= -1236.184484  
 Sum of electronic and thermal Enthalpies= -1236.183540  
 Sum of electronic and thermal Free Energies= -1236.250900

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.647	67.226	141.771



### Xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

C	-3.2882940000	1.0689130000	-0.6380290000
C	-3.6370500000	-0.1060690000	0.0319120000
C	-2.6932420000	-0.8573100000	0.7299670000
C	-1.3683630000	-0.4324780000	0.7378900000

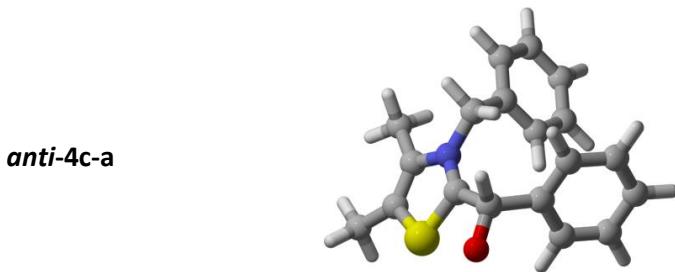
C	-0.9783700000	0.7324080000	0.0527860000
C	-1.9651430000	1.4849580000	-0.6127900000
C	0.4130800000	1.2844440000	0.0378150000
C	1.5457330000	0.4040340000	0.0893520000
O	0.5676890000	2.5288310000	-0.0666930000
N	2.8577320000	0.8318730000	0.1977990000
S	1.5275450000	-1.3301080000	-0.2190420000
C	3.2885240000	-1.3932870000	-0.2424330000
C	3.8174450000	-0.1635280000	-0.0068780000
C	3.2146740000	2.2135610000	0.5461390000
C	5.2781860000	0.1760480000	0.0493780000
C	3.9651890000	-2.7070010000	-0.4857730000
H	-4.0524810000	1.6313390000	-1.1603090000
H	-3.0070140000	-1.7469850000	1.2618370000
H	-0.6452240000	-0.9977030000	1.3161310000
H	-1.6638910000	2.4030860000	-1.1046180000
H	4.2279000000	2.2214420000	0.9471780000
H	2.5209300000	2.5906720000	1.2941550000
H	3.1507710000	2.8660740000	-0.3273100000
H	5.8781760000	-0.6911700000	-0.2303700000
H	5.5914600000	0.4811630000	1.0554600000
H	5.5302600000	0.9905290000	-0.6393030000
H	5.0527800000	-2.5994060000	-0.4886830000
H	3.6707850000	-3.1369880000	-1.4511390000
H	3.7068980000	-3.4388110000	0.2901390000
N	-5.0323880000	-0.5544030000	0.0124530000
O	-5.3107580000	-1.5954220000	0.6118630000
O	-5.8486420000	0.1338450000	-0.6034540000

### Thermodynamic data

Zero-point correction=	0.244307 (Hartree/Particle)
Thermal correction to Energy=	0.262594
Thermal correction to Enthalpy=	0.263538
Thermal correction to Gibbs Free Energy=	0.195691
Sum of electronic and zero-point Energies=	-1236.207592
Sum of electronic and thermal Energies=	-1236.189305
Sum of electronic and thermal Enthalpies=	-1236.188361
Sum of electronic and thermal Free Energies=	-1236.256208

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.780	67.188	142.796

**B.2.2.3 B3LYP/6-31G\* RSE and BDES for 2a with 1c, 1d**



**xyz-matrix**

41

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3299590000	-0.8585870000	0.5264440000
S	-2.7520890000	-1.2729030000	-0.3187990000
C	-3.1397030000	0.4475180000	-0.4942190000
C	-2.2041790000	1.2380400000	0.1038410000
N	-1.1714340000	0.4610830000	0.6777210000
C	-4.3840780000	0.8664950000	-1.2190600000
C	-2.1818100000	2.7326290000	0.2272330000
C	-0.0258660000	1.0387630000	1.4128400000
C	0.9459470000	1.8242680000	0.5519140000
C	1.3457510000	3.1046340000	0.9525090000
C	2.2800630000	3.8245900000	0.2059200000
C	2.8190980000	3.2701970000	-0.9552840000
C	2.4250260000	1.9927040000	-1.3599270000
C	1.4975880000	1.2695180000	-0.6104390000
C	-0.6300900000	-2.1919950000	0.9498900000
C	0.8186600000	-2.2292330000	0.4119640000
O	-1.4284400000	-3.1407450000	0.4754630000
C	1.9292930000	-1.9623560000	1.2172340000
C	3.2246960000	-2.0341090000	0.6949000000
C	3.4176590000	-2.3787330000	-0.6428080000
C	2.3110690000	-2.6711020000	-1.4485160000
C	1.0224460000	-2.6082920000	-0.9207470000
H	-4.5468060000	1.9461830000	-1.1601360000
H	-5.2690460000	0.3726360000	-0.8009710000
H	-4.3330980000	0.5958360000	-2.2807540000
H	-1.3198940000	3.1752860000	-0.2822390000
H	-2.1473360000	3.0544020000	1.2757660000
H	-3.0879190000	3.1540660000	-0.2120970000
H	0.4810940000	0.1965590000	1.8874720000
H	-0.4261440000	1.6733450000	2.2096010000
H	0.9257060000	3.5424750000	1.8557150000

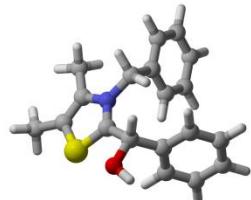
H	2.5806500000	4.8172900000	0.5298280000
H	3.5439070000	3.8289890000	-1.5410340000
H	2.8470900000	1.5503760000	-2.2579400000
H	1.2137120000	0.2695180000	-0.9244840000
H	1.7854250000	-1.7241940000	2.2709320000
H	4.0797810000	-1.8326420000	1.3356740000
H	4.4231070000	-2.4390030000	-1.0517560000
H	2.4583100000	-2.9648530000	-2.4853650000
H	0.1518310000	-2.8854170000	-1.5081280000
H	-0.5490550000	-2.1157170000	2.0708040000

### thermodynamic data

Zero-point correction= 0.333784 (Hartree/Particle)  
 Thermal correction to Energy= 0.353980  
 Thermal correction to Enthalpy= 0.354925  
 Thermal correction to Gibbs Free Energy= 0.283279  
 Sum of electronic and zero-point Energies= -1263.227226  
 Sum of electronic and thermal Energies= -1263.207030  
 Sum of electronic and thermal Enthalpies= -1263.206086  
 Sum of electronic and thermal Free Energies= -1263.277732

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	222.126	77.452	150.791

*anti-3c-a-H*



### xyz-matrix

42

XYZ file generated by gabedit : coordinates in Angstrom

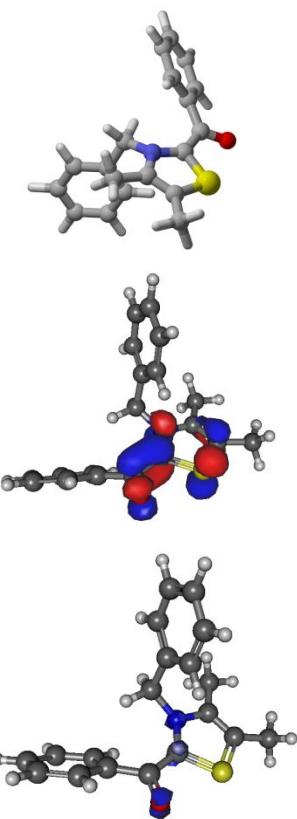
C	-1.2857180000	-0.9545170000	0.5299960000
S	-2.6720620000	-1.3923340000	-0.3636560000
C	-3.1265360000	0.2822580000	-0.5577140000
C	-2.2312380000	1.1001630000	0.0709910000
N	-1.1870260000	0.3686740000	0.6730590000
C	-4.3758910000	0.6339840000	-1.3096300000
C	-2.2919890000	2.5917840000	0.1923630000
C	-0.0849390000	1.0321060000	1.4304300000
C	0.8134800000	1.9141540000	0.5857060000
C	1.1728430000	3.1760480000	1.0751330000
C	2.0495270000	3.9886780000	0.3551700000
C	2.5636420000	3.5502460000	-0.8658260000
C	2.2051610000	2.2940100000	-1.3596520000

C	1.3392200000	1.4744520000	-0.6358750000
C	-0.3670590000	-2.0303780000	1.0831520000
C	0.9833750000	-2.1004240000	0.3833300000
O	-1.1257330000	-3.2220670000	0.9314220000
C	2.1626940000	-1.9249930000	1.1160060000
C	3.4042610000	-2.0319830000	0.4862730000
C	3.4718310000	-2.3233090000	-0.8764070000
C	2.2968500000	-2.5135980000	-1.6103730000
C	1.0558550000	-2.4034300000	-0.9853850000
H	-4.4569140000	1.7135930000	-1.4501720000
H	-5.2696790000	0.2947970000	-0.7738470000
H	-4.3840550000	0.1690250000	-2.3010590000
H	-1.4437890000	3.0751860000	-0.2999660000
H	-2.2978760000	2.9083990000	1.2416430000
H	-3.2109160000	2.9628580000	-0.2630780000
H	0.4881610000	0.2335000000	1.9025310000
H	-0.5551610000	1.6121750000	2.2291510000
H	0.7710310000	3.5258220000	2.0235100000
H	2.3230690000	4.9642340000	0.7457040000
H	3.2404100000	4.1843370000	-1.4306880000
H	2.6049790000	1.9475230000	-2.3080940000
H	1.0809900000	0.4938900000	-1.0253780000
H	2.1161840000	-1.7200520000	2.1835350000
H	4.3145190000	-1.8977630000	1.0626300000
H	4.4372090000	-2.4112200000	-1.3657270000
H	2.3482700000	-2.7532570000	-2.6683400000
H	0.1459260000	-2.5664490000	-1.5573690000
H	-0.2039240000	-1.8200230000	2.1517620000
H	-0.5126280000	-3.9749180000	0.9128410000

#### thermodynamic data

Zero-point correction= 0.347966 (Hartree/Particle)  
 Thermal correction to Energy= 0.368644  
 Thermal correction to Enthalpy= 0.369588  
 Thermal correction to Gibbs Free Energy= 0.296424  
 Sum of electronic and zero-point Energies= -1263.665564  
 Sum of electronic and thermal Energies= -1263.644886  
 Sum of electronic and thermal Enthalpies= -1263.643942  
 Sum of electronic and thermal Free Energies= -1263.717106

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	231.328	78.949	153.988



**7c-a**

**xyz-matrix**

40

XYZ file generated by gabedit : coordinates in Angstrom

C	0.3034210000	-1.3052870000	-0.3017330000
S	-0.5558730000	-2.7215450000	-0.8890590000
C	-1.8411800000	-2.4522630000	0.2953430000
C	-1.6257630000	-1.3299930000	1.0208690000
N	-0.4450610000	-0.6481520000	0.6675620000
C	-2.9469320000	-3.4561720000	0.4045110000
C	-2.5032530000	-0.7504050000	2.0912230000
C	-0.3303240000	0.7954980000	0.9145810000
C	-1.3619420000	1.6430660000	0.1845310000
C	-1.9108020000	2.7542600000	0.8379850000
C	-2.7889600000	3.6098990000	0.1731150000
C	-3.1329620000	3.3595490000	-1.1568350000
C	-2.5912160000	2.2532610000	-1.8126640000
C	-1.7105330000	1.3976930000	-1.1485780000
C	1.5992370000	-1.0660330000	-0.8668770000
C	2.6231990000	-0.1753290000	-0.2319740000
O	1.8988790000	-1.6896850000	-1.9141140000
C	2.8090090000	-0.0983820000	1.1569690000
C	3.8412970000	0.6730900000	1.6925910000
C	4.7005880000	1.3771490000	0.8479580000
C	4.5333640000	1.2937240000	-0.5374290000
C	3.5134950000	0.5120040000	-1.0729170000

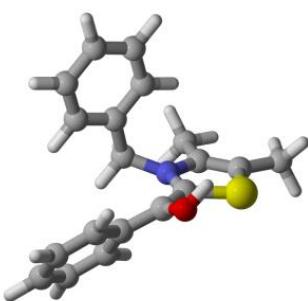
H	-3.6804530000	-3.1640820000	1.1601600000
H	-2.5601130000	-4.4454440000	0.6775320000
H	-3.4790510000	-3.5676430000	-0.5491830000
H	-2.8889490000	0.2333680000	1.8017080000
H	-1.9617320000	-0.6320270000	3.0388230000
H	-3.3579050000	-1.4017110000	2.2812880000
H	0.6754440000	1.1042540000	0.6289160000
H	-0.4051030000	0.9688300000	1.9934620000
H	-1.6509370000	2.9486460000	1.8771010000
H	-3.2103700000	4.4647860000	0.6950090000
H	-3.8188630000	4.0222490000	-1.6772130000
H	-2.8559710000	2.0477740000	-2.8464770000
H	-1.3030230000	0.5333500000	-1.6678500000
H	2.1568620000	-0.6633520000	1.8180840000
H	3.9819190000	0.7134060000	2.7697610000
H	5.5029760000	1.9794360000	1.2658610000
H	5.2058200000	1.8326250000	-1.1997190000
H	3.3893500000	0.4128450000	-2.1463640000

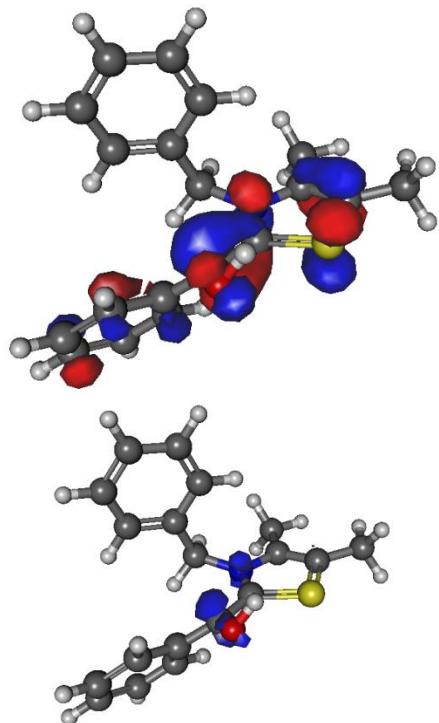
#### thermodynamic data

Zero-point correction= 0.323126 (Hartree/Particle)  
 Thermal correction to Energy= 0.343253  
 Thermal correction to Enthalpy= 0.344198  
 Thermal correction to Gibbs Free Energy= 0.271636  
 Sum of electronic and zero-point Energies= -1262.670136  
 Sum of electronic and thermal Energies= -1262.650009  
 Sum of electronic and thermal Enthalpies= -1262.649065  
 Sum of electronic and thermal Free Energies= -1262.721626

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	215.395	76.876	152.719

7c-a-H





**xyz-matrix**

41

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7086060000	0.9632890000	0.4744380000
S	-2.0908870000	1.6367560000	1.3070210000
C	-3.1682090000	1.1055720000	0.0360550000
C	-2.4745400000	0.4570960000	-0.9492170000
N	-1.1023450000	0.3568080000	-0.6889780000
C	-4.6300460000	1.4196440000	0.1377950000
C	-3.0559800000	-0.1177880000	-2.2073270000
C	-0.2357910000	-0.6184080000	-1.4111110000
C	0.0533600000	-1.8700280000	-0.6022540000
C	1.3615210000	-2.3646660000	-0.5563410000
C	1.6444650000	-3.5509890000	0.1235280000
C	0.6239640000	-4.2453200000	0.7732850000
C	-0.6830100000	-3.7527330000	0.7378990000
C	-0.9681640000	-2.5736860000	0.0504120000
C	0.5857510000	1.0727890000	1.0294160000
C	1.8393740000	1.2392270000	0.3207760000
O	0.6847520000	1.2027500000	2.3746200000
C	1.8895010000	1.8461600000	-0.9545460000
C	3.1100360000	2.0449870000	-1.5890920000
C	4.2983510000	1.6519600000	-0.9631900000
C	4.2622690000	1.0688830000	0.3079940000
C	3.0473120000	0.8676930000	0.9521830000
H	-5.1944910000	0.9346450000	-0.6609180000
H	-4.8105840000	2.4988050000	0.0706550000

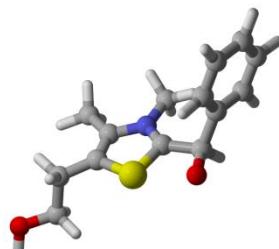
H	-5.0401790000	1.0732520000	1.0928720000
H	-2.5738200000	0.3014490000	-3.0974530000
H	-4.1188630000	0.1166870000	-2.2706820000
H	-2.9568620000	-1.2084250000	-2.2461290000
H	0.6915160000	-0.1189590000	-1.6889510000
H	-0.7567820000	-0.8560810000	-2.3388440000
H	2.1619060000	-1.8255730000	-1.0568350000
H	2.6627750000	-3.9275700000	0.1480580000
H	0.8436590000	-5.1665370000	1.3045820000
H	-1.4818330000	-4.2910550000	1.2396280000
H	-1.9915650000	-2.2057560000	0.0282090000
H	-0.0593590000	0.7732390000	2.8331870000
H	0.9758050000	2.2046610000	-1.4204200000
H	3.1402180000	2.5260900000	-2.5618690000
H	5.2504650000	1.8116250000	-1.4601940000
H	5.1852940000	0.7726900000	0.7967150000
H	3.0159500000	0.4169630000	1.9377320000

### thermodynamic data

Zero-point correction= 0.336027 (Hartree/Particle)  
 Thermal correction to Energy= 0.356284  
 Thermal correction to Enthalpy= 0.357228  
 Thermal correction to Gibbs Free Energy= 0.284577  
 Sum of electronic and zero-point Energies= -1263.051720  
 Sum of electronic and thermal Energies= -1263.031464  
 Sum of electronic and thermal Enthalpies= -1263.030520  
 Sum of electronic and thermal Free Energies= -1263.103170

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	223.571	78.166	152.906

*anti-4d-a*



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

S	1.0938750000	-1.2340900000	0.1471050000
C	-0.0928260000	-0.0864870000	0.5727570000
N	0.2928600000	1.1755340000	0.3576010000
C	1.5926370000	1.3020470000	-0.1744070000

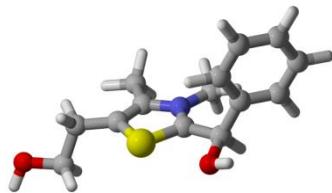
C	2.1715750000	0.0817180000	-0.3620350000
C	-0.5543740000	2.3289460000	0.6735000000
C	2.1478080000	2.6657750000	-0.4603340000
C	3.5483440000	-0.2139990000	-0.8844670000
C	-1.3186050000	-0.8636120000	1.1412250000
O	-0.9599820000	-2.1402930000	1.0466240000
C	-2.5966680000	-0.4772880000	0.3620180000
C	-3.5590550000	0.3918680000	0.8851640000
C	-4.7158830000	0.6973770000	0.1601330000
C	-4.9188840000	0.1284330000	-1.0968520000
C	-3.9704220000	-0.7606260000	-1.6153430000
C	-2.8238330000	-1.0682260000	-0.8863590000
C	4.5527620000	-0.5429440000	0.2263440000
O	5.8040280000	-0.7784800000	-0.4033270000
H	-0.5584940000	3.0239210000	-0.1686170000
H	-0.1775350000	2.8408950000	1.5643660000
H	-1.5711850000	1.9812680000	0.8467320000
H	3.1708570000	2.5814010000	-0.8318210000
H	2.1735570000	3.2954520000	0.4376730000
H	1.5630540000	3.1983460000	-1.2210280000
H	3.9369100000	0.6350270000	-1.4575090000
H	3.5161470000	-1.0648210000	-1.5754540000
H	-3.4191180000	0.8102900000	1.8817810000
H	-5.4618110000	1.3653430000	0.5845490000
H	-5.8181000000	0.3594440000	-1.6624000000
H	-4.1358850000	-1.2233880000	-2.5855310000
H	-2.1008090000	-1.7949370000	-1.2454080000
H	4.2077170000	-1.4249580000	0.7877890000
H	4.6074610000	0.2992960000	0.9353830000
H	6.4348950000	-1.0599980000	0.2761290000
H	-1.4475210000	-0.4536000000	2.1820370000

### thermodynamic data

Zero-point correction= 0.285735 (Hartree/Particle)  
 Thermal correction to Energy= 0.304077  
 Thermal correction to Enthalpy= 0.305022  
 Thermal correction to Gibbs Free Energy= 0.237376  
 Sum of electronic and zero-point Energies= -1146.741691  
 Sum of electronic and thermal Energies= -1146.723349  
 Sum of electronic and thermal Enthalpies= -1146.722404  
 Sum of electronic and thermal Free Energies= -1146.790050

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.811	67.738	142.372

*anti*-4d-a-H



**xyz-matrix**

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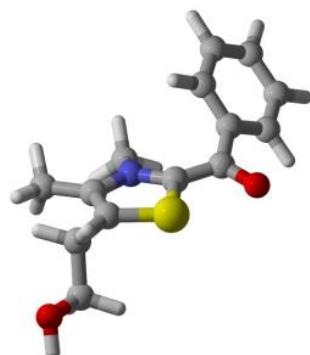
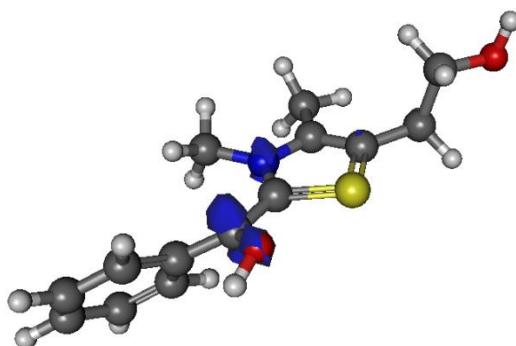
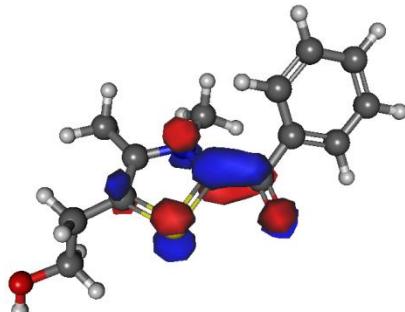
XYZ file generated by gabedit : coordinates in Angstrom

S	1.1527360000	-1.2087890000	0.1236180000
C	-0.0688510000	-0.1255460000	0.6146250000
N	0.3039490000	1.1443890000	0.4472210000
C	1.5937530000	1.3120010000	-0.0891380000
C	2.2003520000	0.1133000000	-0.3390120000
C	-0.5389500000	2.2960700000	0.8202510000
C	2.1362410000	2.6885910000	-0.3218100000
C	3.5654420000	-0.1625360000	-0.8981950000
C	-1.3772200000	-0.6353900000	1.1850690000
O	-1.1374730000	-2.0214380000	1.3857650000
C	-2.5772770000	-0.3621400000	0.2889950000
C	-3.7117970000	0.2638470000	0.8219770000
C	-4.8417600000	0.4654740000	0.0268960000
C	-4.8441100000	0.0376860000	-1.3012340000
C	-3.7177910000	-0.5958840000	-1.8351120000
C	-2.5876780000	-0.7969110000	-1.0451580000
C	4.5817930000	-0.6390440000	0.1531310000
O	5.7905110000	-0.8297190000	-0.5489510000
H	-0.4780610000	3.0504870000	0.0357950000
H	-0.1860280000	2.7186340000	1.7648480000
H	-1.5736700000	1.9741770000	0.9144240000
H	3.1682250000	2.6295940000	-0.6697660000
H	2.1306650000	3.2866280000	0.5962270000
H	1.5616610000	3.2298550000	-1.0828750000
H	3.9603120000	0.7403670000	-1.3728550000
H	3.5063380000	-0.9230460000	-1.6853230000
H	-1.9876170000	-2.4891430000	1.3500710000
H	-3.7194840000	0.5809790000	1.8628970000
H	-5.7188610000	0.9473120000	0.4480750000
H	-5.7233320000	0.1916550000	-1.9195300000
H	-3.7221640000	-0.9357860000	-2.8663910000
H	-1.7195410000	-1.3004100000	-1.4630170000
H	4.2245360000	-1.5703980000	0.6232890000
H	4.6753300000	0.1178320000	0.9485400000
H	6.4717060000	-1.1316960000	0.0713850000
H	-1.5386240000	-0.1349910000	2.1535500000

**thermodynamic data**

Zero-point correction= 0.300014 (Hartree/Particle)  
Thermal correction to Energy= 0.318732  
Thermal correction to Enthalpy= 0.319676  
Thermal correction to Gibbs Free Energy= 0.251434  
Sum of electronic and zero-point Energies= -1147.178544  
Sum of electronic and thermal Energies= -1147.159826  
Sum of electronic and thermal Enthalpies= -1147.158882  
Sum of electronic and thermal Free Energies= -1147.227123

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.007	69.136	143.627

*anti-7d-a***xyz-matrix**

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XYZ file generated by gabedit : coordinates in Angstrom

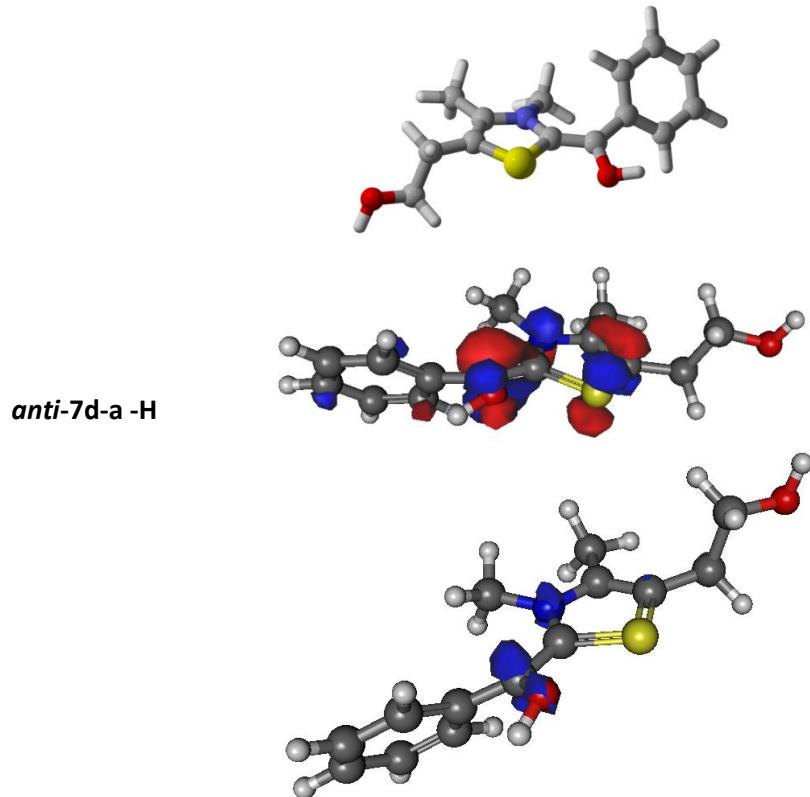
S	1.3865540000	-1.3231840000	-0.3941520000
C	-0.0660620000	-0.4231240000	0.0017890000

N	0.2402250000	0.9078370000	0.2450660000
C	1.5872480000	1.2286710000	0.0174580000
C	2.3470520000	0.1609300000	-0.3433760000
C	-0.6616550000	1.8084970000	0.9630820000
C	2.0463580000	2.6477860000	0.1839950000
C	3.8152550000	0.1067320000	-0.6494180000
C	-1.2940460000	-1.1582780000	0.0538990000
O	-1.2243980000	-2.4118130000	0.0957480000
C	-2.6375630000	-0.4987890000	-0.0137330000
C	-3.6967830000	-1.0669090000	0.7123350000
C	-4.9813270000	-0.5365450000	0.6236680000
C	-5.2365190000	0.5533990000	-0.2143170000
C	-4.1982780000	1.1037980000	-0.9680080000
C	-2.9079040000	0.5816510000	-0.8684570000
C	4.6452850000	-0.5344240000	0.4689200000
O	6.0025640000	-0.5040640000	0.0474490000
H	-1.2639870000	2.4179000000	0.2820620000
H	-0.0797140000	2.4655020000	1.6118180000
H	-1.3387630000	1.2171220000	1.5802060000
H	3.0583100000	2.7665450000	-0.2076340000
H	2.0674210000	2.9579330000	1.2367240000
H	1.3944200000	3.3467530000	-0.3528610000
H	4.2052930000	1.1148070000	-0.8257110000
H	3.9941550000	-0.4598720000	-1.5718750000
H	-3.4915030000	-1.9320200000	1.3350860000
H	-5.7890750000	-0.9779690000	1.2018760000
H	-6.2410550000	0.9614290000	-0.2892600000
H	-4.3954180000	1.9315860000	-1.6446280000
H	-2.1105460000	0.9915970000	-1.4833470000
H	4.2998960000	-1.5647330000	0.6458260000
H	4.4979130000	0.0282870000	1.4048050000
H	6.5345220000	-0.9621270000	0.7152850000

#### thermodynamic data

Zero-point correction=	0.275275 (Hartree/Particle)
Thermal correction to Energy=	0.293384
Thermal correction to Enthalpy=	0.294328
Thermal correction to Gibbs Free Energy=	0.227229
Sum of electronic and zero-point Energies=	-1146.184879
Sum of electronic and thermal Energies=	-1146.166771
Sum of electronic and thermal Enthalpies=	-1146.165827
Sum of electronic and thermal Free Energies=	-1146.232926

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	184.101	67.031	141.221



#### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

S	1.3611030000	-1.3107690000	-0.4560950000
C	-0.0500070000	-0.3983030000	0.0085420000
N	0.2870130000	0.9068710000	0.2646590000
C	1.6280710000	1.2061510000	0.0279520000
C	2.3608090000	0.1174030000	-0.3705240000
C	-0.6232130000	1.8755630000	0.8966300000
C	2.1376510000	2.6009770000	0.2292200000
C	3.8267600000	0.0262470000	-0.6742250000
C	-1.3019900000	-1.0277710000	0.0869990000
O	-1.1968830000	-2.3752990000	0.1887770000
C	-2.6330440000	-0.4334170000	0.0068000000
C	-3.6782040000	-0.9702170000	0.7902450000
C	-4.9707400000	-0.4683810000	0.6712830000
C	-5.2433520000	0.5605840000	-0.2348030000
C	-4.2182860000	1.0878940000	-1.0272460000
C	-2.9217560000	0.5972740000	-0.9121150000
C	4.6707430000	-0.4887300000	0.5050560000
O	6.0049780000	-0.4902850000	0.0448580000
H	-1.1358060000	2.4829310000	0.1465890000
H	-0.0445870000	2.5221730000	1.5551720000
H	-1.3627810000	1.3385170000	1.4877980000
H	3.1505530000	2.6904500000	-0.1656680000
H	2.1768660000	2.8718120000	1.2914420000
H	1.5110350000	3.3376530000	-0.2845870000
H	4.2095040000	1.0096190000	-0.9641700000
H	3.9982640000	-0.6361030000	-1.5300460000

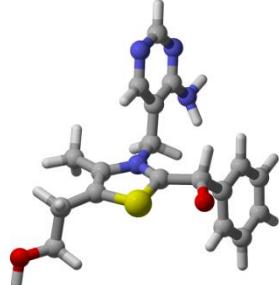
H	-2.0385060000	-2.7931570000	-0.0677380000
H	-3.4649420000	-1.7506430000	1.5162230000
H	-5.7649140000	-0.8754300000	1.2894080000
H	-6.2537610000	0.9464970000	-0.3288920000
H	-4.4362210000	1.8692590000	-1.7488930000
H	-2.1390030000	0.9740600000	-1.5642930000
H	4.3300260000	-1.4962530000	0.7941820000
H	4.5313950000	0.1707670000	1.3769340000
H	6.5807210000	-0.8249260000	0.7494930000

### thermodynamic data

Zero-point correction= 0.288105 (Hartree/Particle)  
 Thermal correction to Energy= 0.306389  
 Thermal correction to Enthalpy= 0.307333  
 Thermal correction to Gibbs Free Energy= 0.239383  
 Sum of electronic and zero-point Energies= -1146.571154  
 Sum of electronic and thermal Energies= -1146.552870  
 Sum of electronic and thermal Enthalpies= -1146.551926  
 Sum of electronic and thermal Free Energies= -1146.619875

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	192.262	68.299	143.012

**anti-4e-a**



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	0.6002090000	-0.5299330000	-0.6874640000
S	2.2007090000	-0.7117480000	-1.2369110000
C	2.7244920000	0.5555500000	-0.1086560000
C	1.6785160000	1.0430490000	0.6190850000
N	0.4713130000	0.4048640000	0.2627060000
C	4.1716630000	0.9458580000	-0.0171250000
C	1.6826150000	2.0919800000	1.6920070000
C	-0.8297730000	0.6967810000	0.8796700000
C	-1.6188020000	1.7894810000	0.1933430000
C	-2.9756160000	2.0069460000	0.5445410000
N	-3.6843540000	3.0109730000	0.0069610000
C	-3.0537810000	3.7817900000	-0.8809790000
N	-1.7999080000	3.6587660000	-1.3173530000
C	-1.1031110000	2.6521090000	-0.7638880000
N	-3.6160500000	1.2381560000	1.4869110000
C	5.0144960000	-0.0555450000	0.7815730000

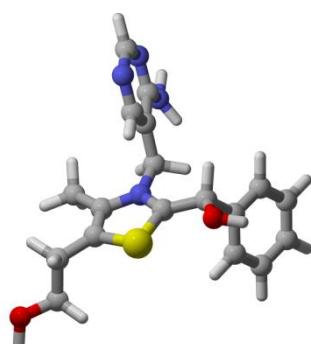
O	6.3412870000	0.4494760000	0.8052910000
C	-0.3028960000	-1.5042750000	-1.5031250000
C	-1.1804640000	-2.3485990000	-0.5505570000
C	-2.5435380000	-2.0877880000	-0.3643050000
C	-3.3144920000	-2.8870100000	0.4879780000
C	-2.7238560000	-3.9576870000	1.1608040000
C	-1.3675340000	-4.2368410000	0.9600040000
C	-0.6058970000	-3.4450130000	0.1023270000
O	0.5522810000	-2.1891470000	-2.2530300000
H	4.2774490000	1.9309030000	0.4504050000
H	4.6048920000	1.0301320000	-1.0209530000
H	1.4806520000	1.6666300000	2.6835600000
H	0.9374590000	2.8735740000	1.5047180000
H	2.6621240000	2.5721610000	1.7375650000
H	-0.6552220000	0.9519990000	1.9303980000
H	-1.3817970000	-0.2469180000	0.8724200000
H	-3.6375330000	4.5982460000	-1.3021110000
H	-0.0778640000	2.5362060000	-1.1111420000
H	-4.6156330000	1.3977460000	1.5274240000
H	-3.3433580000	0.2685780000	1.5878560000
H	4.9647110000	-1.0459390000	0.3027970000
H	4.6003990000	-0.1586590000	1.7979080000
H	6.9048380000	-0.2027120000	1.2479870000
H	-3.0109250000	-1.2717610000	-0.9149670000
H	-4.3778160000	-2.6888680000	0.6050420000
H	-3.3193510000	-4.5845150000	1.8195850000
H	-0.9094210000	-5.0841400000	1.4647210000
H	0.4342580000	-3.6761470000	-0.1092070000
H	-1.0081440000	-0.8156200000	-2.0474960000

### thermodynamic data

Zero-point correction= 0.360995 (Hartree/Particle)  
 Thermal correction to Energy= 0.384714  
 Thermal correction to Enthalpy= 0.385659  
 Thermal correction to Gibbs Free Energy= 0.304215  
 Sum of electronic and zero-point Energies= -1465.157694  
 Sum of electronic and thermal Energies= -1465.133974  
 Sum of electronic and thermal Enthalpies= -1465.133030  
 Sum of electronic and thermal Free Energies= -1465.214474

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	241.412	89.288	171.412

*anti-4e-a-H*



**xyz-matrix**

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XYZ file generated by gabedit : coordinates in Angstrom

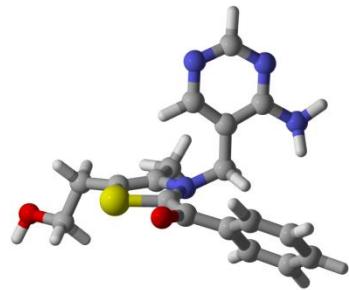
C	0.5221090000	-0.5579680000	-0.7391240000
S	2.1427840000	-0.5657860000	-1.2657710000
C	2.5607860000	0.7062750000	-0.1415660000
C	1.4628310000	1.0909030000	0.5760470000
N	0.3198410000	0.3554300000	0.2137320000
C	3.9718580000	1.2111440000	-0.0585040000
C	1.3828110000	2.1449580000	1.6372450000
C	-1.0120950000	0.6209480000	0.8049130000
C	-1.7547840000	1.7498730000	0.1249460000
C	-2.8863360000	2.3334540000	0.7535540000
N	-3.5275680000	3.3709650000	0.1969140000
C	-3.0712430000	3.8107490000	-0.9750890000
N	-2.0403390000	3.3260880000	-1.6744350000
C	-1.3975580000	2.3023870000	-1.1004440000
N	-3.3439940000	1.9175880000	1.9756280000
C	4.8859880000	0.3489700000	0.8281310000
O	6.1479570000	0.9786130000	0.7966980000
C	-0.5085440000	-1.4800580000	-1.3590410000
C	-1.0196220000	-2.5520630000	-0.4053960000
C	-2.3993920000	-2.7156260000	-0.2231580000
C	-2.8841110000	-3.7370670000	0.5966040000
C	-1.9924420000	-4.6008640000	1.2336950000
C	-0.6150770000	-4.4472020000	1.0479960000
C	-0.1280360000	-3.4287480000	0.2312500000
O	0.1653060000	-2.0191340000	-2.4871760000
H	3.9765730000	2.2326680000	0.3338510000
H	4.4161040000	1.2636670000	-1.0586110000
H	1.1907740000	1.7107570000	2.6259210000
H	0.5939370000	2.8734510000	1.4237130000
H	2.3291120000	2.6847600000	1.6963080000
H	-0.8503650000	0.8541500000	1.8619410000
H	-1.5634460000	-0.3241680000	0.7752910000
H	-3.6017820000	4.6543870000	-1.4103400000
H	-0.5402580000	1.9188940000	-1.6532030000
H	-4.2102420000	2.3536210000	2.2698100000
H	-3.2314700000	0.9563590000	2.2640120000
H	4.9250350000	-0.6797750000	0.4331320000
H	4.4709390000	0.2963710000	1.8478210000
H	6.7703030000	0.4673330000	1.3363470000
H	-3.0963410000	-2.0562260000	-0.7365950000
H	-3.9548090000	-3.8630940000	0.7263210000
H	-2.3680780000	-5.3980320000	1.8681410000
H	0.0784690000	-5.1252420000	1.5362900000
H	0.9431160000	-3.3240750000	0.0787160000
H	-1.3595040000	-0.8583140000	-1.6805780000
H	-0.2671690000	-2.8516500000	-2.7373610000

**thermodynamic data**

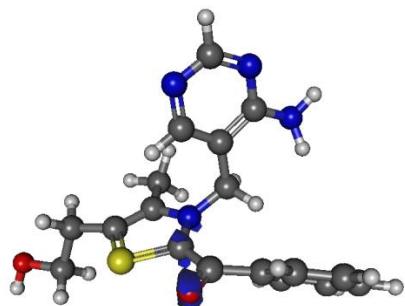
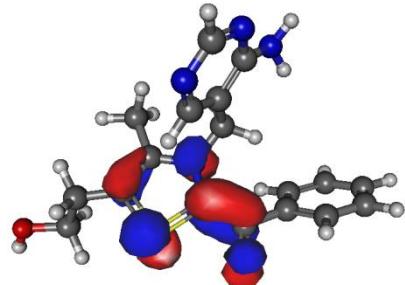
Zero-point correction=	0.374932 (Hartree/Particle)
Thermal correction to Energy=	0.399112
Thermal correction to Enthalpy=	0.400056
Thermal correction to Gibbs Free Energy=	0.318078
Sum of electronic and zero-point Energies=	-1465.592128

Sum of electronic and thermal Energies= -1465.567949  
 Sum of electronic and thermal Enthalpies= -1465.567005  
 Sum of electronic and thermal Free Energies= -1465.648983

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	250.446	90.916	172.538



*anti-7e-a*



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4471930000	1.0234110000	-0.4600720000
S	-2.0276400000	1.2482160000	-1.1899880000
C	-2.7508400000	0.1385540000	-0.0164440000
C	-1.8131700000	-0.3946380000	0.8081520000
N	-0.5072810000	0.0687610000	0.5529180000
C	-4.2352010000	-0.0808670000	-0.0254890000
C	-2.0382710000	-1.3809260000	1.9163710000
C	0.6556810000	-0.7304960000	0.9486400000
C	0.9196220000	-1.9534790000	0.0930530000
C	1.9720570000	-2.8368930000	0.4399740000
N	2.2155050000	-3.9545250000	-0.2592060000
C	1.4229450000	-4.1839050000	-1.3088410000

N	0.4256270000	-3.4207870000	-1.7542470000
C	0.1932550000	-2.3077120000	-1.0356200000
N	2.7638770000	-2.6193930000	1.5456970000
C	-5.0293720000	1.0939840000	0.5576650000
O	-6.4028450000	0.7343550000	0.4988610000
C	0.6189910000	1.8179040000	-0.9959780000
C	1.9204580000	2.0458940000	-0.2872750000
C	3.0791600000	2.1951580000	-1.0655680000
C	4.3028510000	2.4837500000	-0.4664060000
C	4.3857580000	2.6551710000	0.9188630000
C	3.2342670000	2.5406860000	1.7000670000
C	2.0096490000	2.2377580000	1.1014250000
O	0.4161720000	2.3950490000	-2.0912590000
H	-4.4923040000	-0.9816960000	0.5412780000
H	-4.5840600000	-0.2511590000	-1.0519510000
H	-1.7043740000	-0.9819020000	2.8824220000
H	-1.5055320000	-2.3231670000	1.7411740000
H	-3.1004160000	-1.6144750000	2.0051080000
H	0.5153430000	-1.0372920000	1.9917000000
H	1.5254610000	-0.0704980000	0.9441590000
H	1.6239280000	-5.0971470000	-1.8663020000
H	-0.6203590000	-1.6770210000	-1.3865800000
H	3.5758160000	-3.2236590000	1.5870280000
H	2.9403010000	-1.6645310000	1.8273640000
H	-4.8241140000	2.0068640000	-0.0225900000
H	-4.7023980000	1.2804370000	1.5935240000
H	-6.9245920000	1.4869440000	0.8154450000
H	2.9952470000	2.0894950000	-2.1424240000
H	5.1941140000	2.5836850000	-1.0803660000
H	5.3395930000	2.8895590000	1.3840520000
H	3.2849550000	2.7027290000	2.7738790000
H	1.1110450000	2.1776180000	1.7108470000

#### thermodynamic data

Zero-point correction=	0.350503 (Hartree/Particle)
Thermal correction to Energy=	0.374076
Thermal correction to Enthalpy=	0.375021
Thermal correction to Gibbs Free Energy=	0.293649
Sum of electronic and zero-point Energies=	-1464.601280
Sum of electronic and thermal Energies=	-1464.577706
Sum of electronic and thermal Enthalpies=	-1464.576762
Sum of electronic and thermal Free Energies=	-1464.658134

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.736	88.659	171.261

**B.2.1.2 B3LYP/6-31G\* RSE and BDES for 7g-a and 7h-a**

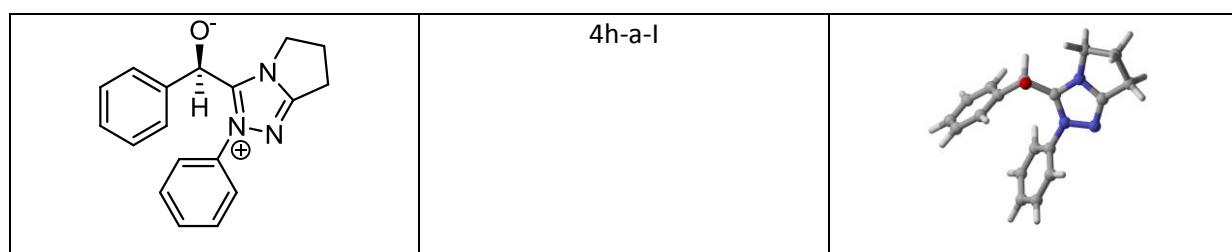
**Table 6**

entry	cmpd	$\Delta H_{(I-II)}$ [kcal/mol]	BDE [kcal/mol]	RSE [kcal/mol]
1	4h-a-I	-2.5	45.5 (min) <sup>a</sup>	—
2	4h-a-II		48.1 (max) <sup>b</sup>	
3	4h-a-H-I		48.0 (prob) <sup>c</sup>	
4	4h-a-H-II	0.2	71.1(min) <sup>a</sup>	—
5	7h-a -I		74.4 (max) <sup>b</sup>	
6	7h-a-II		71.3 (prob) <sup>c</sup>	
7	7h-a-H-I	-2.5	—	—
8	7h-a-H-II		—	—
			—	-54.2 (min) <sup>b</sup>
			—	-59.3 (max) <sup>a</sup>
			—	-56.8 (prob) <sup>c</sup>
			—	-30.4 (min) <sup>b</sup>
			—	-30.6 (max) <sup>a</sup>
			—	-33.5 (prob) <sup>c</sup>

<sup>a</sup> determined from least stable conformer of closed shell species **5** and most stable radical species **4**.<sup>b</sup>

determined from most stable conformer of closed shell species **5** and least stable radical species **4**.<sup>c</sup>

determined from most stable conformer of closed shell species **5** and most stable radical species **4**.



**xyz-matrix**

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XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4059660000	-1.7052360000	0.3106440000
H	-0.7974280000	-2.5303960000	-0.3468680000
O	-0.8784250000	-1.006557060000	1.54744300
C	1.1179310000	-1.7276300000	0.1353680000
C	1.9236960000	-1.4285770000	1.2346200000
C	3.3139990000	-1.4768750000	1.1223470000
C	3.9087850000	-1.8352200000	-0.0899250000
C	3.1058560000	-2.1564820000	-1.1882000000

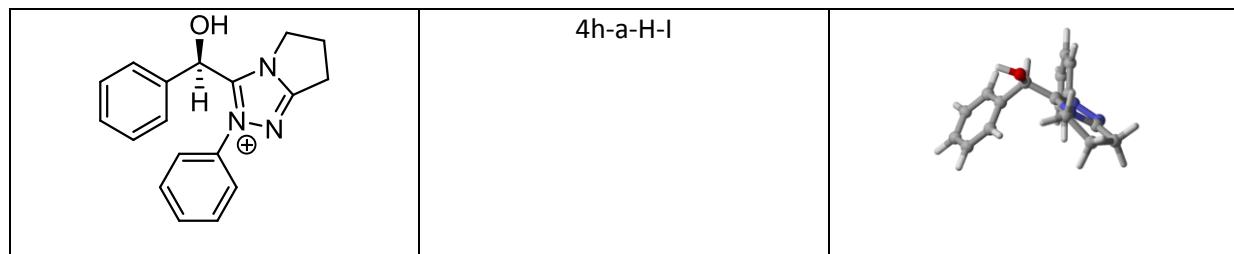
C	1.7160060000	-2.1084880000	-1.0703190000
H	1.4253270000	-1.1765540000	2.1657520000
H	3.9362870000	-1.2415490000	1.9826810000
H	4.9918490000	-1.8793910000	-0.1757470000
H	3.5628510000	-2.4566180000	-2.1284870000
H	1.0887640000	-2.3772820000	-1.9203790000
C	-1.1198410000	-0.4279330000	-0.2611070000
N	-0.8360250000	0.8980050000	-0.2462090000
N	-1.9874450000	1.7024810000	-0.2514510000
N	-2.4726680000	-0.4508670000	-0.3901690000
C	-2.9463650000	0.8290610000	-0.3316250000
C	0.4300660000	1.5580160000	-0.1601360000
C	1.4172740000	1.3154480000	-1.1144000000
C	0.6317360000	2.4836170000	0.8655360000
C	2.6351970000	1.9874030000	-1.0199420000
C	1.8468730000	3.1614760000	0.9412290000
C	2.8512030000	2.9117460000	0.0033600000
H	1.2370850000	0.6025080000	-1.9103280000
H	-0.1576860000	2.6603500000	1.5877390000
H	3.4117440000	1.7898870000	-1.7527630000
H	2.0104710000	3.8802670000	1.7390690000
H	3.7996670000	3.4374000000	0.0696780000
C	-3.4889870000	-1.4770890000	-0.1597870000
C	-4.4419730000	0.8311210000	-0.2945540000
C	-4.7353610000	-0.6180710000	0.2073190000
H	-3.1342820000	-2.1079660000	0.6599460000
H	-3.6379160000	-2.0769340000	-1.0629920000
H	-4.8525280000	1.0065930000	-1.2966630000

H	-4.8406330000	1.6025790000	0.3678880000
H	-4.8503510000	-0.6055130000	1.2951370000
H	-5.6536330000	-1.0267920000	-0.2209810000

### thermodynamic data

Zero-point correction= 0.317518 (Hartree/Particle)  
 Thermal correction to Energy= 0.335353  
 Thermal correction to Enthalpy= 0.336297  
 Thermal correction to Gibbs Free Energy= 0.269869  
 Sum of electronic and zero-point Energies= -935.232998  
 Sum of electronic and thermal Energies= -935.215163  
 Sum of electronic and thermal Enthalpies= -935.214219  
 Sum of electronic and thermal Free Energies= -935.280647

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	-0.2175660000	-0.8281140000	-1.3559060000
H	0.4954120000	-0.3257040000	-2.0232680000
O	-1.2741310000	-1.4260310000	-2.0928630000
H	-0.9266100000	-2.2343990000	-2.5045940000
C	0.5505510000	-1.8105010000	-0.4799230000
C	-0.1368300000	-2.7028360000	0.3555400000
C	0.5706100000	-3.6161650000	1.1344720000
C	1.9673580000	-3.6434810000	1.0860560000

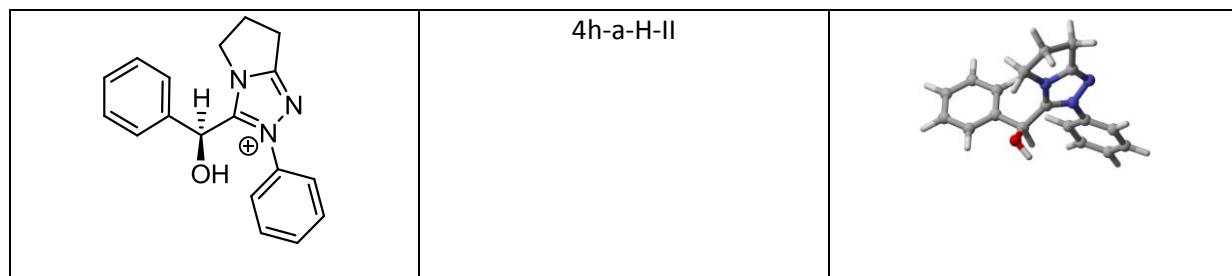
C	2.6548410000	-2.7587240000	0.2543470000
C	1.9485940000	-1.8437830000	-0.5282600000
H	-1.2233630000	-2.6965200000	0.3843650000
H	0.0343240000	-4.3093740000	1.7756810000
H	2.5167650000	-4.3582130000	1.6914660000
H	3.7393110000	-2.7844460000	0.2069870000
H	2.4860640000	-1.1589480000	-1.1793750000
C	-0.8976700000	0.2431570000	-0.5328030000
N	-0.3211800000	1.2886720000	0.0832510000
N	-1.2293650000	2.0270190000	0.8146660000
N	-2.1982920000	0.3124290000	-0.2020200000
C	-2.3598700000	1.4072820000	0.6125490000
C	1.0662700000	1.6804960000	0.0591770000
C	1.6269290000	2.1307820000	-1.1369710000
C	1.7982620000	1.6295280000	1.2449120000
C	2.9676860000	2.5167920000	-1.1449190000
C	3.1341310000	2.0278590000	1.2233290000
C	3.7186460000	2.4643680000	0.0316400000
H	1.0222000000	2.2040170000	-2.0361150000
H	1.3281870000	1.2883630000	2.1611740000
H	3.4173450000	2.8743730000	-2.0658770000
H	3.7170600000	1.9967280000	2.1383540000
H	4.7591990000	2.7739800000	0.0218860000
C	-3.4768650000	-0.3706280000	-0.5114230000
C	-3.7936780000	1.5971350000	0.9887720000
C	-4.4178500000	0.2340160000	0.5644000000
H	-3.3592420000	-1.4502180000	-0.4412850000
H	-3.7621920000	-0.1168850000	-1.5349540000

H	-4.2154530000	2.4382200000	0.4259620000
H	-3.9213460000	1.8154970000	2.0514420000
H	-4.4605030000	-0.4350630000	1.4286220000
H	-5.4335500000	0.3468940000	0.1812010000

### thermodynamic data

Zero-point correction= 0.332195 (Hartree/Particle)  
 Thermal correction to Energy= 0.350224  
 Thermal correction to Enthalpy= 0.351168  
 Thermal correction to Gibbs Free Energy= 0.284026  
 Sum of electronic and zero-point Energies= -935.673274  
 Sum of electronic and thermal Energies= -935.655245  
 Sum of electronic and thermal Enthalpies= -935.654301  
 Sum of electronic and thermal Free Energies= -935.721442

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	219.769	71.143	141.311



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6292840000	-0.5259050000	1.1233350000
H	0.1383850000	-1.2766810000	1.3515650000
O	-1.1425560000	0.0438870000	2.3230330000
H	-0.4428660000	0.0446920000	2.9963480000
C	-1.7717150000	-1.1724010000	0.3452660000
C	-2.8060860000	-1.7905940000	1.0582750000

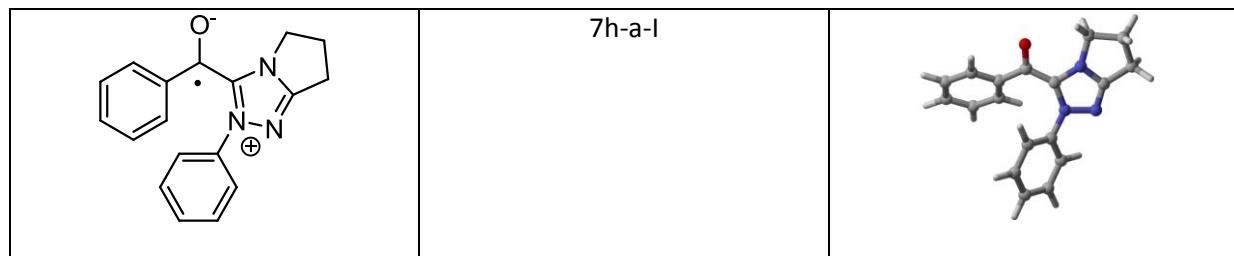
C	-3.8349880000	-2.4378340000	0.3748900000
C	-3.8402520000	-2.4777790000	-1.0211590000
C	-2.8119330000	-1.8630600000	-1.7354840000
C	-1.7817050000	-1.2104580000	-1.0552170000
H	-2.8070980000	-1.7544930000	2.1419560000
H	-4.6342660000	-2.9125430000	0.9362000000
H	-4.6428670000	-2.9837480000	-1.5492140000
H	-2.8095500000	-1.8861570000	-2.8211690000
H	-0.9921560000	-0.7321270000	-1.6313590000
C	0.0394440000	0.5852040000	0.3415830000
N	1.2941610000	0.6709490000	-0.1371710000
N	1.5548260000	1.9111660000	-0.6865130000
N	-0.5124500000	1.7831770000	0.0858860000
C	0.4299810000	2.5593280000	-0.5305530000
C	2.3356820000	-0.3214500000	-0.1080680000
C	2.0562250000	-1.6369720000	-0.4860440000
C	3.6165880000	0.0759100000	0.2817490000
C	3.0838410000	-2.5799410000	-0.4414850000
C	4.6329090000	-0.8763380000	0.3084780000
C	4.3677000000	-2.2023070000	-0.0452020000
H	1.0683890000	-1.9180230000	-0.8376760000
H	3.8073420000	1.1089400000	0.5506700000
H	5.6331930000	-0.5809240000	0.6087980000
H	5.1648990000	-2.9386860000	-0.0207090000
H	2.8802250000	-3.6047950000	-0.7350550000
C	-1.8116320000	2.4593090000	0.2737510000
C	-0.1215290000	3.9087870000	-0.8626500000
C	-1.4276300000	3.9390110000	-0.0079290000

H	-2.1801010000	2.2743730000	1.2827570000
H	-2.5238620000	2.0505290000	-0.4484760000
H	-0.3289410000	3.9714770000	-1.9374220000
H	0.5714280000	4.7156830000	-0.6139850000
H	-1.2343460000	4.4504070000	0.9390700000
H	-2.2368270000	4.4688830000	-0.5131880000

### thermodynamic data

Zero-point correction= 0.332315 (Hartree/Particle)  
 Thermal correction to Energy= 0.350247  
 Thermal correction to Enthalpy= 0.351191  
 Thermal correction to Gibbs Free Energy= 0.284509  
 Sum of electronic and zero-point Energies= -935.671161  
 Sum of electronic and thermal Energies= -935.653229  
 Sum of electronic and thermal Enthalpies= -935.652285  
 Sum of electronic and thermal Free Energies= -935.718967

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	219.783	71.049	140.344



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	-0.2033950000	-1.5917650000	0.3342850000
O	-0.7672570000	-2.5956060000	0.8554080000
C	1.2311790000	-1.6668640000	-0.0634790000
C	2.0369330000	-2.6117050000	0.5949880000
C	3.3694630000	-2.7857920000	0.2322200000
C	3.9185780000	-2.0325120000	-0.8095460000
C	3.1211000000	-1.1076810000	-1.4865440000
C	1.7892000000	-0.9246830000	-1.1171940000

H	1.5877960000	-3.2065130000	1.3836230000
H	3.9816790000	-3.5141410000	0.7582300000
H	4.9578660000	-2.1708240000	-1.0962590000
H	3.5347560000	-0.5296260000	-2.3088750000
H	1.1777860000	-0.2151520000	-1.6659660000
C	-1.0191960000	-0.4322880000	0.1078140000
N	-0.7852060000	0.9155050000	-0.1863560000
N	-1.9828340000	1.5928220000	-0.4930690000
N	-2.4003460000	-0.5146070000	0.0806520000
C	-2.8966470000	0.6856040000	-0.3231170000
C	0.3431250000	1.7195150000	0.1148050000
C	0.5511640000	2.8909690000	-0.6272240000
C	1.2202860000	1.3791430000	1.1514900000
C	1.6398740000	3.7072800000	-0.3332180000
C	2.3104350000	2.2021920000	1.4280700000
C	2.5282280000	3.3667490000	0.6904040000
H	-0.1478870000	3.1516250000	-1.4135000000
H	1.0470730000	0.4842280000	1.7376640000
H	1.7957190000	4.6139320000	-0.9116190000
H	2.9872230000	1.9307430000	2.2334410000
H	3.3794230000	4.0042280000	0.9117090000
C	-3.4019250000	-1.5760240000	0.1520700000
C	-4.3803160000	0.6060890000	-0.5187040000
C	-4.7159380000	-0.7488660000	0.1725470000
H	-3.2404010000	-2.1911220000	1.0355050000
H	-3.3235280000	-2.2236190000	-0.7297810000
H	-4.6132660000	0.5839780000	-1.5905220000
H	-4.9116310000	1.4567520000	-0.0842970000
H	-5.0120520000	-0.5656870000	1.2103820000
H	-5.5366890000	-1.2761490000	-0.3195820000

#### thermodynamic data

Zero-point correction= 0.306463 (Hartree/Particle)

Thermal correction to Energy= 0.324014

Thermal correction to Enthalpy= 0.324958

Thermal correction to Gibbs Free Energy= 0.259041

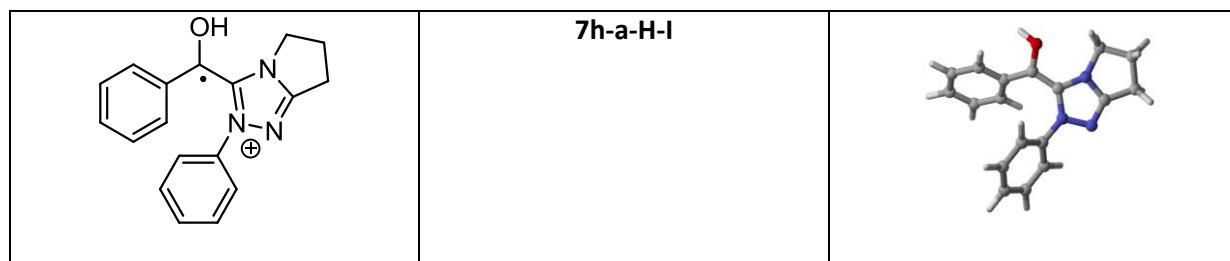
Sum of electronic and zero-point Energies= -934.673782

Sum of electronic and thermal Energies= -934.656232

Sum of electronic and thermal Enthalpies= -934.655287

Sum of electronic and thermal Free Energies= -934.721204

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total 203.322	69.424	138.734



**xyz-matrix**

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XYZ file generated by gabedit : coordinates in Angstrom

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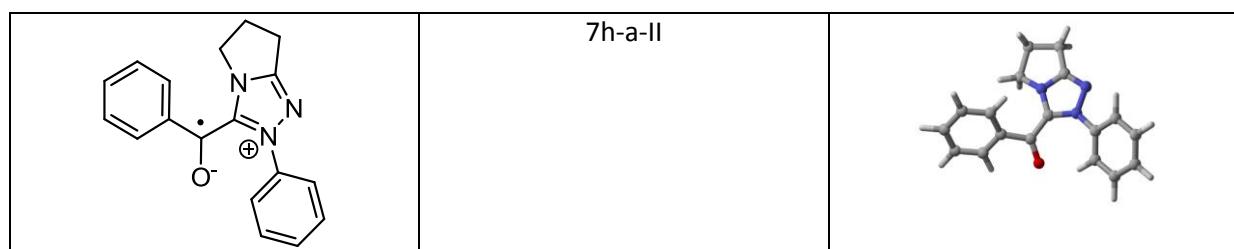
C   -0.2234200000    1.4900800000   -0.2869170000
O   -0.8681070000    2.5477240000   -0.8509260000
H   -0.3440980000    3.3555460000   -0.7046540000
C   1.1758000000    1.6114430000    0.0757810000
C   2.0096680000    2.4732850000   -0.6728940000
C   3.3356300000    2.6677460000   -0.3010330000
C   3.8529720000    2.0122350000    0.8198970000
C   3.0367120000    1.1583930000    1.5695310000
C   1.7104760000    0.9580060000    1.2072870000
H   1.6310210000    2.9524470000   -1.5726020000
H   3.9695230000    3.3216860000   -0.8919180000
H   4.8879260000    2.1666270000    1.1092690000
H   3.4338360000    0.6593160000    2.4480280000
H   1.0776890000    0.3197490000    1.8149750000
C   -1.0818680000   0.3774440000   -0.1014970000
N   -0.8042880000   -0.9594530000   0.0502240000
N   -1.9475790000   -1.6944630000   0.2959330000
N   -2.4473650000   0.4424470000   -0.0185130000
C   -2.9094310000   -0.8127510000   0.2483060000
C   0.4198210000   -1.6742020000   -0.1699070000
C   0.7803900000   -2.6675850000    0.7435190000
C   1.1867000000   -1.4139140000   -1.3077260000
C   1.9447950000   -3.3988140000    0.5173060000
C   2.3524680000   -2.1487130000   -1.5157020000
C   2.7335160000   -3.1375260000   -0.6059320000
H   0.1511020000   -2.8659840000    1.6043800000
H   0.8704570000   -0.6655320000   -2.0267060000
H   2.2338310000   -4.1743410000    1.2196910000
H   2.9532850000   -1.9584350000   -2.3995210000
H   3.6389210000   -3.7114420000   -0.7776420000
C   -3.5045360000   1.4720750000    0.0107790000
C   -4.3894090000   -0.8144440000   0.4570020000
C   -4.7859830000   0.5979730000   -0.0667820000
H   -3.3904400000   2.1582050000   -0.8269840000
H   -3.4272450000   2.0367670000    0.9456510000
H   -4.6119780000   -0.9377310000   1.5235930000
H   -4.8856020000   -1.6272770000   -0.0782510000
H   -5.1122780000   0.5262470000   -1.1080480000
H   -5.6022830000   1.0382440000   0.5085250000

```

**thermodynamic data**

Zero-point correction= 0.319505 (Hartree/Particle)  
 Thermal correction to Energy= 0.337298  
 Thermal correction to Enthalpy= 0.338242  
 Thermal correction to Gibbs Free Energy= 0.272020  
 Sum of electronic and zero-point Energies= -935.061505  
 Sum of electronic and thermal Energies= -935.043712  
 Sum of electronic and thermal Enthalpies= -935.042768  
 Sum of electronic and thermal Free Energies= -935.108990

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	211.658	70.726	139.376



### xyz-matrix

38

XYZ file generated by gabedit : coordinates in Angstrom

```

C   -0.6194490000   -0.9876500000   -0.5497370000
O   -0.0691250000   -1.9381400000   -1.1667910000
C   -2.0239990000   -1.1648330000   -0.0608220000
C   -2.5036880000   -0.6092430000   1.1378750000
C   -3.7989940000   -0.8795690000   1.5821790000
C   -4.6358810000   -1.7143500000   0.8389680000
C   -4.1613520000   -2.2899950000   -0.3439040000
C   -2.8669820000   -2.0268430000   -0.7832660000
H   -1.8480140000   0.0128780000   1.7424010000
H   -4.1479060000   -0.4517960000   2.5188860000
H   -5.6441100000   -1.9260280000   1.1850340000
H   -4.8030530000   -2.9507930000   -0.9213370000
H   -2.4773260000   -2.4885600000   -1.6847420000
C   0.0403220000   0.2652800000   -0.3089110000
N   1.4059110000   0.5863850000   -0.2345040000
N   1.5969320000   1.9689550000   -0.1215560000
N   -0.5771890000   1.5075790000   -0.1888110000
C   0.3992980000   2.4604340000   -0.1169640000
C   2.5590720000   -0.2223270000   -0.0041780000
C   2.7368050000   -1.4606810000   -0.6317140000
C   3.5541890000   0.2840950000   0.8479090000
C   3.8987870000   -2.1906510000   -0.3826050000
C   4.7127380000   -0.4535690000   1.0740880000
C   4.8916010000   -1.6971000000   0.4642220000
H   1.9587280000   -1.8415370000   -1.2799010000
H   3.4128370000   1.2495160000   1.3180030000
H   5.4755380000   -0.0539960000   1.7371730000
H   5.7954040000   -2.2722020000   0.6459460000
H   4.0270170000   -3.1535670000   -0.8697860000

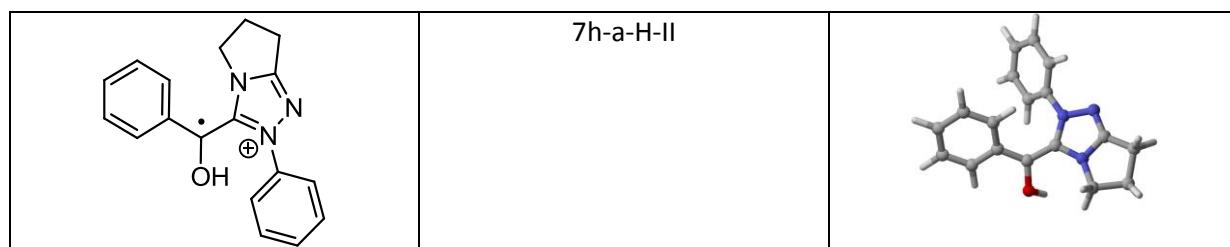
```

C	-1.8745880000	2.0744750000	-0.5701620000
C	-0.1745690000	3.8403530000	-0.2174980000
C	-1.7013590000	3.5559260000	-0.1484510000
H	-2.6950780000	1.5777320000	-0.0524080000
H	-2.0248830000	1.9550430000	-1.6512470000
H	0.1160650000	4.2907770000	-1.1739930000
H	0.1745280000	4.5061200000	0.5765760000
H	-2.0545700000	3.6815770000	0.8799630000
H	-2.2834590000	4.2270140000	-0.7843200000

### Thermodynamic data

Zero-point correction= 0.306530 (Hartree/Particle)  
 Thermal correction to Energy= 0.324031  
 Thermal correction to Enthalpy= 0.324975  
 Thermal correction to Gibbs Free Energy= 0.258442  
 Sum of electronic and zero-point Energies= -934.668560  
 Sum of electronic and thermal Energies= -934.651059  
 Sum of electronic and thermal Enthalpies= -934.650115  
 Sum of electronic and thermal Free Energies= -934.716649

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	203.332	69.251	140.031



### xyz-matrix

39

XYZ file generated by gabedit : coordinates in Angstrom

C	0.1598080000	1.4242040000	0.5067170000
O	0.7032050000	2.4403290000	1.2468020000
H	1.2690430000	2.0903350000	1.9552770000
C	-1.1619630000	1.6503650000	-0.0098750000
C	-1.9857600000	2.6240810000	0.6079600000
C	-3.2528950000	2.8886400000	0.1072930000
C	-3.7266210000	2.1993740000	-1.0148740000
C	-2.9183750000	1.2431600000	-1.6423990000
C	-1.6494600000	0.9707400000	-1.1532790000
H	-1.6173150000	3.1563040000	1.4772820000
H	-3.8773360000	3.6326820000	0.5921660000
H	-4.7181770000	2.4105470000	-1.4036470000
H	-3.2779250000	0.7212920000	-2.5238090000
H	-1.0225680000	0.2511080000	-1.6687660000
C	1.0340320000	0.3384120000	0.2018920000
N	0.7860820000	-0.9934200000	-0.0089340000
N	1.9369080000	-1.6841150000	-0.3396360000
N	2.3949600000	0.4447840000	0.0748090000

C	2.8780040000	-0.7829310000	-0.2836870000
C	-0.4196180000	-1.7453810000	0.1910610000
C	-1.2270810000	-1.4990300000	1.3037770000
C	-0.7263800000	-2.7546700000	-0.7251960000
C	-2.3757250000	-2.2668740000	1.4849150000
C	-1.8748870000	-3.5178120000	-0.5258430000
C	-2.7020270000	-3.2731310000	0.5730290000
H	-0.9591520000	-0.7342870000	2.0246640000
H	-0.0693070000	-2.9398300000	-1.5677090000
H	-2.1217840000	-4.3048480000	-1.2314170000
H	-3.5952270000	-3.8714950000	0.7234510000
H	-3.0072820000	-2.0863520000	2.3490490000
C	3.3969180000	1.5204450000	-0.0724010000
C	4.3380080000	-0.7217240000	-0.6007420000
C	4.7166430000	0.7041880000	-0.1008040000
H	3.3432380000	2.2300380000	0.7534090000
H	3.2032320000	2.0600480000	-1.0051780000
H	4.4833550000	-0.8330600000	-1.6816550000
H	4.9078500000	-1.5143590000	-0.1099730000
H	5.1287260000	0.6440990000	0.9104230000
H	5.4636090000	1.1820520000	-0.7369110000

#### Thermodynamic data

Zero-point correction=	0.319153 (Hartree/Particle)
Thermal correction to Energy=	0.337012
Thermal correction to Enthalpy=	0.337956
Thermal correction to Gibbs Free Energy=	0.271759
Sum of electronic and zero-point Energies=	-935.053648
Sum of electronic and thermal Energies=	-935.035789
Sum of electronic and thermal Enthalpies=	-935.034845
Sum of electronic and thermal Free Energies=	-935.101042

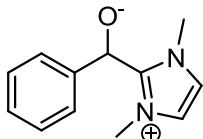
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	211.478	71.027	139.324

**Table 7**

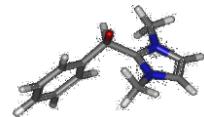
entry	cmpd	$\Delta H_{(I-II)}$ [kcal/mol]	BDE [kcal/mol]	RSE [kcal/mol]
1	4g-a-I	0	45.2 (min) <sup>a</sup>	—
2	4g-a-II		45.2 (max) <sup>b</sup>	
3	4g-a-H-I		45.2 (prob) <sup>c</sup>	
4	4g-a-H-II	-0.6	69.2 (min) <sup>a</sup>	—
5	7g-a-I		73.9 (max) <sup>b</sup>	
6	7g-a-II		69.9 (prob) <sup>c</sup>	
7	7g-a-H-I	-4.1	—	-59.6 (min) <sup>b</sup>
8	7g-a-H-II			-59.6 (max) <sup>a</sup>
				-59.6 (prob) <sup>c</sup>
				-35.6 (min) <sup>b</sup>
				-39.9 (max) <sup>a</sup>

			-34.9 (prob) <sup>c</sup>
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<sup>a</sup> determined from least stable conformer of closed shell species **5** and most stable radical species **4**.<sup>b</sup>  
determined from most stable conformer of closed shell species **5** and least stable radical species **4**.<sup>c</sup>  
determined from most stable conformer of closed shell species **5** and most stable radical species **4**.



**4g-a-I**



### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

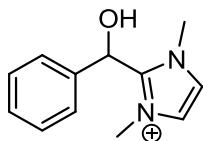
C	-0.0501060000	-0.0097340000	1.2087890000
H	-0.1879840000	-0.9827120000	1.7616970000
O	-0.1689610000	1.0821010000	1.9444870000
C	1.2911790000	-0.1910080000	0.4398840000
C	2.3336210000	0.6828320000	0.7494000000
C	3.5785240000	0.5489690000	0.1303270000
C	3.7905750000	-0.4621880000	-0.8093710000
C	2.7512810000	-1.3430640000	-1.1227690000
C	1.5113290000	-1.2077270000	-0.4964170000
H	2.1270120000	1.4529510000	1.4874660000
H	4.3859860000	1.2334130000	0.3813940000
H	4.7584450000	-0.5670230000	-1.2936390000
H	2.9090390000	-2.1343360000	-1.8524400000
H	0.7086140000	-1.9039030000	-0.7432180000
C	-1.2237990000	-0.0020330000	0.1814700000
N	-1.5328300000	1.0578710000	-0.5983820000
C	-2.7686410000	0.8673390000	-1.1871260000
N	-2.2679160000	-0.8622950000	0.0842450000
C	-3.2341250000	-0.3361120000	-0.7655680000
H	-3.2070880000	1.6054690000	-1.8403150000
H	-4.1533140000	-0.8576720000	-0.9810880000
C	-2.3643450000	-2.1638650000	0.7393670000
C	-0.7174110000	2.2735150000	-0.6660800000
H	-1.7529840000	-2.9091710000	0.2224310000
H	-3.4090300000	-2.4806760000	0.7220780000
H	-2.0301310000	-2.0810260000	1.7745100000
H	-0.3158540000	2.4068620000	0.3472260000
H	-1.3586070000	3.1043020000	-0.9677740000
H	0.0943170000	2.1461280000	-1.3866990000

### Thermodynamic data

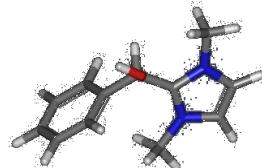
Zero-point correction=	0.240468 (Hartree/Particle)
Thermal correction to Energy=	0.254309
Thermal correction to Enthalpy=	0.255253
Thermal correction to Gibbs Free Energy=	0.196549
Sum of electronic and zero-point Energies=	-650.124217
Sum of electronic and thermal Energies=	-650.110377
Sum of electronic and thermal Enthalpies=	-650.109433

Sum of electronic and thermal Free Energies= -650.168137

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	159.581	52.180	123.554



**4g-a-H-I**



#### xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.1774070000	-1.0758070000	-0.0543170000
H	-0.3601360000	-1.6523000000	-0.9765950000
O	-0.4584640000	-1.8799350000	1.0886540000
H	0.1791120000	-2.6150230000	1.0969530000
C	1.2568840000	-0.5767620000	-0.1087970000
C	2.0149860000	-0.4587700000	1.0621900000
C	3.3365660000	-0.0142420000	0.9958620000
C	3.9048580000	0.3173190000	-0.2359930000
C	3.1538020000	0.1908410000	-1.4076400000
C	1.8361200000	-0.2638940000	-1.3454900000
H	1.5719100000	-0.7201770000	2.0188650000
H	3.9229490000	0.0685950000	1.9061540000
H	4.9338470000	0.6605120000	-0.2853200000
H	3.5983480000	0.4287590000	-2.3693430000
H	1.2632380000	-0.3835560000	-2.2631590000
C	-1.2637690000	-0.0137320000	-0.0360410000
N	-1.2006750000	1.3182630000	0.1810290000
C	-2.4766930000	1.8447170000	0.1038010000
N	-2.5625510000	-0.3250710000	-0.2421020000
C	-3.3277220000	0.8172630000	-0.1591240000
H	-2.6646910000	2.8970890000	0.2467820000
H	-4.3984870000	0.8014810000	-0.2898190000
C	-3.0905200000	-1.6705340000	-0.5168110000
C	-0.0217100000	2.1514730000	0.4846840000
H	-2.9038640000	-1.9403070000	-1.5598530000
H	-4.1650240000	-1.6570540000	-0.3345360000
H	-2.6109030000	-2.3811890000	0.1552250000
H	0.4307280000	1.8342460000	1.4234190000
H	-0.3687430000	3.1807310000	0.5749510000
H	0.7096320000	2.0780950000	-0.3194050000

#### Thermodynamic data

Zero-point correction= 0.255807 (Hartree/Particle)

Thermal correction to Energy= 0.269669

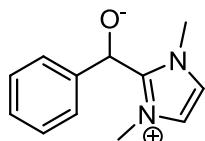
Thermal correction to Enthalpy= 0.270613

Thermal correction to Gibbs Free Energy= 0.214798

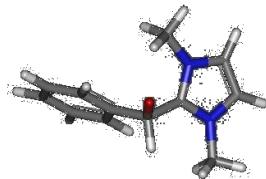
Sum of electronic and zero-point Energies= -650.556793

Sum of electronic and thermal Energies= -650.542930  
 Sum of electronic and thermal Enthalpies= -650.541986  
 Sum of electronic and thermal Free Energies= -650.597801

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.220	53.228	117.472



**4g-a-II**



### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

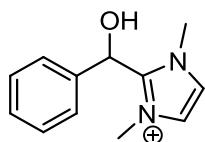
C	0.0500970000	0.0101860000	-1.2083920000
H	0.1879680000	0.9834210000	-1.7608980000
O	0.1691120000	-1.0813650000	-1.9445560000
C	-1.2912680000	0.1910620000	-0.4395740000
C	-2.3336540000	-0.6826210000	-0.7497430000
C	-3.5786940000	-0.5490040000	-0.1309070000
C	-3.7909330000	0.4617180000	0.8092190000
C	-2.7516850000	1.3424010000	1.1232940000
C	-1.5115790000	1.2073200000	0.4971770000
H	-2.1268560000	-1.4523650000	-1.4881480000
H	-4.3861250000	-1.2332980000	-0.3824850000
H	-4.7589200000	0.5663670000	1.2932930000
H	-2.9095950000	2.1333270000	1.8533070000
H	-0.7089070000	1.9033470000	0.7445310000
C	1.2238170000	0.0021020000	-0.1812460000
N	1.5331870000	-1.0579910000	0.5981980000
C	2.7690650000	-0.8673960000	1.1867640000
N	2.2677310000	0.8625720000	-0.0839050000
C	3.2342240000	0.3362770000	0.7654970000
C	0.7180020000	-2.2738060000	0.6657110000
C	2.3640530000	2.1639390000	-0.7395120000
H	2.0336060000	2.0799350000	-1.7757920000
H	3.4080780000	2.4826620000	-0.7186690000
H	1.7495260000	2.9084070000	-0.2251580000
H	0.3160300000	-2.4067670000	-0.3474680000
H	-0.0933860000	-2.1469370000	1.3868040000
H	1.3594940000	-3.1046330000	0.9666810000
H	3.2077440000	-1.6056360000	1.8396720000
H	4.1533420000	0.8579630000	0.9810010000

### Thermodynamic data

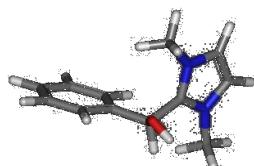
Zero-point correction=	0.240467 (Hartree/Particle)
Thermal correction to Energy=	0.254310
Thermal correction to Enthalpy=	0.255254
Thermal correction to Gibbs Free Energy=	0.196145

Sum of electronic and zero-point Energies= -650.124219  
 Sum of electronic and thermal Energies= -650.110376  
 Sum of electronic and thermal Enthalpies= -650.109432  
 Sum of electronic and thermal Free Energies= -650.168541

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	159.582	52.180	124.405



**4g-a-H-II**



### **xyz-matrix**

30

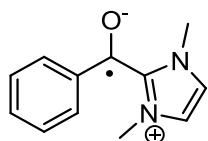
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0417260000	-0.1599790000	-1.1694210000
H	0.1693890000	0.6127330000	-1.9406860000
O	0.0107410000	-1.4484030000	-1.7672020000
H	0.5570350000	-1.4442240000	-2.5691180000
C	-1.2693040000	0.0957560000	-0.4251530000
C	-2.4215750000	-0.6100080000	-0.7881520000
C	-3.6340690000	-0.3363900000	-0.1522610000
C	-3.7064490000	0.6418350000	0.8402560000
C	-2.5586170000	1.3500200000	1.2012350000
C	-1.3441940000	1.0772260000	0.5721360000
H	-2.3658080000	-1.3684370000	-1.5604110000
H	-4.5236030000	-0.8901620000	-0.4374220000
H	-4.6519960000	0.8523640000	1.3307530000
H	-2.6064150000	2.1128130000	1.9726120000
H	-0.4589130000	1.6365810000	0.8688020000
C	1.2437050000	-0.0765000000	-0.2477210000
N	1.5692520000	-0.9810370000	0.6948630000
C	2.7400560000	-0.5883700000	1.3129860000
N	2.1900880000	0.8858370000	-0.2328980000
C	3.1288860000	0.5813730000	0.7368930000
C	0.8218970000	-2.2101410000	1.0129430000
C	2.2300830000	2.0795060000	-1.0914300000
H	1.3042860000	2.6487320000	-0.9906570000
H	2.3845500000	1.7928230000	-2.1342050000
H	3.0649550000	2.7005960000	-0.7674300000
H	-0.2451320000	-1.9894970000	1.0335880000
H	1.1469860000	-2.5547390000	1.9946530000
H	1.0218700000	-2.9696850000	0.2565380000
H	3.1900580000	-1.1695660000	2.1027940000
H	3.9785690000	1.2173220000	0.9301890000

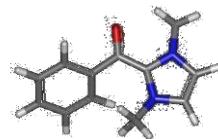
### **Thermodynamic data**

Zero-point correction= 0.255038 (Hartree/Particle)  
 Thermal correction to Energy= 0.269352  
 Thermal correction to Enthalpy= 0.270297  
 Thermal correction to Gibbs Free Energy= 0.212568  
 Sum of electronic and zero-point Energies= -650.556275  
 Sum of electronic and thermal Energies= -650.541960  
 Sum of electronic and thermal Enthalpies= -650.541016  
 Sum of electronic and thermal Free Energies= -650.598745

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.021	53.731	121.500



**7g-a-I**



#### **xyz-matrix**

28

XYZ file generated by gabedit : coordinates in Angstrom

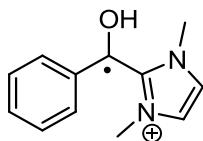
C	-0.0921690000	-0.9355180000	0.2535650000
O	-0.2597540000	-2.1571310000	0.5574310000
C	1.2833480000	-0.4118460000	0.0312880000
C	2.3483460000	-1.0435420000	0.7013510000
C	3.6636310000	-0.6442100000	0.4868560000
C	3.9531820000	0.3828930000	-0.4181820000
C	2.9101710000	0.9960630000	-1.1157120000
C	1.5903550000	0.6000820000	-0.8979460000
H	2.1125790000	-1.8547050000	1.3827280000
H	4.4707650000	-1.1374370000	1.0232940000
H	4.9815480000	0.6905080000	-0.5886490000
H	3.1259290000	1.7720770000	-1.8464620000
H	0.7923620000	1.0519980000	-1.4824830000
C	-1.2405440000	-0.0845590000	0.0864860000
N	-1.3637880000	1.2862490000	0.2950670000
C	-2.6887860000	1.6574450000	0.0866180000
N	-2.5165320000	-0.5314130000	-0.2177080000
C	-3.3876140000	0.5448000000	-0.2363070000
H	-3.0124920000	2.6793270000	0.2081540000
H	-4.4311260000	0.4196990000	-0.4809150000
C	-2.8536710000	-1.8658260000	-0.6988290000
C	-0.4033720000	2.1244460000	0.9984040000
H	-2.6860010000	-1.9427530000	-1.7807530000
H	-3.9090680000	-2.0557250000	-0.4854770000
H	-2.2164000000	-2.5822100000	-0.1823010000
H	-0.9405360000	2.9641660000	1.4457080000
H	0.3759280000	2.5038400000	0.3315740000
H	0.0795260000	1.5430470000	1.7890690000

#### **thermodynamic data**

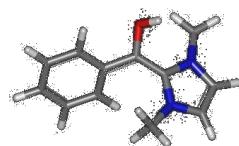
Zero-point correction= 0.229240 (Hartree/Particle)

Thermal correction to Energy= 0.242870  
 Thermal correction to Enthalpy= 0.243814  
 Thermal correction to Gibbs Free Energy= 0.188088  
 Sum of electronic and zero-point Energies= -649.554117  
 Sum of electronic and thermal Energies= -649.540487  
 Sum of electronic and thermal Enthalpies= -649.539543  
 Sum of electronic and thermal Free Energies= -649.595270

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.403	51.870	117.287



7g-a-H-I



### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

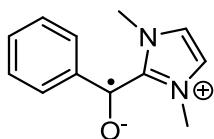
C	-0.0342780000	0.7990700000	-0.3952550000
O	-0.1560630000	2.0813160000	-0.8613390000
H	-0.9031120000	2.1576760000	-1.4794410000
C	1.2940980000	0.3569150000	-0.0761680000
C	2.4086390000	0.9911030000	-0.6815280000
C	3.6992710000	0.5901760000	-0.3652530000
C	3.9155480000	-0.4401310000	0.5576520000
C	2.8254020000	-1.0630790000	1.1784220000
C	1.5297960000	-0.6692860000	0.8745790000
H	2.2406170000	1.7867410000	-1.3984580000
H	4.5441070000	1.0791100000	-0.8405420000
H	4.9275380000	-0.7485100000	0.8013410000
H	2.9927030000	-1.8412390000	1.9169630000
H	0.6949720000	-1.1182600000	1.4059050000
C	-1.2423430000	0.0657060000	-0.1390910000
N	-2.4140610000	0.5738400000	0.3564630000
C	-3.3601400000	-0.4304020000	0.3967880000
N	-1.4755310000	-1.2533890000	-0.4188780000
C	-2.7770340000	-1.5634380000	-0.0789160000
H	-4.3587780000	-0.2562840000	0.7671990000
H	-3.1808820000	-2.5538630000	-0.2213950000
C	-0.5641920000	-2.1699210000	-1.1137890000
C	-2.6075740000	1.8911480000	0.9828250000
H	-1.1640900000	-2.9315130000	-1.6129540000
H	0.1239270000	-2.6414970000	-0.4094650000
H	0.0103840000	-1.6142000000	-1.8561040000
H	-2.6980490000	1.7678150000	2.0650140000
H	-3.5205850000	2.3429430000	0.5882720000
H	-1.7562640000	2.5302320000	0.7596820000

### thermodynamic data

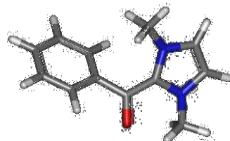
Zero-point correction= 0.242502 (Hartree/Particle)

Thermal correction to Energy= 0.256404  
 Thermal correction to Enthalpy= 0.257348  
 Thermal correction to Gibbs Free Energy= 0.201083  
 Sum of electronic and zero-point Energies= -649.941011  
 Sum of electronic and thermal Energies= -649.927109  
 Sum of electronic and thermal Enthalpies= -649.926165  
 Sum of electronic and thermal Free Energies= -649.982430

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.896	53.269	118.420



7g-a-II



### xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

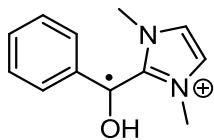
C	-0.0921350000	0.9354170000	0.2537440000
O	-0.2596020000	2.1569490000	0.5578330000
C	1.2833770000	0.4116690000	0.0313630000
C	2.3483940000	1.0434500000	0.7013040000
C	3.6636920000	0.6442020000	0.4866920000
C	3.9532050000	-0.3829210000	-0.4183260000
C	2.9101570000	-0.9961740000	-1.1157360000
C	1.5903390000	-0.6002380000	-0.8978890000
H	2.1126450000	1.8546370000	1.3826580000
H	4.4708420000	1.1374900000	1.0230480000
H	4.9815650000	-0.6905010000	-0.5888880000
H	3.1258940000	-1.7722050000	-1.8464720000
H	0.7923180000	-1.0522590000	-1.4823030000
C	-1.2405430000	0.0845580000	0.0864530000
N	-1.3637490000	-1.2863400000	0.2945700000
C	-2.6888850000	-1.6573290000	0.0862700000
N	-2.5165270000	0.5315850000	-0.2174660000
C	-3.3876730000	-0.5446000000	-0.2363140000
C	-0.4038380000	-2.1242340000	0.9989410000
C	-2.8533510000	1.8659590000	-0.6991880000
H	-2.2163930000	2.5824480000	-0.1824340000
H	-3.9088570000	2.0559180000	-0.4864360000
H	-2.6850640000	1.9425090000	-1.7810280000
H	0.0781040000	-1.5427570000	1.7901500000
H	0.3762650000	-2.5033970000	0.3329080000
H	-0.9411560000	-2.9641710000	1.4456480000
H	-3.0126630000	-2.6791920000	0.2078030000
H	-4.4311790000	-0.4193810000	-0.4809170000

### thermodynamic data

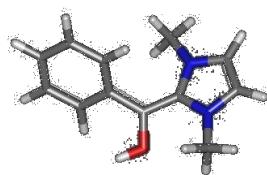
Zero-point correction= 0.229238 (Hartree/Particle)

Thermal correction to Energy= 0.242870  
 Thermal correction to Enthalpy= 0.243814  
 Thermal correction to Gibbs Free Energy= 0.188083  
 Sum of electronic and zero-point Energies= -649.554119  
 Sum of electronic and thermal Energies= -649.540488  
 Sum of electronic and thermal Enthalpies= -649.539543  
 Sum of electronic and thermal Free Energies= -649.595274

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.403	51.871	117.295



7g-a-H-II



### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.0736450000	-0.8242290000	0.2379740000
C	1.2870520000	-0.3699020000	0.0300370000
C	-1.2568090000	-0.0458410000	0.0951200000
O	-0.3116000000	-2.1131440000	0.6059320000
H	0.4732100000	-2.6543220000	0.4064050000
N	-1.4098000000	1.2919960000	0.3613970000
N	-2.4902940000	-0.5137230000	-0.2816390000
C	-2.7217880000	1.6470240000	0.1296490000
C	-3.3898540000	0.5282210000	-0.2638530000
H	-3.0716430000	2.6567270000	0.2776850000
H	-4.4248900000	0.3903550000	-0.5352800000
C	-2.8174370000	-1.8732780000	-0.7308410000
C	-0.4212020000	2.1887000000	0.9699530000
H	-0.9607240000	3.0011980000	1.4576880000
H	0.2561830000	2.5959530000	0.2169220000
H	0.1572400000	1.6411710000	1.7152170000
H	-2.0993180000	-2.1965370000	-1.4863330000
H	-3.8145060000	-1.8461540000	-1.1709380000
H	-2.7988870000	-2.5671720000	0.1097280000
C	2.3408160000	-0.9531030000	0.7727420000
C	1.6032430000	0.5857770000	-0.9631110000
C	3.6594660000	-0.5802590000	0.5355170000
C	2.9245580000	0.9537770000	-1.1890680000
C	3.9564020000	0.3743450000	-0.4421070000
H	2.1180090000	-1.6633520000	1.5651400000
H	0.8139530000	0.9979010000	-1.5860070000
H	4.4572610000	-1.0259140000	1.1216700000
H	3.1558110000	1.6777960000	-1.9645120000
H	4.9869600000	0.6621980000	-0.6252280000

### thermodynamic data

Zero-point correction= 0.242964 (Hartree/Particle)  
 Thermal correction to Energy= 0.256681  
 Thermal correction to Enthalpy= 0.257625  
 Thermal correction to Gibbs Free Energy= 0.202009  
 Sum of electronic and zero-point Energies= -649.947418  
 Sum of electronic and thermal Energies= -649.933701  
 Sum of electronic and thermal Enthalpies= -649.932757  
 Sum of electronic and thermal Free Energies= -649.988372

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	161.070	52.997	117.053

## B.2.2 M06-2X/6-31++G\*\*

### **methane**

#### **Xyz-matrix**

5

XYZ file generated by gabedit : coordinates in Angstrom

C	0.0000000000	-0.0000150000	0.0000000000
H	-0.3653850000	1.0275710000	0.0000000000
H	-0.8469880000	-0.6871060000	0.0000000000
H	0.6061870000	-0.1701890000	0.8905660000
H	0.6061870000	-0.1701890000	-0.8905660000

#### **Thermodynamic data**

Zero-point correction= 0.045059 (Hartree/Particle)  
 Thermal correction to Energy= 0.047927  
 Thermal correction to Enthalpy= 0.048871  
 Thermal correction to Gibbs Free Energy= 0.025395  
 Sum of electronic and zero-point Energies= -40.442871  
 Sum of electronic and thermal Energies= -40.440003  
 Sum of electronic and thermal Enthalpies= -40.439059  
 Sum of electronic and thermal Free Energies= -40.462534

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	30.074	6.463	49.408

### **methyl radical**

#### **Xyz-matrix**

4

XYZ file generated by gabedit : coordinates in Angstrom

C	0.0000000000	-0.0000660000	0.0002630000
H	0.9356660000	-0.5393180000	-0.0005240000
H	-0.9352320000	-0.5400690000	-0.0005240000

H -0.0004340000 1.0797800000 -0.0005270000

### Thermodynamic data

Zero-point correction= 0.029799 (Hartree/Particle)  
Thermal correction to Energy= 0.032936  
Thermal correction to Enthalpy= 0.033880  
Thermal correction to Gibbs Free Energy= 0.009959  
Sum of electronic and zero-point Energies= -39.782117  
Sum of electronic and thermal Energies= -39.778980  
Sum of electronic and thermal Enthalpies= -39.778036  
Sum of electronic and thermal Free Energies= -39.801957

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	20.667	7.588	50.347

### hydrogen atom

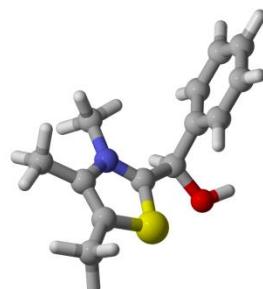
### Xyz-matrix

### Thermodynamic data

Zero-point correction= 0.000000 (Hartree/Particle)  
Thermal correction to Energy= 0.001416  
Thermal correction to Enthalpy= 0.002360  
Thermal correction to Gibbs Free Energy= -0.010654  
Sum of electronic and zero-point Energies= -0.498302  
Sum of electronic and thermal Energies= -0.496886  
Sum of electronic and thermal Enthalpies= -0.495941  
Sum of electronic and thermal Free Energies= -0.508956

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	0.889	2.981	27.392

*anti-4a-a-H*



### Xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

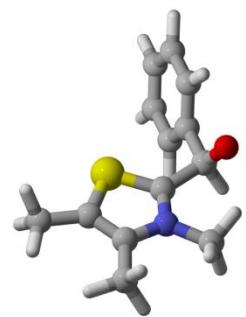
C 4.0691750000 0.7882920000 -0.1512100000

C	4.0751580000	0.5932420000	1.2281510000
C	3.0011070000	-0.0450610000	1.8508920000
C	1.9175540000	-0.4827960000	1.0956020000
C	1.9059910000	-0.2820600000	-0.2882990000
C	2.9852720000	0.3488320000	-0.9103430000
C	0.7565140000	-0.8053460000	-1.1296130000
C	-0.5880060000	-0.3869350000	-0.5812650000
O	0.6878330000	-2.2137610000	-1.1580990000
N	-1.0661480000	0.8475470000	-0.5230470000
S	-1.6787240000	-1.5159830000	0.0545730000
C	-2.8235700000	-0.2659310000	0.4215580000
C	-2.3429840000	0.9509710000	0.0438100000
C	-0.3511020000	2.0267690000	-1.0330470000
C	-2.9930040000	2.2905350000	0.1702690000
C	-4.1263930000	-0.6070320000	1.0771460000
H	4.9070690000	1.2760870000	-0.6378670000
H	4.9194960000	0.9318660000	1.8194200000
H	3.0113650000	-0.2043010000	2.9239880000
H	1.0885790000	-0.9933430000	1.5807860000
H	2.9843300000	0.4921420000	-1.9889860000
H	0.8447130000	-0.4047350000	-2.1517680000
H	1.5806900000	-2.5824040000	-1.1632230000
H	-0.8127850000	2.3526900000	-1.9673610000
H	0.6947020000	1.7758220000	-1.1937820000
H	-0.4106330000	2.8221440000	-0.2906960000
H	-4.0072400000	2.1761630000	0.5500470000
H	-3.0518010000	2.7986830000	-0.7964010000
H	-2.4483290000	2.9339890000	0.8680550000
H	-4.8125740000	0.2390860000	1.0317600000
H	-3.9763860000	-0.8687670000	2.1281490000
H	-4.6054980000	-1.4530210000	0.5789370000

### Thermodynamic data

Zero-point correction= 0.268309 (Hartree/Particle)  
 Thermal correction to Energy= 0.284404  
 Thermal correction to Enthalpy= 0.285348  
 Thermal correction to Gibbs Free Energy= 0.223765  
 Sum of electronic and zero-point Energies= -1032.418191  
 Sum of electronic and thermal Energies= -1032.402095  
 Sum of electronic and thermal Enthalpies= -1032.401151  
 Sum of electronic and thermal Free Energies= -1032.462735

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.466	60.256	129.614



**4a-a**

### Xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	-3.8662690000	0.2354510000	-1.0698880000
C	-4.2673120000	0.9661800000	0.0483890000
C	-3.5143660000	0.9084880000	1.2222980000
C	-2.3631660000	0.1246790000	1.2683950000
C	-1.9518150000	-0.5955190000	0.1446330000
C	-2.7109650000	-0.5450710000	-1.0222300000
C	-0.6715540000	-1.4409800000	0.1505680000
C	0.5365310000	-0.4581470000	0.1861870000
O	-0.4800670000	-2.2330770000	-0.8952810000
N	1.7956220000	-0.8785480000	0.2423350000
S	0.4808790000	1.2187230000	-0.1148140000
C	2.2187870000	1.3287140000	-0.1677170000
C	2.7699230000	0.1074170000	0.0512240000
C	2.0988700000	-2.3050540000	0.4322200000
C	4.2186850000	-0.2591630000	0.1031150000
C	2.8914590000	2.6392750000	-0.4362130000
H	-4.4592810000	0.2699800000	-1.9793650000
H	-5.1680300000	1.5717120000	0.0111090000
H	-3.8291280000	1.4660400000	2.0997220000
H	-1.7799460000	0.0677220000	2.1873170000
H	-2.3682110000	-1.1399940000	-1.8641580000
H	-0.6387150000	-1.9383680000	1.1591890000
H	1.2761980000	-2.8531480000	-0.0431110000
H	2.1779860000	-2.5252530000	1.4994350000
H	3.0405190000	-2.5336240000	-0.0642030000
H	4.8337490000	0.6401140000	0.0842300000
H	4.5043540000	-0.8804410000	-0.7513870000
H	4.4528260000	-0.8097120000	1.0188340000
H	3.9744410000	2.5459900000	-0.3407320000
H	2.5556850000	3.4050310000	0.2684350000
H	2.6718360000	2.9912270000	-1.4482730000

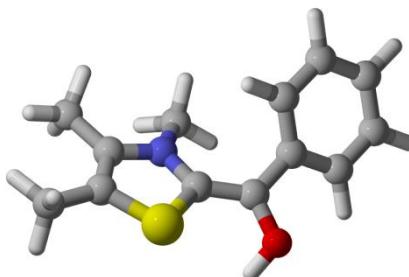
### Thermodynamic data

Zero-point correction=	0.254281 (Hartree/Particle)
Thermal correction to Energy=	0.269842
Thermal correction to Enthalpy=	0.270786
Thermal correction to Gibbs Free Energy=	0.210808

Sum of electronic and zero-point Energies= -1031.987808  
 Sum of electronic and thermal Energies= -1031.972248  
 Sum of electronic and thermal Enthalpies= -1031.971304  
 Sum of electronic and thermal Free Energies= -1032.031282

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.328	58.613	126.234

*anti-7a-a-H*



### Xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3225060000	-0.1945860000	-0.3715300000
C	4.3634640000	0.9053090000	0.4870410000
C	3.2006800000	1.3459160000	1.1241090000
C	1.9948860000	0.7004850000	0.8892400000
C	1.9428120000	-0.3941230000	0.0068230000
C	3.1222030000	-0.8524400000	-0.6065120000
C	0.6980980000	-1.1055030000	-0.2218870000
C	-0.5971540000	-0.5579030000	-0.1349890000
O	0.8289980000	-2.4294540000	-0.4018280000
N	-0.9894130000	0.7191620000	-0.3954630000
S	-1.9526030000	-1.5163560000	0.3645910000
C	-3.0200330000	-0.1518430000	0.2425940000
C	-2.3405230000	0.9605500000	-0.1571660000
C	-0.1472700000	1.7157930000	-1.0709160000
C	-2.8971190000	2.3317440000	-0.3744750000
C	-4.4714040000	-0.3197470000	0.5648050000
H	5.2300470000	-0.5413080000	-0.8539490000
H	5.3052830000	1.4113240000	0.6721810000
H	3.2427840000	2.1790970000	1.8175350000
H	1.0993020000	1.0109910000	1.4219760000
H	3.0825060000	-1.7131030000	-1.2656170000
H	0.0586010000	-2.8355640000	-0.8256510000
H	-0.7586080000	2.2417240000	-1.8031760000
H	0.6686710000	1.2079500000	-1.5808290000
H	0.2655000000	2.4270260000	-0.3525510000
H	-3.8922190000	2.4061580000	0.0613470000
H	-2.9809780000	2.5668940000	-1.4401710000
H	-2.2666880000	3.0897180000	0.0979280000
H	-4.9975080000	0.6307560000	0.4769780000

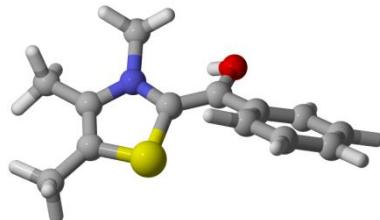
H	-4.6078970000	-0.6914730000	1.5837800000
H	-4.9401220000	-1.0289160000	-0.1231910000

### Thermodynamic data

Zero-point correction= 0.255948 (Hartree/Particle)  
 Thermal correction to Energy= 0.271624  
 Thermal correction to Enthalpy= 0.272568  
 Thermal correction to Gibbs Free Energy= 0.212247  
 Sum of electronic and zero-point Energies= -1031.798433  
 Sum of electronic and thermal Energies= -1031.782757  
 Sum of electronic and thermal Enthalpies= -1031.781812  
 Sum of electronic and thermal Free Energies= -1031.842134

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.447	59.718	126.958

*syn-7a-q-H*



### Xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3458440000	0.2083000000	-0.5837790000
C	4.4947600000	-0.9040950000	0.2467310000
C	3.4045400000	-1.3938270000	0.9677590000
C	2.1631200000	-0.7844670000	0.8507420000
C	1.9990610000	0.3229510000	-0.0030160000
C	3.1096550000	0.8266110000	-0.7064330000
C	0.7155310000	0.9816690000	-0.1554980000
C	-0.5266190000	0.3356390000	-0.0272230000
O	0.7776640000	2.2896370000	-0.4712030000
N	-1.7318560000	0.9455210000	0.1839890000
S	-0.7582440000	-1.3530090000	-0.3444410000
C	-2.4821520000	-1.1843300000	-0.2277080000
C	-2.8322440000	0.1036040000	0.0493600000
C	-1.8675350000	2.2948070000	0.7545320000
C	-4.2126510000	0.6485200000	0.2352770000
C	-3.3575410000	-2.3817140000	-0.4246770000
H	5.1965820000	0.5919170000	-1.1366450000
H	5.4643470000	-1.3816570000	0.3427050000
H	3.5286310000	-2.2383920000	1.6368600000
H	1.3358030000	-1.1374690000	1.4583760000

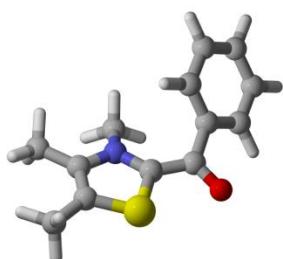
H	2.9870480000	1.6896080000	-1.3515620000
H	-0.0022460000	2.5912870000	-0.9568120000
H	-2.1408750000	3.0222790000	-0.0154070000
H	-0.9305240000	2.5817400000	1.2284090000
H	-2.6505520000	2.2745060000	1.5117300000
H	-4.9474210000	-0.0573730000	-0.1493000000
H	-4.3402250000	1.5897080000	-0.3059730000
H	-4.4370010000	0.8247170000	1.2922040000
H	-4.3918800000	-2.1492850000	-0.1707570000
H	-3.0343990000	-3.2069110000	0.2153900000
H	-3.3263220000	-2.7242780000	-1.4628590000

### Thermodynamic data

Zero-point correction= 0.255743 (Hartree/Particle)  
 Thermal correction to Energy= 0.271542  
 Thermal correction to Enthalpy= 0.272486  
 Thermal correction to Gibbs Free Energy= 0.211798  
 Sum of electronic and zero-point Energies= -1031.796966  
 Sum of electronic and thermal Energies= -1031.781167  
 Sum of electronic and thermal Enthalpies= -1031.780222  
 Sum of electronic and thermal Free Energies= -1031.840910

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.395	59.894	127.728

*anti-7a-a*



### Xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	4.2909740000	-0.1991810000	-0.4788400000
C	4.3707480000	0.8871670000	0.3939660000
C	3.2406490000	1.2900270000	1.1044330000
C	2.0306540000	0.6228140000	0.9253760000
C	1.9405010000	-0.4535670000	0.0364630000
C	3.0859550000	-0.8745590000	-0.6468940000
C	0.6774090000	-1.2401280000	-0.1269960000
C	-0.5977980000	-0.5962010000	-0.1145180000
O	0.7246510000	-2.4857200000	-0.2095070000
N	-0.9429470000	0.7212770000	-0.3283020000

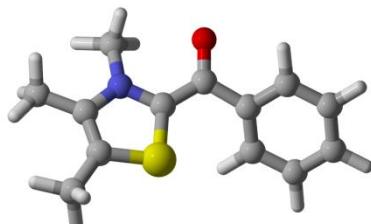
S	-2.0093710000	-1.5580170000	0.2225620000
C	-3.0202220000	-0.1247370000	0.1858620000
C	-2.3028070000	0.9808790000	-0.1217210000
C	-0.0865140000	1.6632300000	-1.0437600000
C	-2.8070430000	2.3843290000	-0.2626710000
C	-4.4844190000	-0.2540430000	0.4647590000
H	5.1731330000	-0.5233560000	-1.0225720000
H	5.3136440000	1.4077270000	0.5301960000
H	3.3051310000	2.1157840000	1.8067540000
H	1.1534360000	0.9207550000	1.4959050000
H	3.0115630000	-1.7392440000	-1.2993380000
H	-0.6987440000	2.2594120000	-1.7218170000
H	0.6446890000	1.1047170000	-1.6286330000
H	0.4521360000	2.3256720000	-0.3603740000
H	-3.8027980000	2.4724920000	0.1715260000
H	-2.8720610000	2.6927880000	-1.3115110000
H	-2.1502350000	3.0886080000	0.2566350000
H	-4.9915050000	0.7072070000	0.3645930000
H	-4.6632600000	-0.6309720000	1.4766500000
H	-4.9502900000	-0.9526700000	-0.2375900000

#### Thermodynamic data

Zero-point correction= 0.242778 (Hartree/Particle)  
 Thermal correction to Energy= 0.258474  
 Thermal correction to Enthalpy= 0.259419  
 Thermal correction to Gibbs Free Energy= 0.198573  
 Sum of electronic and zero-point Energies= -1031.424641  
 Sum of electronic and thermal Energies= -1031.408944  
 Sum of electronic and thermal Enthalpies= -1031.408000  
 Sum of electronic and thermal Free Energies= -1031.468846

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.195	58.462	128.061

*syn*-7a-a



#### Xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	-4.2823430000	0.2409720000	-0.7598100000
C	-4.5089450000	-0.8670110000	0.0583160000
C	-3.4866100000	-1.3432910000	0.8760000000
C	-2.2362610000	-0.7270520000	0.8650070000
C	-1.9980560000	0.3730420000	0.0346540000
C	-3.0383630000	0.8619860000	-0.7641610000
C	-0.6939780000	1.1089640000	-0.0099920000
C	0.5264360000	0.3713410000	0.0923010000
O	-0.6901130000	2.3475630000	-0.1861830000
N	1.7726680000	0.9564140000	0.1724510000
S	0.7005690000	-1.3538640000	-0.1446090000
C	2.4471610000	-1.2087880000	-0.2007670000
C	2.8344030000	0.0763850000	-0.0160250000
C	1.9550920000	2.3622300000	0.5324870000
C	4.2393650000	0.5940650000	0.0008220000
C	3.2708920000	-2.4382100000	-0.4169090000
H	-5.0790720000	0.6220400000	-1.3914140000
H	-5.4814600000	-1.3497810000	0.0659650000
H	-3.6643510000	-2.1891670000	1.5331520000
H	-1.4580030000	-1.0866050000	1.5321290000
H	-2.8473940000	1.7379420000	-1.3762030000
H	2.9585530000	2.4907930000	0.9361460000
H	1.2193090000	2.6346580000	1.2874510000
H	1.8036590000	3.0106910000	-0.3320710000
H	4.9307100000	-0.1875950000	-0.3121590000
H	4.5373740000	0.9249230000	1.0008870000
H	4.3529340000	1.4388640000	-0.6849230000
H	4.3367220000	-2.2050110000	-0.3976500000
H	3.0436320000	-2.9030100000	-1.3816450000
H	3.0777560000	-3.1801250000	0.3648420000

### Thermodynamic data

Zero-point correction= 0.242710 (Hartree/Particle)  
 Thermal correction to Energy= 0.258407  
 Thermal correction to Enthalpy= 0.259351  
 Thermal correction to Gibbs Free Energy= 0.198446  
 Sum of electronic and zero-point Energies= -1031.428756  
 Sum of electronic and thermal Energies= -1031.413060  
 Sum of electronic and thermal Enthalpies= -1031.412115  
 Sum of electronic and thermal Free Energies= -1031.473020

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.153	58.491	128.186

### 6a

#### Xyz-matrix

11

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3872360000	0.7434980000	0.0973310000
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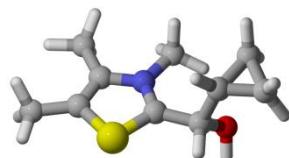
C	-0.1981000000	-0.0000090000	-0.4768280000
C	1.0414060000	-0.0000540000	0.3272430000
O	2.1605590000	0.0000270000	-0.1270940000
C	-1.3872850000	-0.7434670000	0.0972800000
H	-2.0173510000	1.2678450000	-0.6110250000
H	-1.2429010000	1.2524880000	1.0452920000
H	-0.0538820000	0.0000290000	-1.5514360000
H	0.8773760000	-0.0001310000	1.4296680000
H	-2.0174390000	-1.2677230000	-0.6111080000
H	-1.2429850000	-1.2525300000	1.0452070000

### Thermodynamic data

Zero-point correction= 0.091848 (Hartree/Particle)  
 Thermal correction to Energy= 0.096837  
 Thermal correction to Enthalpy= 0.097781  
 Thermal correction to Gibbs Free Energy= 0.063970  
 Sum of electronic and zero-point Energies= -231.036721  
 Sum of electronic and thermal Energies= -231.031732  
 Sum of electronic and thermal Enthalpies= -231.030788  
 Sum of electronic and thermal Free Energies= -231.064599

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	60.766	17.198	71.161

**3b-H**



### Xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.5457030000	-0.7436150000	0.4976500000
C	-0.0675140000	-0.4346350000	0.2985930000
O	-2.0708400000	-0.0226930000	1.5872950000
N	0.4903980000	0.7656470000	0.2055290000
S	1.0829190000	-1.6613200000	0.0765510000
C	2.3541080000	-0.5143470000	-0.1587430000
C	1.8631130000	0.7521260000	-0.0548520000
C	-0.2513380000	2.0346960000	0.3274790000
C	2.6332690000	2.0254050000	-0.1863330000
C	3.7665880000	-0.9395550000	-0.4284610000
C	-2.3299860000	-0.4251380000	-0.7650660000
C	-3.8279320000	-0.5047220000	-0.7241300000
C	-3.1568660000	0.8279380000	-0.8849740000

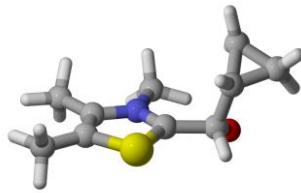
H	-1.6081710000	-1.8248410000	0.6811800000
H	-1.9970800000	-0.5306360000	2.4037240000
H	0.3605820000	2.7359290000	0.8933870000
H	-1.1803030000	1.8476800000	0.8570270000
H	-0.4488780000	2.4278930000	-0.6718160000
H	3.6501560000	1.8014590000	-0.5098750000
H	2.6944300000	2.5576270000	0.7680460000
H	2.1825460000	2.6917080000	-0.9269440000
H	4.0895580000	-0.5957940000	-1.4148260000
H	3.8644690000	-2.0258550000	-0.4039360000
H	4.4421370000	-0.5254930000	0.3242390000
H	-1.8500210000	-0.7875900000	-1.6707020000
H	-4.2861950000	-0.6963750000	0.2404210000
H	-4.3310250000	-0.9463030000	-1.5758840000
H	-3.1899560000	1.3135600000	-1.8536950000
H	-3.2114560000	1.4912450000	-0.0291990000

### Thermodynamic data

Zero-point correction=	0.249907 (Hartree/Particle)
Thermal correction to Energy=	0.264304
Thermal correction to Enthalpy=	0.265248
Thermal correction to Gibbs Free Energy=	0.208812
Sum of electronic and zero-point Energies=	-918.122495
Sum of electronic and thermal Energies=	-918.108098
Sum of electronic and thermal Enthalpies=	-918.107153
Sum of electronic and thermal Free Energies=	-918.163589

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.853	53.448	118.780

*syn-3b*



### Xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.6369080000	-1.5020890000	1.2970190000
O	-2.0982860000	0.4969040000	1.5189790000
H	4.0089440000	-1.7215840000	0.4399880000
S	0.9523530000	-1.6392000000	0.2510670000
C	-1.6386400000	-0.5021820000	0.7891250000
H	-4.2428580000	-0.1371310000	0.3654960000

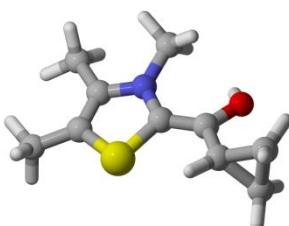
C	-0.1317600000	-0.3262450000	0.4149280000
C	3.6443810000	-1.1414970000	-0.4124510000
C	2.2826870000	-0.5845160000	-0.1361390000
C	-3.8324700000	-0.4922730000	-0.5744190000
H	3.6309660000	-1.7968230000	-1.2877500000
C	-2.3545180000	-0.7285040000	-0.5672820000
N	0.5025050000	0.8179060000	0.2062040000
H	-1.1289670000	1.9361270000	0.7944840000
H	4.3596280000	-0.3396730000	-0.6014510000
H	-4.4588660000	-1.1499430000	-1.1673800000
C	1.8656290000	0.7058350000	-0.1114890000
H	-1.9810960000	-1.5489640000	-1.1796190000
H	0.4543490000	2.8172620000	0.8277980000
C	-0.1791340000	2.1249310000	0.2720700000
H	-2.7874070000	1.4294410000	-0.8035520000
H	2.7649480000	2.5467010000	0.5403320000
C	-2.9158110000	0.4660870000	-1.2865170000
C	2.6649420000	1.9432860000	-0.3670770000
H	3.6650040000	1.6803840000	-0.7105070000
H	-0.3356150000	2.4913550000	-0.7451630000
H	-2.9068390000	0.4686290000	-2.3714880000
H	2.1939910000	2.5634070000	-1.1350350000

### Thermodynamic data

Zero-point correction= 0.235008 (Hartree/Particle)  
 Thermal correction to Energy= 0.249021  
 Thermal correction to Enthalpy= 0.249965  
 Thermal correction to Gibbs Free Energy= 0.194063  
 Sum of electronic and zero-point Energies= -917.695166  
 Sum of electronic and thermal Energies= -917.681154  
 Sum of electronic and thermal Enthalpies= -917.680210  
 Sum of electronic and thermal Free Energies= -917.736111

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.263	52.019	117.655

*syn-4b-H*



### Xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

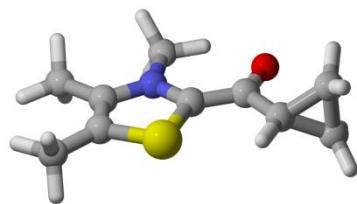
C	-1.5176310000	0.3489070000	0.0369430000
C	-0.1473540000	0.0929360000	-0.0380340000
O	-2.0216600000	1.5434390000	0.3863640000
N	0.8835240000	0.9992010000	-0.0223260000
S	0.4775490000	-1.5259290000	-0.0538530000
C	2.1112180000	-0.9426070000	0.0109300000
C	2.1470940000	0.4206170000	0.0307820000
C	0.7018790000	2.4341240000	-0.2739390000
C	3.3648100000	1.2875640000	0.0868190000
C	3.2435450000	-1.9199670000	0.0456500000
C	-2.5188830000	-0.6685580000	-0.2522830000
C	-3.7162000000	-0.8030420000	0.6893290000
C	-3.9198920000	-0.2290610000	-0.6603950000
H	-1.4064410000	2.0834090000	0.8981770000
H	0.6198430000	2.9938120000	0.6637150000
H	-0.1819970000	2.5840710000	-0.8935580000
H	1.5658700000	2.8079360000	-0.8204100000
H	4.2327400000	0.6919950000	0.3660530000
H	3.2507260000	2.0775010000	0.8339220000
H	3.5750110000	1.7517990000	-0.8821330000
H	4.1954330000	-1.4151130000	-0.1200540000
H	3.1269870000	-2.6742510000	-0.7367390000
H	3.2884640000	-2.4345800000	1.0099580000
H	-2.1465530000	-1.5778270000	-0.7098140000
H	-3.7370850000	-0.1246410000	1.5348810000
H	-4.0453550000	-1.8160730000	0.8885920000
H	-4.3909860000	-0.8386880000	-1.4222070000
H	-4.0903560000	0.8381090000	-0.7381680000

#### Thermodynamic data

Zero-point correction= 0.237201 (Hartree/Particle)  
 Thermal correction to Energy= 0.251518  
 Thermal correction to Enthalpy= 0.252462  
 Thermal correction to Gibbs Free Energy= 0.195243  
 Sum of electronic and zero-point Energies= -917.505265  
 Sum of electronic and thermal Energies= -917.490949  
 Sum of electronic and thermal Enthalpies= -917.490005  
 Sum of electronic and thermal Free Energies= -917.547223

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	157.830	53.167	120.427

*syn*-4b



### Xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.2408780000	2.8868610000	0.8881850000
H	0.2971940000	2.7163550000	0.0013130000
H	-3.4033810000	1.9006540000	0.8859290000
C	-0.7606370000	2.4691610000	-0.0015210000
H	-1.2352540000	2.8841440000	-0.8955810000
H	3.9265290000	0.4992160000	1.2366490000
C	-3.3692430000	1.2582310000	0.0008090000
H	-3.4025930000	1.9028420000	-0.8827360000
O	2.0021310000	1.6248580000	0.0014760000
N	-0.8920630000	1.0131910000	0.0004170000
H	4.2611500000	-1.3134950000	1.2670740000
H	-4.2649310000	0.6382490000	-0.0003380000
C	3.8339000000	-0.4638340000	0.7464790000
C	-2.1418990000	0.4011600000	0.0003200000
C	1.5653520000	0.4527640000	0.0001370000
C	0.1740320000	0.1315620000	-0.0000940000
C	2.5395830000	-0.6857720000	-0.0009580000
H	2.1466550000	-1.6970990000	-0.0027600000
C	-2.0915290000	-0.9521860000	-0.0000160000
H	-4.1735500000	-1.4650350000	-0.0001270000
S	-0.4306920000	-1.5122760000	-0.0003620000
C	3.8348320000	-0.4615920000	-0.7460620000
H	-3.1475060000	-2.5994890000	0.8846640000
H	3.9280950000	0.5029260000	-1.2332140000
C	-3.1991400000	-1.9563970000	0.0000660000
H	4.2627440000	-1.3096920000	-1.2686550000
H	-3.1473060000	-2.5998010000	-0.8842910000

### Thermodynamic data

Zero-point correction=	0.223517 (Hartree/Particle)
Thermal correction to Energy=	0.237299
Thermal correction to Enthalpy=	0.238243
Thermal correction to Gibbs Free Energy=	0.179728
Sum of electronic and zero-point Energies=	-917.140494
Sum of electronic and thermal Energies=	-917.126713
Sum of electronic and thermal Enthalpies=	-917.125768
Sum of electronic and thermal Free Energies=	-917.184283

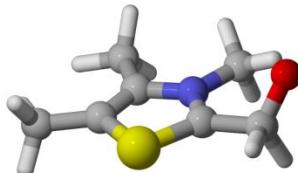
E (Thermal)

CV

S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	148.907	49.876	123.155

**3c**



### Xyz-matrix

21

XYZ file generated by gabedit : coordinates in Angstrom

S	-0.3340840000	-1.6649530000	-0.0855850000
C	0.9075280000	-0.5005990000	-0.1966800000
N	0.3970530000	0.7215660000	-0.1291780000
C	-0.9962420000	0.7906610000	-0.0053320000
C	-1.5682320000	-0.4400230000	0.0327450000
C	1.2654200000	1.9086780000	-0.2093950000
C	-1.6625620000	2.1267000000	0.0706840000
C	-3.0106410000	-0.8151440000	0.1737500000
C	2.4288560000	-0.7990440000	-0.2250580000
O	3.0569950000	-0.0929720000	0.7020230000
H	1.2805690000	2.2717990000	-1.2400000000
H	2.2574390000	1.5716270000	0.1305100000
H	0.8691070000	2.6782400000	0.4523210000
H	-2.7454950000	2.0102470000	0.0409360000
H	-1.3656150000	2.7608660000	-0.7695910000
H	-1.4028260000	2.6475390000	0.9974150000
H	-3.6417170000	0.0748710000	0.1787410000
H	-3.1855780000	-1.3563690000	1.1079270000
H	-3.3337720000	-1.4526120000	-0.6537910000
H	2.7073340000	-0.5906240000	-1.2956780000
H	2.4858060000	-1.9108910000	-0.1356570000

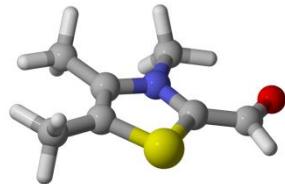
### Thermodynamic data

Zero-point correction=	0.171935 (Hartree/Particle)
Thermal correction to Energy=	0.183047
Thermal correction to Enthalpy=	0.183991
Thermal correction to Gibbs Free Energy=	0.135036
Sum of electronic and zero-point Energies=	-801.091740
Sum of electronic and thermal Energies=	-801.080628
Sum of electronic and thermal Enthalpies=	-801.079684
Sum of electronic and thermal Free Energies=	-801.128640

E (Thermal)      CV      S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	114.864	39.956	103.036

*syn-4c*



### Xyz-matrix

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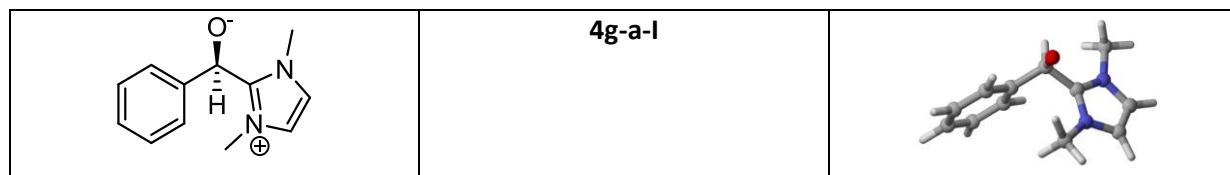
XYZ file generated by gabedit : coordinates in Angstrom

S	0.3226560000	-1.7082570000	-0.0000500000
C	-0.9724770000	-0.5120020000	-0.0000540000
N	-0.4284440000	0.7620290000	-0.0000520000
C	0.9660120000	0.7959910000	-0.0000120000
C	1.5487110000	-0.4326030000	0.0000140000
C	-1.2518960000	1.9738160000	0.0000430000
C	1.6620090000	2.1244520000	-0.0000470000
C	2.9967510000	-0.8114270000	0.0000940000
C	-2.3409570000	-0.8897910000	0.0000410000
O	-3.3290790000	-0.1250290000	0.0000310000
H	-1.0436720000	2.5750120000	0.8918550000
H	-2.2953050000	1.6612380000	0.0000930000
H	-1.0437120000	2.5751090000	-0.8917120000
H	2.7449570000	1.9915990000	0.0001250000
H	1.3982650000	2.7182730000	0.8834520000
H	1.3984940000	2.7180870000	-0.8837440000
H	3.6378400000	0.0741790000	-0.0002610000
H	3.2556160000	-1.4089340000	-0.8834490000
H	3.2557170000	-1.4083230000	0.8840210000
H	-2.4878790000	-1.9887210000	0.0000740000

### Thermodynamic data

Zero-point correction=	0.160909 (Hartree/Particle)
Thermal correction to Energy=	0.171792
Thermal correction to Enthalpy=	0.172737
Thermal correction to Gibbs Free Energy=	0.124121
Sum of electronic and zero-point Energies=	-800.535535
Sum of electronic and thermal Energies=	-800.524652
Sum of electronic and thermal Enthalpies=	-800.523707
Sum of electronic and thermal Free Energies=	-800.572323

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	107.801	39.573	102.320



**xyz-matrix**

29

XYZ file generated by gabedit : coordinates in Angstrom

```

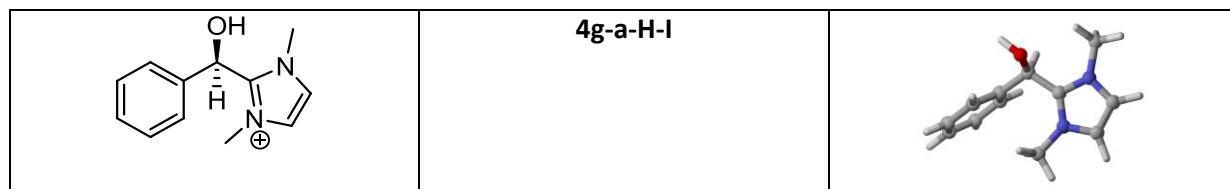
C   -0.1178760000    -0.5675100000    1.0867610000
H   -0.2969330000    -1.6717040000    1.1667690000
O   -0.2525630000     0.1208890000    2.2146360000
C   1.2410290000    -0.4387050000    0.3639990000
C   2.2863030000     0.1869260000    1.0375830000
C   3.5317370000     0.3270730000    0.4237550000
C   3.7368230000    -0.1551830000    -0.8688120000
C   2.6923820000    -0.7882410000    -1.5452680000
C   1.4519800000    -0.9311390000    -0.9254820000
H   2.0787300000     0.5579700000    2.0382700000
H   4.3449540000     0.8158750000    0.9530110000
H   4.7049060000    -0.0411370000    -1.3473640000
H   2.8462920000    -1.1691750000    -2.5508820000
H   0.6376780000    -1.4282890000    -1.4545360000
C   -1.2169380000   -0.0678210000    0.1338230000
N   -1.3150650000    1.1948080000    -0.3075680000
C   -2.5397820000    1.3852310000    -0.9090060000
N   -2.3680720000   -0.6830810000    -0.1854420000
C   -3.2071360000    0.2049800000    -0.8346810000
H   -2.8286080000    2.3352060000    -1.3293350000
H   -4.1885120000   -0.0795170000    -1.1778260000
C   -2.7037070000   -2.0553570000    0.1797300000
C   -0.3047760000    2.2208710000    -0.0485610000
H   -2.0579330000   -2.7590160000    -0.3475830000
H   -3.7417160000   -2.2352030000    -0.0992860000
H   -2.5866190000   -2.1810860000    1.2571860000
H   0.0159320000     2.0938350000    0.9896400000
H   -0.7678150000    3.1958650000    -0.2016380000
H   0.5418770000     2.0904130000    -0.7254820000

```

**thermodynamic data**

Zero-point correction=	0.242845 (Hartree/Particle)
Thermal correction to Energy=	0.256407
Thermal correction to Enthalpy=	0.257351
Thermal correction to Gibbs Free Energy=	0.201592
Sum of electronic and zero-point Energies=	-649.885802
Sum of electronic and thermal Energies=	-649.872240
Sum of electronic and thermal Enthalpies=	-649.871296
Sum of electronic and thermal Free Energies=	-649.927055

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.898	51.542	117.356



**xyz-matrix**

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XYZ file generated by gabedit : coordinates in Angstrom

```

C -0.2053720000 -1.1197450000 -0.0243690000
H -0.4110810000 -1.7151800000 -0.9287660000
O -0.4967230000 -1.8722010000 1.1358370000
H 0.0991130000 -2.6332740000 1.1796830000
C 1.2261480000 -0.6345680000 -0.1063010000
C 2.0035120000 -0.5111720000 1.0450060000
C 3.3055640000 -0.0213000000 0.9518100000
C 3.8288360000 0.3458600000 -0.2871210000
C 3.0568250000 0.2049630000 -1.4409840000
C 1.7598490000 -0.2948330000 -1.3515630000
H 1.5883720000 -0.7851760000 2.0111760000
H 3.9116190000 0.0704790000 1.8472540000
H 4.8421180000 0.7273240000 -0.3570430000
H 3.4694990000 0.4693360000 -2.4090500000
H 1.1641870000 -0.4196710000 -2.2539440000
C -1.2412590000 -0.0173160000 -0.0289300000
N -1.1264140000 1.3003820000 0.2069310000
C -2.3739430000 1.8777170000 0.1130190000
N -2.5379650000 -0.2754580000 -0.2620520000
C -3.2595290000 0.8893960000 -0.1801680000
H -2.5221560000 2.9347880000 0.2668010000
H -4.3268170000 0.9165900000 -0.3334060000
C -3.0971890000 -1.5993270000 -0.5582060000
C 0.0745680000 2.0744030000 0.5664150000
H -2.8489440000 -1.8855030000 -1.5820870000
H -4.1788480000 -1.5370380000 -0.4521380000
H -2.6978900000 -2.3204150000 0.1540410000
H 0.4606710000 1.7326400000 1.5253640000
H -0.2317180000 3.1163830000 0.6425140000
H 0.8382470000 1.9673940000 -0.2028930000

```

**thermodynamic data**

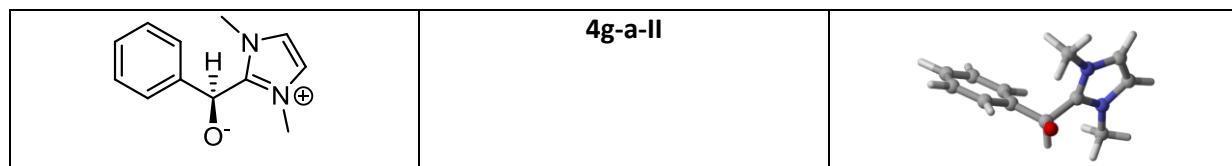
Zero-point correction=	0.257895 (Hartree/Particle)
Thermal correction to Energy=	0.271398
Thermal correction to Enthalpy=	0.272342
Thermal correction to Gibbs Free Energy=	0.217554
Sum of electronic and zero-point Energies=	-650.313698
Sum of electronic and thermal Energies=	-650.300195
Sum of electronic and thermal Enthalpies=	-650.299251
Sum of electronic and thermal Free Energies=	-650.354039

E (Thermal)

CV

S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	170.305	52.527	115.311



### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

```

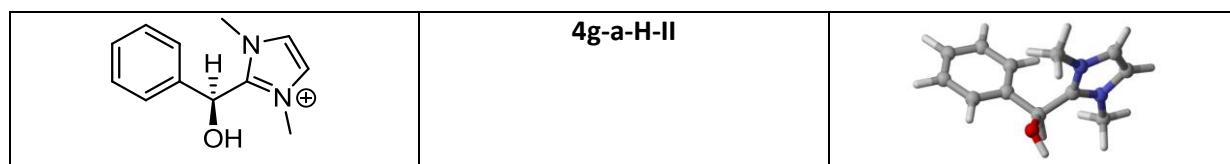
C   -0.1015240000   -0.7235690000   1.1216610000
H   -0.0543190000   -0.1396250000   2.0865620000
O   -0.3507970000   -2.0102510000   1.2515080000
C   1.2130040000   -0.3939790000   0.3834860000
C   2.3174350000   0.1037640000   1.0722930000
C   3.5218250000   0.3462380000   0.4093220000
C   3.6279940000   0.0929460000   -0.9567380000
C   2.5299430000   -0.4178320000   -1.6524790000
C   1.3351960000   -0.6649020000   -0.9819210000
H   2.2339330000   0.2940780000   2.1407630000
H   4.3771940000   0.7281830000   0.9593540000
H   4.5624740000   0.2827170000   -1.4758710000
H   2.6112710000   -0.6288060000   -2.7149200000
H   0.4856850000   -1.0904720000   -1.5144250000
C   -1.2208220000   0.0438720000   0.3455230000
N   -2.2982560000   -0.4802550000   -0.2566110000
C   -3.0588080000   0.5293770000   -0.8130410000
N   -1.2969640000   1.3798610000   0.1779190000
C   -2.4295000000   1.7000290000   -0.5414230000
C   -2.6484780000   -1.9060850000   -0.3523800000
C   -0.2952430000   2.3349160000   0.6384520000
H   -0.0189410000   2.1027020000   1.6682140000
H   -0.7312960000   3.3329450000   0.5921190000
H   0.5953060000   2.2770710000   0.0094100000
H   -2.6208190000   -2.1987610000   -1.4040490000
H   -3.6558850000   -2.0377950000   0.0467240000
H   -1.9002490000   -2.4455110000   0.2392000000
H   -3.9740260000   0.3205000000   -1.3436640000
H   -2.6835410000   2.7188840000   -0.7871610000

```

### thermodynamic data

Zero-point correction=	0.242087 (Hartree/Particle)
Thermal correction to Energy=	0.255645
Thermal correction to Enthalpy=	0.256589
Thermal correction to Gibbs Free Energy=	0.201067
Sum of electronic and zero-point Energies=	-649.883926
Sum of electronic and thermal Energies=	-649.870368
Sum of electronic and thermal Enthalpies=	-649.869424
Sum of electronic and thermal Free Energies=	-649.924946

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.419	51.697	116.856



#### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

```

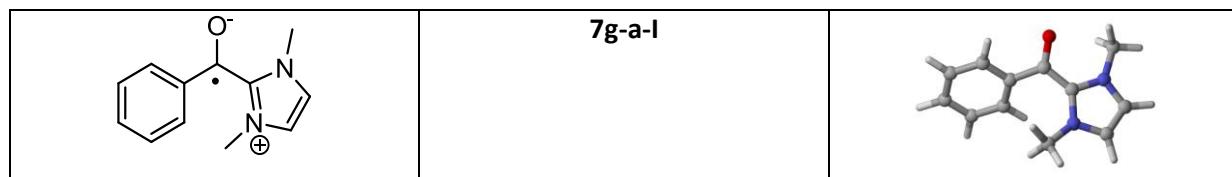
C    0.0550330000   -0.2506740000   -1.1927760000
H    0.1886940000    0.4687980000   -2.0116240000
O    0.0076110000   -1.5695720000   -1.6898550000
H    0.4866170000   -1.6378060000   -2.5241250000
C   -1.2383130000    0.0748100000   -0.4539930000
C   -2.4062430000   -0.6211820000   -0.7656540000
C   -3.5980400000   -0.2948760000   -0.1196180000
C   -3.6286340000    0.7234190000    0.8306870000
C   -2.4611230000    1.4192290000    1.1410570000
C   -1.2673890000    1.0936980000    0.5019430000
H   -2.3765140000   -1.4176660000   -1.5009560000
H   -4.5039840000   -0.8405600000   -0.3617630000
H   -4.5582520000    0.9738040000    1.3307520000
H   -2.4783640000    2.2117970000    1.8819170000
H   -0.3618300000    1.6398520000    0.7618330000
C    1.2396530000   -0.1129640000   -0.2663920000
N    1.5236350000   -0.9453530000    0.7409750000
C    2.6586680000   -0.5041760000    1.3824520000
N    2.1666930000    0.8555460000   -0.2756060000
C    3.0626920000    0.6290370000    0.7481650000
C    0.7540950000   -2.1429990000    1.1068690000
C    2.2157110000    1.9862000000   -1.2092890000
H    1.2731310000    2.5348190000   -1.1807140000
H    2.4191240000    1.6295190000   -2.2200600000
H    3.0221550000    2.6461320000   -0.8942060000
H   -0.3101340000   -1.9266100000    1.0113490000
H    0.9912060000   -2.3851010000    2.1416150000
H    1.0226020000   -2.9663050000    0.4458630000
H    3.0777730000   -1.0284470000    2.2270830000
H    3.8979290000    1.2858600000    0.9335850000

```

#### thermodynamic data

Zero-point correction=	0.256752 (Hartree/Particle)
Thermal correction to Energy=	0.270831
Thermal correction to Enthalpy=	0.271775
Thermal correction to Gibbs Free Energy=	0.214883
Sum of electronic and zero-point Energies=	-650.314005
Sum of electronic and thermal Energies=	-650.299926
Sum of electronic and thermal Enthalpies=	-650.298982
Sum of electronic and thermal Free Energies=	-650.355874

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	169.949	53.192	119.739



### xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

```

C   -0.1078680000   -0.9490320000   0.2269350000
O   -0.3067610000   -2.1679810000   0.5025970000
C   1.2701090000   -0.4345670000   0.0164150000
C   2.3252010000   -1.0639010000   0.6935120000
C   3.6380090000   -0.6510680000   0.4963590000
C   3.9256380000   0.3861410000   -0.3937180000
C   2.8871690000   0.9952730000   -1.0976980000
C   1.5712590000   0.5845310000   -0.8987770000
H   2.0849170000   -1.8826740000   1.3646750000
H   4.4439450000   -1.1418000000   1.0341040000
H   4.9515680000   0.7047160000   -0.5501410000
H   3.1041330000   1.7794240000   -1.8174660000
H   0.7710540000   1.0349650000   -1.4828590000
C   -1.2339790000   -0.0745640000   0.0865900000
N   -1.3352970000   1.2853840000   0.3002410000
C   -2.6512720000   1.6756510000   0.0998940000
N   -2.5033890000   -0.5065140000   -0.2134570000
C   -3.3646140000   0.5712500000   -0.2194110000
H   -2.9612880000   2.7013020000   0.2195410000
H   -4.4109930000   0.4579270000   -0.4543000000
C   -2.8422650000   -1.8498870000   -0.6604000000
C   -0.3479710000   2.1129850000   0.9724130000
H   -2.2033470000   -2.1298190000   -1.5016910000
H   -3.8862530000   -1.8399530000   -0.9771360000
H   -2.6822430000   -2.5680280000   0.1417330000
H   -0.8744930000   2.9029900000   1.5105380000
H   0.3606120000   2.5562060000   0.2688220000
H   0.2107800000   1.4996330000   1.6832340000

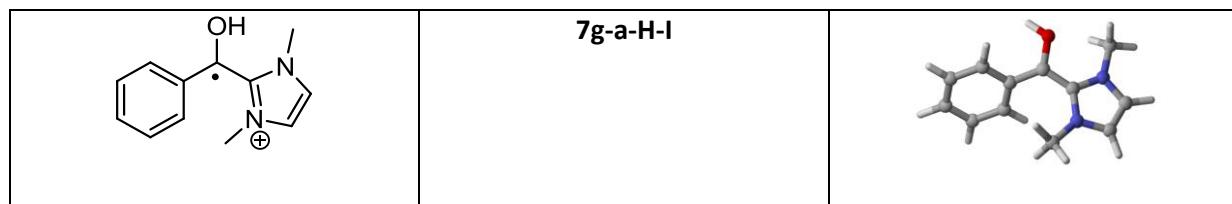
```

### thermodynamic data

Zero-point correction=	0.230875 (Hartree/Particle)
Thermal correction to Energy=	0.244273
Thermal correction to Enthalpy=	0.245217
Thermal correction to Gibbs Free Energy=	0.190108
Sum of electronic and zero-point Energies=	-649.311300
Sum of electronic and thermal Energies=	-649.297902
Sum of electronic and thermal Enthalpies=	-649.296957

Sum of electronic and thermal Free Energies= -649.352067

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	153.283	51.338	115.987



#### xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	0.0854460000	-0.8527780000	-0.2383770000
O	0.3413630000	-2.1310690000	-0.5879290000
H	-0.4336780000	-2.6880860000	-0.4209340000
C	-1.2735260000	-0.3973400000	-0.0249770000
C	-2.3313700000	-0.9777730000	-0.7510280000
C	-3.6416360000	-0.5816490000	-0.5119490000
C	-3.9164770000	0.3924020000	0.4486920000
C	-2.8742550000	0.9679950000	1.1790540000
C	-1.5624010000	0.5752840000	0.9513890000
H	-2.1247310000	-1.7051300000	-1.5324290000
H	-4.4498440000	-1.0261360000	-1.0829830000
H	-4.9408410000	0.6980000000	0.6332890000
H	-3.0891900000	1.7084470000	1.9424770000
H	-0.7587240000	0.9882690000	1.5566890000
C	1.2527360000	-0.0475720000	-0.1043630000
N	1.3699870000	1.2813550000	-0.3747610000
C	2.6680110000	1.6706380000	-0.1398220000
N	2.4816460000	-0.4858960000	0.2777550000
C	3.3592300000	0.5702260000	0.2605490000
H	2.9929630000	2.6877700000	-0.2930950000
H	4.3956750000	0.4536600000	0.5360040000
C	2.8190870000	-1.8372160000	0.7342310000
C	0.3576810000	2.1461900000	-0.9844810000
H	2.0767620000	-2.1709810000	1.4597750000
H	3.7968800000	-1.7878320000	1.2108210000
H	2.8436430000	-2.5248730000	-0.1099080000
H	-0.2530920000	1.5574440000	-1.6688770000
H	0.8779510000	2.9255440000	-1.5398770000
H	-0.2812560000	2.5938070000	-0.2219830000

#### thermodynamic data

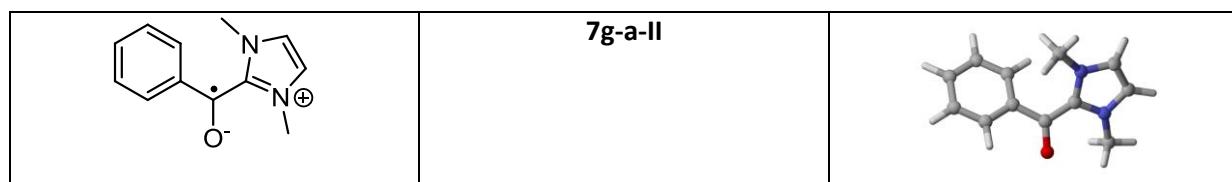
Zero-point correction= 0.244430 (Hartree/Particle)

Thermal correction to Energy= 0.257938

Thermal correction to Enthalpy= 0.258883

Thermal correction to Gibbs Free Energy= 0.203698  
 Sum of electronic and zero-point Energies= -649.697824  
 Sum of electronic and thermal Energies= -649.684315  
 Sum of electronic and thermal Enthalpies= -649.683371  
 Sum of electronic and thermal Free Energies= -649.738555

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.859	52.540	116.145



#### xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

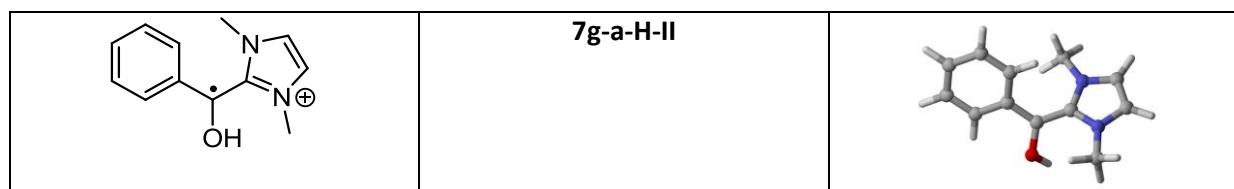
C	-0.1078740000	0.9490910000	0.2268600000
O	-0.3067330000	2.1680900000	0.5024800000
C	1.2701020000	0.4345750000	0.0163720000
C	2.3252300000	1.0641630000	0.6931590000
C	3.6380480000	0.6512910000	0.4960470000
C	3.9256480000	-0.3861880000	-0.3936990000
C	2.8871290000	-0.9955530000	-1.0974400000
C	1.5712320000	-0.5848240000	-0.8985180000
H	2.0849880000	1.8831530000	1.3640710000
H	4.4439980000	1.1422460000	1.0335710000
H	4.9515710000	-0.7047890000	-0.5501070000
H	3.1040800000	-1.7798960000	-1.8170020000
H	0.7709900000	-1.0354740000	-1.4823870000
C	-1.2339950000	0.0746390000	0.0865680000
N	-1.3351670000	-1.2853300000	0.3002190000
C	-2.6510790000	-1.6757520000	0.0997570000
N	-2.5033860000	0.5063910000	-0.2137300000
C	-3.3645250000	-0.5714490000	-0.2196660000
C	-0.3479910000	-2.1128030000	0.9728440000
C	-2.8425520000	1.8498890000	-0.6600540000
H	-2.6823010000	2.5677210000	0.1423350000
H	-3.8866940000	1.8400520000	-0.9762870000
H	-2.2039820000	2.1302090000	-1.5014650000
H	0.2106990000	-1.4992840000	1.6835360000
H	0.3606120000	-2.5562740000	0.2694220000
H	-0.8746540000	-2.9026060000	1.5111410000
H	-2.9609220000	-2.7014890000	0.2191440000
H	-4.4108950000	-0.4581960000	-0.4546310000

#### thermodynamic data

Zero-point correction= 0.230876 (Hartree/Particle)  
 Thermal correction to Energy= 0.244274  
 Thermal correction to Enthalpy= 0.245218

Thermal correction to Gibbs Free Energy= 0.190102  
 Sum of electronic and zero-point Energies= -649.311298  
 Sum of electronic and thermal Energies= -649.297901  
 Sum of electronic and thermal Enthalpies= -649.296956  
 Sum of electronic and thermal Free Energies= -649.352072

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	153.284	51.338	116.001



#### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

```

C 0.0440620000 0.8219790000 0.3914300000
O 0.1768530000 2.0960440000 0.8378090000
H 0.9224870000 2.1985670000 1.4443760000
C -1.2810570000 0.3717840000 0.0714430000
C -2.3958770000 1.0258420000 0.6380920000
C -3.6800520000 0.6044120000 0.3256590000
C -3.8793940000 -0.4619900000 -0.5542140000
C -2.7824200000 -1.1027080000 -1.1377450000
C -1.4942280000 -0.6897810000 -0.8358010000
H -2.2359880000 1.8521450000 1.3218950000
H -4.5322110000 1.1071040000 0.7704630000
H -4.8863850000 -0.7850300000 -0.7959100000
H -2.9381640000 -1.9097020000 -1.8458440000
H -0.6489040000 -1.1575970000 -1.3349530000
C 1.2398140000 0.0637360000 0.1455400000
N 2.3929170000 0.5499900000 -0.3807380000
C 3.3279530000 -0.4580570000 -0.4265620000
N 1.4558820000 -1.2436660000 0.4358940000
C 2.7411330000 -1.5774860000 0.0747150000
C 2.5761480000 1.8894330000 -0.9485790000
C 0.5345310000 -2.1402450000 1.1381560000
H -0.0538400000 -2.7193770000 0.4248050000
H -0.1349610000 -1.5451900000 1.7587720000
H 1.1255990000 -2.8055960000 1.7666780000
H 1.6181270000 2.2560910000 -1.3157680000
H 3.2804020000 1.8123830000 -1.7760240000
H 2.9715400000 2.5744170000 -0.1963820000
H 4.3201940000 -0.2992370000 -0.8195400000
H 3.1320020000 -2.5731160000 0.2160540000

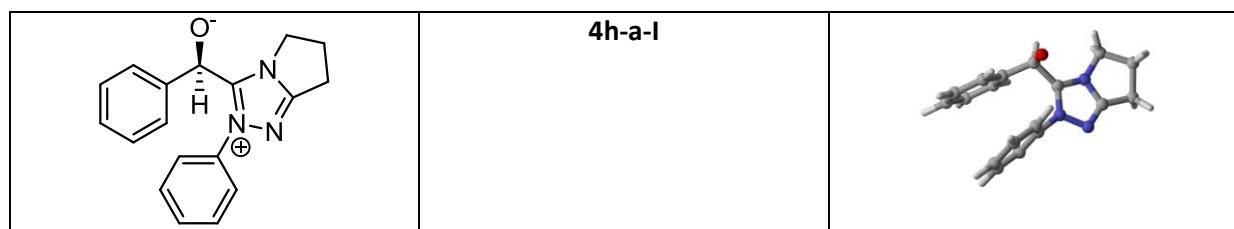
```

#### thermodynamic data

Zero-point correction= 0.244142 (Hartree/Particle)  
 Thermal correction to Energy= 0.257799

Thermal correction to Enthalpy= 0.258743  
 Thermal correction to Gibbs Free Energy= 0.203446  
 Sum of electronic and zero-point Energies= -649.691513  
 Sum of electronic and thermal Energies= -649.677856  
 Sum of electronic and thermal Enthalpies= -649.676912  
 Sum of electronic and thermal Free Energies= -649.732210

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.771	52.870	116.383



### xyz-matrix

39

XYZ file generated by gabedit : coordinates in Angstrom

```

C   -0.3818650000   -1.4365870000   0.8948810000
H   -0.9081560000   -2.4095870000   0.6993260000
O   -0.4889540000   -0.9567260000   2.1297110000
C   1.0269850000   -1.5993150000   0.3040930000
C   2.1284460000   -1.2542530000   1.0798960000
C   3.4136060000   -1.3389300000   0.5439490000
C   3.6007690000   -1.7764350000   -0.7670330000
C   2.4978850000   -2.1445170000   -1.5399600000
C   1.2166920000   -2.0600520000   -0.9997170000
H   1.9356010000   -0.9030940000   2.0901420000
H   4.2719230000   -1.0571220000   1.1476280000
H   4.6015510000   -1.8385650000   -1.1843560000
H   2.6393990000   -2.4986340000   -2.5572100000
H   0.3528950000   -2.3463580000   -1.6006120000
C   -1.1677140000   -0.4170120000   0.0571220000
N   -0.7972010000   0.8099010000   -0.3362760000
N   -1.8631310000   1.5973220000   -0.7195860000
N   -2.4977920000   -0.4226160000   -0.1149030000
C   -2.8814470000   0.8067070000   -0.5722970000
C   0.5071410000   1.3866450000   -0.1622130000
C   1.3673500000   1.4789500000   -1.2487220000
C   0.8707440000   1.8024500000   1.1137170000
C   2.6387820000   2.0091810000   -1.0492450000
C   2.1410460000   2.3431300000   1.2964980000
C   3.0210220000   2.4437050000   0.2199070000
H   1.0491420000   1.1180830000   -2.2213340000
H   0.1865450000   1.6355300000   1.9399360000
H   3.3327110000   2.0723050000   -1.8808540000
H   2.4498810000   2.6650860000   2.2855580000
H   4.0152830000   2.8524550000   0.3714720000
C   -3.6057560000   -1.3216860000   0.1914250000

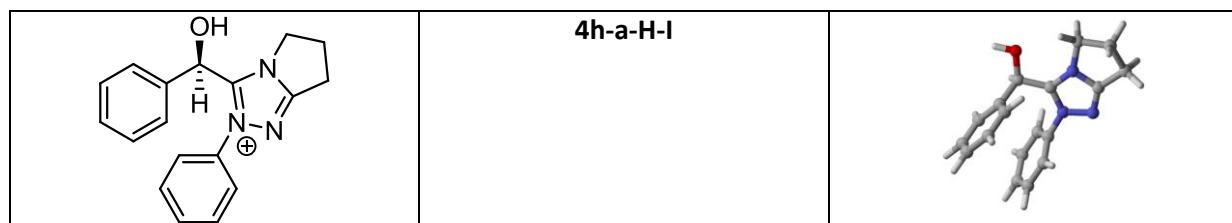
```

C	-4.3663940000	0.8558260000	-0.7358080000
C	-4.8042590000	-0.3378360000	0.1579030000
H	-3.4443370000	-1.7792800000	1.1690620000
H	-3.6750920000	-2.0993740000	-0.5740420000
H	-4.6330380000	0.6974010000	-1.7859140000
H	-4.7894460000	1.8077110000	-0.4140530000
H	-4.9913560000	0.0238890000	1.1719520000
H	-5.7131940000	-0.8187190000	-0.2053990000

### thermodynamic data

Zero-point correction= 0.320164 (Hartree/Particle)  
 Thermal correction to Energy= 0.337642  
 Thermal correction to Enthalpy= 0.338586  
 Thermal correction to Gibbs Free Energy= 0.273903  
 Sum of electronic and zero-point Energies= -934.898292  
 Sum of electronic and thermal Energies= -934.880814  
 Sum of electronic and thermal Enthalpies= -934.879869  
 Sum of electronic and thermal Free Energies= -934.944553

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	211.874	69.211	136.137



### xyz-matrix

40

XYZ file generated by gabedit : coordinates in Angstrom

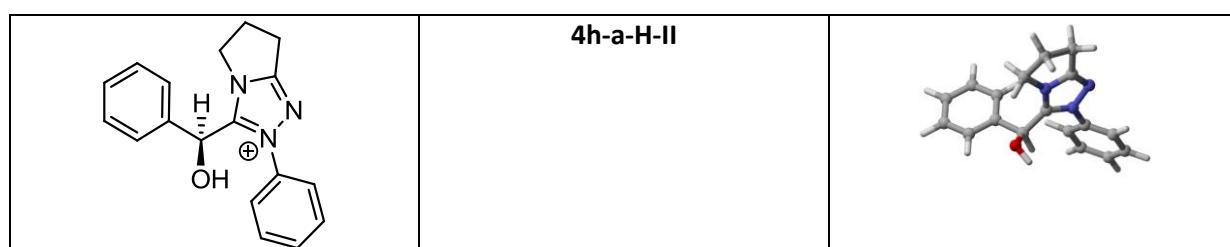
C	-0.2931490000	-0.9913830000	-1.3195100000
H	0.1148830000	-0.4835950000	-2.2057280000
O	-1.2376980000	-1.9742200000	-1.6852890000
H	-0.7696730000	-2.7389190000	-2.0454720000
C	0.8538730000	-1.5180760000	-0.4789370000
C	0.5846060000	-2.1577230000	0.7344000000
C	1.6342590000	-2.6129140000	1.5258880000
C	2.9533830000	-2.4270100000	1.1071600000
C	3.2212720000	-1.7968940000	-0.1059940000
C	2.1702560000	-1.3432520000	-0.9017980000
H	-0.4450960000	-2.3044810000	1.0553930000
H	1.4275730000	-3.1126560000	2.4665580000
H	3.7716670000	-2.7798220000	1.7264490000
H	4.2458710000	-1.6570570000	-0.4346050000
H	2.3770500000	-0.8380240000	-1.8423420000
C	-1.0939760000	0.0203780000	-0.5394230000
N	-0.6234980000	1.1290820000	0.0359150000
N	-1.5885690000	1.8083250000	0.7212300000
N	-2.3917100000	-0.0197770000	-0.2243710000

C	-2.6576070000	1.0882750000	0.5390570000
C	0.7467650000	1.5715470000	0.0211720000
C	1.2657590000	2.1023700000	-1.1535370000
C	1.5112880000	1.4077500000	1.1705520000
C	2.6110290000	2.4647600000	-1.1808280000
C	2.8516560000	1.7782010000	1.1300100000
C	3.4000500000	2.2977370000	-0.0437670000
H	0.6280950000	2.2389570000	-2.0223470000
H	1.0661230000	0.9852000000	2.0657490000
H	3.0365490000	2.8854970000	-2.0854790000
H	3.4692310000	1.6560990000	2.0133520000
H	4.4467040000	2.5826730000	-0.0684950000
C	-3.5915610000	-0.8454530000	-0.4803150000
C	-4.1041430000	1.1542310000	0.9012070000
C	-4.5662510000	-0.2925940000	0.5854800000
H	-3.3518820000	-1.8997580000	-0.3630960000
H	-3.9198360000	-0.6635190000	-1.5060830000
H	-4.6032510000	1.8940320000	0.2672780000
H	-4.2591250000	1.4388730000	1.9421930000
H	-4.4941760000	-0.9026210000	1.4891890000
H	-5.5977340000	-0.3302360000	0.2354810000

#### thermodynamic data

Zero-point correction= 0.334204 (Hartree/Particle)  
 Thermal correction to Energy= 0.352022  
 Thermal correction to Enthalpy= 0.352966  
 Thermal correction to Gibbs Free Energy= 0.287181  
 Sum of electronic and zero-point Energies= -935.333692  
 Sum of electronic and thermal Energies= -935.315874  
 Sum of electronic and thermal Enthalpies= -935.314930  
 Sum of electronic and thermal Free Energies= -935.380715

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	220.897	70.658	138.456



#### xyz-matrix

40

XYZ file generated by gabedit : coordinates in Angstrom

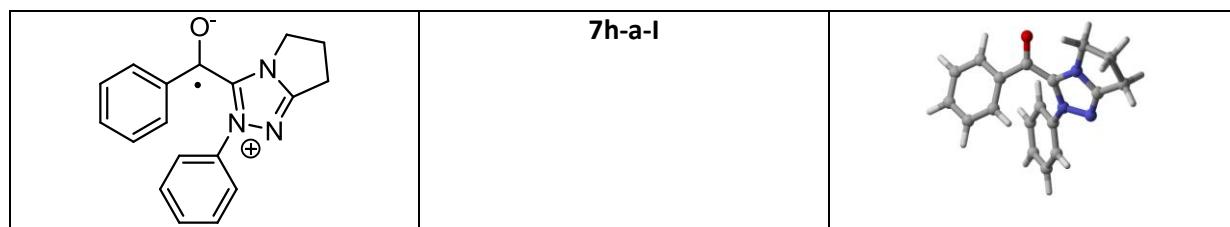
C	-0.2123520000	-1.1861230000	0.1156090000
H	0.2992750000	-1.7271510000	-0.6900160000
O	0.2749440000	-1.5666150000	1.3779110000
H	1.1959940000	-1.8505020000	1.3128220000
C	-1.7007930000	-1.4376270000	0.0152960000
C	-2.4616790000	-1.6574990000	1.1623480000

C	-3.8434990000	-1.8139180000	1.0506630000
C	-4.4600700000	-1.7530540000	-0.1983070000
C	-3.6927540000	-1.5522850000	-1.3462780000
C	-2.3129330000	-1.3969950000	-1.2390980000
H	-1.9712730000	-1.7164800000	2.1283530000
H	-4.4369640000	-1.9935200000	1.9412840000
H	-5.5344900000	-1.8807950000	-0.2805490000
H	-4.1659600000	-1.5310460000	-2.3226740000
H	-1.7135220000	-1.2542700000	-2.1372410000
C	0.0872670000	0.2947680000	-0.0707390000
N	1.3161070000	0.8162510000	-0.1470120000
N	1.3086590000	2.1784920000	-0.1763180000
N	-0.7364160000	1.3500290000	-0.0591950000
C	0.0420010000	2.4767510000	-0.1280930000
C	2.5531250000	0.0806950000	-0.1438750000
C	2.8729130000	-0.7037040000	-1.2483050000
C	3.3870090000	0.1786100000	0.9659260000
C	4.0598720000	-1.4325440000	-1.2271010000
C	4.5752700000	-0.5477010000	0.9678300000
C	4.9063360000	-1.3544530000	-0.1216580000
H	2.2172800000	-0.7251970000	-2.1138830000
H	3.1070250000	0.8112730000	1.8021110000
H	5.2412220000	-0.4840130000	1.8214450000
H	5.8321320000	-1.9196900000	-0.1119020000
H	4.3284940000	-2.0470150000	-2.0793630000
C	-2.1845420000	1.6627040000	-0.0411250000
C	-0.7958490000	3.7113370000	-0.1555410000
C	-2.1610810000	3.1617750000	0.3317400000
H	-2.7051410000	1.0331060000	0.6793200000
H	-2.5862490000	1.4725760000	-1.0393800000
H	-0.8473470000	4.0945050000	-1.1797340000
H	-0.3940560000	4.4984240000	0.4828950000
H	-2.2296670000	3.2640150000	1.4175350000
H	-3.0042020000	3.6908780000	-0.1123920000

#### thermodynamic data

Zero-point correction=	0.334740 (Hartree/Particle)
Thermal correction to Energy=	0.352497
Thermal correction to Enthalpy=	0.353441
Thermal correction to Gibbs Free Energy=	0.287787
Sum of electronic and zero-point Energies=	-935.327977
Sum of electronic and thermal Energies=	-935.310221
Sum of electronic and thermal Enthalpies=	-935.309277
Sum of electronic and thermal Free Energies=	-935.374931

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.195	70.482	138.181



**xyz-matrix**

38

XYZ file generated by gabedit : coordinates in Angstrom

```

C   -0.3336950000    -1.6033430000    -0.2684290000
O   -0.9280980000    -2.6175720000    -0.7244230000
C   1.1011820000    -1.6646870000    0.1201890000
C   1.6280930000    -0.9195480000    1.1815070000
C   2.9754540000    -1.0225010000    1.5139140000
C   3.8117850000    -1.8713450000    0.7891090000
C   3.2882160000    -2.6327250000    -0.2565780000
C   1.9385140000    -2.5376530000    -0.5827580000
H   0.9812200000    -0.2608210000    1.7553450000
H   3.3728480000    -0.4395270000    2.3392460000
H   4.8646450000    -1.9454600000    1.0437040000
H   3.9334010000    -3.3029310000    -0.8167660000
H   1.5069060000    -3.1337560000    -1.3812470000
C   -1.0919800000    -0.4026040000    -0.1220660000
N   -0.7777950000    0.9323420000    0.0893590000
N   -1.9180110000    1.7071100000    0.2880430000
N   -2.4660060000    -0.3991450000    -0.1163360000
C   -2.8899050000    0.8618390000    0.1496910000
C   0.4433350000    1.6034230000    -0.1639760000
C   1.2991980000    1.1600330000    -1.1728590000
C   0.7677160000    2.7209500000    0.6065220000
C   2.5022780000    1.8245250000    -1.3869810000
C   1.9685880000    3.3836900000    0.3730640000
C   2.8440560000    2.9342410000    -0.6154950000
H   1.0284810000    0.2998380000    -1.7757160000
H   0.0755360000    3.0573820000    1.3707470000
H   3.1724770000    1.4712350000    -2.1639370000
H   2.2237540000    4.2518860000    0.9723950000
H   3.7846550000    3.4476200000    -0.7858120000
C   -3.5343460000    -1.3841560000    -0.2321860000
C   -4.3841780000    0.9102450000    0.1937340000
C   -4.7353480000    -0.5940990000    0.3468000000
H   -3.2852660000    -2.2841190000    0.3293440000
H   -3.6622190000    -1.6636420000    -1.2818180000
H   -4.7635210000    1.3243250000    -0.7460640000
H   -4.7575640000    1.5264400000    1.0123280000
H   -4.8416580000    -0.8325890000    1.4085750000
H   -5.6699980000    -0.8551690000    -0.1516100000

```

**thermodynamic data**

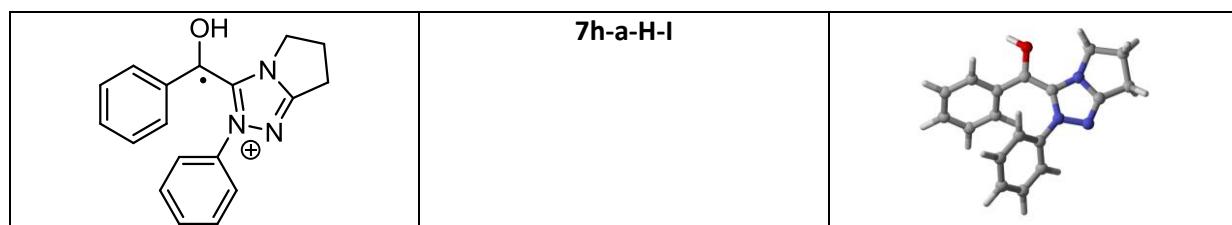
Zero-point correction= 0.308407 (Hartree/Particle)

Thermal correction to Energy= 0.325975

Thermal correction to Enthalpy= 0.326919

Thermal correction to Gibbs Free Energy= 0.260377  
 Sum of electronic and zero-point Energies= -934.333250  
 Sum of electronic and thermal Energies= -934.315681  
 Sum of electronic and thermal Enthalpies= -934.314737  
 Sum of electronic and thermal Free Energies= -934.381279

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.552	69.017	140.050



#### xyz-matrix

39

XYZ file generated by gabedit : coordinates in Angstrom

```

C   -0.3134700000    1.5080010000   -0.1691740000
O   -0.9777900000    2.5937980000   -0.6139480000
H   -0.4534400000    3.3940800000   -0.4603130000
C   1.1021630000    1.5820970000   0.1498730000
C   1.9420490000    2.3950050000   -0.6309350000
C   3.2978070000    2.4810070000   -0.3355850000
C   3.8253210000    1.7628420000   0.7374130000
C   2.9932710000    0.9628700000   1.5240530000
C   1.6381870000    0.8735780000   1.2382140000
H   1.5449900000    2.9196860000   -1.4969700000
H   3.9442730000    3.0987970000   -0.9496170000
H   4.8841840000    1.8291780000   0.9644170000
H   3.4021670000    0.4165610000   2.3675170000
H   0.9897940000    0.2695860000   1.8663750000
C   -1.1404530000   0.3646920000   -0.0673570000
N   -0.8099360000   -0.9562370000   0.0025850000
N   -1.9107640000   -1.7482590000   0.1797020000
N   -2.4979150000   0.3735690000   -0.0061040000
C   -2.9093460000   -0.9129050000   0.1716200000
C   0.4662420000   -1.5706390000   -0.2141380000
C   0.8999700000   -2.5355300000   0.6890050000
C   1.2277450000   -1.1956030000   -1.3173610000
C   2.1470490000   -3.1215350000   0.4900350000
C   2.4776350000   -1.7802540000   -1.4959960000
C   2.9385020000   -2.7377880000   -0.5925570000
H   0.2684920000   -2.8186030000   1.5248450000
H   0.8494440000   -0.4629620000   -2.0238690000
H   2.5007600000   -3.8768030000   1.1835020000
H   3.0837830000   -1.4976700000   -2.3498330000
H   3.9111650000   -3.1951780000   -0.7394740000
C   -3.5946480000   1.3523950000   0.0741430000
C   -4.3889100000   -0.9801560000   0.3580870000
C   -4.8239490000   0.4319450000   -0.1133520000

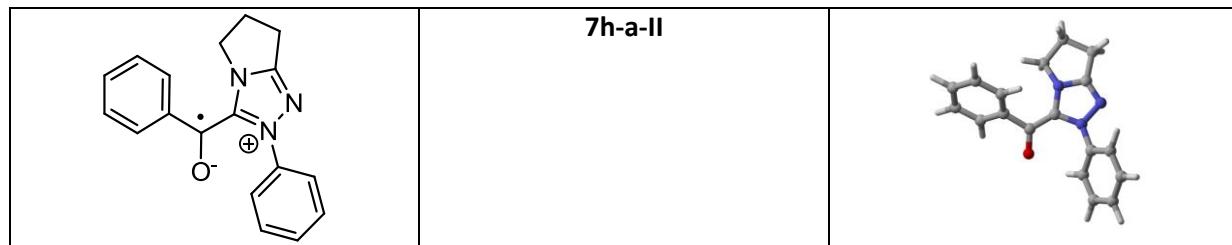
```

H	-3.4885660000	2.1070080000	-0.7027880000
H	-3.5653860000	1.8350550000	1.0555350000
H	-4.6115740000	-1.1481520000	1.4166200000
H	-4.8444440000	-1.7870840000	-0.2165690000
H	-5.0858990000	0.3979500000	-1.1734490000
H	-5.6881060000	0.8045200000	0.4364530000

### thermodynamic data

Zero-point correction= 0.322236 (Hartree/Particle)  
 Thermal correction to Energy= 0.339814  
 Thermal correction to Enthalpy= 0.340759  
 Thermal correction to Gibbs Free Energy= 0.275399  
 Sum of electronic and zero-point Energies= -934.714328  
 Sum of electronic and thermal Energies= -934.696750  
 Sum of electronic and thermal Enthalpies= -934.695806  
 Sum of electronic and thermal Free Energies= -934.761166

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.237	70.068	137.561



### xyz-matrix

38

XYZ file generated by gabedit : coordinates in Angstrom

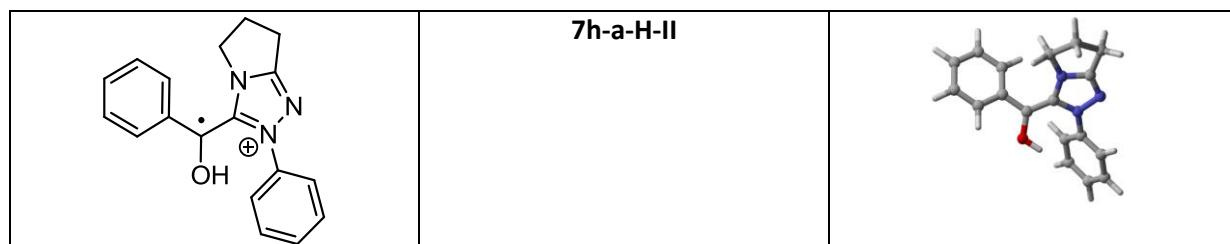
C	-0.5399320000	-1.0228990000	-0.4848000000
O	0.0883680000	-1.9823550000	-0.9929280000
C	-1.9558670000	-1.2143950000	-0.0399230000
C	-2.4599990000	-0.6539100000	1.1402340000
C	-3.7652890000	-0.9196430000	1.5491410000
C	-4.5822280000	-1.7502950000	0.7824410000
C	-4.0793690000	-2.3286870000	-0.3842010000
C	-2.7721630000	-2.0724170000	-0.7858490000
H	-1.8175380000	-0.0244320000	1.7527300000
H	-4.1400490000	-0.4912980000	2.4741320000
H	-5.5995130000	-1.9577080000	1.0998350000
H	-4.7075640000	-2.9861120000	-0.9776230000
H	-2.3546410000	-2.5354300000	-1.6747360000
C	0.0447640000	0.2677650000	-0.3173560000
N	1.3850560000	0.6338920000	-0.2748850000
N	1.5341150000	2.0079830000	-0.1472010000
N	-0.6186430000	1.4756130000	-0.1923820000
C	0.3251920000	2.4607970000	-0.1288930000
C	2.5444930000	-0.1613410000	-0.0312870000
C	2.8625390000	-1.2603370000	-0.8286050000
C	3.3910080000	0.2362760000	1.0065510000

C	4.0255140000	-1.9767470000	-0.5556800000
C	4.5550220000	-0.4816320000	1.2586880000
C	4.8736090000	-1.5943950000	0.4818330000
H	2.1925530000	-1.5587880000	-1.6235340000
H	3.1324740000	1.1074680000	1.5977730000
H	5.2097560000	-0.1722830000	2.0671340000
H	5.7795310000	-2.1576360000	0.6820460000
H	4.2706090000	-2.8379140000	-1.1689380000
C	-1.9263050000	1.9976300000	-0.5889970000
C	-0.3019730000	3.8155630000	-0.2274140000
C	-1.8081900000	3.4688070000	-0.1355160000
H	-2.7396530000	1.4640950000	-0.0982290000
H	-2.0419310000	1.8949850000	-1.6754050000
H	-0.0430690000	4.2599460000	-1.1936250000
H	0.0342210000	4.4947180000	0.5575740000
H	-2.1401740000	3.5463550000	0.9035100000
H	-2.4306100000	4.1296220000	-0.7401620000

#### thermodynamic data

Zero-point correction= 0.308803 (Hartree/Particle)  
 Thermal correction to Energy= 0.326252  
 Thermal correction to Enthalpy= 0.327196  
 Thermal correction to Gibbs Free Energy= 0.260905  
 Sum of electronic and zero-point Energies= -934.325080  
 Sum of electronic and thermal Energies= -934.307632  
 Sum of electronic and thermal Enthalpies= -934.306688  
 Sum of electronic and thermal Free Energies= -934.372979

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.726	68.789	139.521



#### xyz-matrix

39

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5133080000	-0.8648900000	0.4094870000
O	0.2123860000	-1.8130810000	1.0145480000
H	1.1157440000	-1.5365650000	1.2322880000
C	-1.9000470000	-1.2031850000	0.1463280000
C	-2.5705950000	-2.0918260000	1.0056270000
C	-3.8944000000	-2.4285560000	0.7552030000
C	-4.5564700000	-1.9021170000	-0.3555990000
C	-3.8861830000	-1.0458020000	-1.2310270000
C	-2.5637140000	-0.6993850000	-0.9869340000
H	-2.0492580000	-2.4987420000	1.8657020000

H	-4.4132700000	-3.1044530000	1.4265930000
H	-5.5896040000	-2.1714290000	-0.5488820000
H	-4.3894070000	-0.6680820000	-2.1150150000
H	-2.0262600000	-0.0788120000	-1.7000570000
C	0.0459410000	0.3957330000	0.0745910000
N	1.3592710000	0.7305640000	-0.0826050000
N	1.5369390000	2.0790390000	-0.2271940000
N	-0.6097560000	1.5864030000	-0.0217320000
C	0.3302340000	2.5617950000	-0.1891680000
C	2.4947370000	-0.1403960000	-0.1375310000
C	2.4533480000	-1.2796530000	-0.9414240000
C	3.6235130000	0.1964950000	0.6081400000
C	3.5667250000	-2.1152240000	-0.9713410000
C	4.7329140000	-0.6416140000	0.5534550000
C	4.7028890000	-1.7974640000	-0.2273910000
H	1.5728760000	-1.5043910000	-1.5365300000
H	3.6262200000	1.1020700000	1.2053660000
H	5.6197560000	-0.3919820000	1.1255080000
H	5.5697660000	-2.4485410000	-0.2613180000
H	3.5493660000	-3.0061380000	-1.5893390000
C	-1.9622450000	2.1237250000	0.2067410000
C	-0.3057380000	3.9114360000	-0.2130250000
C	-1.6535090000	3.6120830000	0.4922370000
H	-2.4407600000	1.6014080000	1.0369470000
H	-2.5646270000	1.9801280000	-0.6936700000
H	-0.4468210000	4.2347210000	-1.2496070000
H	0.2965400000	4.6604350000	0.3009120000
H	-1.5396790000	3.7570140000	1.5694580000
H	-2.4593940000	4.2590340000	0.1457640000

### thermodynamic data

Zero-point correction= 0.321822 (Hartree/Particle)  
 Thermal correction to Energy= 0.339413  
 Thermal correction to Enthalpy= 0.340358  
 Thermal correction to Gibbs Free Energy= 0.274684  
 Sum of electronic and zero-point Energies= -934.710121  
 Sum of electronic and thermal Energies= -934.692530  
 Sum of electronic and thermal Enthalpies= -934.691586  
 Sum of electronic and thermal Free Energies= -934.757260

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	212.985	70.217	138.222

### B.2.3 M06-2X/6-31++G\*\* SCRF=(PCM; Solvent=2-Propanol)

#### H atom

#### Xyz-matrix

-

**Thermodynamic data**

Zero-point correction=	0.000000 (Hartree/Particle)
Thermal correction to Energy=	0.001416
Thermal correction to Enthalpy=	0.002360
Thermal correction to Gibbs Free Energy=	-0.010654
Sum of electronic and zero-point Energies=	-0.498327
Sum of electronic and thermal Energies=	-0.496911
Sum of electronic and thermal Enthalpies=	-0.495967
Sum of electronic and thermal Free Energies=	-0.508981

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	0.889	2.981	27.392

**methane****Xyz-matrix**

5

XYZ file generated by gabedit : coordinates in Angstrom

C	0.0000000000	-0.0000150000	0.0000000000
H	-0.3653850000	1.0275710000	0.0000000000
H	-0.8469880000	-0.6871060000	0.0000000000
H	0.6061870000	-0.1701890000	0.8905660000
H	0.6061870000	-0.1701890000	-0.8905660000

**Thermodynamic data**

Zero-point correction=	0.044883 (Hartree/Particle)
Thermal correction to Energy=	0.047753
Thermal correction to Enthalpy=	0.048698
Thermal correction to Gibbs Free Energy=	0.025220
Sum of electronic and zero-point Energies=	-40.443244
Sum of electronic and thermal Energies=	-40.440374
Sum of electronic and thermal Enthalpies=	-40.439430
Sum of electronic and thermal Free Energies=	-40.462908

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	29.966	6.486	49.413

**Methyl radical****xyz-matrix**

4

XYZ file generated by gabedit : coordinates in Angstrom

C	0.0000000000	-0.0000660000	0.0002630000
H	0.9356660000	-0.5393180000	-0.0005240000
H	-0.9352320000	-0.5400690000	-0.0005240000

H	-0.0004340000	1.0797800000	-0.0005270000
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### Thermodynamic data

Zero-point correction=	0.029712 (Hartree/Particle)
Thermal correction to Energy=	0.032860
Thermal correction to Enthalpy=	0.033804
Thermal correction to Gibbs Free Energy=	0.009864
Sum of electronic and zero-point Energies=	-39.782874
Sum of electronic and thermal Energies=	-39.779726
Sum of electronic and thermal Enthalpies=	-39.778782
Sum of electronic and thermal Free Energies=	-39.802722

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	20.620	7.620	50.387

### 4aa

### Xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	-3.8347070000	0.3507940000	-1.0713860000
C	-4.2569570000	0.9873270000	0.0959080000
C	-3.5278190000	0.8251700000	1.2758260000
C	-2.3811800000	0.0319910000	1.2812540000
C	-1.9495750000	-0.6018360000	0.1124000000
C	-2.6860520000	-0.4426350000	-1.0606000000
C	-0.6745590000	-1.4577290000	0.0945240000
C	0.5342370000	-0.4919230000	0.0729910000
O	-0.5602960000	-2.3222610000	-0.9277950000
N	1.7905660000	-0.8942230000	0.1976390000
S	0.4700450000	1.1724330000	-0.2733320000
C	2.2033950000	1.3095410000	-0.2446420000
C	2.7611680000	0.1010950000	0.0306720000
C	2.1343540000	-2.2905980000	0.5036190000
C	4.2081590000	-0.2472790000	0.1635040000
C	2.8669560000	2.6260460000	-0.5026370000
H	-4.4027290000	0.4689740000	-1.9897110000
H	-5.1524550000	1.6012840000	0.0900610000
H	-3.8564440000	1.3103360000	2.1902600000
H	-1.8158360000	-0.0983270000	2.2029390000
H	-2.3427570000	-0.9586360000	-1.9523330000
H	-0.6152190000	-1.9236050000	1.1103550000
H	1.2891100000	-2.9073980000	0.2014060000
H	2.3465340000	-2.3859140000	1.5701900000
H	3.0135190000	-2.5690010000	-0.0754790000
H	4.8144610000	0.6568650000	0.1343550000
H	4.5338040000	-0.9004600000	-0.6515440000
H	4.4024230000	-0.7564930000	1.1113800000

H	3.9489370000	2.5342450000	-0.4036590000
H	2.5216930000	3.3821810000	0.2069620000
H	2.6467450000	2.9806780000	-1.5128650000

### Thermodynamic data

Zero-point correction= 0.254806 (Hartree/Particle)  
 Thermal correction to Energy= 0.270305  
 Thermal correction to Enthalpy= 0.271249  
 Thermal correction to Gibbs Free Energy= 0.211286  
 Sum of electronic and zero-point Energies= -1032.014096  
 Sum of electronic and thermal Energies= -1031.998597  
 Sum of electronic and thermal Enthalpies= -1031.997653  
 Sum of electronic and thermal Free Energies= -1032.057616

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	169.619	58.508	126.202

### 4aa-anti-H

#### Xyz-matrix

32			
XYZ file generated by gabedit : coordinates in Angstrom			
C	4.0446100000	0.8040170000	-0.1396880000
C	4.0303740000	0.6448660000	1.2448700000
C	2.9490480000	0.0156600000	1.8657730000
C	1.8811440000	-0.4489670000	1.1034370000
C	1.8918210000	-0.2862730000	-0.2849260000
C	2.9762930000	0.3360780000	-0.9049640000
C	0.7557160000	-0.8359220000	-1.1299340000
C	-0.5915680000	-0.4185560000	-0.5956520000
O	0.7125680000	-2.2488460000	-1.1274490000
N	-1.0527460000	0.8185840000	-0.5301590000
S	-1.6939500000	-1.5360770000	0.0409360000
C	-2.8195660000	-0.2740570000	0.4184210000
C	-2.3222950000	0.9367080000	0.0444830000
C	-0.3258510000	1.9968940000	-1.0216890000
C	-2.9477760000	2.2854160000	0.1832240000
C	-4.1268250000	-0.6000360000	1.0696600000
H	4.8840030000	1.2901840000	-0.6258730000
H	4.8606990000	1.0086340000	1.8417040000
H	2.9385780000	-0.1118660000	2.9432610000
H	1.0434300000	-0.9437550000	1.5890190000
H	2.9867610000	0.4566350000	-1.9855530000
H	0.8522190000	-0.4580290000	-2.1574250000
H	1.5896240000	-2.5916750000	-1.3435800000
H	-0.9155270000	2.4710160000	-1.8064620000
H	0.6374810000	1.6919560000	-1.4198990000
H	-0.1707930000	2.6864620000	-0.1911830000
H	-3.9346370000	2.1906380000	0.6335440000
H	-3.0635460000	2.7703180000	-0.7897670000
H	-2.3448110000	2.9340280000	0.8243660000
H	-4.7781670000	0.2740010000	1.0743530000

H	-3.9737770000	-0.9227300000	2.1026730000
H	-4.6381610000	-1.4019240000	0.5326140000

### Thermodynamic data

Zero-point correction= 0.268261 (Hartree/Particle)

Thermal correction to Energy= 0.284331

Thermal correction to Enthalpy= 0.285275

Thermal correction to Gibbs Free Energy= 0.223768

Sum of electronic and zero-point Energies= -1032.482849

Sum of electronic and thermal Energies= -1032.466779

Sum of electronic and thermal Enthalpies= -1032.465835

Sum of electronic and thermal Free Energies= -1032.527342

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.421	60.370	129.453

### 4aa-syn-H

#### Xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

C	3.7803450000	-0.4836400000	1.2770330000
C	4.2836450000	-0.9776110000	0.0733310000
C	3.6171400000	-0.7130440000	-1.1236190000
C	2.4473370000	0.0443830000	-1.1193840000
C	1.9435860000	0.5398080000	0.0864560000
C	2.6104380000	0.2739220000	1.2836660000
C	0.6607250000	1.3468060000	0.0999440000
C	-0.5552490000	0.4475730000	0.1017560000
O	0.5016450000	2.1741460000	-1.0365590000
N	-1.7963040000	0.8826630000	0.1785540000
S	-0.4975990000	-1.2376080000	-0.0423500000
C	-2.2202860000	-1.3516820000	-0.0117320000
C	-2.7700560000	-0.1113800000	0.1004280000
C	-2.1583950000	2.2991030000	0.3317170000
C	-4.2169790000	0.2542090000	0.1132950000
C	-2.9109130000	-2.6742360000	-0.1396860000
H	4.3011580000	-0.6803190000	2.2084600000
H	5.1955340000	-1.5660010000	0.0676120000
H	4.0094280000	-1.0935810000	-2.0611470000
H	1.9257340000	0.2585970000	-2.0479910000
H	2.2218390000	0.6687340000	2.2190860000
H	0.6308910000	1.9391960000	1.0265060000
H	1.2177780000	2.8245840000	-1.0469720000
H	-2.7067970000	2.6198160000	-0.5546270000
H	-1.2558310000	2.8940870000	0.4286970000
H	-2.7863300000	2.4030290000	1.2161520000
H	-4.8242560000	-0.6432350000	0.0037460000
H	-4.4537500000	0.9264780000	-0.7162780000
H	-4.4969130000	0.7500690000	1.0467740000
H	-3.8934480000	-2.6330030000	0.3324100000
H	-2.3367840000	-3.4636760000	0.3482940000
H	-3.0411450000	-2.9409640000	-1.1919320000

**Thermodynamic data**

Zero-point correction= 0.268431 (Hartree/Particle)  
 Thermal correction to Energy= 0.283597  
 Thermal correction to Enthalpy= 0.284541  
 Thermal correction to Gibbs Free Energy= 0.225764  
 Sum of electronic and zero-point Energies= -1032.481725  
 Sum of electronic and thermal Energies= -1032.466559  
 Sum of electronic and thermal Enthalpies= -1032.465615  
 Sum of electronic and thermal Free Energies= -1032.524392

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.960	58.127	123.706

**7aa-anti****Xyz-matrix**

30

XYZ file generated by gabedit : coordinates in Angstrom

C	4.2855420000	-0.1944950000	-0.5052140000
C	4.3754870000	0.8797690000	0.3827000000
C	3.2524220000	1.2738610000	1.1107330000
C	2.0403260000	0.6076920000	0.9393330000
C	1.9398520000	-0.4599780000	0.0391550000
C	3.0777030000	-0.8677770000	-0.6676900000
C	0.6736430000	-1.2378890000	-0.1098720000
C	-0.5978870000	-0.5957940000	-0.1109530000
O	0.7176500000	-2.4988350000	-0.1567680000
N	-0.9483120000	0.7097150000	-0.3424400000
S	-2.0084740000	-1.5505770000	0.2505210000
C	-3.0259550000	-0.1250170000	0.1909080000
C	-2.3058020000	0.9760560000	-0.1343150000
C	-0.0783460000	1.6809530000	-1.0062200000
C	-2.8101460000	2.3758850000	-0.2986190000
C	-4.4907590000	-0.2540020000	0.4655870000
H	5.1590620000	-0.5070550000	-1.0691420000
H	5.3189970000	1.4006280000	0.5125240000
H	3.3219400000	2.0949830000	1.8175350000
H	1.1705020000	0.9058860000	1.5201550000
H	3.0009300000	-1.7114050000	-1.3471030000
H	-0.6726590000	2.2616370000	-1.7112990000
H	0.6970670000	1.1480490000	-1.5542730000
H	0.3930800000	2.3535100000	-0.2852140000
H	-3.8084100000	2.4676630000	0.1277390000
H	-2.8667270000	2.6633090000	-1.3532070000
H	-2.1564440000	3.0871550000	0.2135800000
H	-4.9942130000	0.7065230000	0.3490230000
H	-4.6720920000	-0.6154610000	1.4822010000
H	-4.9527180000	-0.9625020000	-0.2287290000

**Thermodynamic data**

Zero-point correction= 0.243025 (Hartree/Particle)  
 Thermal correction to Energy= 0.258555  
 Thermal correction to Enthalpy= 0.259500

Thermal correction to Gibbs Free Energy= 0.199316  
 Sum of electronic and zero-point Energies= -1031.440429  
 Sum of electronic and thermal Energies= -1031.424899  
 Sum of electronic and thermal Enthalpies= -1031.423954  
 Sum of electronic and thermal Free Energies= -1031.484138

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	162.246	58.325	126.668

### 7aa-syn

#### Xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	-4.2613360000	0.1653370000	-0.8005300000
C	-4.4819310000	-0.8981630000	0.0773890000
C	-3.4641200000	-1.3071410000	0.9381500000
C	-2.2256440000	-0.6667800000	0.9130160000
C	-1.9928480000	0.3922640000	0.0271370000
C	-3.0281980000	0.8107560000	-0.8187910000
C	-0.6985350000	1.1447670000	-0.0169130000
C	0.5205510000	0.4112640000	0.0634890000
O	-0.7158160000	2.3954570000	-0.1740580000
N	1.7698590000	0.9728560000	0.1680120000
S	0.6698940000	-1.3095260000	-0.2078240000
C	2.4176740000	-1.1944330000	-0.2436270000
C	2.8234220000	0.0812390000	-0.0272740000
C	1.9806180000	2.3631160000	0.5746990000
C	4.2340690000	0.5787130000	0.0240870000
C	3.2249830000	-2.4328970000	-0.4707700000
H	-5.0521050000	0.4913020000	-1.4693200000
H	-5.4448170000	-1.3992500000	0.0960230000
H	-3.6357260000	-2.1186070000	1.6386010000
H	-1.4490010000	-0.9759310000	1.6069890000
H	-2.8490390000	1.6458710000	-1.4892650000
H	2.9562900000	2.4426540000	1.0506020000
H	1.2060800000	2.6448960000	1.2843780000
H	1.9291210000	3.0337660000	-0.2848510000
H	4.9177260000	-0.1970140000	-0.3178140000
H	4.5234690000	0.8586500000	1.0416380000
H	4.3627750000	1.4525390000	-0.6206430000
H	4.2922450000	-2.2092920000	-0.4511830000
H	2.9897520000	-2.8855990000	-1.4387080000
H	3.0228750000	-3.1774500000	0.3054520000

#### Thermodynamic data

Zero-point correction= 0.242544 (Hartree/Particle)  
 Thermal correction to Energy= 0.258265  
 Thermal correction to Enthalpy= 0.259210  
 Thermal correction to Gibbs Free Energy= 0.198077  
 Sum of electronic and zero-point Energies= -1031.441459  
 Sum of electronic and thermal Energies= -1031.425737

Sum of electronic and thermal Enthalpies= -1031.424793  
 Sum of electronic and thermal Free Energies= -1031.485925

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	162.064	58.491	128.664

### 7aa-anti-H

#### Xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3247320000	-0.1945460000	-0.3430020000
C	4.3558360000	0.9044890000	0.5182250000
C	3.1829440000	1.3438100000	1.1361320000
C	1.9795150000	0.6967750000	0.8857880000
C	1.9381530000	-0.3964630000	0.0024180000
C	3.1261910000	-0.8498440000	-0.5975450000
C	0.6956210000	-1.1076220000	-0.2478790000
C	-0.6018130000	-0.5620300000	-0.1476480000
O	0.8296560000	-2.4305660000	-0.4452870000
N	-0.9911400000	0.7101520000	-0.4100490000
S	-1.9472500000	-1.5118910000	0.3794790000
C	-3.0105720000	-0.1482420000	0.2649390000
C	-2.3348640000	0.9599660000	-0.1543090000
C	-0.1527960000	1.7036560000	-1.0946140000
C	-2.8900160000	2.3282700000	-0.3826890000
C	-4.4589790000	-0.3061010000	0.6003960000
H	5.2376150000	-0.5396570000	-0.8170220000
H	5.2944750000	1.4120770000	0.7152200000
H	3.2097030000	2.1826130000	1.8235530000
H	1.0762670000	1.0148840000	1.3994240000
H	3.0937000000	-1.7027240000	-1.2669470000
H	0.0732880000	-2.8212910000	-0.9094870000
H	-0.7669890000	2.2168970000	-1.8325430000
H	0.6629870000	1.1927480000	-1.6003860000
H	0.2497600000	2.4239870000	-0.3802860000
H	-3.8731230000	2.4140550000	0.0771220000
H	-2.9972190000	2.5376920000	-1.4512860000
H	-2.2410230000	3.0896110000	0.0564900000
H	-4.9684140000	0.6561880000	0.5549480000
H	-4.5849920000	-0.7154180000	1.6055750000
H	-4.9444520000	-0.9832020000	-0.1077010000

#### Thermodynamic data

Zero-point correction= 0.255718 (Hartree/Particle)  
 Thermal correction to Energy= 0.271370  
 Thermal correction to Enthalpy= 0.272314  
 Thermal correction to Gibbs Free Energy= 0.212169  
 Sum of electronic and zero-point Energies= -1031.863206  
 Sum of electronic and thermal Energies= -1031.847554  
 Sum of electronic and thermal Enthalpies= -1031.846610  
 Sum of electronic and thermal Free Energies= -1031.906755

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	170.287	59.799	126.585

### 7aa-syn-H

#### Xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3411020000	0.1862800000	-0.5864880000
C	4.4851030000	-0.9142010000	0.2611910000
C	3.3899190000	-1.3846710000	0.9870540000
C	2.1511050000	-0.7672390000	0.8613360000
C	1.9936340000	0.3281210000	-0.0064870000
C	3.1069710000	0.8103890000	-0.7184120000
C	0.7117740000	0.9999300000	-0.1627970000
C	-0.5315980000	0.3512280000	-0.0432630000
O	0.7910810000	2.3074030000	-0.4695810000
N	-1.7330380000	0.9448780000	0.1910170000
S	-0.7523810000	-1.3313930000	-0.3884290000
C	-2.4726250000	-1.1807790000	-0.2471930000
C	-2.8276460000	0.1012740000	0.0550800000
C	-1.8790110000	2.2975530000	0.7512290000
C	-4.2065670000	0.6349020000	0.2692870000
C	-3.3429510000	-2.3798060000	-0.4478590000
H	5.1930880000	0.5556360000	-1.1476490000
H	5.4514710000	-1.3970410000	0.3638530000
H	3.5043220000	-2.2227550000	1.6662380000
H	1.3184010000	-1.1101880000	1.4669250000
H	2.9880500000	1.6614590000	-1.3800040000
H	0.0246190000	2.6221690000	-0.9712190000
H	-2.1836960000	3.0059990000	-0.0224390000
H	-0.9360400000	2.6029420000	1.1987300000
H	-2.6410620000	2.2655040000	1.5282020000
H	-4.9429670000	-0.0751700000	-0.1032170000
H	-4.3450850000	1.5784530000	-0.2640360000
H	-4.4048730000	0.8049900000	1.3317950000
H	-4.3788530000	-2.1457110000	-0.2034130000
H	-3.0196220000	-3.2012260000	0.1964400000
H	-3.3003260000	-2.7227150000	-1.4851200000

#### Thermodynamic data

Zero-point correction=	0.255297 (Hartree/Particle)
Thermal correction to Energy=	0.271256
Thermal correction to Enthalpy=	0.272200
Thermal correction to Gibbs Free Energy=	0.210803
Sum of electronic and zero-point Energies=	-1031.862508
Sum of electronic and thermal Energies=	-1031.846549
Sum of electronic and thermal Enthalpies=	-1031.845605
Sum of electronic and thermal Free Energies=	-1031.907002

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	170.215	59.996	129.220
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### **4ab**

#### **Xyz-matrix**

28

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.6369080000	-1.5020890000	1.2970190000
O	-2.0982860000	0.4969040000	1.5189790000
H	4.0089440000	-1.7215840000	0.4399880000
S	0.9523530000	-1.6392000000	0.2510670000
C	-1.6386400000	-0.5021820000	0.7891250000
H	-4.2428580000	-0.1371310000	0.3654960000
C	-0.1317600000	-0.3262450000	0.4149280000
C	3.6443810000	-1.1414970000	-0.4124510000
C	2.2826870000	-0.5845160000	-0.1361390000
C	-3.8324700000	-0.4922730000	-0.5744190000
H	3.6309660000	-1.7968230000	-1.2877500000
C	-2.3545180000	-0.7285040000	-0.5672820000
N	0.5025050000	0.8179060000	0.2062040000
H	-1.1289670000	1.9361270000	0.7944840000
H	4.3596280000	-0.3396730000	-0.6014510000
H	-4.4588660000	-1.1499430000	-1.1673800000
C	1.8656290000	0.7058350000	-0.1114890000
H	-1.9810960000	-1.5489640000	-1.1796190000
H	0.4543490000	2.8172620000	0.8277980000
C	-0.1791340000	2.1249310000	0.2720700000
H	-2.7874070000	1.4294410000	-0.8035520000
H	2.7649480000	2.5467010000	0.5403320000
C	-2.9158110000	0.4660870000	-1.2865170000
C	2.6649420000	1.9432860000	-0.3670770000
H	3.6650040000	1.6803840000	-0.7105070000
H	-0.3356150000	2.4913550000	-0.7451630000
H	-2.9068390000	0.4686290000	-2.3714880000
H	2.1939910000	2.5634070000	-1.1350350000

#### **Thermodynamic data**

Zero-point correction=	0.235250 (Hartree/Particle)
Thermal correction to Energy=	0.249206
Thermal correction to Enthalpy=	0.250150
Thermal correction to Gibbs Free Energy=	0.194254
Sum of electronic and zero-point Energies=	-917.718372
Sum of electronic and thermal Energies=	-917.704416
Sum of electronic and thermal Enthalpies=	-917.703472
Sum of electronic and thermal Free Energies=	-917.759368

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	156.379	51.886	117.644

ERROR

***syn-4ab-H***

## Xyz-matrix

### Thermodynamic data

### 7ab

## Xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.4596390000	2.9777110000	0.5527190000
H	0.2506740000	2.7639800000	0.0990990000
H	-3.4229140000	1.8512870000	0.9886790000
C	-0.7700320000	2.4730990000	-0.1245920000
H	-1.0131650000	2.7443390000	-1.1573650000
H	3.9041560000	0.3291410000	1.3550180000
C	-3.3732460000	1.2567150000	0.0714760000
H	-3.3962040000	1.9440160000	-0.7790740000
O	2.0091930000	1.6409130000	0.1473090000
N	-0.8906340000	1.0248220000	0.0529770000
H	4.2013330000	-1.4788650000	1.1749120000
H	-4.2637200000	0.6315130000	0.0263660000
C	3.8070960000	-0.5640130000	0.7472690000
C	-2.1410360000	0.4078430000	0.0474260000
C	1.5648880000	0.4681150000	0.0385450000
C	0.1759640000	0.1500550000	0.0140690000
C	2.5341420000	-0.6701700000	-0.0617010000
H	2.1328430000	-1.6687280000	-0.1964210000
C	-2.0836150000	-0.9459530000	0.0266360000
H	-4.1599860000	-1.4709250000	-0.0174930000
S	-0.4209310000	-1.4963460000	0.0012530000
C	3.8567630000	-0.3883090000	-0.7351630000
H	-3.1577780000	-2.5603160000	0.9499070000
H	3.9861000000	0.6211930000	-1.1095850000
C	-3.1852580000	-1.9570580000	0.0371720000
H	4.2855430000	-1.1816950000	-1.3367020000
H	-3.0989420000	-2.6368590000	-0.8159300000

### Thermodynamic data

Zero-point correction=	0.223861 (Hartree/Particle)
Thermal correction to Energy=	0.238211
Thermal correction to Enthalpy=	0.239155
Thermal correction to Gibbs Free Energy=	0.180804
Sum of electronic and zero-point Energies=	-917.150307
Sum of electronic and thermal Energies=	-917.135957
Sum of electronic and thermal Enthalpies=	-917.135013
Sum of electronic and thermal Free Energies=	-917.193364

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	149.480	51.815	122.811

### ***syn-7ab-H***

#### **Xyz-matrix**

28

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.5160860000	0.3627150000	0.0239850000
C	-0.1470620000	0.1033350000	-0.0462390000
O	-2.0309970000	1.5549220000	0.3585850000
N	0.8859820000	1.0009570000	-0.0366010000
S	0.4688190000	-1.5200410000	-0.0508600000
C	2.1037990000	-0.9437770000	0.0152370000
C	2.1445100000	0.4198500000	0.0240190000
C	0.7094630000	2.4416850000	-0.2576170000
C	3.3630380000	1.2842410000	0.0708820000
C	3.2317140000	-1.9241890000	0.0529060000
C	-2.5143950000	-0.6682500000	-0.2518880000
C	-3.6967950000	-0.8039940000	0.6995590000
C	-3.9146710000	-0.2449660000	-0.6601190000
H	-1.4245190000	2.1081820000	0.8695330000
H	0.6250080000	2.9753120000	0.6931330000
H	-0.1697500000	2.6051100000	-0.8788910000
H	1.5764400000	2.8213440000	-0.7934450000
H	4.2320590000	0.6875940000	0.3429520000
H	3.2493850000	2.0755420000	0.8158260000
H	3.5598190000	1.7462010000	-0.9013860000
H	4.1901360000	-1.4101530000	-0.0162610000
H	3.1619480000	-2.6228590000	-0.7848500000
H	3.2147790000	-2.5026850000	0.9805980000
H	-2.1389900000	-1.5800470000	-0.7008600000
H	-3.7155270000	-0.1152060000	1.5367600000
H	-4.0206130000	-1.8164130000	0.9095950000
H	-4.3882500000	-0.8691070000	-1.4083590000
H	-4.0949440000	0.8197800000	-0.7479920000

#### **Thermodynamic data**

Zero-point correction=	0.223861 (Hartree/Particle)
Thermal correction to Energy=	0.238211
Thermal correction to Enthalpy=	0.239155
Thermal correction to Gibbs Free Energy=	0.180804
Sum of electronic and zero-point Energies=	-917.150307
Sum of electronic and thermal Energies=	-917.135957
Sum of electronic and thermal Enthalpies=	-917.135013
Sum of electronic and thermal Free Energies=	-917.193364

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	149.480	51.815	122.811

### **4ac**

#### **Xyz-matrix**

21

XYZ file generated by gabedit : coordinates in Angstrom

S	-0.3340840000	-1.6649530000	-0.0855850000
C	0.9075280000	-0.5005990000	-0.1966800000
N	0.3970530000	0.7215660000	-0.1291780000
C	-0.9962420000	0.7906610000	-0.0053320000
C	-1.5682320000	-0.4400230000	0.0327450000
C	1.2654200000	1.9086780000	-0.2093950000
C	-1.6625620000	2.1267000000	0.0706840000
C	-3.0106410000	-0.8151440000	0.1737500000
C	2.4288560000	-0.7990440000	-0.2250580000
O	3.0569950000	-0.0929720000	0.7020230000
H	1.2805690000	2.2717990000	-1.2400000000
H	2.2574390000	1.5716270000	0.1305100000
H	0.8691070000	2.6782400000	0.4523210000
H	-2.7454950000	2.0102470000	0.0409360000
H	-1.3656150000	2.7608660000	-0.7695910000
H	-1.4028260000	2.6475390000	0.9974150000
H	-3.6417170000	0.0748710000	0.1787410000
H	-3.1855780000	-1.3563690000	1.1079270000
H	-3.3337720000	-1.4526120000	-0.6537910000
H	2.7073340000	-0.5906240000	-1.2956780000
H	2.4858060000	-1.9108910000	-0.1356570000

### Thermodynamic data

Zero-point correction= 0.172402 (Hartree/Particle)

Thermal correction to Energy= 0.182577

Thermal correction to Enthalpy= 0.183521

Thermal correction to Gibbs Free Energy= 0.137121

Sum of electronic and zero-point Energies= -801.118772

Sum of electronic and thermal Energies= -801.108597

Sum of electronic and thermal Enthalpies= -801.107653

Sum of electronic and thermal Free Energies= -801.154053

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	114.569	37.721	97.656

7ac

NIMag=1; -63 cm-1

### Xyz-matrix

20

XYZ file generated by gabedit : coordinates in Angstrom

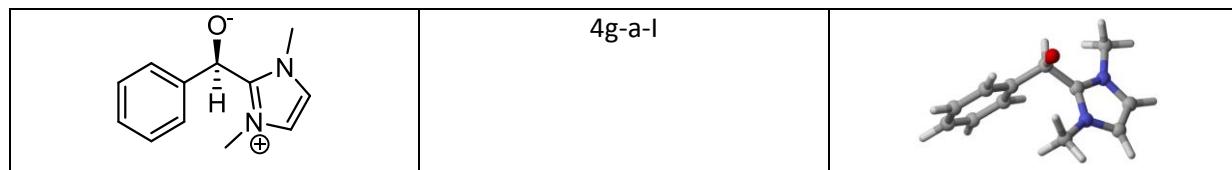
S	0.3191370000	-1.6909330000	0.0001170000
C	-0.9651040000	-0.5058680000	0.0001130000
N	-0.4318880000	0.7588060000	0.0000430000
C	0.9613450000	0.7965570000	0.0000210000
C	1.5383620000	-0.4310800000	0.0000520000
C	-1.2337590000	1.9826040000	0.0000300000
C	1.6495330000	2.1244070000	-0.0000500000
C	2.9845720000	-0.8110300000	0.0000640000
C	-2.3224700000	-0.9050720000	0.0001430000
O	-3.3308460000	-0.1545910000	-0.0001110000
H	-1.0068240000	2.5724830000	0.8913620000
H	-2.2829510000	1.7027790000	0.0000040000
H	-1.0067750000	2.5724910000	-0.8912830000
H	2.7300710000	1.9902950000	-0.0000050000

H	1.3791240000	2.7080070000	0.8848420000
H	1.3791750000	2.7078870000	-0.8850370000
H	3.6178650000	0.0769410000	-0.0001760000
H	3.2343040000	-1.4050030000	-0.8842390000
H	3.2343980000	-1.4046040000	0.8846110000
H	-2.4536620000	-2.0003780000	-0.0000370000

### Thermodynamic data

Zero-point correction= 0.160720 (Hartree/Particle)  
 Thermal correction to Energy= 0.171144  
 Thermal correction to Enthalpy= 0.172088  
 Thermal correction to Gibbs Free Energy= 0.124272  
 Sum of electronic and zero-point Energies= -800.547732  
 Sum of electronic and thermal Energies= -800.537308  
 Sum of electronic and thermal Enthalpies= -800.536363  
 Sum of electronic and thermal Free Energies= -800.584180

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	107.395	37.883	100.638



**xyz-matrix**

29

XYZ file generated by gabedit : coordinates in Angstrom

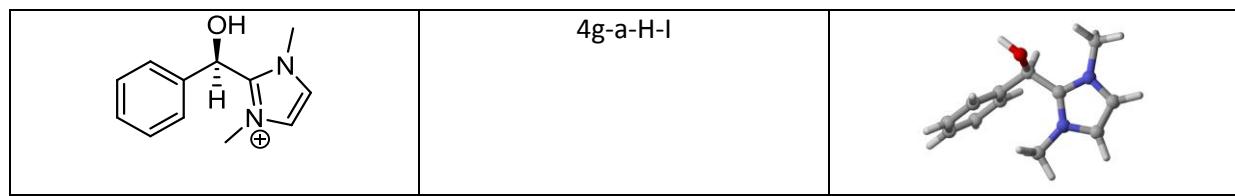
C	-0.1325600000	-0.6661780000	1.0719030000
H	-0.3210370000	-1.7608430000	1.0048900000
O	-0.2179720000	-0.1634380000	2.3147960000
C	1.2181670000	-0.4677170000	0.3511610000
C	2.2794130000	0.1188630000	1.0302470000
C	3.5077670000	0.3026300000	0.3963370000
C	3.6815780000	-0.1011190000	-0.9242160000
C	2.6221570000	-0.6966900000	-1.6084230000
C	1.3998060000	-0.8802910000	-0.9700450000
H	2.1135230000	0.4343300000	2.0538460000

H	4.3293720000	0.7651210000	0.9322840000
H	4.6350720000	0.0449370000	-1.4185150000
H	2.7508190000	-1.0171280000	-2.6360630000
H	0.5771760000	-1.3476900000	-1.5069060000
C	-1.2236150000	-0.0474260000	0.1937900000
N	-1.2913170000	1.2388430000	-0.1715080000
C	-2.4790340000	1.4712570000	-0.8318320000
N	-2.3549850000	-0.6345230000	-0.2192480000
C	-3.1493770000	0.2942580000	-0.8628400000
H	-2.7394290000	2.4442860000	-1.2111610000
H	-4.1094840000	0.0356140000	-1.2742760000
C	-2.7126830000	-2.0374140000	-0.0075980000
C	-0.2594000000	2.2391510000	0.1006890000
H	-2.0853880000	-2.6828200000	-0.6200760000
H	-3.7536580000	-2.1623000000	-0.2947270000
H	-2.5953280000	-2.2888370000	1.0445570000
H	-0.7183990000	3.2231460000	0.0378080000
H	0.5430360000	2.1512380000	-0.6317410000
H	0.1283000000	2.0622630000	1.1019750000

#### thermodynamic data

Zero-point correction=	0.242378 (Hartree/Particle)
Thermal correction to Energy=	0.255954
Thermal correction to Enthalpy=	0.256898
Thermal correction to Gibbs Free Energy=	0.201414
Sum of electronic and zero-point Energies=	-650.056360
Sum of electronic and thermal Energies=	-650.042784
Sum of electronic and thermal Enthalpies=	-650.041840
Sum of electronic and thermal Free Energies=	-650.097324

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.614	51.581	116.777



**xyz-matrix**

30

XYZ file generated by gabedit : coordinates in Angstrom

```

C   -0.1457180000   -0.8088160000   0.8886710000
H   -0.3596350000   -1.8746420000   0.7566930000
O   -0.2383450000   -0.4494060000   2.2506090000
H   0.2604020000   -1.0845250000   2.7766940000
C   1.2121510000   -0.5158350000   0.2600260000
C   2.2562320000   0.0112210000   1.0120610000
C   3.4841790000   0.2745010000   0.4080250000
C   3.6690430000   0.0159690000   -0.9453650000
C   2.6235750000   -0.5149260000   -1.6983010000
C   1.4001420000   -0.7827900000   -1.0964660000
H   2.1111640000   0.2340310000   2.0623540000
H   4.2933410000   0.6874880000   0.9983350000
H   4.6232930000   0.2248520000   -1.4137960000
H   2.7620740000   -0.7213060000   -2.7526970000
H   0.5891470000   -1.1987160000   -1.6872220000
C   -1.2388880000   -0.0525280000   0.1858480000
N   -1.2669220000   1.2654940000   -0.0339890000
C   -2.4324560000   1.5860070000   -0.6878010000
N   -2.3666180000   -0.5760480000   -0.3067530000
C   -3.1227320000   0.4301220000   -0.8612790000

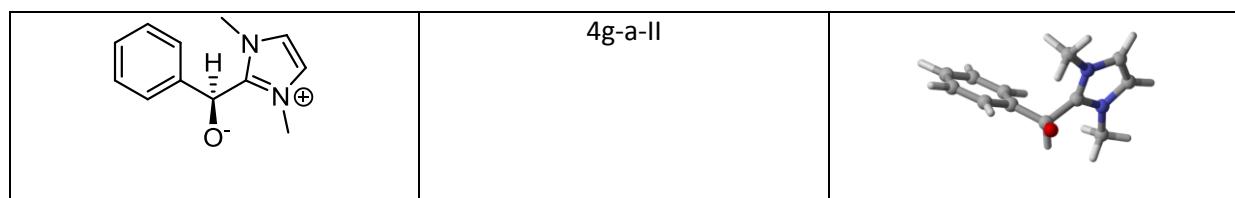
```

H	-2.6686340000	2.5993200000	-0.9635500000
H	-4.0767330000	0.2388660000	-1.3209650000
C	-2.7563130000	-1.9891950000	-0.2560890000
C	-0.2250770000	2.2248740000	0.3477400000
H	-2.1091210000	-2.5775190000	-0.9037160000
H	-3.7822600000	-2.0607230000	-0.6061420000
H	-2.7005800000	-2.3464700000	0.7699600000
H	-0.6712460000	3.2158950000	0.3413620000
H	0.5958760000	2.1762480000	-0.3667000000
H	0.1296150000	1.9847140000	1.3472970000

### thermodynamic data

Zero-point correction= 0.256844 (Hartree/Particle)  
 Thermal correction to Energy= 0.270521  
 Thermal correction to Enthalpy= 0.271466  
 Thermal correction to Gibbs Free Energy= 0.216486  
 Sum of electronic and zero-point Energies= -650.523664  
 Sum of electronic and thermal Energies= -650.509987  
 Sum of electronic and thermal Enthalpies= -650.509042  
 Sum of electronic and thermal Free Energies= -650.564022

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	169.755	52.847	115.715



### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

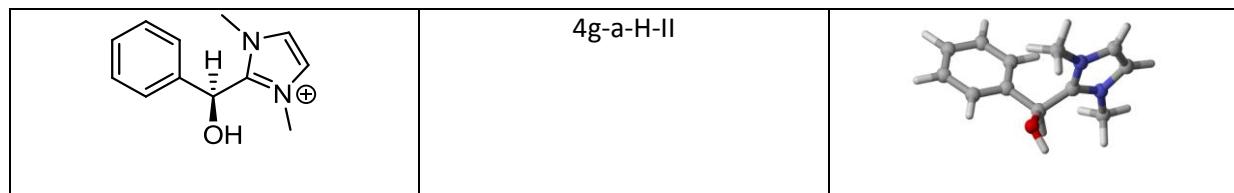
C	-0.1325970000	0.6673520000	1.0711300000
---	---------------	--------------	--------------

H	-0.3210850000	1.7619410000	1.0027730000
O	-0.2180570000	0.1661170000	2.3146130000
C	1.2181740000	0.4681060000	0.3507150000
C	1.3998320000	0.8792810000	-0.9709280000
C	2.6221800000	0.6950040000	-1.6090900000
C	3.6816000000	0.1001920000	-0.9242050000
C	3.5077550000	-0.3021920000	0.3967480000
C	2.2793670000	-0.1177920000	1.0304380000
H	0.5771950000	1.3461420000	-1.5082520000
H	2.7508800000	1.0143440000	-2.6370660000
H	4.6351140000	-0.0463570000	-1.4183210000
H	4.3293580000	-0.7640930000	0.9332060000
H	2.1134790000	-0.4321320000	2.0543860000
C	-1.2235970000	0.0475750000	0.1936860000
N	-1.2912070000	-1.2390300000	-0.1704420000
C	-2.4789410000	-1.4721200000	-0.8305230000
N	-2.3550240000	0.6342100000	-0.2198450000
C	-3.1493630000	-0.2952020000	-0.8625830000
C	-0.2592740000	-2.2390620000	0.1026710000
C	-2.7128740000	2.0372300000	-0.0092460000
H	-2.5957510000	2.2893610000	1.0427700000
H	-3.7538130000	2.1618320000	-0.2966320000
H	-2.0854880000	2.6822590000	-0.6220200000
H	0.5434870000	-2.1513930000	-0.6294300000
H	-0.7181220000	-3.2231420000	0.0400350000
H	0.1279650000	-2.0617000000	1.1040480000
H	-2.7392640000	-2.4455080000	-1.2089760000
H	-4.1094650000	-0.0369880000	-1.2743010000

### thermodynamic data

Zero-point correction= 0.242380 (Hartree/Particle)  
Thermal correction to Energy= 0.255954  
Thermal correction to Enthalpy= 0.256899  
Thermal correction to Gibbs Free Energy= 0.201419  
Sum of electronic and zero-point Energies= -650.056357  
Sum of electronic and thermal Energies= -650.042784  
Sum of electronic and thermal Enthalpies= -650.041839  
Sum of electronic and thermal Free Energies= -650.097319

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.614	51.579	116.767



**xyz-matrix**

30

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.1142680000	0.9094380000	0.7967100000
H	-0.3081540000	1.9623640000	0.5680970000
O	-0.0654250000	0.7099980000	2.1926470000
H	-0.7857300000	1.1953800000	2.6091230000
C	1.2180690000	0.5157280000	0.1779020000
C	1.3176510000	0.3622580000	-1.2054260000
C	2.5330590000	0.0172920000	-1.7846780000
C	3.6557550000	-0.1796460000	-0.9843080000
C	3.5560550000	-0.0252910000	0.3940350000
C	2.3402560000	0.3235250000	0.9777120000
H	0.4471810000	0.5060970000	-1.8389710000

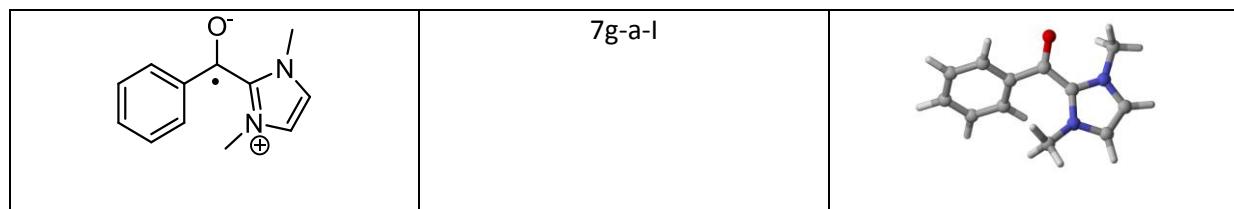
H	2.6013260000	-0.1013910000	-2.8593520000
H	4.6022800000	-0.4532770000	-1.4347590000
H	4.4258150000	-0.1783820000	1.0217830000
H	2.2602370000	0.4395150000	2.0507310000
C	-1.2373680000	0.1004910000	0.1976310000
N	-1.3201700000	-1.2334180000	0.2046110000
C	-2.4844760000	-1.6142550000	-0.4179490000
N	-2.3284690000	0.5774410000	-0.4117740000
C	-3.1186950000	-0.4783520000	-0.8055590000
C	-0.3158670000	-2.1517980000	0.7521940000
C	-2.6606770000	1.9937590000	-0.6055730000
H	-2.8128570000	2.4723240000	0.3604040000
H	-3.5805710000	2.0400750000	-1.1816690000
H	-1.8655120000	2.4904930000	-1.1575810000
H	0.4647250000	-2.3203090000	0.0109190000
H	-0.8169050000	-3.0860640000	0.9928810000
H	0.1075360000	-1.7152300000	1.6530940000
H	-2.7582450000	-2.6494860000	-0.5259560000
H	-4.0542270000	-0.3291520000	-1.3159270000

### thermodynamic data

Zero-point correction=	0.256615 (Hartree/Particle)
Thermal correction to Energy=	0.270423
Thermal correction to Enthalpy=	0.271368
Thermal correction to Gibbs Free Energy=	0.215785
Sum of electronic and zero-point Energies=	-650.524588
Sum of electronic and thermal Energies=	-650.510780
Sum of electronic and thermal Enthalpies=	-650.509836
Sum of electronic and thermal Free Energies=	-650.565419

E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
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Total 169.693 53.021 116.984



**xyz-matrix**

28

XYZ file generated by gabedit : coordinates in Angstrom

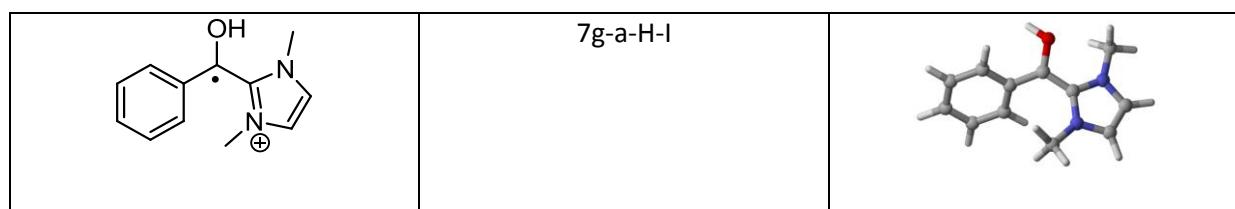
C	-0.0933850000	-0.9435290000	0.3087150000
O	-0.2878020000	-2.1510960000	0.6626910000
C	1.2643970000	-0.4286740000	0.0509260000
C	2.3585910000	-1.0560380000	0.6700370000
C	3.6571910000	-0.6362610000	0.4154230000
C	3.9000220000	0.4119740000	-0.4725570000
C	2.8249070000	1.0256720000	-1.1140850000
C	1.5244350000	0.6071950000	-0.8621180000
H	2.1663070000	-1.8731600000	1.3549690000
H	4.4869550000	-1.1276850000	0.9113820000
H	4.9140620000	0.7372240000	-0.6721550000
H	3.0020500000	1.8221490000	-1.8280530000
H	0.7024560000	1.0659060000	-1.4027740000
C	-1.2344190000	-0.0843490000	0.1171430000
N	-1.3622040000	1.2556830000	0.3586550000
C	-2.6638130000	1.6430030000	0.0932820000
N	-2.4663360000	-0.5209070000	-0.2713130000
C	-3.3452040000	0.5422000000	-0.2943590000
H	-2.9873440000	2.6612660000	0.2228320000
H	-4.3728830000	0.4203690000	-0.5903270000

C	-2.7705770000	-1.8609390000	-0.7579600000
C	-0.3911750000	2.1074460000	1.0319960000
H	-2.0003780000	-2.1722270000	-1.4629000000
H	-3.7349660000	-1.8203080000	-1.2602110000
H	-2.8000320000	-2.5688180000	0.0666290000
H	-0.9368400000	2.8652780000	1.5908890000
H	0.2790070000	2.5880390000	0.3189770000
H	0.1979850000	1.5011100000	1.7191610000

### thermodynamic data

Zero-point correction= 0.230112 (Hartree/Particle)  
 Thermal correction to Energy= 0.243502  
 Thermal correction to Enthalpy= 0.244446  
 Thermal correction to Gibbs Free Energy= 0.189227  
 Sum of electronic and zero-point Energies= -649.469708  
 Sum of electronic and thermal Energies= -649.456318  
 Sum of electronic and thermal Enthalpies= -649.455374  
 Sum of electronic and thermal Free Energies= -649.510593

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	152.800	51.273	116.218



### xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

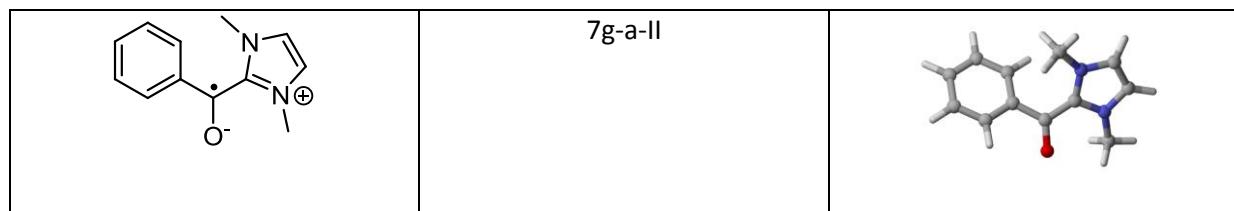
C	-0.0738240000	0.8503430000	0.2918830000
O	-0.3271990000	2.1072430000	0.7075490000
H	0.4166820000	2.6901650000	0.5046200000

C	1.2716690000	0.3938300000	0.0427160000
C	2.3590160000	1.0003130000	0.6990220000
C	3.6555780000	0.5898690000	0.4266620000
C	3.8930760000	-0.4265330000	-0.4964110000
C	2.8221710000	-1.0289960000	-1.1568980000
C	1.5236100000	-0.6222520000	-0.8986700000
H	2.1872800000	1.7656020000	1.4482050000
H	4.4837940000	1.0580710000	0.9445020000
H	4.9072250000	-0.7446160000	-0.7046040000
H	3.0031070000	-1.8062260000	-1.8893720000
H	0.7000260000	-1.0635760000	-1.4497750000
C	-1.2487790000	0.0538330000	0.1229300000
N	-2.4467230000	0.5051620000	-0.3160910000
C	-3.3413100000	-0.5344570000	-0.3233580000
N	-1.3953080000	-1.2632010000	0.4037480000
C	-2.6859360000	-1.6377260000	0.1200550000
H	-4.3590010000	-0.4041810000	-0.6485980000
H	-3.0290280000	-2.6463680000	0.2727400000
C	-0.4145440000	-2.1384510000	1.0480140000
C	-2.7333270000	1.8546360000	-0.8074470000
H	0.1715490000	-2.6703950000	0.3001090000
H	-0.9600680000	-2.8475820000	1.6657630000
H	0.2420370000	-1.5380570000	1.6734990000
H	-2.8565670000	2.5390640000	0.0283990000
H	-3.6480790000	1.8034570000	-1.3919000000
H	-1.9115530000	2.1865190000	-1.4385890000

#### thermodynamic data

Zero-point correction= 0.243585 (Hartree/Particle)  
 Thermal correction to Energy= 0.257173  
 Thermal correction to Enthalpy= 0.258117  
 Thermal correction to Gibbs Free Energy= 0.202836  
 Sum of electronic and zero-point Energies= -649.903640  
 Sum of electronic and thermal Energies= -649.890052  
 Sum of electronic and thermal Enthalpies= -649.889108  
 Sum of electronic and thermal Free Energies= -649.944389

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	161.379	52.639	116.349



**xyz-matrix**

28

XYZ file generated by gabedit : coordinates in Angstrom

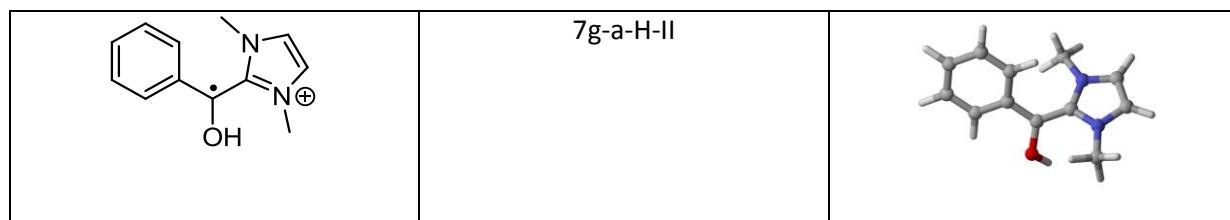
C	-0.0934070000	0.9435550000	0.3086160000
O	-0.2877710000	2.1512030000	0.6623390000
C	1.2644000000	0.4286680000	0.0509240000
C	2.3585530000	1.0560040000	0.6701090000
C	3.6571660000	0.6362550000	0.4155120000
C	3.9000250000	-0.4119210000	-0.4725270000
C	2.8249440000	-1.0255790000	-1.1141410000
C	1.5244630000	-0.6071210000	-0.8621930000
H	2.1662380000	1.8730910000	1.3550740000
H	4.4869150000	1.1276480000	0.9115260000
H	4.9140760000	-0.7371480000	-0.6721160000
H	3.0021230000	-1.8220030000	-1.8281600000
H	0.7024860000	-1.0658010000	-1.4028800000

C	-1.2344200000	0.0843550000	0.1171420000
N	-1.3621000000	-1.2557140000	0.3586060000
C	-2.6636820000	-1.6431160000	0.0932500000
N	-2.4663740000	0.5208280000	-0.2713080000
C	-3.3451450000	-0.5423590000	-0.2943910000
C	-0.3910700000	-2.1073670000	1.0320860000
C	-2.7708760000	1.8609040000	-0.7576660000
H	-2.8000540000	2.5686780000	0.0670200000
H	-3.7354910000	1.8202690000	-1.2594930000
H	-2.0010360000	2.1723620000	-1.4629230000
H	0.1974780000	-1.5011190000	1.7198600000
H	0.2797040000	-2.5873770000	0.3192350000
H	-0.9367110000	-2.8656780000	1.5903520000
H	-2.9871040000	-2.6614310000	0.2226720000
H	-4.3728520000	-0.4205700000	-0.5902800000

### thermodynamic data

Zero-point correction= 0.230120 (Hartree/Particle)  
 Thermal correction to Energy= 0.243505  
 Thermal correction to Enthalpy= 0.244449  
 Thermal correction to Gibbs Free Energy= 0.189255  
 Sum of electronic and zero-point Energies= -649.469700  
 Sum of electronic and thermal Energies= -649.456315  
 Sum of electronic and thermal Enthalpies= -649.455371  
 Sum of electronic and thermal Free Energies= -649.510564

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	152.802	51.270	116.165



**xyz-matrix**

29

XYZ file generated by gabedit : coordinates in Angstrom

```

C   -0.0738170000   -0.8502340000   0.2915090000
C    1.2717610000   -0.3937840000   0.0426000000
C   -1.2487210000   -0.0536730000   0.1225480000
O   -0.3272450000   -2.1069550000   0.7077310000
H    0.4167290000   -2.6898950000   0.5052800000
N   -1.3954540000    1.2633110000   0.4035520000
N   -2.4467040000   -0.5052390000   -0.3161700000
C   -2.6862860000    1.6375470000   0.1202340000
C   -3.3415580000    0.5342050000   -0.3229890000
H   -3.0294530000    2.6461400000   0.2730630000
H   -4.3592890000    0.4037580000   -0.6480410000
C   -2.7330750000   -1.8548160000   -0.8073840000
C   -0.4147350000    2.1387390000   1.0477140000
H   -0.9605220000    2.8488080000   1.6641440000
H    0.1722230000    2.6695680000   0.2997070000
H    0.2409500000    1.5386560000   1.6744430000
H   -1.9107140000   -2.1869870000   -1.4376170000
H   -3.6472120000   -1.8035940000   -1.3928050000
H   -2.8573230000   -2.5389520000   0.0285530000
C    2.3589360000   -1.0000470000   0.6993760000
C    1.5238800000    0.6218450000   -0.8991670000
C    3.6555420000   -0.5897250000   0.4271220000

```

C	2.8224720000	1.0286980000	-1.1570620000
C	3.8932070000	0.4264840000	-0.4961060000
H	2.1869740000	-1.7649120000	1.4489310000
H	0.7004540000	1.0626120000	-1.4509500000
H	4.4836710000	-1.0579650000	0.9450650000
H	3.0035530000	1.8058640000	-1.8895650000
H	4.9073850000	0.7446080000	-0.7040960000

### **thermodynamic data**

Zero-point correction= 0.243586 (Hartree/Particle)  
 Thermal correction to Energy= 0.257176  
 Thermal correction to Enthalpy= 0.258121  
 Thermal correction to Gibbs Free Energy= 0.202833  
 Sum of electronic and zero-point Energies= -649.903639  
 Sum of electronic and thermal Energies= -649.890049  
 Sum of electronic and thermal Enthalpies= -649.889105  
 Sum of electronic and thermal Free Energies= -649.944392

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	161.381	52.638	116.362