Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

An Electrochemical Release of Free N-heterocyclic Carbene with Iron Bis(dithiolene) N-heterocyclic Carbene Adducts

Jayaraman Selvakumar,[a] Scott M. Simpson,[b] Eva Zurek,[c] and Kuppuswamy Arumugam[a]

[a] Department of Chemistry, Wright State University, 3640 Colonel Glenn Hwy. Dayton, OH 45435 USA. [b] Department of Chemistry, St. Bonaventure University, 3261 West State Road, St. Bonaventure, NY 14778 USA. [c] Department of Chemistry, State University of New York at Buffalo, Buffalo, NY 14260, USA.

kuppuswamy.arumugam@wright.edu

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General experimental conditions

All synthetic manipulations were done in nitrogen filled glove box (Inert Glove box system) unless otherwise noted. All glassware were oven dried at 110 °C for 12 hours prior to use. The compounds 1,3-bis(2,4,6-trimethylphenyl)imidazolinium chloride (**3**) and 1,3-bis(2,4,6-trimethylphenyl)imidazolium chloride (**4**) were prepared according to the literature procedure.[1] Iron bis(dithiolene) dimers $[Fe(S_2C_2Ph_2)_2]_2$ (**1**) and $[Fe(S_2C_2(C_6H_4\text{-}OCH_3)_2)_2]_2$ (**2**) were prepared following the procedure reported by Schrauzer et. al.[2] All other reagents were purchased from commercial sources and used as received, such as sodium bis(trimethylsilyl)amide, *trans*-cinnamaldehyde, *trans*-4-methylcinnamaldehyde, *trans*-4-methoxyylcinnamaldehyde and *trans*-4-chlorocinnamaldehyde. $[N(n\text{Bu})_4][PF_6]$ was purified by recrystallized in ethanol followed by vacuum drying at 80 ^oC for 24 h. Solvents were dried with a solvent purification system from Inert Pure Company (THF, CH_2Cl_2, Et_2O and toluene) and degassed using three freeze–pump–thaw cycles prior to use. All solvents were stored over 4 Å molecular sieves in nitrogen filled glove box. $CDCl_3$ (99.9%) was purchased from Acros Laboratories and dried over 4 Å molecular sieves prior to use.

Instrumentation

UV-Vis spectra were obtained at ambient temperature with a Varian Cary 50 Bio UV-vis spectrophotometer and molar absorptivities were reported in M^{-1} cm^{-1}. ^1H and ^{13}C NMR spectra were recorded on a Bruker 300 MHz NMR spectrometer. Spectra were referenced to the residual solvent as an internal standard, for ^1H NMR: $CDCl_3$, 7.26 ppm; for ^{13}C NMR: $CDCl_3$, 77.16. Coupling constants (J) are expressed in hertz (Hz). Elemental analyses were performed by Midwest Microlab, LLC in Indianapolis, IN. Electrochemical measurements were performed on a CHI620E electrochemical workstation using a silver wire quasi-reference electrode, a platinum disk working electrode, and a Pt wire auxiliary electrode in a gas tight three-electrode cell under nitrogen atmosphere. Unless specified otherwise, the measurements were performed using 1.0 mM solutions of the analyte in dry THF with 0.1 M $[N(n\text{Bu})_4][PF_6]$ as the electrolyte and decamethylferrocene (Fc*) as the internal standard. Differential pulse voltammetry measurements were performed with 50 mV pulse amplitudes and 4 mV data intervals. All potentials listed herein were determined by cyclic voltammetry at 100 mVs^{-1} scan rates and referenced to a saturated calomel electrode (SCE) by in decamethylferrocene 0/+ to 0.102 V (THF).[3] Bulk electrolysis where conducted on two compartment cell separated by glass frit, Pt mesh working electrode, Pt mesh counter electrode and Ag/Ag^+ (in MeCN) non aqueous reference electrode.

X-ray crystallography

Solid-state structure of compounds **5-8** were unambiguously assigned using single crystal X-ray diffraction studies. Dark brown single crystals of **5** and **6** were obtained by diffusing hexanes into a saturated of CH_2Cl_2 solution. Diffraction quality single crystals of **7** and **8** were obtained by diffusing Et_2O into a saturated CH_2Cl_2 solution (Table S1). For single crystal X-ray diffraction analysis (**5-7)**, a suitable crystal with appropriate dimensions was mounted on a loop with Paratone-N oil and transferred to the goniostat bathed in cold nitrogen stream. Intensity data were collected at 183 K on a Bruker SMART X2S bench top diffractometer using equipped with Mo Kα radiation, λ=0.71073Å. For **8** the data were collected with a Oxford Diffraction System equipped with cold nitrogen stream unit supplying nitrogen stream at 100 K. Program(s) used to solve structure: XT. Ver. 2014/4. (Sheldrick, 2015a); program(s) used to refine structure: XL. Ver. 2014/7. (Sheldrick, 2015b); molecular graphics: Olex2 (Dolomanov et al., 2009); software used to prepare material for publication: Olex2 (Dolomanov et al., 2009), Platon (Spek, 2009), Mercury (Macrae et al, 2006)), and POV-ray.

Crystallographic refinement data

Table S1. Crystal and refinement data for compounds **5-8**

	5	**6**	**7**	**8**
CCDC	1946471	1946472	1946473	1946474
solvent	CH_2Cl_2/Hexane	CH_2Cl_2/Hexane	CH_2Cl_2/Et_2O	CH_2Cl_2/Et_2O
formula	$C_{49}H_{44}FeN_2S_4$	$C_{49}H_{46}FeN_2S_4$	$C_{53}H_{51}FeN_2O_4S_4.OEt_2$	$C_{53}H_{54}FeN_2O_4S_4$
Colour, habit	brown, block	brown, prism	brown, plate	green, plate
Formula weight	844.95	846.97	1038.16	967.07
Temperature/K	170	170	170	100(2)
Crystal system	monoclinic	monoclinic	Triclinic	monoclinic
Space group	C2/c	C2/c	P-1	$P2_1/c$
a/Å	27.790(3)	18.4713(16)	8.5800(8)	15.8248(7)
b/Å	7.9364(10)	8.3758(9)	17.5729(18)	23.4741(8)
c/Å	22.386(2)	27.608(3)	19.058(2)	16.4772(6)
α/°	90	90	105.927(3)	90
β/°	120.634(3)	96.178(3)	102.064(3)	108.994(5)
γ/°	90	90	98.133(3)	90
Volume/Å^3	4248.3(8)	4246.4(7)	2641.0(5)	5787.6(4)
Z	4	4	2	4
Reflections coll.	23160	22990	51798	22491
R_{int}	R_{int} = 0.0410	R_{int} = 0.0483	R_{int} = 0.0521	R_{int} = 0.0372
GoF on F^2	1.032	1.043	1.063	1.027
R1, wR2[a]	0.0342, 0.0839	0.0303, 0.0914	0.0440, 0.1160	0.0596, 0.1586

[a]$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b]$R_w = \{[\Sigma w(F_o^2 - F_c^2)/\Sigma w(F_o^2)^2\}^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (xP)^2]$, where $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Index of deviation of geometry in compounds **5-8**[4]

Compound	β	α	τ
5	164.4	151.0	0.22
6	166.2	141.2	0.41
7	174.6	136.8	0.63
8	172.37	135.99	0.60

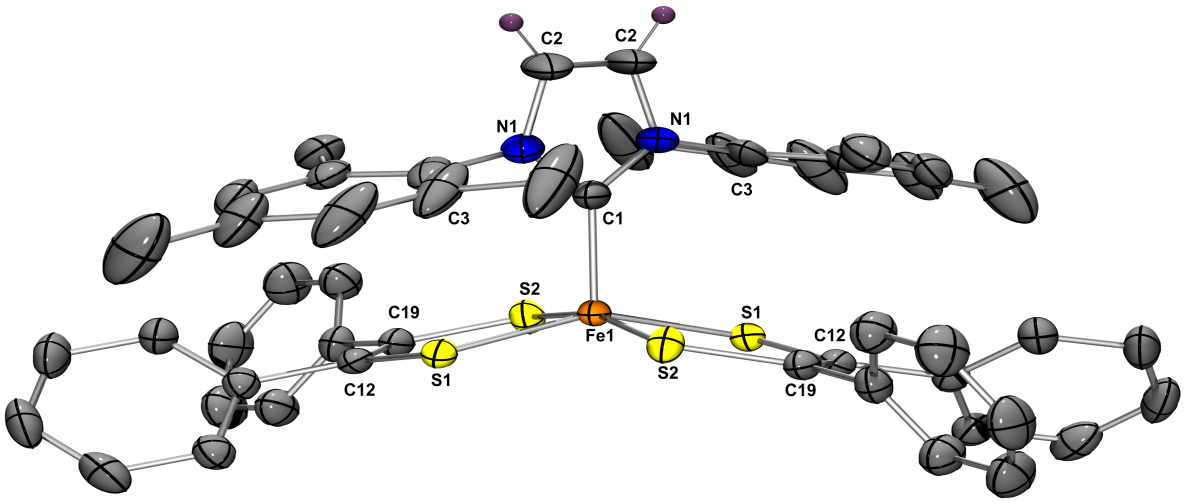


Figure S1. ORTEP diagram of **5** rendered by using POV-Ray. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms and solvent molecules are omitted for clarity. Selected distances [Å] and angles [°]: Fe1–C1, 1.963(3); Fe1–S1, 2.1567 (5); Fe1–S2, 2.1799(6); S2–C19, 1.715(2); C12–C19, 1.381(3); S1–C12, 1.719(2); N1–C1, 1.362(3); N1–C2, 1.385(4), N1–C3, 1.443(4); C1–Fe1–S2, 97.771(18); C1–Fe1–S1, 104.472(18); S2–Fe1–S4, 164.4; S1–Fe1–S3, 151.0. S1–Fe1–S1, 151.05(3); S1–Fe1–S2, 88.25(2).

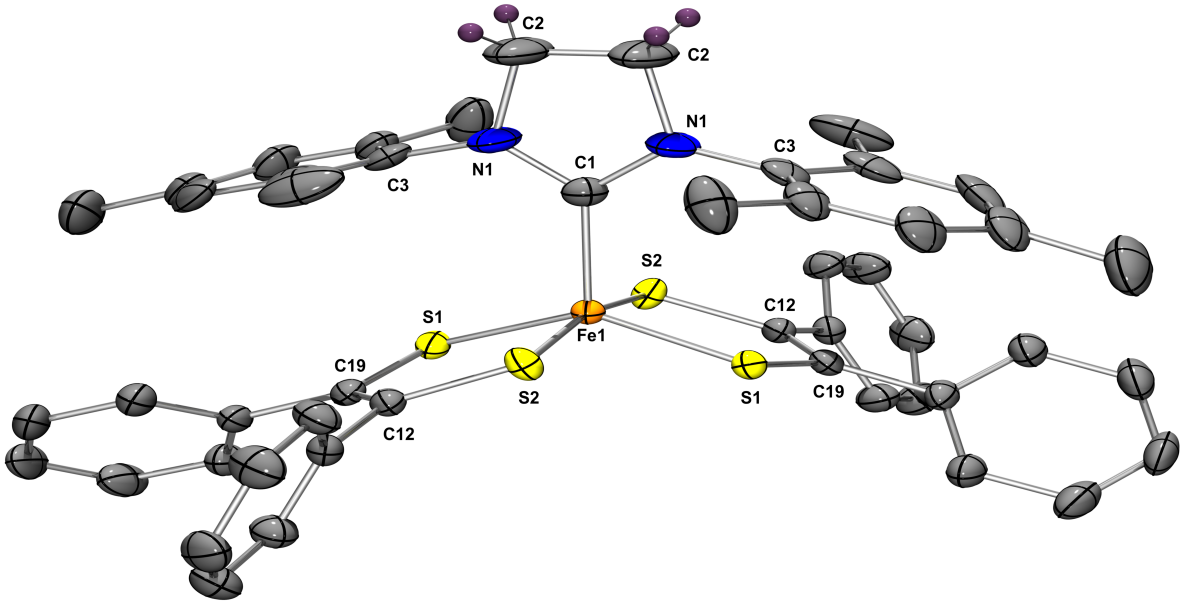


Figure S2. ORTEP diagram of **6** rendered by using POV-Ray. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms and solvent molecules are omitted for clarity. Selected distances [Å] and angles [°]:Fe1–S1, 2.1448(5); Fe1–S2, 2.1927(5); Fe1–C1, 1.960(3); S1–C19, 1.7185(19); S2–C12, 1.7145(18); N1–C1, 1.349(2); N1–C2, 1.471(3); N1–C3, 1.433(3); C19–C12, 1.384(3); S1–Fe1–S1, 141.24(3); S1–Fe1–S2, 88.438(18); C1–Fe1–S1, 109.378(15); N1–C1–N1, 107.2(2).

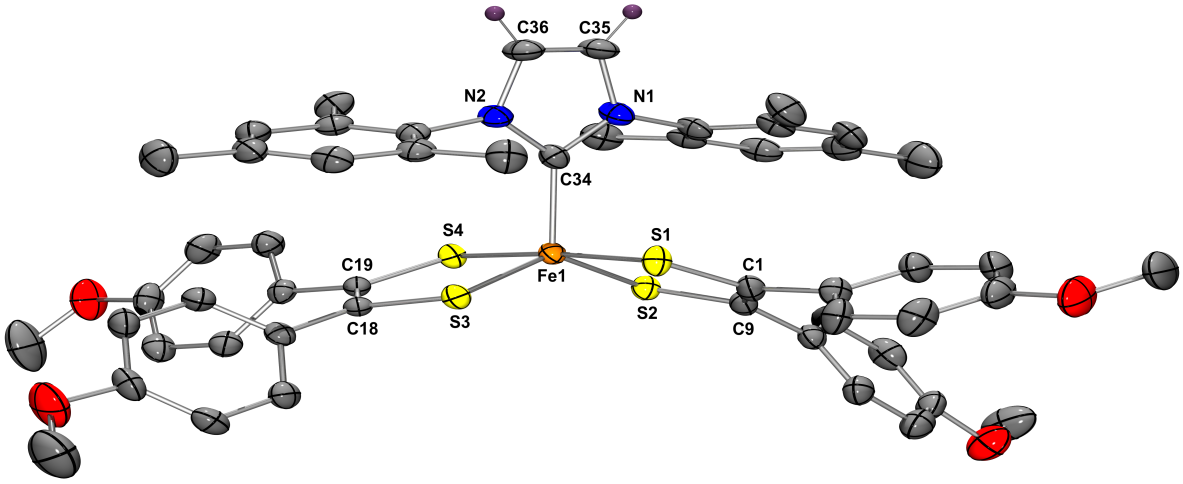


Figure S3. ORTEP diagram of **7** rendered by using POV-Ray. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms and solvent molecules are omitted for clarity. Selected distances [Å] and angles [°]:Fe1–S1, 2.1926(8); Fe1–S2, 2.1520(7); Fe1–S3, 2.1417(8); Fe1–S4, 2.1984(7); Fe1–C34, 1.968(3); S1–C1, 1.717(3); S2–C9, 1.724(3); S3–C18, 1.731(3); S4–C19, 1.736(3); N1–C34, 1.368(3); N1–C35, 1.390(3); N2–C34, 1.371(3); C35–C36, 1.334(4); S1–Fe1–S4, 174.62(3); S2–Fe1–S1, 87.75(3); S2–Fe1–S4, 89.70(3); S3–Fe1–S1, 90.72(3); S3–Fe1–S2, 136.84(3); S3–Fe1–S4, 87.90(3); C34–Fe1–S1, 88.53(8); N1 C34 N2 103.5(2).

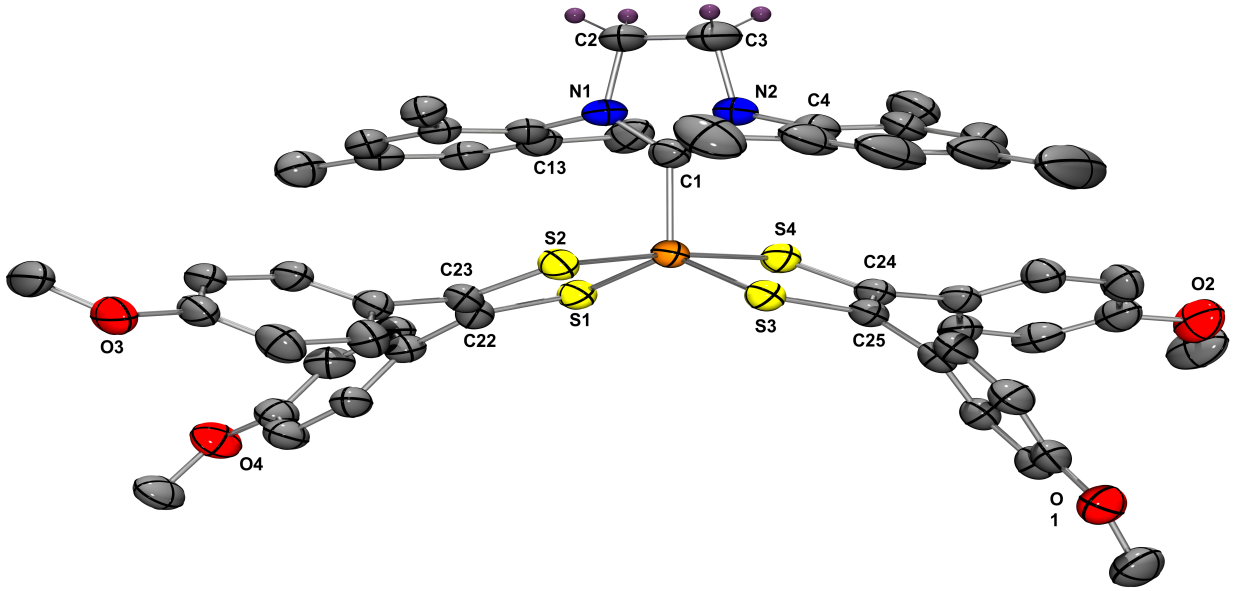


Figure S4. ORTEP diagram of **8** rendered by using POV-Ray. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms and solvent molecules are omitted for clarity. Selected distances [Å] and angles [°]:Fe1–S1, 2.1405(10); Fe1–S2, 2.1917(9); Fe1–S4, 2.2019(9); Fe1–S3, 2.1261(10); Fe1–C1, 1.940(3); N1–C1, 1.342(5); N1–C2, 1.477(4); S1–C22 1.717(3); S2–C23, 1.716(3); S4–C24, 1.717(4); S3–C25, 1.722(3); C2–C3, 1.496(6); S1–Fe1–S2, 87.81(3); S1–Fe1–S4, 90.62(4); C1–Fe1–S1, 113.02(12); C13–N1–C2, 117.2(3); N1–C1–N2, 107.1(3); N2–C1 Fe1, 126.5(3)

Electro- and spectroelectrochemistry

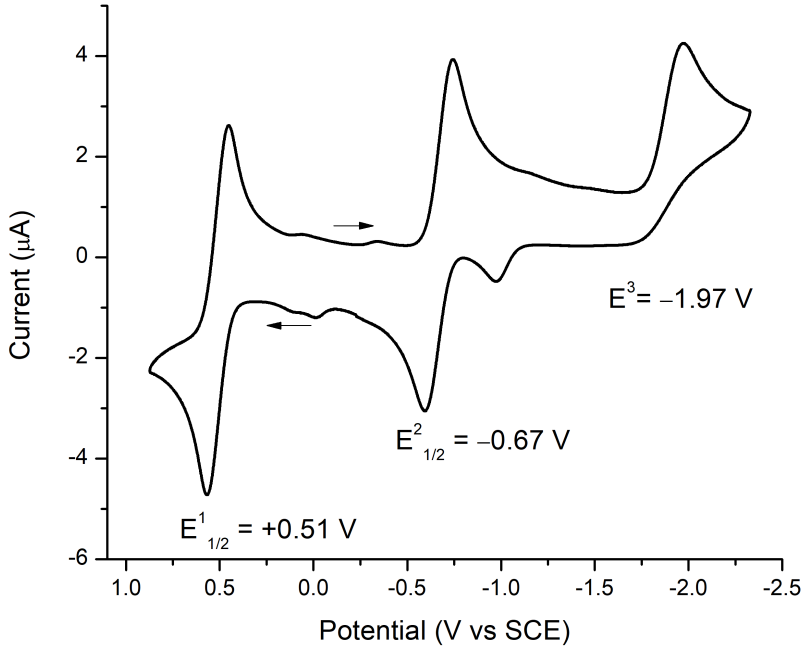


Figure S5. Cyclic voltammogram of **5** with 0.1M $[N(nBu)_4]PF_6$ in THF (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

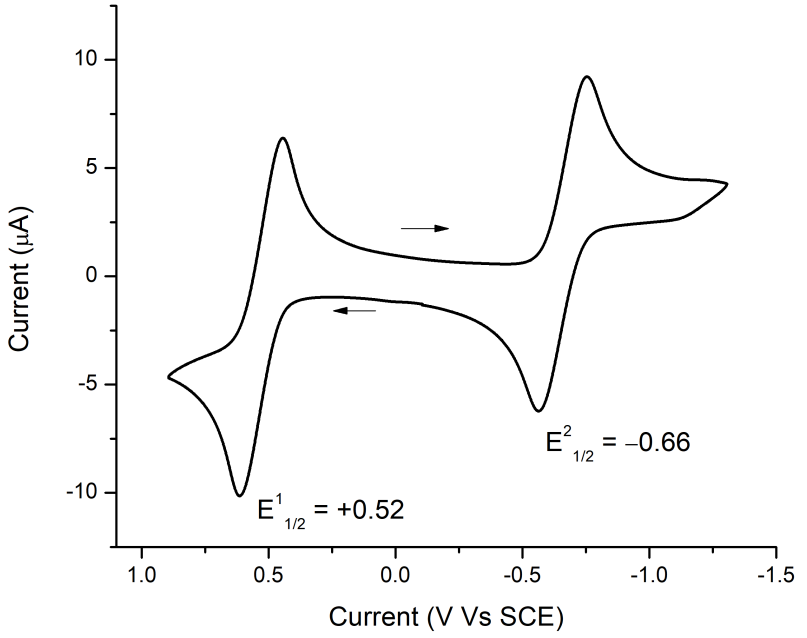


Figure S6. Cyclic voltammogram of **5** (short potential window (+1 to –1.5)) with 0.1M $[N(nBu)_4]PF_6$ in THF (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

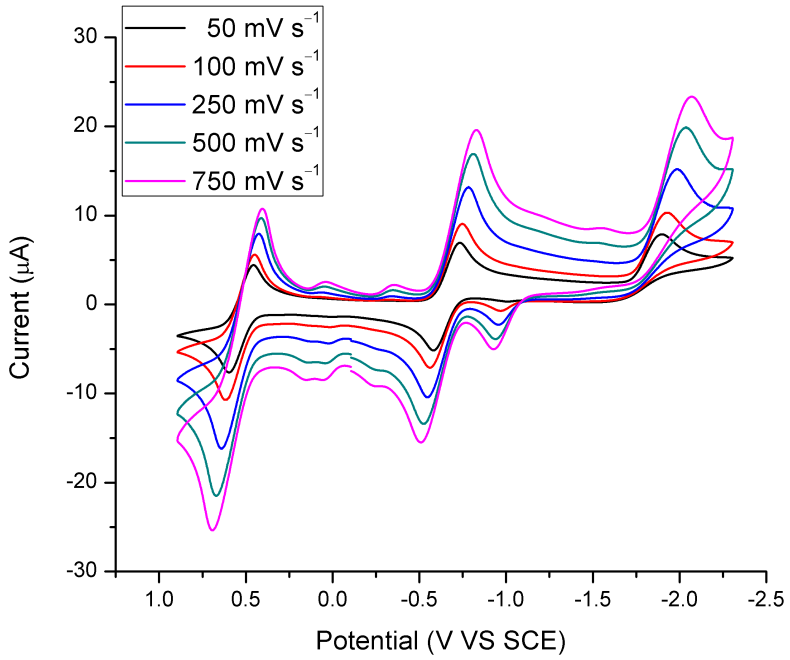


Figure S7. Cyclic voltammogram curves of **5** at various scan rates from 50 to 750 mV S^{-1} with 0.1M $[N(nBu)_4]PF_6$ in THF (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

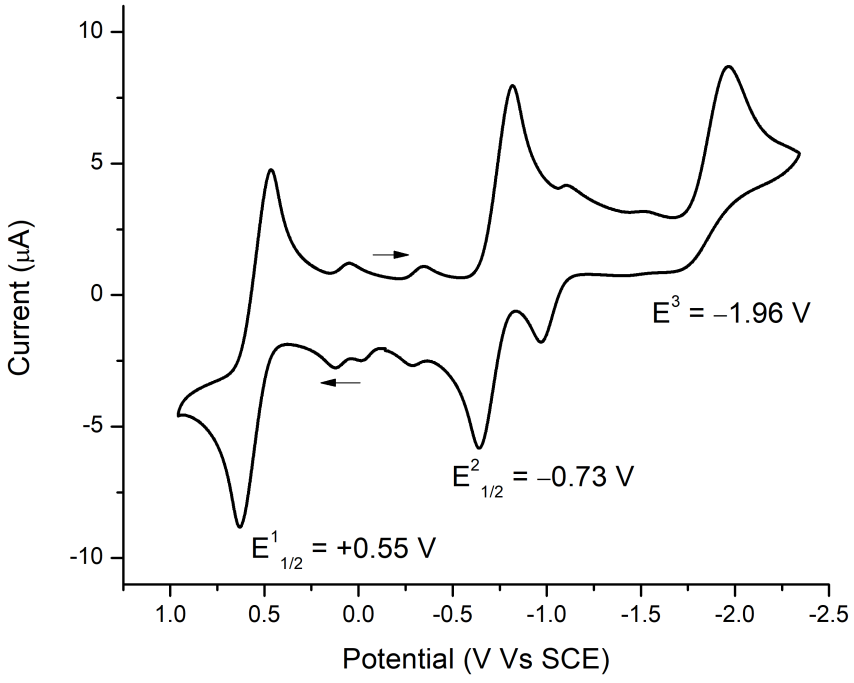


Figure S8. Cyclic voltammogram of **6** with 0.1M $[N(nBu)_4]PF_6$ in THF (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

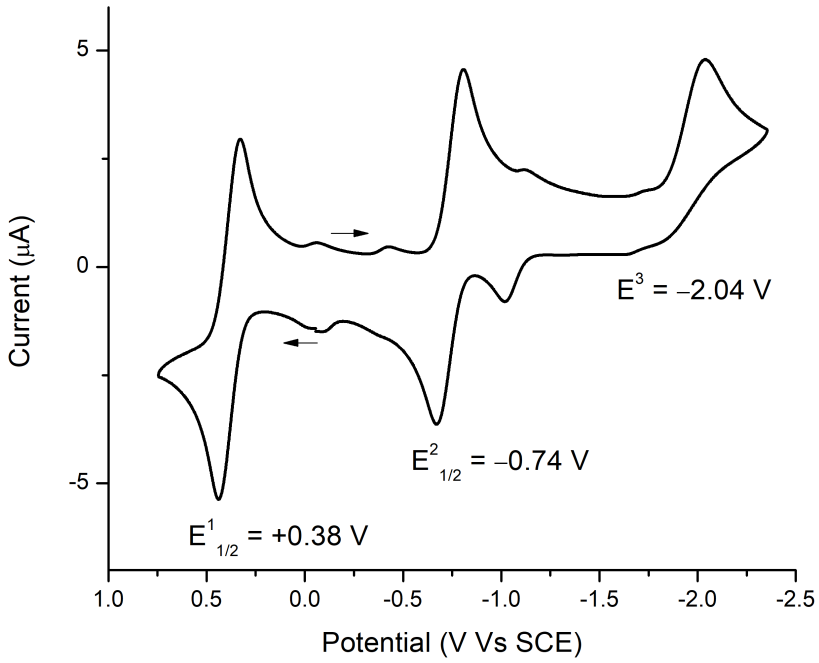


Figure S9. Cyclic voltammogram of **7** with 0.1M $[N(nBu)_4]PF_6$ in THF (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

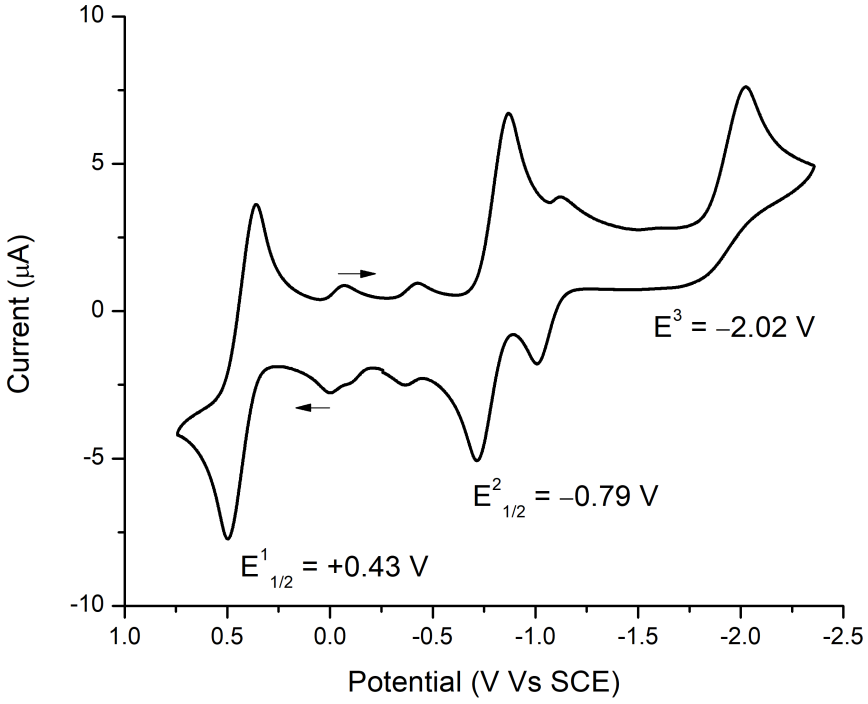


Figure S10. Cyclic voltammogram of **8** with 0.1M $[N(nBu)_4]PF_6$ in THF (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

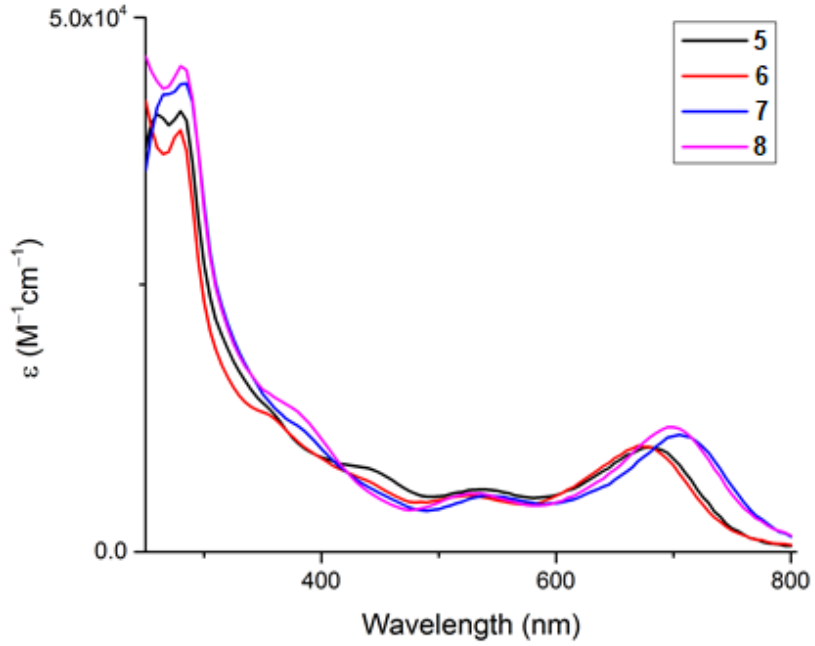


Figure S11. Electronic absorption spectra of adducts **5-8** recorded in tetrahydrofuran solvent.

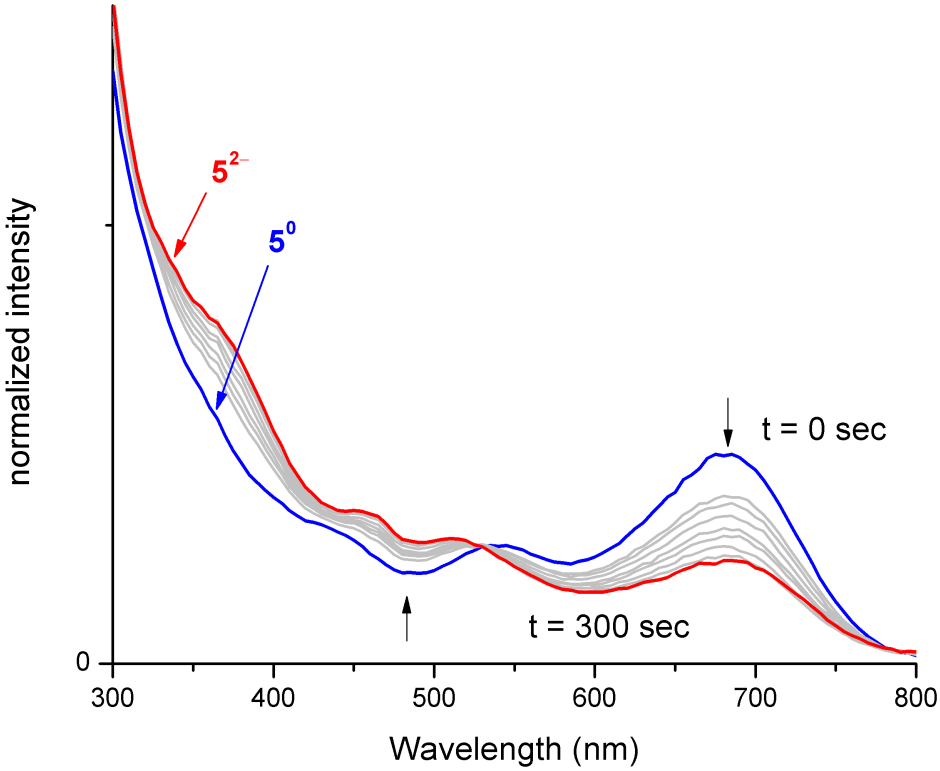


Figure S12: Electronic absorption spectra recorded during bulk reduction of compound **5** **(5→5^{2-})** holding at -2.25 (vs. AgCl) in THF with 0.1 M [N(*n*Bu)$_4$][PF$_6$] as the supporting electrolyte at 25 °C.

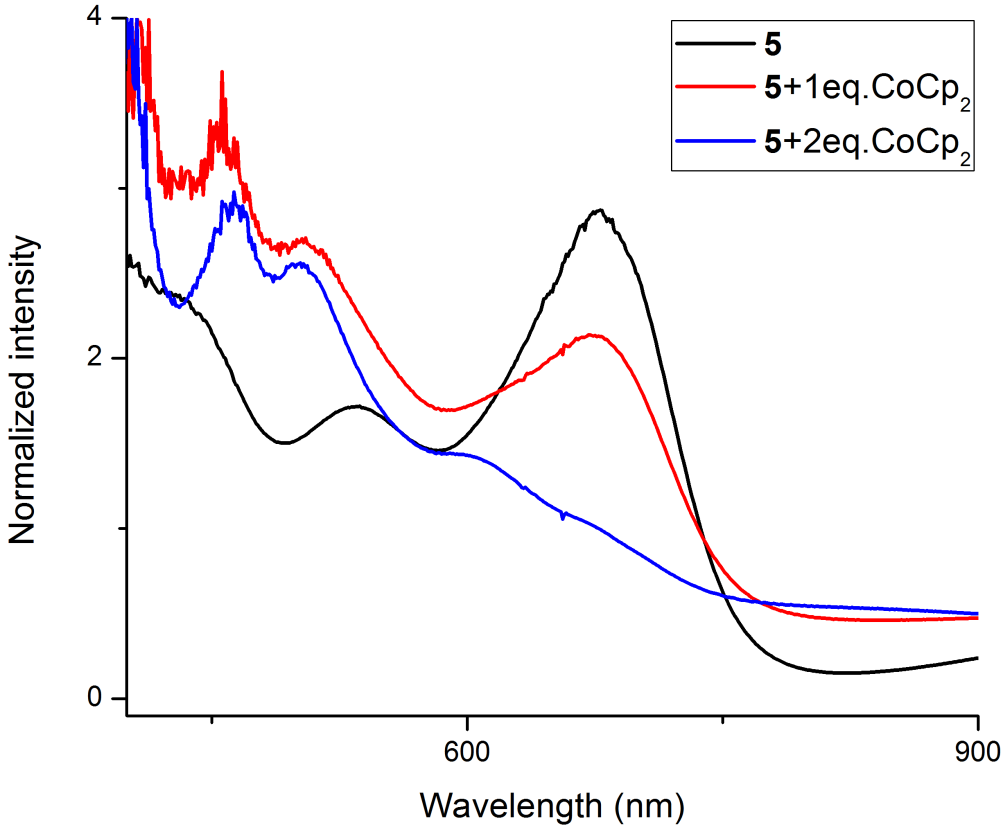
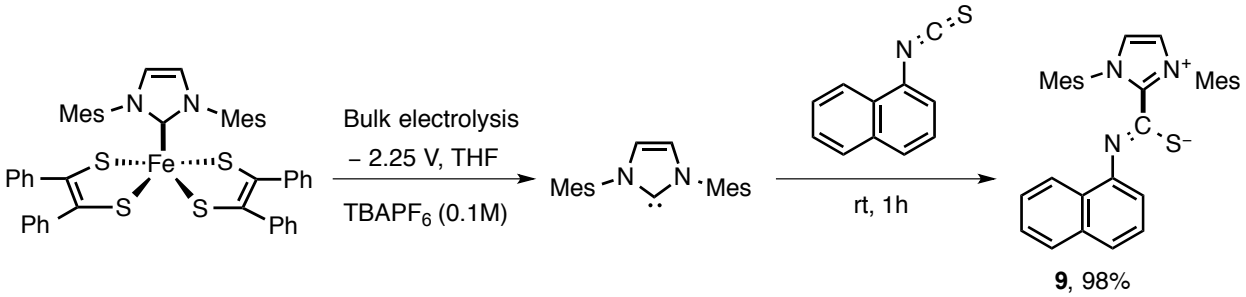


Figure S13. Electronic absorption spectra of **5**, $\mathbf{5}^{1-}$ and $\mathbf{5}^{2-}$ recorded in tetrahydrofuran solvent.

Chemical trapping of electrochemically generated carbene



9, 98%

20 mL of the electrolyte solution $TBAPF_6$ (774 mg, in degassed 20 mL THF) was equally transferred to the both compartment of the electrochemical cell. (17 mg, 0.02 mmol) of the catalyst **1** was dissolved on working electrode compartment. Working electrode (Pt mesh) and reference electrode (Ag/Ag^+ in MeCN) were immersed to one side compartment and Pt mesh counter electrode is immersed on the second compartment. Electrolysis was conducted at -2.25 V potential. After completing the electrolysis, the solution inside the working electrode compartment was transferred in to a 20 mL vial containing 1-naphthylisothiocyanate (0.3 mmol, 5.6 mg, 1.5 equiv.) and the solution was stirred for 1 h. 3 gm of silica gel was added to the mixture and solvent was removed. Resulting slurry was directly loaded in to the silica gel column. Gradual elution of column chromatography from 100% hexane to 30% EtOAc and 70% hexane yield the product **9** as yellow solid 9.5 mg (98% yield. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.63-7.55(m, 3H), 7.29-7.18 (m, 3H), 7.06 (s, 2H), 7.01 (s, 4H), 6.88-6.85 (m, 1H), 2.38 (s, 12H), 2.36 (s, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 165.31, 149.26, 146.92, 140.60, 135.89, 134.39, 131.55, 130.55, 129.47, 127.63, 127.60, 127.47, 125.06, 123.60, 123.34, 120.23, 117.48, 21.32, 18.53; LC-MS (ESI) for $[C_{32}H_{31}N_3S]^+$ $[M]^+$ Calcd. 489.22 Found. 489.22.

Faraday's Law of electrolysis calculation was used to calculated number of moles of electrons used for bulk electrolysis.

$Q = n(e^-)F$

Q = Quantity of electron measured in Coulombs (C)
$n(e^-)$ = moles of electrons used
F = Faraday constant (96500 C mol^{-1}).

Q = 3.817 C; F = 96500 C mol^{-1}
$n(e^-)$ = 3.817/96500= 3.9554×10^{-5}mole = **0.0395 mmol of electrons**

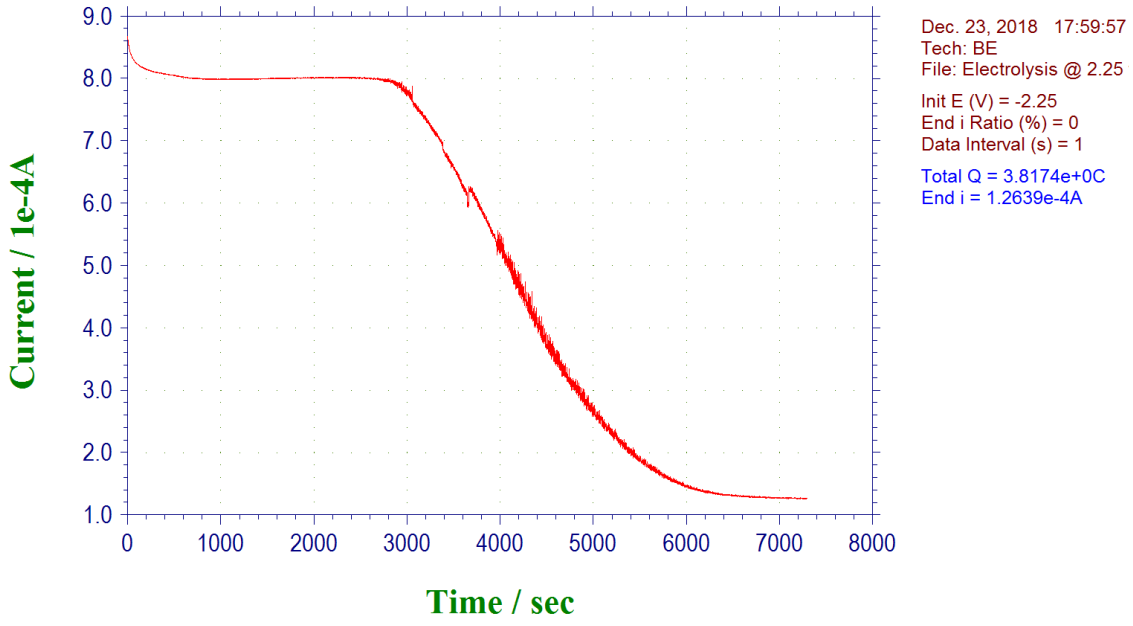
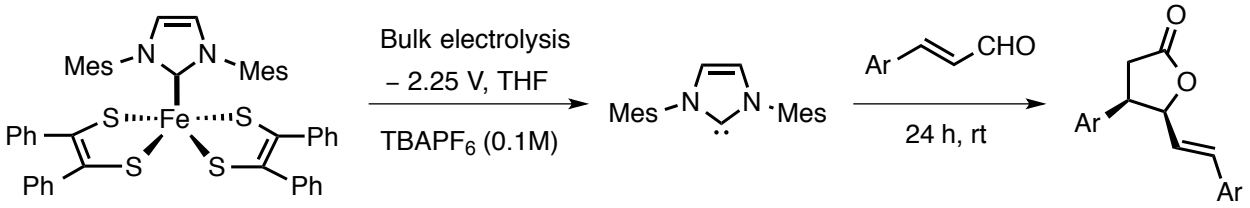
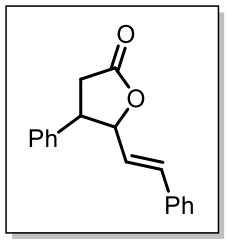


Figure S14: Current versus time output of bulk reduction of compound **5** **(5→5^{2-})** holding at -2.25 (vs. AgCl) in THF with 0.1 M [N(*n*Bu)$_4$][PF$_6$] as the supporting electrolyte at 25 °C.

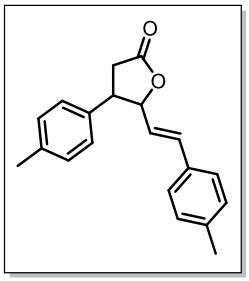
***In situ* organocatalysis of electrochemically generated carbene: synthesis of γ-butyrolactone**



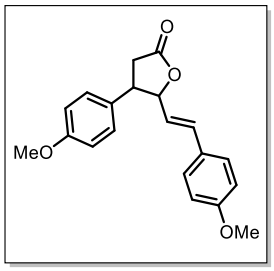
20 mL of the electrolyte solution TBAPF$_6$ (774 mg, in degassed 20 mL THF) was equally transferred to the both compartment of the electrochemical cell. (17 mg, 0.02 mmol) of the catalyst **1** was dissolved on working electrode compartment. Working electrode (Pt mesh) and reference electrode (Ag/Ag$^+$ in MeCN) were immersed to one side compartment and Pt mesh counter electrode is immersed on the second compartment. Electrolysis was conducted at –2.25 V potential. After completing the electrolysis, the solution inside the working electrode compartment was transferred in to a 20 mL vial containing cinnamaldehyde derivative (0.4 mmol, 53 mg) and the solution was stirred for 24 h. 3 gm of silica gel was added to the mixture and solvent was removed. Resulting slurry was directly loaded in to the silica gel column. Gradual elution of column chromatography from 100% hexane to 15% EtOAc and 85% hexane offered the γ-butyrolactones (**10-13**).



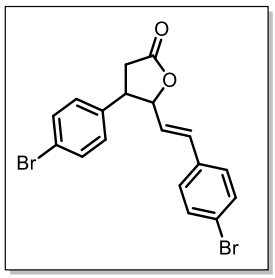
By following the above general procedure *trans*-cinnamaldehyde produced γ-butyrolactone **10** in 34% yield (18 mg), 1:0.16 *dr*. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.21-7.07 (m, 10H), 6.55 (d, *J* = 15.8 Hz, 1H), 5.58 (dd, *J* = 15.8, 6.5 Hz, 1H), 5.35-5.30 (m, 1H), 3.88 (q, J = 7.5 Hz, 1H), 2.95-2.79 (m, 1H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 176.45, 137.02, 135.87, 133.49, 128.93, 128.67, 128.29, 127.96, 127.88, 126.74, 123.90, 83.59, 45.70, 34.36. GC-MS (ESI) for $[C_{18}H_{16}O_2]^+$ $[M]^+$ Calcd. 264.1 Found. 264.1.



By following the above general procedure *trans*-4-methyl-cinnamaldehyde produced γ-butyrolactone **11** in 33% yield (18 mg), 1:0.5 *dr*. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.08-7.05 (m, 2H), 6.99-6.96 (m, 6H), 6.54-6.48 (m, 1H), 5.58-5.50 (m, 1H), 5.29-5.24 (m, 1H), 3.85-3.78 (m, 1H), 2.84-2.80 (m, 2H), 2.26 (s, 3H), 2.23 (s, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 176.46, 151.51, 138.12, 137.40, 133.81, 133.31, 133.09, 129.46, 129.25, 127.75, 126.60, 122.78, 83.76, 45.33, 34.39, 21.18, 21.04. GC-MS (ESI) for $[C_{20}H_{20}O_2]^+$ $[M]^+$ Calcd. 292.14 Found. 292.1.



By following the above general procedure *trans*-4-methoxy-cinnamaldehyde produced γ-butyrolactone **12** in 21% yield (18 mg), 1:0.5 *dr*. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.13-7.07 (m, 4H), 6.88-6.77 (m, 4H) 6.58-6.53 (m, 1H), 5.55-5.48 (m, 1H), 5.34-5.29 (m, 1H), 3.87-3.80 (m, 1 H), 3.80 (s, 3H), 3.78 (s, 3H), 2.92-2.85 (m, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 176.48, 159.69, 159.02, 133.03, 128.93, 127.93, 121.54, 114.15, 113.99, 84.04, 55.27, 44.98, 34.61. GC-MS (ESI) for $[C_{20}H_{20}O4]^+$ $[M]^+$ Calcd. 324.13 Found. 324.1.



By following the above general procedure *trans*-4-bromo-cinnamaldehyde produced γ-butyrolactone **13** in 24% yield (18 mg), 1:0 *dr*. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.40-7.35 (m, 4H), 7.08-7.01 (m, 4H), 6.58-6.53 (m, 1H), 5.65-5.58 (m, 1H), 5.37-5.32 (m, 1H), 3.93-3.86 (m, 1H), 3.01-2.69 (m, 2 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 175.75, 135.92, 132.62, 132.04, 131.83, 129.53, 128.17, 124.06, 122.35, 121.86, 82.92, 45.11, 34.35. GC-MS (ESI) for $[C_{18}H_{14}Br_2O_2]^+$ $[M]^+$ Calcd. 421.93 Found. 421.9.

Control experiments

In order to confirm electrochemically generated IMes carbene was the organocatalyst yielded the γ-butyrolactones following blank experiments were conducted.

1. Blank bulk electrolysis was conducted at −2.25 V without catalyst (only electrolyte) **5** (Fe(pdt)2IMes) for **3200 sec**. After completing the electrolysis, the solution inside the working electrode compartment was transferred into 20 mL vial containing cinnamaldehyde (0.4 mmol, 53 mg) and stirred for 24 h.

2. Complex **5** (3.5 mg, 0.04 mmol), Cinnamaldehyde (0.4 mmol, 53 mg) and 5 mL THF was stirred in 10 mL vial for 24 h.

Comparing butyrolactone **10** with aliquots from control experiment **1** and **2** in thin layer chromatography and ^{1}H-NMR confirm no butyrolactone **10** was formed during the blank experiments 1 and 2.

References

1. (a). Arduengo, A. J., III; Goerlich, J. R.; Marshall, W. J. *J. Am. Chem. Soc*. **1995**, *117*, 11027. (b). Kuhn, K. M.; Grubbs, R. H. *Org. Lett.* **2008**, *10*, 2075.
2. Schrauzer, G. N.; Mayweg, V. P.; Finck, H. W.; Heinrich, W. *J. Am. Chem. Soc.* **1966**, *88*, 4604.
3. Aranzaes, J. R.; Daniel, M. C.; Astruc, D. *Can. J. Chem.* **2006**, *84*, 288.
4. Addison, A. W.; Rao, T. N.; Reedijk, J.; van Rijn, J.; Verschoor, G. C. *J. Chem. Soc., Dalton Trans*. **1984**, 1349.

^{1}H and ^{13}C NMR of Compounds 5-8

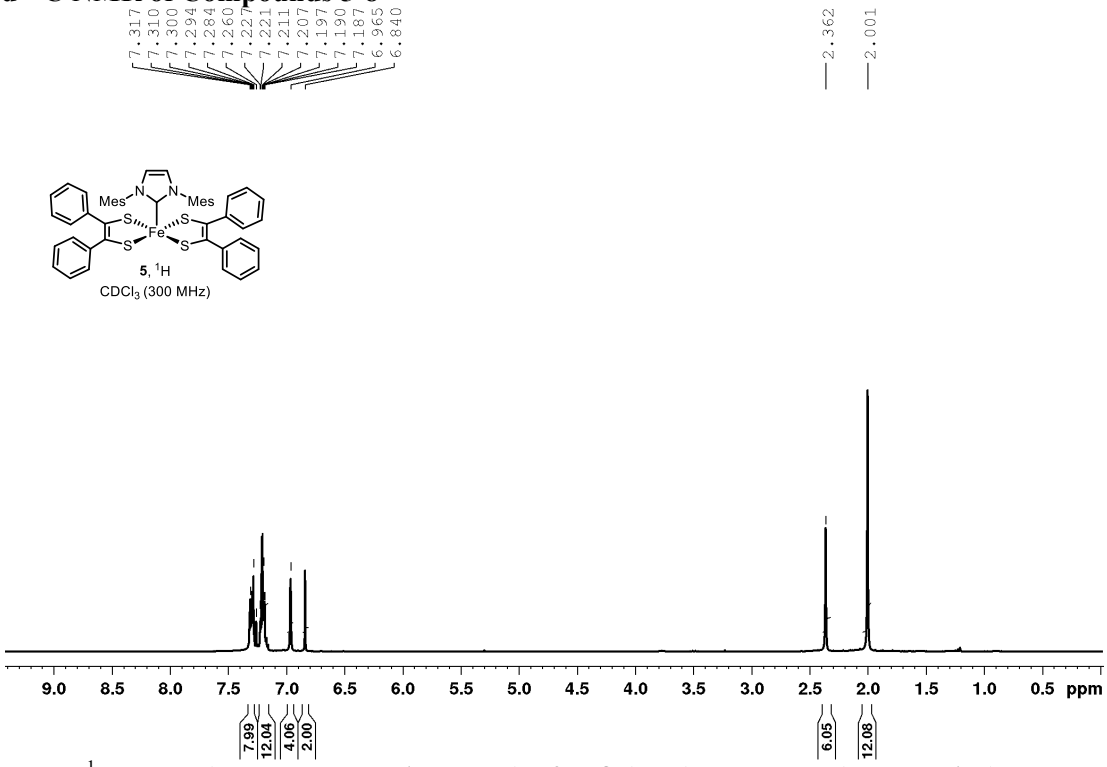


Figure S15. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **5**, δ (ppm): 7.31-7.28 (m, 8H, Ph*H*), 7.22-7.18 (m, 12H, Ph*H*), 6.96 (s, 4H, Ph*H*), 6.84 (s, 2H, C*H*=C*H*), 2.36 (s, 6H, CH_3), 2.00 (s, 12H, CH_3).

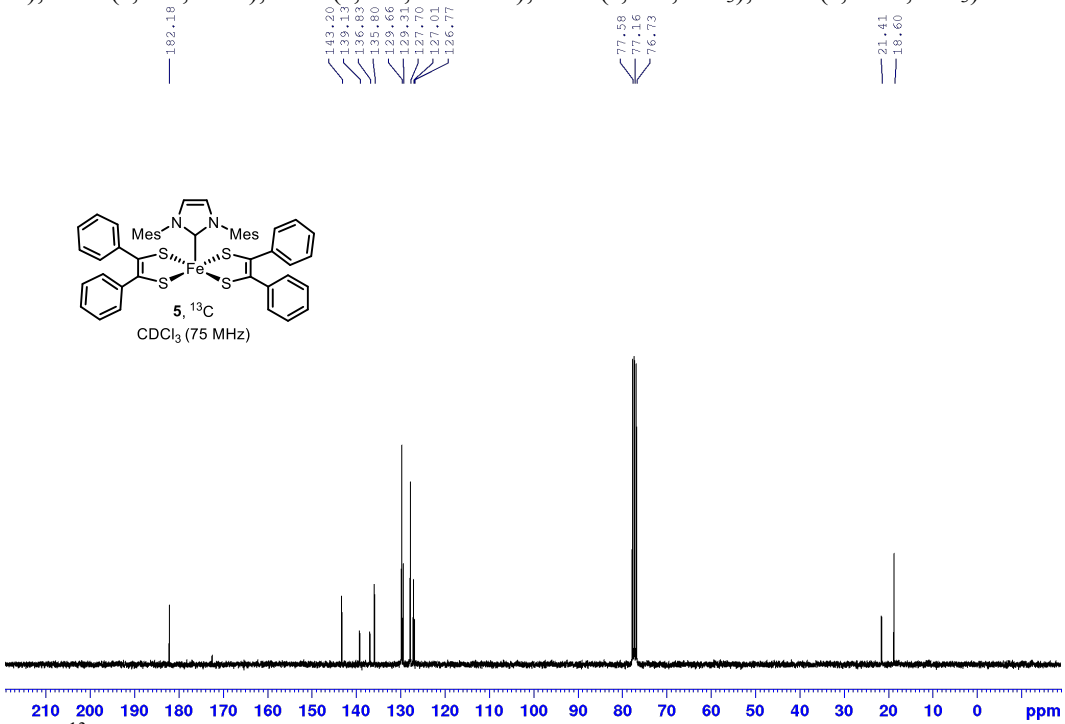


Figure S16. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **5**, δ (ppm): 182.18 (aromatic), 143.19 (aromatic), 139.13 (aromatic), 136.82 (aromatic), 135.80 (aromatic), 129.65 (aromatic), 129.31 (aromatic), 127.69(aromatic), 127.00 (aromatic), 126.77 (CH=CH), 21.41 (CH_3), 18.60 (CH_3).

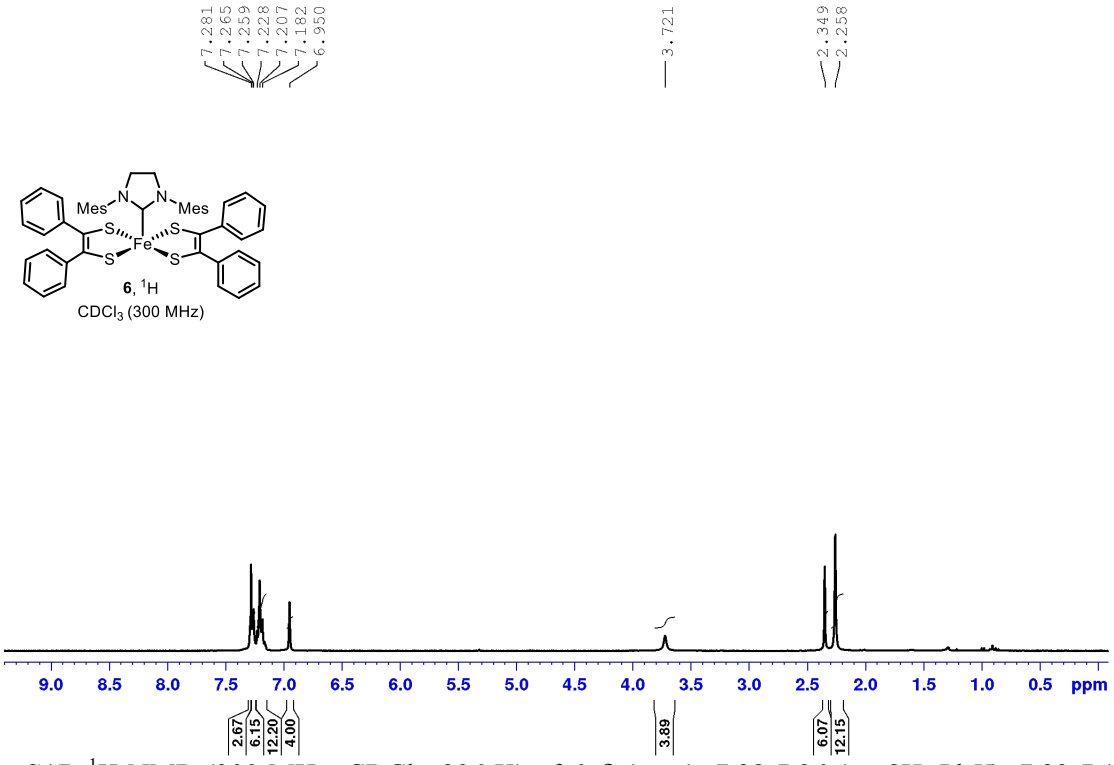


Figure S17. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **6**, δ (ppm): 7.28-7.26 (m, 8H, Ph*H*), 7.23-7.18 (m, 12H, Ph*H*), 6.95 (s, 4H, Ph*H*), 3.72 (s, 4H, CH_2-CH_2), 2.34 (s, 6H, CH_3), 2.26 (s, 12H, CH_3).

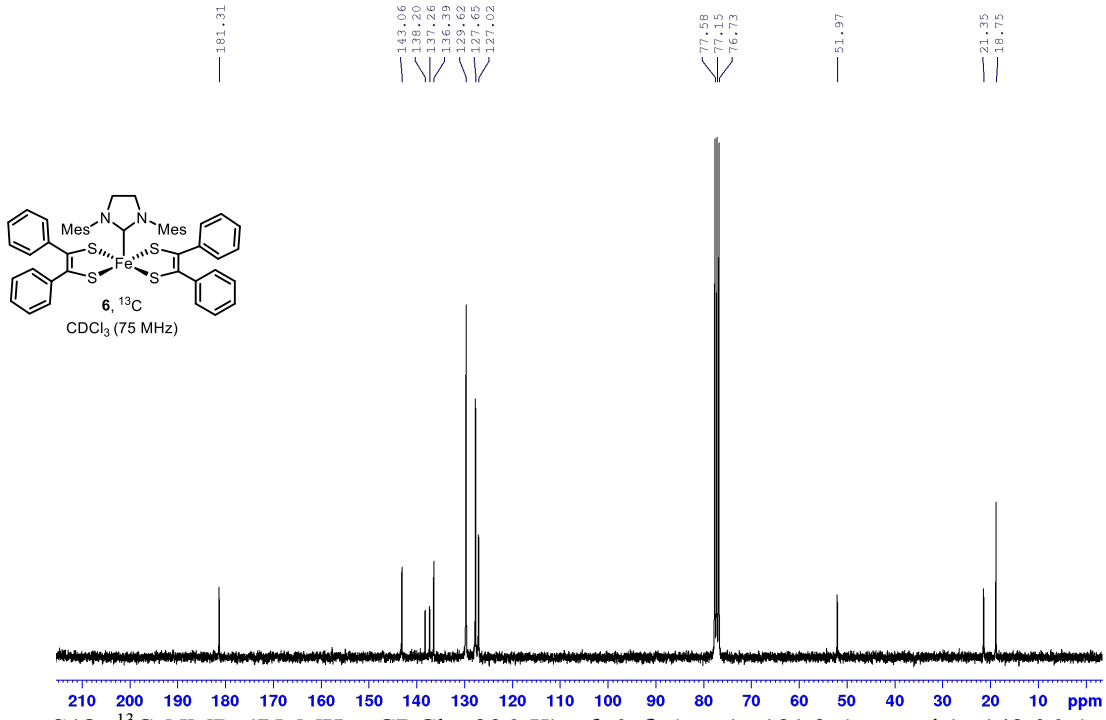


Figure S18. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **6**, δ (ppm): 181.3 (aromatic), 143.06 (aromatic), 138.20 (aromatic), 137.26 (aromatic), 136.39 (aromatic), 129.62 (aromatic), 127.65 (aromatic), 127.02 (aromatic), 51.97 (CH_2-CH_2), 21.35 (CH_3), 18.75 (CH_3).

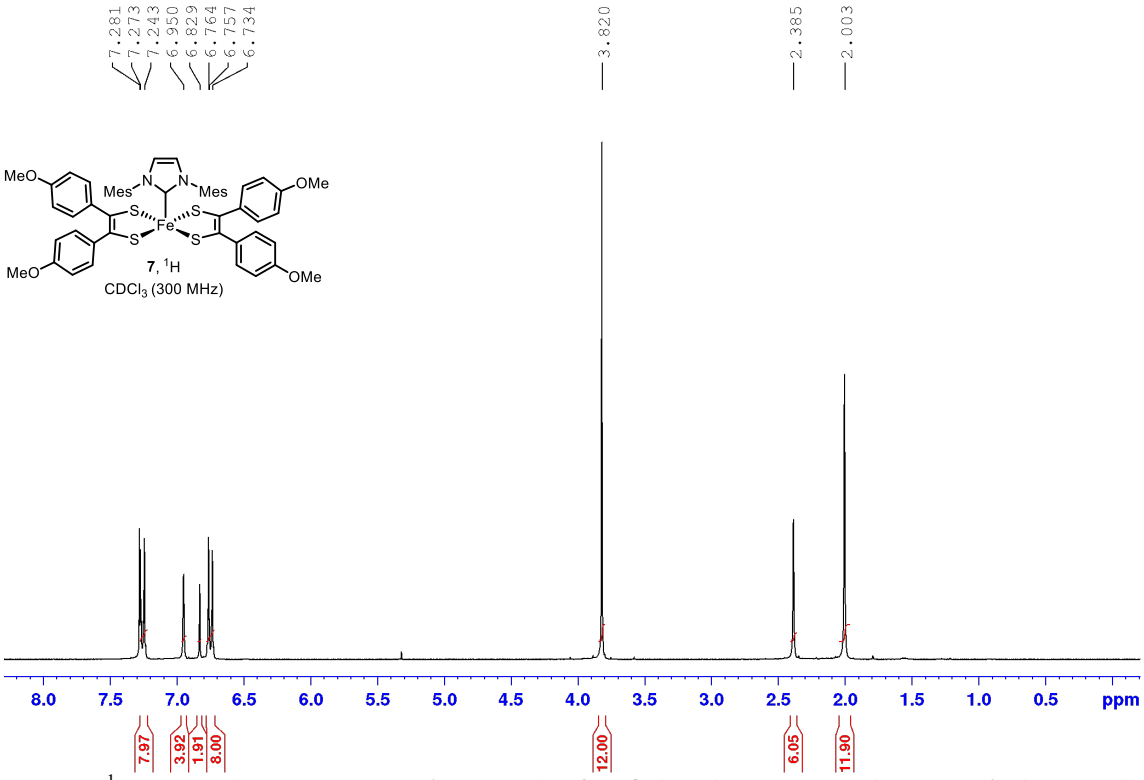


Figure S19. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **7**, δ (ppm): 7.27-7.24 (m, 8H, Ph*H*), 6.94 (s, 4H, Ph*H*), 6.82 (s, 2H, C*H*=C*H*), 6.76-6.73 (m, 8H, Ph*H*), 3.82 (s, 12 H, OCH_3), 2.36 (s, 6H, CH_3), 2.00 (s, 12H, CH_3).

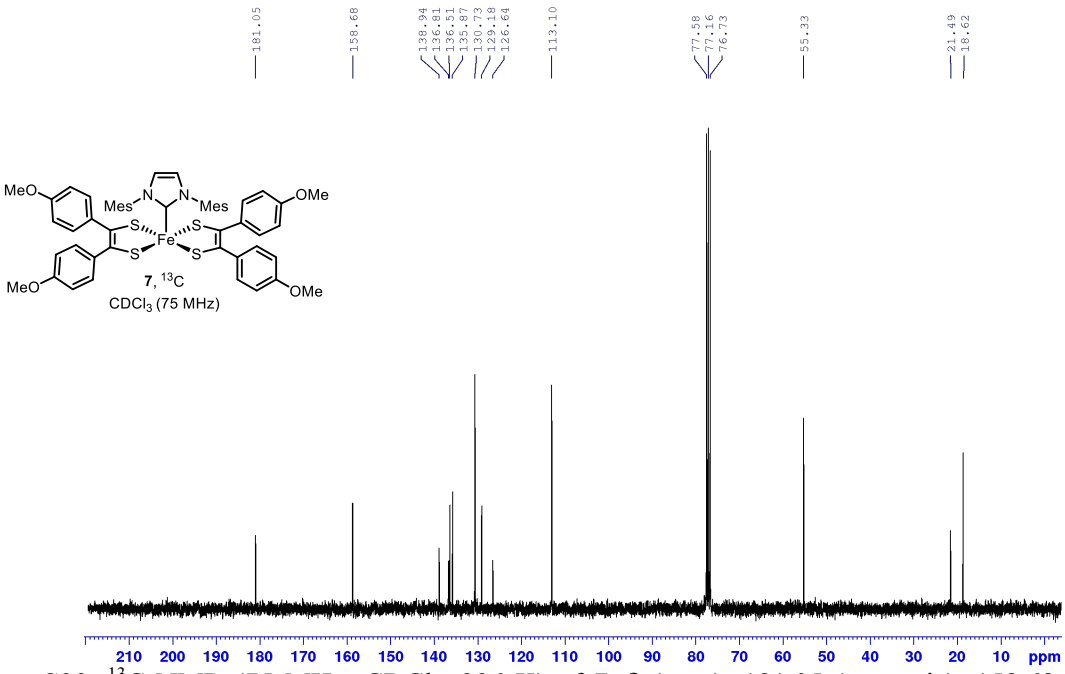


Figure S20. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **7**, δ (ppm): 181.05 (aromatic), 158.68 (aromatic), 138.94 (aromatic), 136.80 (aromatic), 136.51 (aromatic), 135.87 (aromatic), 130.73 (aromatic), 129.17 (aromatic), 126.63 (CH=CH), 113.09 (aromatic), 55.33 (OCH_3), 21.49 (CH_3), 18.62. (CH_3).

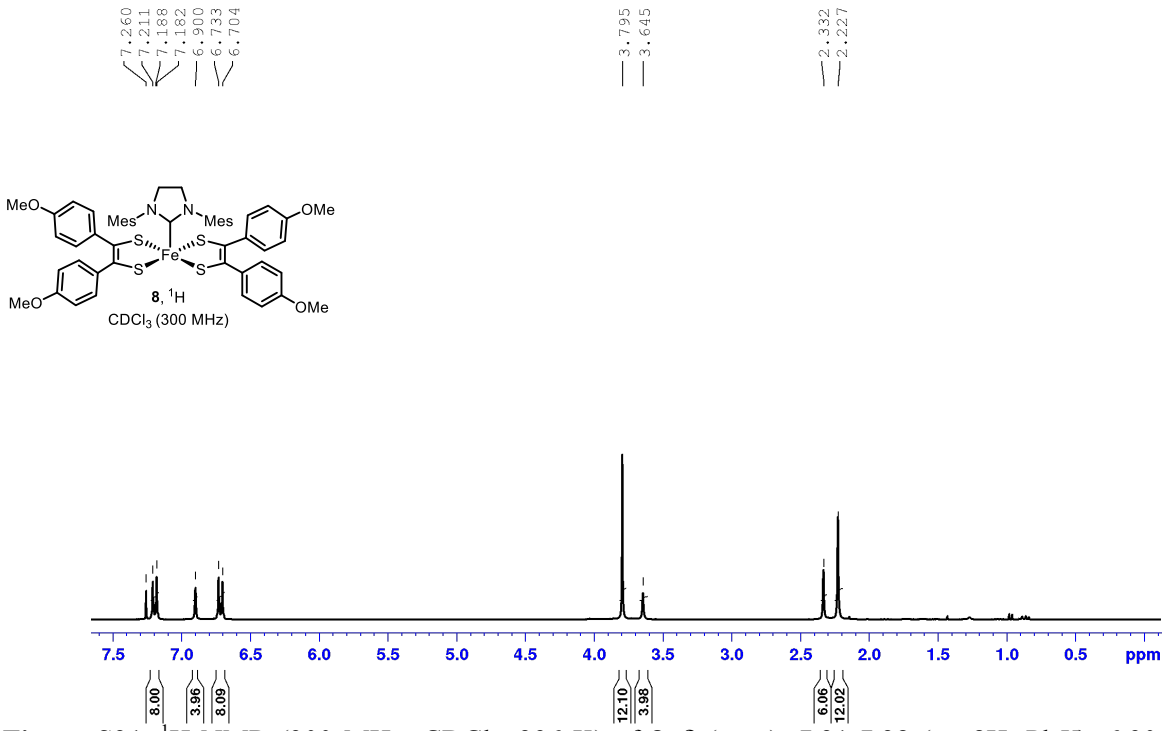


Figure S21. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **8**, δ (ppm): 7.21-7.28 (m, 8H, Ph*H*), 6.90 (s, 4H, Ph*H*), 6.73-6.70 (m, 8H, Ph*H*), 3.79 (s, 12H, OCH_3), 3.64 (s, 4 H, CH_2-CH_2), 2.33 (s, 6H, CH_3), 2.22 (s, 12H, CH_3).

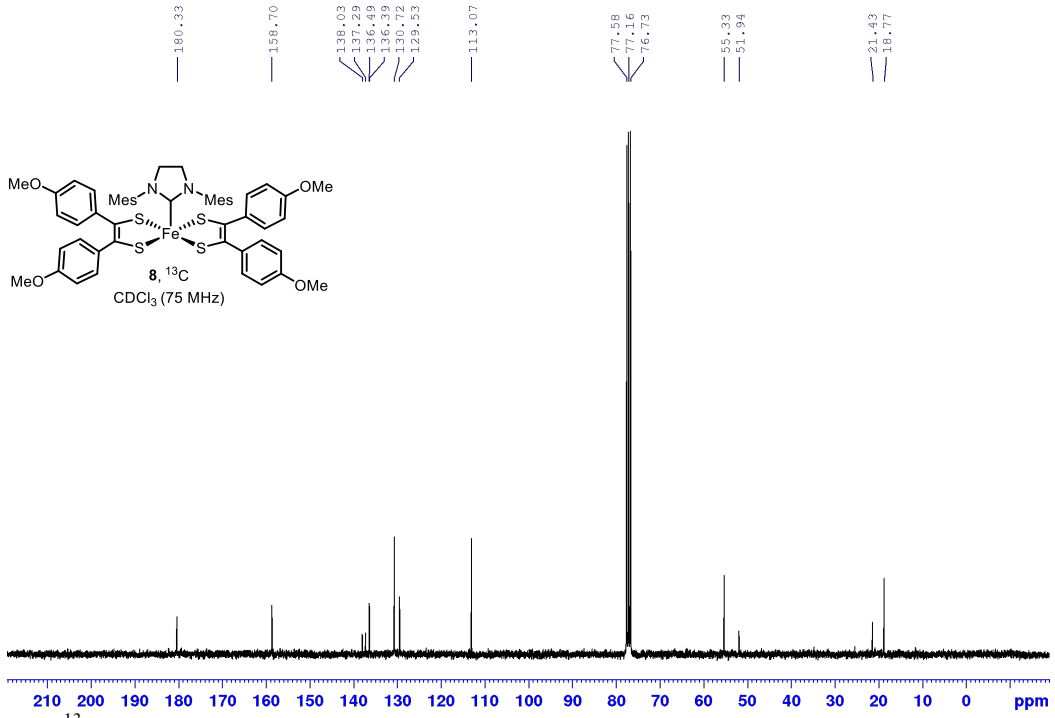


Figure S22. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **8**, δ (ppm): 180.32 (aromatic), 158.70 (aromatic), 138.03 (aromatic), 137.29 (aromatic), 136.48 (aromatic), 136.39 (aromatic), 130.72 (aromatic), 129.53 (aromatic), 113.06 (aromatic), 55.33 (OCH_3), 51.94 (CH_2-CH_2), 21.42 (CH_3), 18.77 (CH_3).

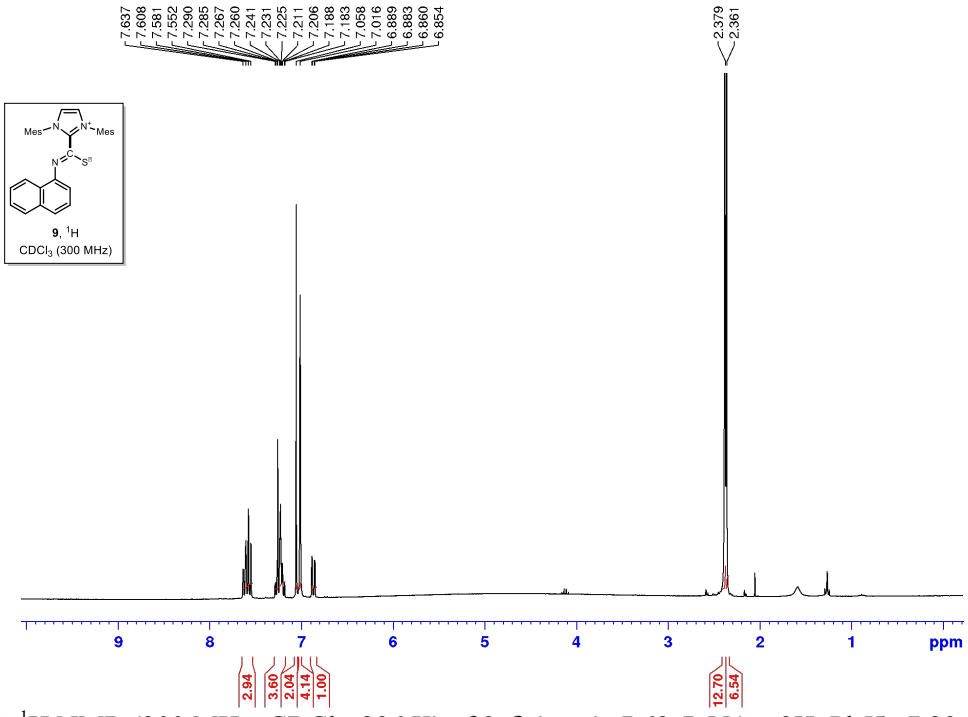


Figure S23. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **9**, δ (ppm): 7.63-7.55(m, 3H, Ph*H*), 7.29-7.18 (m, 3H, Ph*H*), 7.06 (s, 2H, C*H*=C*H*), 7.01 (s, 4H, Ph*H*), 6.88-6.85 (m, 1H, Ph*H*), 2.38 (s, 12H, CH_3), 2.36 (s, 6H, CH_3).

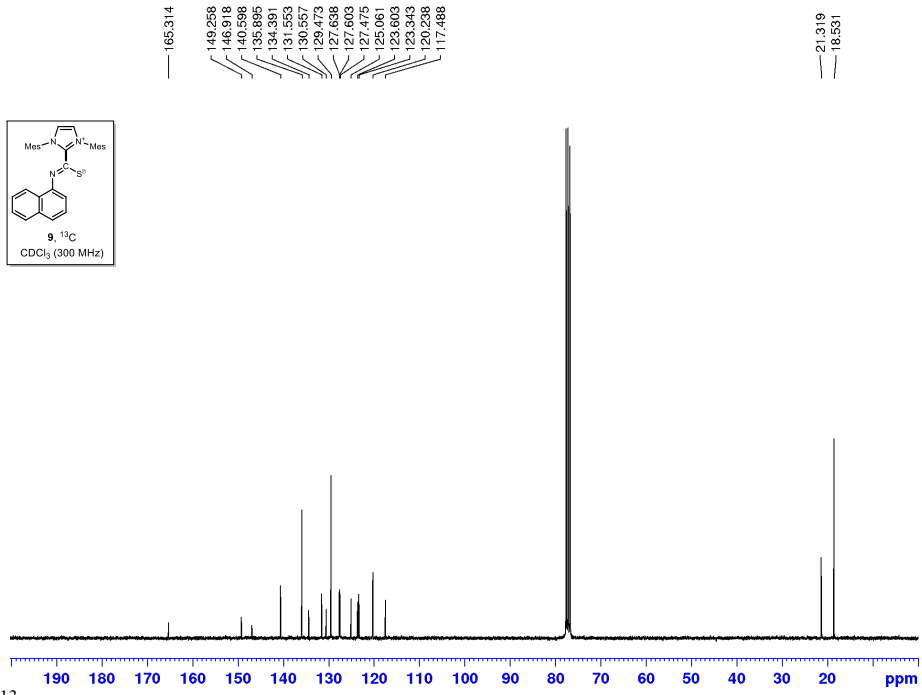


Figure S24. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **9**, δ (ppm): 165.31 (aromatic), 149.26 (aromatic), 146.92 (aromatic), 140.60 (aromatic), 135.89 (aromatic), 134.39 (aromatic), 131.55 (aromatic), 130.55 (aromatic), 129.47 (aromatic), 127.63 (aromatic), 127.60 (aromatic), 127.47 (aromatic), 125.06 (aromatic), 123.60 (aromatic), 123.34 (aromatic), 120.23 (CH=CH), 117.48 (aromatic), 21.32 (CH_3), 18.53 (CH_3).

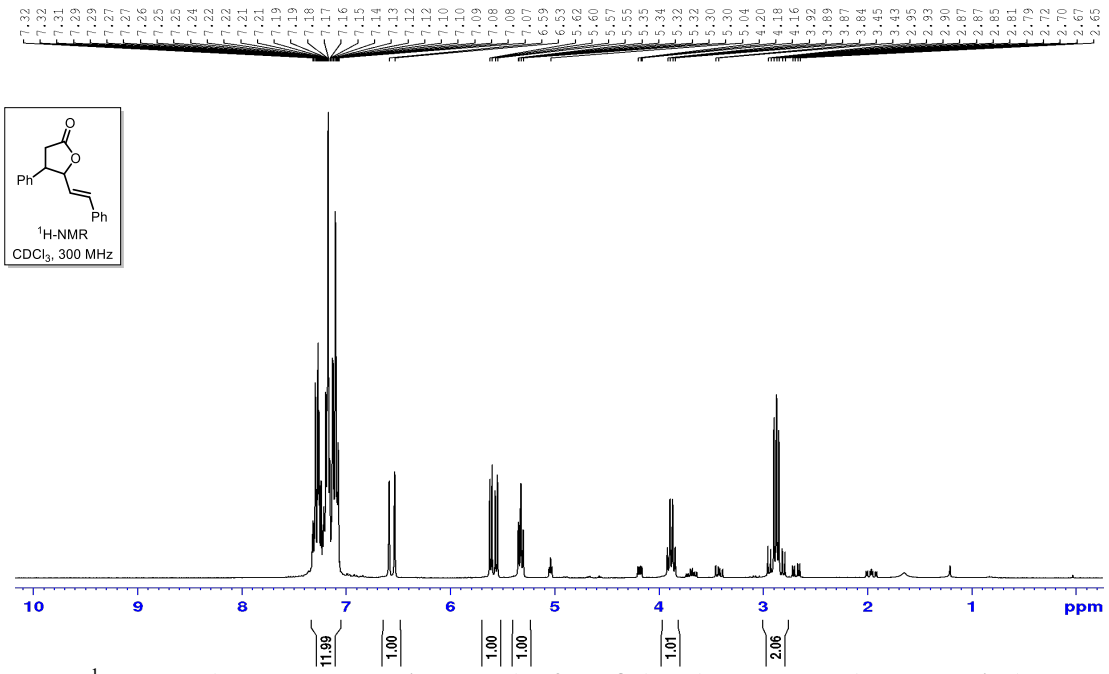


Figure S25. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **10**, δ (ppm): 7.21-7.07 (m, 10H, Ph*H*), 6.55 (d, *J* = 15.8 Hz, 1H, CH=C*H*), 5.58 (dd, *J* = 15.8, 6.5 Hz, 1H, CH-C*H*=CH), 5.35-5.30 (m, 1H, CH=CH-C*H*), 3.88 (q, *J* = 7.5 Hz, 1H, PhC*H*), 2.95-2.79 (m, 2H, CH_2C=O).

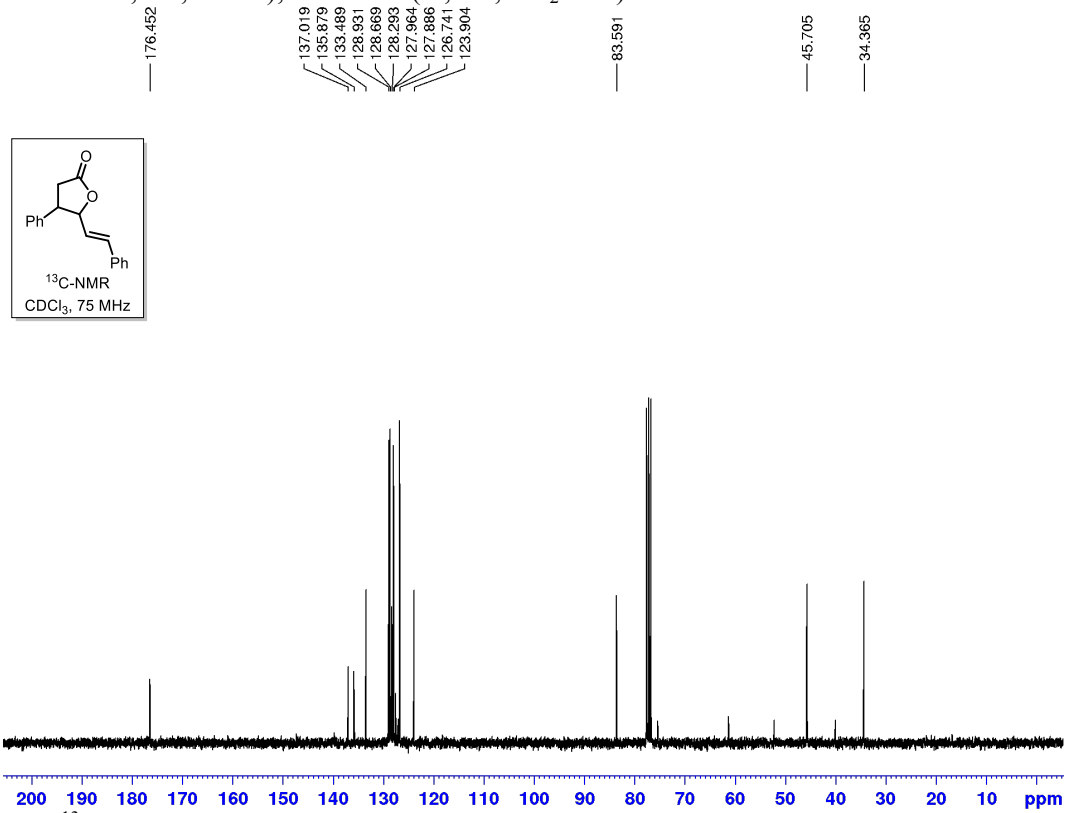


Figure S26. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **10**, δ (ppm): 176.45 (C=O), 137.02 (aromatic), 135.87 (aromatic), 133.49 (aromatic), 128.93 (aromatic), 128.67 (aromatic), 128.29 (aromatic), 127.96 (aromatic), 127.88 (aromatic), 126.74 (Ph*C*H=CH), 123.90 (PhCH=*C*H), 83.59 (CH=CH-*C*H), 45.70 (Ph*C*H), 34.36 (CH_2CO).

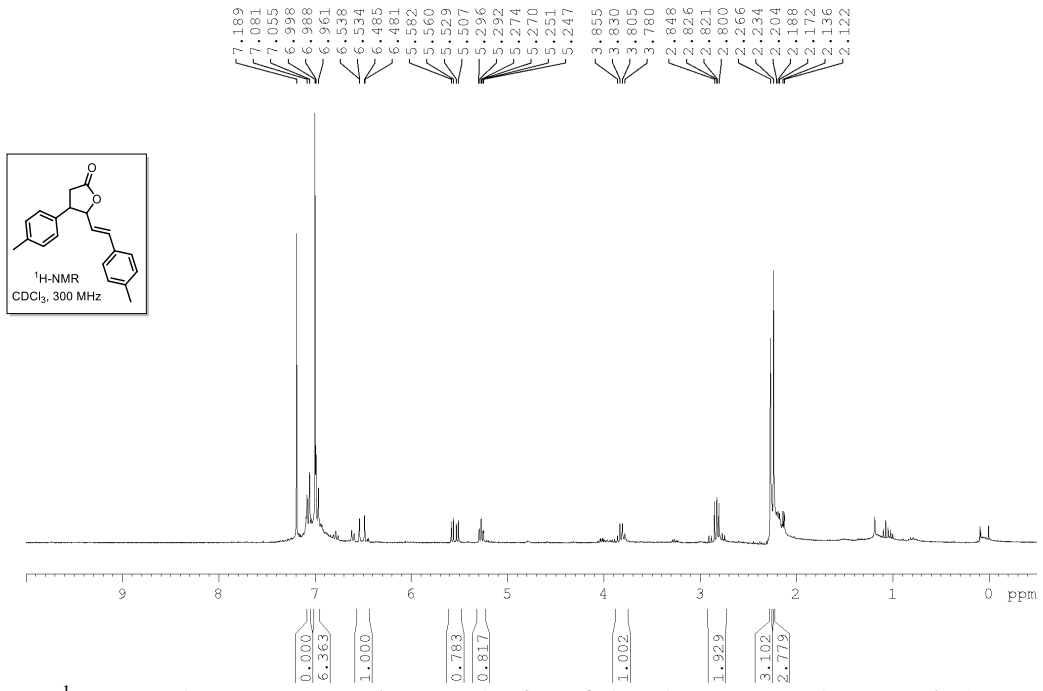


Figure S27. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **11**, δ (ppm): 7.08-7.05 (m, 2H, Ph*H*), 6.99-6.96 (m, 6H, Ph*H*), 6.54-6.48 (m, 1H, PhC*H*=), 5.58-5.50 (m, 1H, PhCH=C*H*), 5.29-5.24 (m, 1H, CH=CH-C*H*), 3.85-3.78 (m, 1H, PhC*H*), 2.84-2.80 (m, 2H, CH_2C=O), 2.26 (s, 3H, CH_3), 2.23 (s, 3H, CH_3).

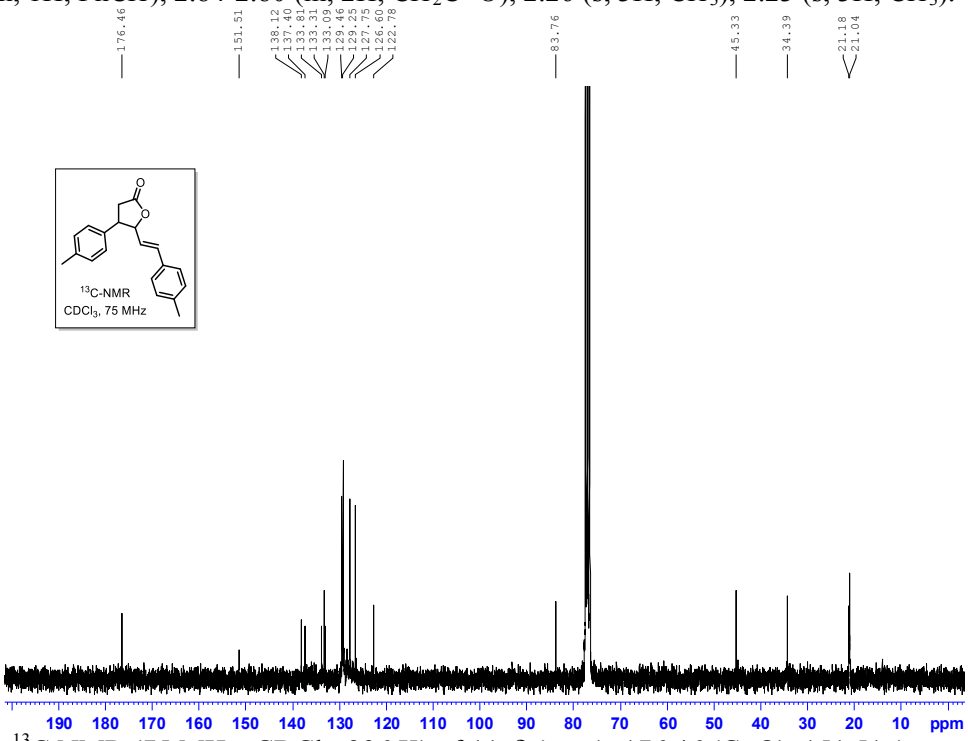


Figure S28. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **11**, δ (ppm): 176.46 (C=O), 151.51 (aromatic), 138.12 (aromatic), 137.40 (aromatic), 133.81 (aromatic), 133.31 (aromatic), 133.09 (aromatic), 129.46 (aromatic), 129.25 (aromatic), 127.75 (aromatic), 126.60 (Ph*C*H=CH), 122.78 (PhCH=*C*H), 83.76 (CH=CH-*C*H), 45.33 (Ph*C*H), 34.39 (CH_2), 21.18 (CH_3), 21.04 (CH_3).

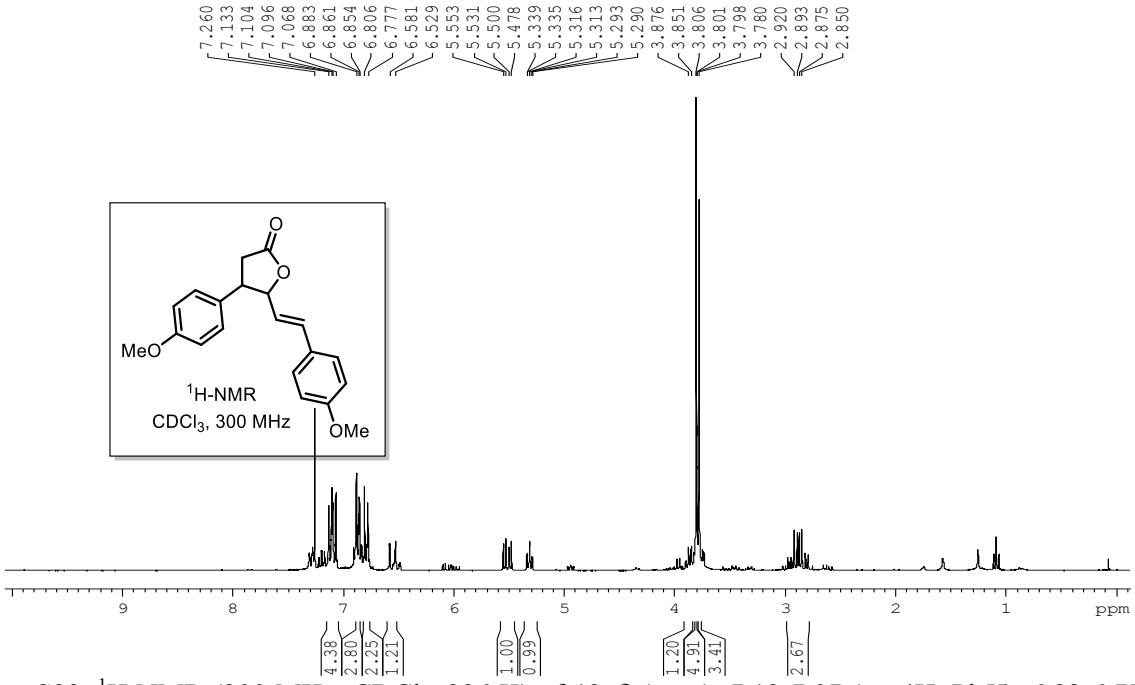


Figure S29. ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **12**, δ (ppm): 7.13-7.07 (m, 4H, Ph*H*), 6.88-6.77 (m, 4H, Ph*H*) 6.58-6.53 (m, 1H, PhC*H*=CH), 5.55-5.48 (PhCH=C*H*) (m, 1H), 5.34-5.29 (m, 1H, CH=CH-C*H*), 3.87-3.80 (m, 1 H, PhC*H*), 3.80 (s, 3H, OCH_3), 3.78 (s, 3H, OCH_3), 2.92-2.85 (m, 2H, CH_2C=O).

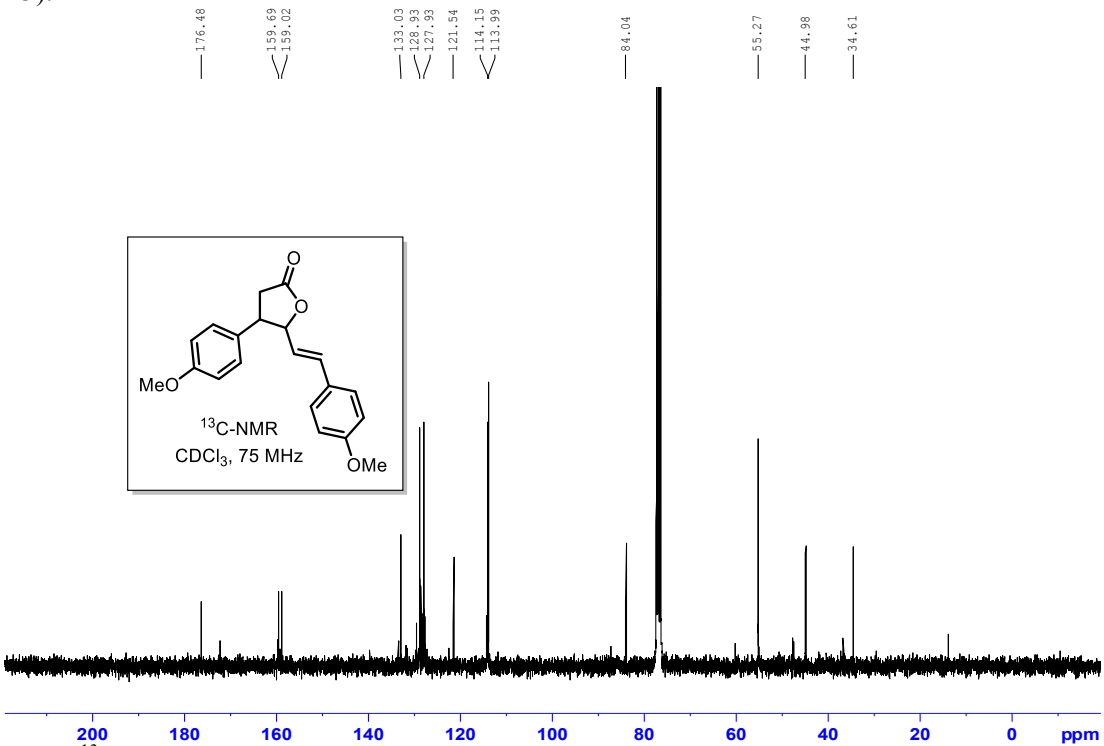


Figure S30. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **12**, δ (ppm): 176.48 (C=O), 159.69 (aromatic), 159.02 (aromatic), 133.03 (aromatic), 128.93 (aromatic), 127.93 (aromatic), 121.54 (aromatic), 114.15 (Ph*C*H=CH), 113.99 (PhCH=*C*H), 84.04 (CH=CH-*C*H), 55.27 (OCH_3), 44.98 (Ph*C*H), 34.61 (CH_2CO).

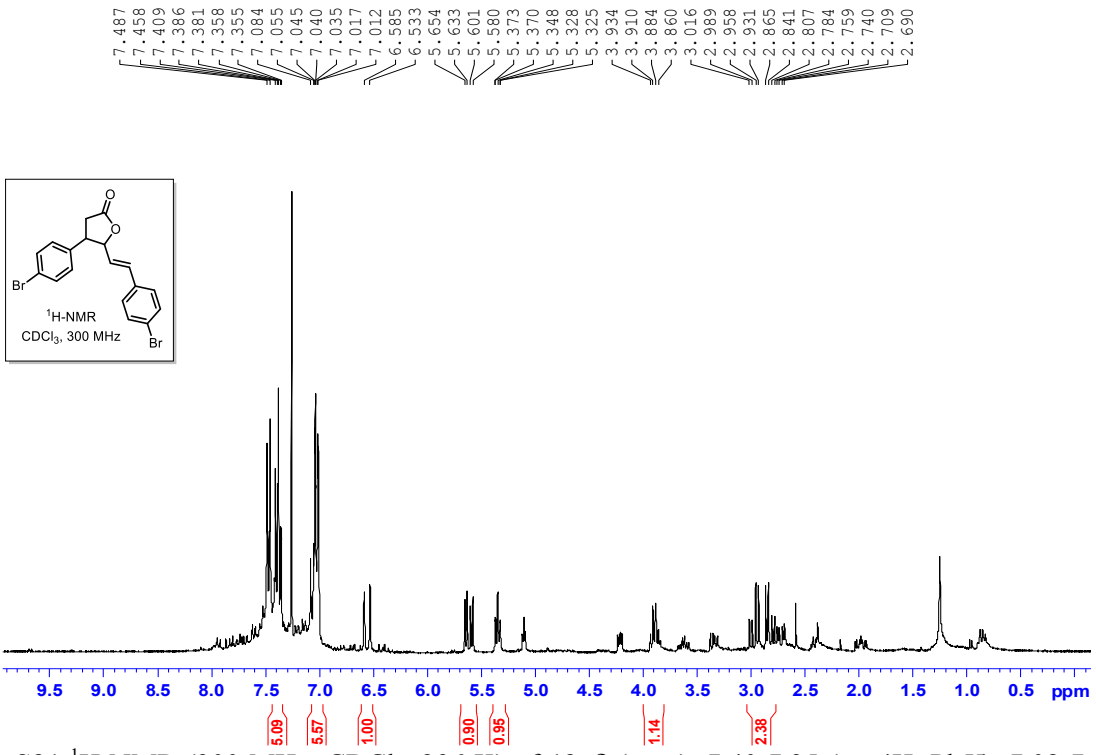


Figure S31 ^{1}H NMR (300 MHz, $CDCl_3$, 296 K) of **13**, δ (ppm): 7.40-7.35 (m, 4H, Ph*H*), 7.08-7.01 (m, 4H, Ph*H*), 6.58-6.53 (m, 1H, PhC*H*=CH), 5.65-5.58 (m, 1H, PhCH=C*H*), 5.37-5.32 (m, 1H, PhCH=CH-C*H*), 3.93-3.86 (m, 1H, PhC*H*), 3.01-2.69 (m, 2 H, CH_2C=O).

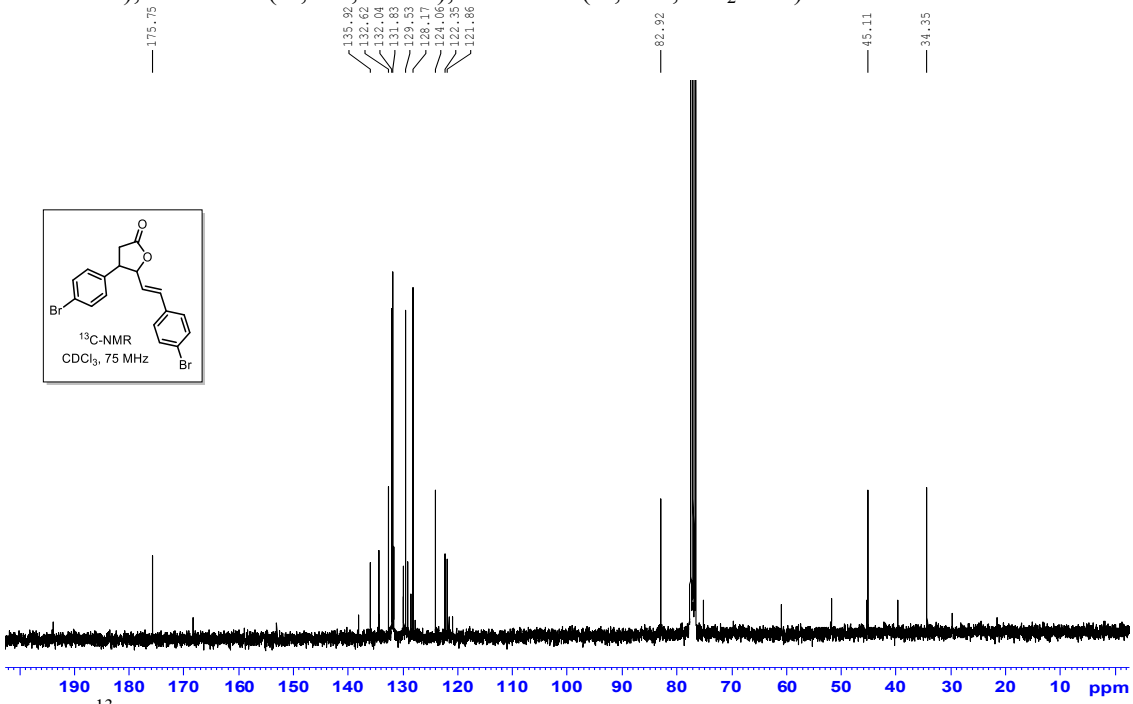


Figure S32. ^{13}C NMR (75 MHz, $CDCl_3$, 296 K) of **13**, δ (ppm): 175.75 (C=O), 135.92 (aromatic), 132.62 (aromatic), 132.04 (aromatic), 131.83 (aromatic), 129.53 (aromatic), 128.17 (aromatic), 124.06 (aromatic), 122.35 (Ph*C*H=CH), 121.86 (PhCH=*C*H), 82.92 (CH=CH-*C*H), 45.11 (Ph*C*H), 34.35 (CH_2C=O).

Comparison of experimental bond lengths with DFT optimized bond lengths

Below are tables that contain the measured bond lengths in the crystal, the bond lengths computed for the molecular complex with an S=0, S=1, and S=2 spin state (Å), and the τ parameter for each of the tested functionals. The S=0* has the same geometry as the S=1 state. The method by Noodleman and the spinflip option in ADF are conducted by taking the converged electron density from the spin unpaired case (S=1) the restarting the calculation to converge to the broken spin-symmetry configuration (S=0*). For each spin state, the mean absolute error (MAE) and root-mean-square error (RMS) is indicated for the measured bonds. The absolute error (AE) for τ is also indicated for each spin state. The utilized functional is indicated above the table.

In our calculations the B3LYP and PBE0 functionals yielded similar results, with the $S = 1$ state being preferred, the $S = 2$ being second lowest in energy, the $S = 0$ the second highest, and the $S = 0$* highest. The decrease of exact exchange in the B3LYP* functional affects the difference in energy between the $S = 0$, $S = 0$*, and $S = 1$ states, and the low spin $S = 0$ is slightly preferred. The GGA functionals, on the other hand, favor the $S = 0$ state. The only tested meta-GGA functional showed that the antiferromagnetically coupled state ($S = 0$*) was preferred over the $S = 0$ state by 0.3 kcal/mol, but otherwise followed a similar trend as the GGA functionals. As shown in the SI, the PBE functional provides the best description of the Fe-S, Fe-C and N-C bond lengths, followed closely by the TPSS functional, while the BP86 functional performed the best at calculating the bond angles, with the B3LYP functional as a close 2nd. However, it should be pointed out that the molecular models used herein cannot mimic the crystal packing and electrostatic effects that are present in the extended compound.

As previously mentioned, there are two possible ways to obtain a diamagnetic solution for **5**. The energetic difference between the Pauli coupled ($S = 0$) and the antiferomagnetically coupled ($S = 0$*) states were calculated to be 2.6, 3.3, 5.8, and 4.8 kcal/mol for the BP86, PBE, PBEsol, and revPBE functionals, respectively, favouring the S=0 state. While the hybrid functionals found that the $S = 1$ state was energetically preferred over both the $S = 0$ and the $S = 0$* states, the energetic difference between the singlet spin states was found to be 0.9, 2.2, and 0.3 kcal/mol, for the B3LYP, B3LYP*, and PBE0 functionals, respectively, with the $S = 0$ being favoured yet again. From all of the tested functionals it was only the TPSS that favoured the antiferromagnetic state by 0.3 kcal/mol. However, the experimentally measured bond lengths extracted from the crystal structure were in better agreement with functionals for which the $S = 0$ state was preferred to the antiferromagnetically coupled state. Therefore, we conclude that the BP86 and PBE functionals utilized herein are better suited to model this system as they had the smallest error between the calculated and experimental bond lengths or bond angles, and these functionals predicted spin states that corresponded to experimental observations. Our functional selection essentially mirrors conclusions about BP86, B3LYP, and B3LYP* results obtained by Jacobsen et al. for similar systems. We therefore studied the electronic structure of **5** using the BP86 functional, as described below.

revPBE				
Length	**Xtal**	**S=0**	**S=1**	**S=2**
Fe-S1	2.180	2.234	2.244	2.308
Fe-S2	2.157	2.183	2.243	2.289
Fe-C	1.963	1.978	2.049	2.267
N-C	1.362	1.394	1.385	1.381
τ	0.22	0.32	0.46	0.39
	MAE(Bonds)	0.032	0.065	0.146
	RMS(bonds)	0.035	0.070	0.178
	AE(τ)	0.094	0.234	0.164

PBE				
Length	**Xtal**	**S=0**	**S=1**	**S=2**
Fe-S1	2.180	2.171	2.228	2.298
Fe-S2	2.157	2.170	2.223	2.274
Fe-C	1.963	1.957	2.015	2.216
N-C	1.362	1.388	1.378	1.374
τ	0.22	0.29	0.38	0.29
	MAE(Bonds)	0.014	0.045	0.125
	RMS(bonds)	0.016	0.049	0.151
	AE(τ)	0.069	0.154	0.065

PBEsol				
Length	**Xtal**	**S=0**	**S=1**	**S=2**
Fe-S1	2.180	2.180	2.195	2.265
Fe-S2	2.157	2.147	2.189	2.243
Fe-C	1.963	1.919	1.964	2.145
N-C	1.362	1.381	1.372	1.366
τ	0.22	0.20	0.38	0.30
	MAE(Bonds)	0.018	0.014	0.089
	RMS(bonds)	0.025	0.019	0.109
	AE(τ)	0.021	0.161	0.075

BP86				
Length	**Xtal**	**S=0**	**S=1**	**S=2**
Fe-S1	2.180	2.221	2.233	2.313
Fe-S2	2.157	2.177	2.227	2.279
Fe-C	1.963	1.960	2.012	2.204
N-C	1.362	1.389	1.379	1.375
τ	0.22	0.23	0.44	0.40
	MAE(Bonds)	0.023	0.047	0.127
	RMS(bonds)	0.026	0.051	0.151
	AE(τ)	0.011	0.217	0.174

B3LYP				
Length	**Xtal**	**S=0**	**S=1**	**S=2**

Fe-S1	2.180	2.233	2.320	2.359
Fe-S2	2.157	2.271	2.320	2.344
Fe-C	1.963	2.019	2.313	2.299
N-C	1.362	1.381	1.370	1.369
τ	0.22	0.24	0.20	0.25
	MAE(Bonds)	0.060	0.165	0.177
	RMS(bonds)	0.069	0.205	0.212
	AE(τ)	0.013	0.028	0.026

B3LYP*				
Length	**Xtal**	**S=0**	**S=1**	**S=2**
Fe-S1	2.180	2.259	2.286	2.347
Fe-S2	2.157	2.218	2.278	2.330
Fe-C	1.963	2.002	2.110	2.275
N-C	1.362	1.382	1.371	1.369
τ	0.22	0.26	0.53	0.25
	MAE(Bonds)	0.049	0.096	0.165
	RMS(bonds)	0.054	0.109	0.197
	AE(τ)	0.039	0.307	0.030

PBE0				
Length	**Xtal**	**S=0**	**S=1**	**S=2**
Fe-S1	2.180	2.214	2.300	2.288
Fe-S2	2.157	2.171	2.279	2.274
Fe-C	1.963	1.957	2.279	2.216
N-C	1.362	1.388	1.363	1.374
τ	0.22	0.29	0.14	0.29
	MAE(Bonds)	0.020	0.140	0.122
	RMS(bonds)	0.023	0.179	0.149
	AE(τ)	0.069	0.081	0.065

TPSS				
Length	**Xtal**	**S=0**	**S=1**	**S=2**
Fe-S1	2.180	2.201	2.206	2.289
Fe-S2	2.157	2.160	2.206	2.277
Fe-C	1.963	1.951	2.000	2.185
N-C	1.362	1.388	1.378	1.375
τ	0.22	0.29	0.43	0.45
	MAE(Bonds)	0.016	0.032	0.116
	RMS(bonds)	0.018	0.034	0.138
	AE(τ)	0.070	0.202	0.224

Fe Spin Density for the reduced forms of compound 5

Below are tables that contain results of spin unrestricted DFT calculations in which molecular symmetry has been disabled. The following information is contained in the tables below: the number of unpaired electrons in the system, the spin state (S) of the system, electronic energy in kcal/mol, relative energy (E_{rel}) in kcal/mol, the α spin density on the Fe atom (χ_α), the β spin density on the Fe atom(χ_β), and the difference between the α and the β density on the Fe atom (χ_{diff}) for the neutral and reduced forms of compound 5. The spin densities were determined from the Mulliken populations. The functional, along with the total charge on the molecule, is indicated above the respective table. The antiferromagnetic case has been labeled with AFM.

Functional: BP86 Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-14569.35	0	4.22	4.22	0.00
AFM	0*	-14564.97	4.38	4.08	4.34	-0.26
2	1	-14562.8	6.55	4.90	3.51	1.40
4	2	-14547.66	21.69	5.52	2.73	2.80

Functional: BP86 Total Charge: -1

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
1	0.5	-14617.93	0	4.50	3.87	0.63
3	1.5	-14613.73	4.2	5.12	3.16	1.97
5	2.5	-14597.38	20.55	5.83	2.19	3.64

Functional: BP86 Total Charge: -2

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-14591.23	0	4.14	4.14	0.00
2	1	-14590.47	0.76	5.12	3.16	1.97
4	2	-14581.42	9.81	5.70	2.29	3.42

Functional: B3LYP* Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-16110.77	1.61	4.12	4.12	0.00
AFM	0*	-16108.61	3.77	3.50	4.68	-1.18
2	1	-16112.38	0	5.18	2.97	2.22
4	2	-16108.8	3.58	5.45	2.59	2.87

Functional: B3LYP* Total Charge: -1

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
1	0.5	-16162.87	10.16	4.51	3.62	0.89
3	1.5	-16173.03	0	5.42	2.65	2.77
5	2.5	-16165.94	7.09	5.85	2.00	3.84

Functional: B3LYP* Total Charge: -2

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-16130.94	14.21	4.03	4.03	0.00
2	1	-16138.21	6.94	5.05	2.96	2.08
4	2	-16145.15	0	5.68	2.10	3.59

Functional: TPSS Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-14905.92	0.34	13.18	13.18	0.00
AFM	0*	-14906.26	0	13.03	13.29	-0.26
2	1	-14900.93	5.33	13.85	12.45	1.41
4	2	-14883.06	23.2	14.49	11.63	2.86

Functional: TPSS Total Charge: -1

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
1	0.5	-14951.15	0	13.46	12.81	0.65
3	1.5	-14947.09	4.06	14.30	11.81	2.49
5	2.5	-14930.31	20.84	14.79	11.08	3.71

Functional: TPSS Total Charge: -2

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-14919.61	0	13.10	13.10	0.00
2	1	-14918.98	0.63	14.06	12.07	1.99
4	2	-14910.35	9.26	14.66	11.19	3.48

Functional: revPBE Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-14307.38	0	4.21	4.21	0.00
AFM	0*	-14302.56	4.82	4.03	4.37	-0.34
2	1	-14303.12	4.26	4.94	3.45	1.49
4	2	-14290.83	16.55	5.54	2.66	2.88

Functional: PBE Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-14776.4	0	4.24	4.24	0.00
AFM	0*	-14773.07	3.33	4.10	4.35	-0.25
2	1	-14772.15	4.25	4.91	3.52	1.39
4	2	-14755.68	20.72	5.53	2.74	2.79

Functional: PBEsol Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-15305.37	0	4.28	4.28	0.00
AFM	0*	-15299.56	5.81	4.20	4.34	-0.15
2	1	-15296.35	9.02	4.91	3.62	1.29
4	2	-15275.37	30.00	5.54	2.83	2.71

Functional: B3LYP Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-16640.2	13.42	4.11	4.11	0.00
AFM	0*	-16639.27	14.35	3.25	4.89	-1.64
2	1	-16653.62	0	5.47	2.62	2.85
4	2	-16646.38	7.24	5.51	2.53	2.98

Functional: PBE0 Total Charge: 0

Unpaired e	S	Energy (kcal/mol)	E_{rel}	χ_α	χ_β	χ_{diff}
0	0	-17943.04	15.73	4.16	4.16	0.00
AFM	0*	-17942.71	16.06	3.25	4.95	-1.69
2	1	-17958.77	0	5.57	2.58	2.99
4	2	-17951.89	6.88	5.58	2.50	3.09

Hirshfeld charges of 5, $[5]^{1-}$, $[5]^{2-}$

Table 3S below contains the Hirshfeld charges (q) of the iron atom (q(Fe)), summed over the NHC ligand (q(NHC)), summed over the bis(dithiolene) ligand (q(bis(dithiolene))), and over the entire molecule (q(sum)) obtained from BP86, B3LYP*, and TPSS calculations.

Table 3S. Hirshfeld charges (q) of the iron atom (q(Fe)), summed over the NHC ligand (q(NHC)), summed over the bis(dithiolene) ligand (q(bis(dithiolene))), and over the entire molecule (q(sum)) obtained from BP86, B3LYP*, and TPSS calculations.

	Compound	**q(Fe)**	**q(NHC)**	**q(bis(ditholene)**	**q(sum)**
BP86	5	-0.10	0.21	-0.11	0
	$[5]^{1-}$	-0.10	-0.00	-0.89	-1
	$[5]^{2-}$	-0.13	-0.27	-1.60	-2
B3LYP*	5	-0.04	0.21	-0.18	0
	$[5]^{1-}$	0.09	0.00	-1.09	-1
	$[5]^{2-}$	0.11	-0.15	-1.95	-2
TPSS	5	-0.10	0.24	-0.14	0
	$[5]^{1-}$	-0.10	0.04	-0.94	-1
	$[5]^{2-}$	-0.13	-0.23	-1.64	-2

Optimized DFT coordinates

Complex 5-revPBE S=0

100

Fe	-34.710289	-11.638589	1.640854
S	-33.000201	-10.969609	0.459801
C	-31.700524	-10.567675	1.547091
C	-30.424743	-10.136332	0.909946
C	-30.424327	-9.193259	-0.142604
H	-31.369246	-8.744179	-0.454319
C	-29.233932	-8.833430	-0.784600
H	-29.258531	-8.098761	-1.593150
C	-28.015526	-9.408802	-0.394682
H	-27.087040	-9.129736	-0.898100
C	-28.001009	-10.346343	0.648174
H	-27.059302	-10.805952	0.959212
C	-29.189466	-10.705947	1.293004
H	-29.165695	-11.444239	2.095123
C	-31.914222	-10.730160	2.923572
C	-30.946596	-10.365965	3.998174
C	-30.332485	-9.094552	4.031614
C	-29.465912	-8.747339	5.074034
H	-29.007686	-7.755232	5.086086
C	-29.188462	-9.660982	6.101561
H	-28.511158	-9.387125	6.913671
C	-29.791736	-10.926527	6.080821
H	-29.583703	-11.646363	6.876278
H	-30.550026	-8.372073	3.243487
C	-30.665019	-11.273143	5.043915
H	-31.136709	-12.257534	5.034913
S	-33.457428	-11.314212	3.460944
C	-34.706860	-13.617378	1.637266
N	-33.973134	-14.487122	0.832088
C	-32.978641	-14.187487	-0.184756
C	-31.616841	-14.162137	0.204646
C	-31.202722	-14.372860	1.645083
H	-30.117844	-14.246801	1.754548
H	-31.704283	-13.657308	2.311663
H	-31.462282	-15.384260	1.996195
C	-30.655278	-13.933112	-0.786139
H	-29.602485	-13.888657	-0.494726
C	-31.005717	-13.736979	-2.134765
C	-29.939725	-13.444464	-3.170398
H	-29.363638	-12.546632	-2.894704
H	-30.379954	-13.274578	-4.163100
H	-29.224204	-14.278974	-3.252787
C	-32.357954	-13.820682	-2.483433
H	-32.649964	-13.695727	-3.530095
C	-33.367714	-14.064452	-1.531697
C	-34.800261	-14.205762	-2.001452
H	-34.886902	-15.052135	-2.701430
H	-35.123819	-13.301065	-2.535691
H	-35.498422	-14.370440	-1.174881
N	-35.442634	-14.490016	2.436934

C	-36.429282	-14.192838	3.461555
C	-36.030034	-14.078936	4.806144
C	-34.594620	-14.228829	5.264353
H	-34.253247	-13.316575	5.774326
H	-34.511983	-15.060199	5.982360
H	-33.907380	-14.421652	4.434557
C	-37.031853	-13.835817	5.766281
H	-36.732073	-13.718442	6.811590
C	-38.386006	-13.742995	5.427180
C	-39.442578	-13.450047	6.472256
H	-38.994084	-13.285798	7.461556
H	-40.017140	-12.549435	6.204901
H	-40.160451	-14.281396	6.557500
C	-38.747023	-13.930014	4.079916
H	-39.801306	-13.877268	3.795650
C	-37.793431	-14.159907	3.081705
C	-38.217078	-14.365815	1.643329
H	-37.715619	-13.652213	0.974840
H	-39.301922	-14.235439	1.539768
H	-37.963686	-15.377998	1.289740
S	-36.419718	-10.969987	2.824006
C	-37.718691	-10.562751	1.737697
C	-38.991442	-10.125109	2.376861
C	-38.984568	-9.183525	3.430874
H	-38.036807	-8.739076	3.740255
C	-40.171447	-8.819756	4.076918
H	-40.140924	-8.085862	4.886136
C	-41.393792	-9.388975	3.689765
H	-42.319262	-9.106317	4.196504
C	-41.415744	-10.323749	2.644339
H	-42.360453	-10.777095	2.333509
C	-40.230576	-10.687477	1.995569
H	-40.260269	-11.424168	1.191914
C	-37.507332	-10.727578	0.361184
C	-38.476268	-10.363641	-0.712078
C	-39.082655	-9.088533	-0.750904
H	-38.856997	-8.362360	0.031711
C	-39.953349	-8.743797	-1.790803
H	-40.406061	-7.749350	-1.807084
C	-40.242704	-9.663210	-2.810024
H	-40.923851	-9.391508	-3.619657
C	-39.645809	-10.931818	-2.784418
H	-39.861720	-11.656090	-3.573935
C	-38.768341	-11.276417	-1.750176
H	-38.301458	-12.263485	-1.737050
S	-35.966585	-11.315757	-0.178443
C	-35.171257	-15.824435	2.127921
C	-34.250320	-15.822975	1.132663
H	-33.766203	-16.636206	0.604667
H	-35.658819	-16.639040	2.650725

Complex 5-revPBE S=1

100

Fe	-34.708030	-11.462955	1.644239
S	-32.969030	-10.618016	0.505927

C	-31.615543	-10.432095	1.619528
C	-30.304113	-10.122437	0.988588
C	-30.220272	-9.193280	-0.074466
H	-31.121977	-8.666150	-0.391333
C	-29.003109	-8.943716	-0.718981
H	-28.964627	-8.217952	-1.535161
C	-27.839488	-9.618780	-0.323347
H	-26.890556	-9.427278	-0.829987
C	-27.906433	-10.544383	0.729502
H	-27.008028	-11.081394	1.044519
C	-29.120918	-10.792254	1.378115
H	-29.159404	-11.521875	2.187398
C	-31.843611	-10.644369	2.971178
C	-30.866470	-10.428168	4.075433
C	-30.134389	-9.224407	4.181924
C	-29.241254	-9.022317	5.240244
H	-28.686512	-8.082944	5.305706
C	-29.059933	-10.013639	6.216272
H	-28.362197	-9.853565	7.041311
C	-29.788254	-11.208612	6.128932
H	-29.657868	-11.987009	6.884822
H	-30.277930	-8.442300	3.434640
C	-30.685723	-11.410666	5.074216
H	-31.252526	-12.341944	5.012100
S	-33.452166	-11.133887	3.474129
C	-34.708582	-13.512428	1.639226
N	-34.005063	-14.369831	0.810116
C	-33.035362	-14.057052	-0.228205
C	-31.669099	-14.022900	0.139086
C	-31.228340	-14.243135	1.570226
H	-30.141539	-14.121856	1.658730
H	-31.713069	-13.530127	2.251357
H	-31.483013	-15.256377	1.919330
C	-30.727070	-13.784539	-0.868122
H	-29.670388	-13.728710	-0.594431
C	-31.103424	-13.591572	-2.209830
C	-30.057458	-13.306086	-3.268045
H	-29.354079	-12.531716	-2.926249
H	-30.518939	-12.961078	-4.203875
H	-29.466260	-14.208836	-3.496853
C	-32.461319	-13.683737	-2.534989
H	-32.772786	-13.559396	-3.575991
C	-33.452751	-13.934765	-1.566690
C	-34.892798	-14.078999	-2.013045
H	-34.966185	-14.831617	-2.813314
H	-35.269036	-13.127497	-2.415832
H	-35.559298	-14.376809	-1.196651
N	-35.414434	-14.372116	2.463666
C	-36.379868	-14.062413	3.506631
C	-35.956556	-13.948870	4.843912
C	-34.514681	-14.099729	5.282609
H	-34.131979	-13.150056	5.683159
H	-34.439741	-14.852701	6.082374
H	-33.854023	-14.400432	4.462762
C	-36.943351	-13.700194	5.817595
H	-36.627441	-13.583509	6.858064

C	-38.302336	-13.602062	5.498465
C	-39.343459	-13.320993	6.562595
H	-38.878060	-12.981538	7.498354
H	-40.047599	-12.544264	6.228099
H	-39.934448	-14.224368	6.788877
C	-38.684684	-13.786475	4.157408
H	-39.742219	-13.726068	3.888360
C	-37.747594	-14.022348	3.145138
C	-38.194898	-14.233937	1.714773
H	-37.712037	-13.517632	1.035844
H	-39.281872	-14.110610	1.631712
H	-37.943024	-15.245416	1.358497
S	-36.446358	-10.617085	2.781976
C	-37.801478	-10.434906	1.669150
C	-39.110544	-10.124323	2.303879
C	-39.187193	-9.198592	3.370572
H	-38.282299	-8.676571	3.686620
C	-40.401129	-8.945870	4.019780
H	-40.434338	-8.222056	4.837728
C	-41.568754	-9.613929	3.624841
H	-42.515715	-9.419262	4.133792
C	-41.508635	-10.536485	2.569770
H	-42.410587	-11.067729	2.255795
C	-40.297317	-10.788360	1.916345
H	-40.264369	-11.515838	1.104941
C	-37.574216	-10.647906	0.317536
C	-38.550096	-10.433137	-0.788303
C	-39.279213	-9.228248	-0.899214
H	-39.138587	-8.446435	-0.151153
C	-40.164690	-9.024059	-1.963759
H	-40.716307	-8.083332	-2.033358
C	-40.341628	-10.014466	-2.941329
H	-41.032909	-9.852377	-3.771546
C	-39.618393	-11.211966	-2.847878
H	-39.745789	-11.990195	-3.604396
C	-38.728885	-11.416443	-1.786792
H	-38.164902	-12.349052	-1.720915
S	-35.964552	-11.134705	-0.185012
C	-35.151946	-15.707100	2.149703
C	-34.270146	-15.705744	1.118474
H	-33.805511	-16.517277	0.570690
H	-35.619464	-16.520120	2.693117

Complex 5-revPBE S=2

100

Fe	-34.719446	-11.487402	1.707754
S	-33.110944	-10.414912	0.482546
C	-31.725767	-10.324425	1.584188
C	-30.412031	-10.060691	0.934967
C	-30.314056	-9.134537	-0.130083
H	-31.205351	-8.587359	-0.442413
C	-29.095288	-8.908500	-0.778958
H	-29.045382	-8.181973	-1.593442
C	-27.942900	-9.606061	-0.388397
H	-26.991774	-9.430209	-0.896850

C	-28.025078	-10.533831	0.660331
H	-27.136537	-11.089028	0.970658
C	-29.241761	-10.758058	1.314104
H	-29.291393	-11.489047	2.121049
C	-31.925470	-10.486909	2.947517
C	-30.896562	-10.278141	4.006920
C	-30.148594	-9.081336	4.068255
C	-29.219463	-8.871286	5.093356
H	-28.658268	-7.934420	5.128787
C	-29.013538	-9.850390	6.076625
H	-28.288424	-9.683880	6.876624
C	-29.754514	-11.039755	6.031492
H	-29.606351	-11.807297	6.795049
H	-30.311034	-8.309648	3.314050
C	-30.691739	-11.248098	5.012997
H	-31.272901	-12.171659	4.987509
S	-33.541493	-10.823116	3.578501
C	-34.641075	-13.753169	1.700115
N	-33.918884	-14.588035	0.870378
C	-32.938737	-14.203532	-0.132146
C	-31.582999	-14.120402	0.262571
C	-31.161930	-14.355191	1.698116
H	-30.074605	-14.249173	1.801268
H	-31.644239	-13.637435	2.376910
H	-31.437976	-15.363990	2.042484
C	-30.633478	-13.813340	-0.719142
H	-29.583958	-13.729995	-0.425863
C	-30.993651	-13.591141	-2.061155
C	-29.941610	-13.230564	-3.089539
H	-29.430994	-12.294483	-2.813712
H	-30.384140	-13.095509	-4.086427
H	-29.170042	-14.014237	-3.161317
C	-32.343379	-13.707559	-2.411213
H	-32.642915	-13.547411	-3.450774
C	-33.340206	-14.028210	-1.469466
C	-34.771008	-14.193783	-1.938254
H	-34.862747	-15.085475	-2.579766
H	-35.081348	-13.325004	-2.535563
H	-35.476711	-14.294656	-1.107875
N	-35.379897	-14.638674	2.459709
C	-36.361672	-14.325310	3.486197
C	-35.941888	-14.189215	4.823908
C	-34.486972	-14.293934	5.227081
H	-33.925848	-13.407328	4.893716
H	-34.396087	-14.364056	6.319295
H	-34.000422	-15.175524	4.784647
C	-36.930505	-13.940502	5.793004
H	-36.620299	-13.815186	6.833858
C	-38.290552	-13.849258	5.466315
C	-39.335957	-13.556122	6.523023
H	-38.881533	-13.439863	7.517234
H	-39.879448	-12.627095	6.286457
H	-40.082541	-14.365092	6.581032
C	-38.665491	-14.027988	4.123776
H	-39.721867	-13.961638	3.849515
C	-37.722952	-14.266816	3.114434

C	-38.159438	-14.435655	1.674681
H	-37.670928	-13.693302	1.026669
H	-39.245932	-14.308730	1.586329
H	-37.902711	-15.432720	1.283690
S	-36.594056	-10.718074	2.859664
C	-37.873784	-10.393357	1.701337
C	-39.181006	-10.011131	2.304308
C	-39.244045	-9.025759	3.314987
H	-38.328236	-8.511276	3.612370
C	-40.460220	-8.703352	3.928297
H	-40.486602	-7.933685	4.703412
C	-41.639324	-9.363534	3.554093
H	-42.587536	-9.115427	4.036988
C	-41.590575	-10.348017	2.555894
H	-42.501886	-10.873993	2.260311
C	-40.377350	-10.668037	1.936720
H	-40.348538	-11.442686	1.169687
C	-37.634200	-10.591197	0.351805
C	-38.590265	-10.307343	-0.754693
C	-39.247123	-9.061141	-0.859557
H	-39.059615	-8.291263	-0.109135
C	-40.120090	-8.800827	-1.922520
H	-40.613961	-7.828300	-1.989100
C	-40.356015	-9.775306	-2.903703
H	-41.035196	-9.568691	-3.733997
C	-39.704583	-11.014219	-2.815728
H	-39.877313	-11.780347	-3.575906
C	-38.827762	-11.274905	-1.757231
H	-38.319718	-12.239344	-1.694887
S	-36.063003	-11.191519	-0.156119
C	-35.121137	-15.964966	2.111321
C	-34.199457	-15.933486	1.110889
H	-33.723796	-16.730308	0.549961
H	-35.614450	-16.794990	2.604536

Complex 5-PBE S=0

100

Fe	-34.703261	-11.518354	1.642104
S	-32.974085	-10.906902	0.480607
C	-31.665268	-10.591282	1.574531
C	-30.365726	-10.244621	0.953122
C	-30.303875	-9.333538	-0.119020
H	-31.221936	-8.846068	-0.452155
C	-29.092893	-9.054265	-0.752484
H	-29.068929	-8.340959	-1.578224
C	-27.915082	-9.681022	-0.333795
H	-26.967594	-9.465387	-0.831665
C	-27.961864	-10.586999	0.729823
H	-27.049709	-11.085849	1.064253
C	-29.170815	-10.866006	1.366843
H	-29.196493	-11.580567	2.189658
C	-31.898054	-10.748517	2.945073
C	-30.915064	-10.477883	4.022232
C	-30.167761	-9.284703	4.054776
C	-29.268360	-9.037363	5.092147

H	-28.702036	-8.103427	5.102926
C	-29.089892	-9.975629	6.114474
H	-28.381413	-9.781761	6.922179
C	-29.830524	-11.160692	6.097717
H	-29.702411	-11.899123	6.892209
H	-30.303908	-8.545834	3.263791
C	-30.737556	-11.406373	5.066065
H	-31.317024	-12.331754	5.054121
S	-33.475788	-11.229710	3.461847
C	-34.708559	-13.475664	1.641814
N	-33.986330	-14.340264	0.832176
C	-33.015034	-14.028383	-0.191034
C	-31.657021	-13.974251	0.185920
C	-31.238675	-14.194867	1.615024
H	-30.152936	-14.078655	1.720546
H	-31.732707	-13.477985	2.287149
H	-31.508385	-15.204520	1.962443
C	-30.712438	-13.700775	-0.804251
H	-29.660014	-13.623413	-0.519162
C	-31.080994	-13.493199	-2.141355
C	-30.039423	-13.163453	-3.179870
H	-29.350595	-12.388497	-2.811517
H	-30.502541	-12.798611	-4.107307
H	-29.432651	-14.048902	-3.431691
C	-32.429435	-13.613653	-2.480859
H	-32.732697	-13.481761	-3.523486
C	-33.420592	-13.897861	-1.527964
C	-34.851333	-14.051704	-1.973327
H	-34.903357	-14.686879	-2.870404
H	-35.285998	-13.072568	-2.228749
H	-35.484060	-14.495995	-1.195331
N	-35.431699	-14.342590	2.449396
C	-36.403884	-14.034955	3.472944
C	-35.999418	-13.909805	4.810588
C	-34.568604	-14.064807	5.255781
H	-34.126347	-13.084154	5.491616
H	-34.518267	-14.683113	6.164335
H	-33.940915	-14.528115	4.484806
C	-36.990659	-13.624005	5.762771
H	-36.688217	-13.495269	6.805954
C	-38.338265	-13.496027	5.422153
C	-39.378455	-13.163041	6.461205
H	-38.914285	-12.800316	7.388661
H	-40.065362	-12.386334	6.093212
H	-39.987538	-14.046740	6.713162
C	-38.706870	-13.699744	4.084218
H	-39.758581	-13.617067	3.798163
C	-37.762098	-13.975505	3.094597
C	-38.179556	-14.190514	1.664270
H	-37.687105	-13.470159	0.994869
H	-39.265386	-14.075375	1.559960
H	-37.908446	-15.198064	1.312638
S	-36.431036	-10.905569	2.803996
C	-37.740184	-10.587714	1.711207
C	-39.039307	-10.246564	2.336672
C	-39.098215	-9.347407	3.419656

H	-38.179244	-8.863783	3.756441
C	-40.307498	-9.073574	4.059321
H	-40.328876	-8.367438	4.892061
C	-41.487472	-9.693603	3.636226
H	-42.433927	-9.480265	4.137394
C	-41.443846	-10.588093	2.562018
H	-42.357421	-11.082307	2.223901
C	-40.236077	-10.861925	1.919025
H	-40.212649	-11.568732	1.088994
C	-37.507156	-10.741902	0.340100
C	-38.491282	-10.473954	-0.736993
C	-39.244051	-9.284258	-0.767786
H	-39.111281	-8.546029	0.024467
C	-40.144285	-9.039044	-1.804775
H	-40.714768	-8.107837	-1.814247
C	-40.315154	-9.974218	-2.830807
H	-41.021933	-9.780516	-3.639860
C	-39.569369	-11.156512	-2.815495
H	-39.692383	-11.893415	-3.612368
C	-38.664020	-11.401766	-1.782267
H	-38.081745	-12.325442	-1.770952
S	-35.928703	-11.220734	-0.177226
C	-35.162232	-15.672326	2.141843
C	-34.253582	-15.670802	1.136855
H	-33.770382	-16.481779	0.604991
H	-35.645342	-16.485097	2.671731

Complex 5-PBE S=1

100

Fe	-34.707746	-11.462323	1.651213
S	-32.976815	-10.690721	0.489576
C	-31.616400	-10.507733	1.586856
C	-30.309223	-10.247785	0.944688
C	-30.223156	-9.403850	-0.180887
H	-31.126622	-8.908698	-0.540670
C	-29.006282	-9.196774	-0.830834
H	-28.964217	-8.532897	-1.696781
C	-27.845526	-9.829492	-0.375603
H	-26.893339	-9.667039	-0.884300
C	-27.915713	-10.673138	0.737868
H	-27.016673	-11.177284	1.099548
C	-29.130568	-10.881059	1.389461
H	-29.174565	-11.547957	2.250448
C	-31.841624	-10.672855	2.940927
C	-30.860349	-10.433839	4.025238
C	-30.083759	-9.259099	4.055955
C	-29.181037	-9.028760	5.093878
H	-28.591439	-8.109315	5.102702
C	-29.034992	-9.962956	6.124804
H	-28.329460	-9.779970	6.937833
C	-29.807886	-11.127911	6.111872
H	-29.707001	-11.861068	6.914696
H	-30.200956	-8.521770	3.260457
C	-30.714729	-11.358462	5.076381
H	-31.319908	-12.267513	5.070098

S	-33.454254	-11.113071	3.459174
C	-34.704816	-13.477241	1.640597
N	-33.989052	-14.326895	0.824922
C	-33.008490	-14.003041	-0.188025
C	-31.659323	-13.923080	0.205597
C	-31.255281	-14.118222	1.642723
H	-30.171895	-13.991975	1.757880
H	-31.761035	-13.394506	2.298503
H	-31.520761	-15.124519	2.002627
C	-30.707306	-13.661403	-0.781840
H	-29.658166	-13.570601	-0.488439
C	-31.063038	-13.499486	-2.127944
C	-30.013754	-13.184801	-3.162992
H	-29.563216	-12.198432	-2.970949
H	-30.440062	-13.173794	-4.175469
H	-29.196813	-13.923697	-3.142107
C	-32.407919	-13.640243	-2.479924
H	-32.699076	-13.547461	-3.529702
C	-33.405390	-13.906946	-1.530579
C	-34.835870	-14.086277	-1.964582
H	-34.887438	-14.256224	-3.047370
H	-35.432710	-13.191419	-1.728734
H	-35.316244	-14.935863	-1.457229
N	-35.420176	-14.332059	2.451264
C	-36.401093	-14.013745	3.465476
C	-36.005720	-13.921668	4.808936
C	-34.575341	-14.098214	5.244179
H	-33.983157	-13.196229	5.021147
H	-34.525282	-14.282212	6.325094
H	-34.088931	-14.938423	4.726527
C	-37.004826	-13.660362	5.758151
H	-36.714986	-13.570957	6.808626
C	-38.349699	-13.520585	5.405140
C	-39.401075	-13.213301	6.440243
H	-38.976064	-13.202795	7.452594
H	-39.857323	-12.229236	6.250980
H	-40.212802	-13.956489	6.417020
C	-38.703515	-13.677502	4.058049
H	-39.752333	-13.586753	3.763626
C	-37.749954	-13.933525	3.070806
C	-38.152595	-14.122872	1.632438
H	-37.645220	-13.397564	0.979566
H	-39.235860	-13.995110	1.516635
H	-37.888016	-15.128372	1.269492
S	-36.438844	-10.686480	2.810787
C	-37.797304	-10.501153	1.711636
C	-39.105338	-10.238459	2.351455
C	-39.194441	-9.385705	3.470423
H	-38.292342	-8.885250	3.827131
C	-40.412419	-9.176018	4.117056
H	-40.456480	-8.504974	4.977295
C	-41.571013	-9.816079	3.666550
H	-42.523811	-9.652459	4.173432
C	-41.497598	-10.669259	2.560940
H	-42.394749	-11.179845	2.204299
C	-40.281949	-10.878400	1.910632

H	-40.235080	-11.552558	1.055204
C	-37.571212	-10.667436	0.357739
C	-38.549759	-10.429770	-0.729692
C	-39.325923	-9.255421	-0.763299
H	-39.209657	-8.517234	0.031382
C	-40.225813	-9.026618	-1.803787
H	-40.814292	-8.106900	-1.814851
C	-40.369546	-9.962236	-2.833769
H	-41.073919	-9.780394	-3.647753
C	-39.595881	-11.126005	-2.819677
H	-39.696347	-11.860218	-3.621734
C	-38.690695	-11.354247	-1.782537
H	-38.085525	-12.262986	-1.775412
S	-35.958955	-11.110145	-0.158312
C	-35.154545	-15.661521	2.140869
C	-34.256135	-15.658637	1.125918
H	-33.777385	-16.467489	0.586600
H	-35.633648	-16.473416	2.675261

Complex 5-PBE S=2

100

Fe	-34.711330	-11.465674	1.670098
S	-33.085795	-10.467859	0.431803
C	-31.715825	-10.402846	1.543251
C	-30.389863	-10.223055	0.909012
C	-30.250199	-9.390640	-0.221162
H	-31.123008	-8.850251	-0.592221
C	-29.019350	-9.249458	-0.861250
H	-28.935687	-8.589318	-1.727893
C	-27.896593	-9.941858	-0.395836
H	-26.933746	-9.832222	-0.898666
C	-28.020119	-10.776070	0.720762
H	-27.152450	-11.327089	1.090916
C	-29.248676	-10.914408	1.365908
H	-29.333117	-11.575433	2.229007
C	-31.937663	-10.509447	2.907766
C	-30.920033	-10.298767	3.965588
C	-30.083229	-9.165608	3.953647
C	-29.156142	-8.956434	4.973973
H	-28.521175	-8.068275	4.951464
C	-29.043580	-9.870976	6.026968
H	-28.316658	-9.704591	6.824491
C	-29.877727	-10.992443	6.057984
H	-29.803213	-11.708593	6.879222
H	-30.174991	-8.443202	3.141449
C	-30.811600	-11.200367	5.042109
H	-31.467393	-12.072565	5.070445
S	-33.564477	-10.768787	3.523347
C	-34.640025	-13.680522	1.666422
N	-33.911429	-14.522175	0.861281
C	-32.919721	-14.141192	-0.118518
C	-31.586597	-13.994928	0.305453
C	-31.202839	-14.178843	1.750481
H	-30.115613	-14.100643	1.872774

H	-31.676813	-13.415245	2.385587
H	-31.520487	-15.160698	2.133217
C	-30.630099	-13.665887	-0.658127
H	-29.593154	-13.526362	-0.342928
C	-30.968330	-13.489541	-2.006672
C	-29.914420	-13.101326	-3.011773
H	-29.438163	-12.150254	-2.727043
H	-30.341753	-12.982913	-4.016360
H	-29.117783	-13.859868	-3.066569
C	-32.299748	-13.678349	-2.387585
H	-32.578468	-13.559945	-3.438050
C	-33.299129	-14.014003	-1.463604
C	-34.721929	-14.213370	-1.914435
H	-34.768202	-14.304144	-3.007771
H	-35.352590	-13.360822	-1.613554
H	-35.169939	-15.116094	-1.473910
N	-35.391567	-14.547297	2.422738
C	-36.369391	-14.197859	3.428265
C	-35.952329	-14.031816	4.757335
C	-34.504895	-14.156616	5.152759
H	-33.908831	-13.346487	4.702733
H	-34.397872	-14.094866	6.242831
H	-34.068895	-15.110035	4.816070
C	-36.934582	-13.726744	5.709518
H	-36.628047	-13.579493	6.748537
C	-38.285100	-13.603659	5.369638
C	-39.320777	-13.248846	6.405607
H	-38.871657	-13.145789	7.402440
H	-39.813056	-12.297018	6.153405
H	-40.107808	-14.016768	6.462684
C	-38.657333	-13.804368	4.033553
H	-39.707556	-13.702613	3.747871
C	-37.718574	-14.102199	3.042742
C	-38.133473	-14.277156	1.606017
H	-37.640760	-13.529679	0.965222
H	-39.219359	-14.159680	1.502557
H	-37.858491	-15.269895	1.218050
S	-36.560829	-10.770568	2.843117
C	-37.866469	-10.465571	1.717658
C	-39.170960	-10.161878	2.349273
C	-39.243094	-9.286891	3.451067
H	-38.330958	-8.796699	3.795824
C	-40.457565	-9.043881	4.093548
H	-40.491486	-8.355592	4.940486
C	-41.626384	-9.672546	3.655159
H	-42.576513	-9.482600	4.158431
C	-41.568292	-10.547901	2.565706
H	-42.474224	-11.049156	2.218385
C	-40.356844	-10.791124	1.919895
H	-40.319489	-11.484502	1.078955
C	-37.634001	-10.614960	0.364236
C	-38.610289	-10.344940	-0.716066
C	-39.358190	-9.152348	-0.743339
H	-39.214182	-8.414866	0.047488
C	-40.265332	-8.905388	-1.773872
H	-40.832923	-7.972607	-1.780772

C	-40.444118	-9.839715	-2.799393
H	-41.154588	-9.643702	-3.604982
C	-39.698663	-11.022419	-2.790843
H	-39.827254	-11.757148	-3.588589
C	-38.787484	-11.269797	-1.763778
H	-38.204433	-12.192852	-1.758306
S	-36.044482	-11.123281	-0.169215
C	-35.137781	-15.873764	2.095986
C	-34.200099	-15.858700	1.111617
H	-33.714341	-16.662954	0.570467
H	-35.643977	-16.694157	2.592128

Complex 5-PBEsol S=0

100

Fe	-34.704200	-11.590907	1.645778
S	-33.001084	-11.041217	0.459445
C	-31.698614	-10.673633	1.526161
C	-30.408738	-10.344710	0.894282
C	-30.360365	-9.517574	-0.239566
H	-31.293115	-9.087498	-0.618936
C	-29.151850	-9.244905	-0.872172
H	-29.136341	-8.589750	-1.749499
C	-27.964552	-9.796085	-0.390257
H	-27.013574	-9.580580	-0.887517
C	-27.999177	-10.621488	0.733448
H	-27.073847	-11.061982	1.119308
C	-29.205978	-10.893373	1.369885
H	-29.226747	-11.544871	2.248735
C	-31.926306	-10.776677	2.900316
C	-30.955087	-10.431582	3.953376
C	-30.191750	-9.255028	3.880473
C	-29.301992	-8.924969	4.896424
H	-28.721163	-7.999623	4.827154
C	-29.153419	-9.760656	6.003711
H	-28.452307	-9.498046	6.801884
C	-29.909843	-10.928180	6.090347
H	-29.802733	-11.589711	6.956111
H	-30.311288	-8.592847	3.018000
C	-30.804582	-11.258570	5.077513
H	-31.401068	-12.174812	5.142310
S	-33.491456	-11.259988	3.427253
C	-34.706532	-13.509929	1.644272
N	-33.959357	-14.372406	0.866001
C	-32.980899	-14.053572	-0.131418
C	-31.637856	-13.953720	0.263739
C	-31.251752	-14.127939	1.697873
H	-30.167061	-13.999012	1.826411
H	-31.770474	-13.389386	2.334566
H	-31.528457	-15.128649	2.073178
C	-30.690920	-13.667920	-0.716372
H	-29.642008	-13.552783	-0.418298
C	-31.049183	-13.496758	-2.057037
C	-30.014185	-13.133862	-3.078106
H	-29.594824	-12.135270	-2.864222
H	-30.439153	-13.114920	-4.093560

H	-29.172026	-13.846379	-3.069146
C	-32.386926	-13.662846	-2.413497
H	-32.678718	-13.562214	-3.465710
C	-33.376042	-13.955715	-1.470032
C	-34.799991	-14.153108	-1.881505
H	-34.880132	-14.232708	-2.975986
H	-35.427243	-13.303478	-1.549778
H	-35.231863	-15.062747	-1.431543
N	-35.457623	-14.371809	2.419716
C	-36.436034	-14.053925	3.417601
C	-36.041469	-13.958294	4.756349
C	-34.617133	-14.151670	5.167983
H	-33.992775	-13.298961	4.838862
H	-34.537198	-14.233097	6.262340
H	-34.181623	-15.058241	4.715909
C	-37.031889	-13.671357	5.700391
H	-36.740815	-13.573888	6.752988
C	-38.370034	-13.508907	5.344451
C	-39.407450	-13.157687	6.367355
H	-38.982844	-13.139201	7.382271
H	-39.836598	-12.163043	6.157854
H	-40.242298	-13.877961	6.356422
C	-38.727189	-13.675926	4.003074
H	-39.776161	-13.562951	3.704943
C	-37.779180	-13.956084	3.022513
C	-38.164618	-14.127137	1.587691
H	-37.649598	-13.384118	0.953276
H	-39.249997	-14.003745	1.459627
H	-37.882477	-15.125383	1.209352
S	-36.407839	-11.041422	2.831561
C	-37.709083	-10.671793	1.763251
C	-38.999073	-10.340718	2.393209
C	-39.048057	-9.508443	3.522560
H	-38.115183	-9.079052	3.901711
C	-40.257628	-9.230591	4.150937
H	-40.274040	-8.571298	5.024717
C	-41.444676	-9.781817	3.669309
H	-42.396366	-9.561088	4.162897
C	-41.409054	-10.614113	2.550981
H	-42.334466	-11.055027	2.165732
C	-40.201440	-10.890764	1.918505
H	-40.179677	-11.546901	1.043313
C	-37.480173	-10.774127	0.389217
C	-38.448810	-10.427029	-0.665311
C	-39.214663	-9.252113	-0.591569
H	-39.099387	-8.592537	0.273358
C	-40.100970	-8.920345	-1.610097
H	-40.683913	-7.996379	-1.539816
C	-40.243430	-9.752323	-2.720936
H	-40.942274	-9.488500	-3.521003
C	-39.484296	-10.917931	-2.808424
H	-39.586429	-11.576250	-3.677159
C	-38.593475	-11.250230	-1.792690
H	-37.994725	-12.164928	-1.858235
S	-35.915228	-11.258466	-0.136321
C	-35.184691	-15.696776	2.123873

C	-34.238908	-15.697222	1.155863
H	-33.734413	-16.509748	0.639009
H	-35.692318	-16.508850	2.638132

Complex 5-PBEsol S=1

100

Fe	-34.703547	-11.473398	1.641168
S	-32.988976	-10.728338	0.501858
C	-31.636289	-10.570888	1.595991
C	-30.329660	-10.331759	0.964966
C	-30.230414	-9.507100	-0.168241
H	-31.132671	-9.009593	-0.538141
C	-29.011447	-9.321537	-0.812621
H	-28.956911	-8.668438	-1.689335
C	-27.864004	-9.960595	-0.344686
H	-26.905299	-9.816936	-0.853382
C	-27.947875	-10.784769	0.778123
H	-27.053689	-11.294351	1.151659
C	-29.163972	-10.968024	1.426485
H	-29.223749	-11.620261	2.301775
C	-31.870171	-10.743782	2.944361
C	-30.893766	-10.540226	4.028207
C	-30.060853	-9.409915	4.049573
C	-29.160789	-9.214089	5.090297
H	-28.523392	-8.323702	5.094493
C	-29.075444	-10.137901	6.132361
H	-28.368655	-9.978942	6.952690
C	-29.904557	-11.258477	6.128352
H	-29.849155	-11.986059	6.944161
H	-30.133735	-8.679171	3.238951
C	-30.808812	-11.454850	5.089284
H	-31.465055	-12.332059	5.083798
S	-33.484334	-11.161328	3.439956
C	-34.705942	-13.437310	1.639690
N	-34.005224	-14.283660	0.819192
C	-33.048463	-13.937801	-0.192292
C	-31.705961	-13.817766	0.200545
C	-31.309147	-14.020068	1.628665
H	-30.229105	-13.858272	1.757593
H	-31.848547	-13.318788	2.290103
H	-31.548373	-15.041464	1.973243
C	-30.769992	-13.495922	-0.777123
H	-29.722969	-13.360786	-0.480899
C	-31.138192	-13.311438	-2.114147
C	-30.108352	-12.943156	-3.138644
H	-29.493265	-12.098179	-2.788522
H	-30.575087	-12.659244	-4.093479
H	-29.422640	-13.785416	-3.334109
C	-32.473935	-13.490216	-2.465931
H	-32.773392	-13.371299	-3.514274
C	-33.455721	-13.815688	-1.523379
C	-34.876845	-14.009092	-1.952244
H	-34.918551	-14.501866	-2.935901
H	-35.390987	-13.034293	-2.035470

H	-35.449094	-14.612278	-1.231623
N	-35.405642	-14.285454	2.459878
C	-36.364083	-13.940723	3.470350
C	-35.959339	-13.820236	4.802537
C	-34.539670	-14.016114	5.235081
H	-34.024025	-13.042638	5.319933
H	-34.501807	-14.509152	6.218446
H	-33.966097	-14.619900	4.516289
C	-36.942378	-13.493867	5.743404
H	-36.644594	-13.375605	6.792315
C	-38.277446	-13.313298	5.389543
C	-39.308785	-12.944171	6.412159
H	-38.843067	-12.660730	7.368459
H	-39.921937	-12.097676	6.060452
H	-39.996572	-13.785979	6.606133
C	-38.643407	-13.497509	4.051849
H	-39.689834	-13.361862	3.753835
C	-37.706070	-13.819495	3.075579
C	-38.101021	-14.021049	1.646812
H	-37.558925	-13.321286	0.985741
H	-39.180463	-13.855977	1.516666
H	-37.864665	-15.043109	1.302683
S	-36.416968	-10.732002	2.784687
C	-37.770891	-10.570321	1.692349
C	-39.076801	-10.335024	2.326396
C	-39.172985	-9.520463	3.467790
H	-38.269749	-9.027189	3.840882
C	-40.390647	-9.339344	4.116041
H	-40.442984	-8.693622	4.998903
C	-41.539596	-9.973192	3.644764
H	-42.497407	-9.831972	4.156447
C	-41.458496	-10.787493	2.513608
H	-42.353483	-11.292857	2.137058
C	-40.243941	-10.966111	1.860154
H	-40.186472	-11.610576	0.977801
C	-37.537701	-10.736729	0.343045
C	-38.516113	-10.532338	-0.738378
C	-39.354797	-9.406549	-0.755017
H	-39.283979	-8.677660	0.057732
C	-40.256979	-9.211351	-1.794811
H	-40.898314	-8.323790	-1.795921
C	-40.341367	-10.133302	-2.838353
H	-41.052040	-9.976547	-3.656167
C	-39.507322	-11.249750	-2.837912
H	-39.562374	-11.976479	-3.654440
C	-38.599879	-11.444369	-1.801074
H	-37.940916	-12.319256	-1.798137
S	-35.923373	-11.150184	-0.155518
C	-35.145540	-15.609806	2.153141
C	-34.263125	-15.609089	1.125311
H	-33.788703	-16.419661	0.578332
H	-35.616700	-16.421404	2.701385

Complex 5-PBEsol S=2

100

Fe	-34.700603	-11.524871	1.687939
S	-33.114350	-10.526658	0.455843
C	-31.747288	-10.477845	1.554030
C	-30.427925	-10.306344	0.926081
C	-30.294337	-9.515860	-0.228450
H	-31.180020	-9.008285	-0.624914
C	-29.063287	-9.373962	-0.859542
H	-28.982718	-8.742898	-1.750754
C	-27.936031	-10.025253	-0.359880
H	-26.967829	-9.915132	-0.858582
C	-28.054585	-10.819773	0.780990
H	-27.177905	-11.342079	1.178741
C	-29.283419	-10.959654	1.416359
H	-29.368321	-11.592545	2.303998
C	-31.968217	-10.588745	2.915661
C	-30.953538	-10.391624	3.966389
C	-30.086835	-9.286703	3.936897
C	-29.162736	-9.087105	4.955867
H	-28.502265	-8.214599	4.923546
C	-29.081143	-9.985453	6.020681
H	-28.351976	-9.825488	6.821154
C	-29.943235	-11.079480	6.066449
H	-29.890983	-11.785484	6.901676
H	-30.156000	-8.577435	3.106846
C	-30.877753	-11.275332	5.054125
H	-31.563495	-12.128733	5.089218
S	-33.590209	-10.832131	3.522203
C	-34.637392	-13.668714	1.687727
N	-33.921351	-14.500940	0.874764
C	-32.961049	-14.091684	-0.109390
C	-31.638227	-13.881296	0.303131
C	-31.246117	-14.054743	1.737299
H	-30.156154	-13.966560	1.853868
H	-31.725496	-13.287851	2.372183
H	-31.557338	-15.038356	2.128899
C	-30.712551	-13.494776	-0.663303
H	-29.678740	-13.298647	-0.355359
C	-31.074564	-13.326790	-2.003156
C	-30.059034	-12.885169	-3.012681
H	-29.581916	-11.941091	-2.698221
H	-30.517107	-12.728838	-4.001624
H	-29.254868	-13.633470	-3.124368
C	-32.395052	-13.578880	-2.372064
H	-32.691078	-13.462503	-3.421433
C	-33.363120	-13.970468	-1.443311
C	-34.776908	-14.219689	-1.864936
H	-34.842122	-14.332737	-2.958131
H	-35.425190	-13.372927	-1.565548
H	-35.196269	-15.124185	-1.393357
N	-35.377698	-14.531446	2.446491
C	-36.342391	-14.161421	3.442136
C	-35.920799	-13.976565	4.761812
C	-34.481676	-14.120651	5.144477
H	-33.886625	-13.295380	4.709419
H	-34.364625	-14.090847	6.238305
H	-34.049505	-15.065012	4.772651

C	-36.890643	-13.618230	5.702080
H	-36.580310	-13.453528	6.740809
C	-38.231517	-13.455519	5.355161
C	-39.251740	-13.045766	6.373390
H	-38.791274	-12.879990	7.359042
H	-39.756346	-12.113436	6.067613
H	-40.034955	-13.815644	6.487422
C	-38.607994	-13.671369	4.026279
H	-39.654932	-13.530841	3.732003
C	-37.680683	-14.023961	3.049139
C	-38.080195	-14.193546	1.617825
H	-37.580613	-13.434412	0.987549
H	-39.168007	-14.078008	1.502309
H	-37.791963	-15.182674	1.222562
S	-36.532286	-10.853957	2.838557
C	-37.827151	-10.560077	1.715406
C	-39.130973	-10.267764	2.332614
C	-39.209365	-9.429197	3.456757
H	-38.291298	-8.963233	3.830325
C	-40.428980	-9.189703	4.082137
H	-40.469222	-8.525532	4.951787
C	-41.594306	-9.788033	3.603774
H	-42.553459	-9.599887	4.096411
C	-41.528467	-10.630645	2.493086
H	-42.436913	-11.111317	2.114573
C	-40.311758	-10.869668	1.864159
H	-40.263030	-11.537275	0.998846
C	-37.584520	-10.707276	0.366102
C	-38.541253	-10.426230	-0.715786
C	-39.341949	-9.272385	-0.695004
H	-39.252062	-8.577278	0.144997
C	-40.228522	-9.007287	-1.732533
H	-40.840019	-8.099663	-1.703007
C	-40.332060	-9.883522	-2.813261
H	-41.028687	-9.671331	-3.630508
C	-39.533022	-11.025451	-2.851791
H	-39.603048	-11.715813	-3.698612
C	-38.642983	-11.291675	-1.816794
H	-38.012961	-12.187463	-1.844451
S	-35.996749	-11.213094	-0.141948
C	-35.129835	-15.850816	2.115805
C	-34.204725	-15.832202	1.120498
H	-33.721189	-16.635060	0.569049
H	-35.632539	-16.673885	2.618120

Complex 5-BP86 S=0

100

Fe -34.7057100000 -11.5261750000 1.6448770000
S -32.9689670000 -10.8986220000 0.4925610000
C -31.6692480000 -10.5726000000 1.5984680000
C -30.3702940000 -10.1971520000 0.9881700000
C -30.3115800000 -9.2468630000 -0.0503770000
H -31.2310550000 -8.7548130000 -0.3706530000
C -29.0992690000 -8.9329930000 -0.6665780000
H -29.0776430000 -8.1898030000 -1.4655680000

C -27.9176240000 -9.5648240000 -0.2653690000
H -26.9706880000 -9.3227910000 -0.7506480000
C -27.9615830000 -10.5117390000 0.7628530000
H -27.0473040000 -11.0161560000 1.0814120000
C -29.1715410000 -10.8239140000 1.3840820000
H -29.1952080000 -11.5676290000 2.1802770000
C -31.9051320000 -10.7428670000 2.9667030000
C -30.9223210000 -10.4742870000 4.0462670000
C -30.1812830000 -9.2769170000 4.0868750000
C -29.2800560000 -9.0321360000 5.1242550000
H -28.7188280000 -8.0962580000 5.1404700000
C -29.0963000000 -9.9754380000 6.1407650000
H -28.3874260000 -9.7833520000 6.9482240000
C -29.8299360000 -11.1655900000 6.1156380000
H -29.6953360000 -11.9091470000 6.9033610000
H -30.3230240000 -8.5333120000 3.3027920000
C -30.7362920000 -11.4101180000 5.0825120000
H -31.3069410000 -12.3398080000 5.0630850000
S -33.4828710000 -11.2414800000 3.4767440000
C -34.7070330000 -13.4856700000 1.6413560000
N -33.9895420000 -14.3508420000 0.8255780000
C -33.0270980000 -14.0442720000 -0.2097980000
C -31.6639150000 -13.9935850000 0.1504200000
C -31.2272160000 -14.1967850000 1.5776230000
H -30.1367980000 -14.1178390000 1.6604970000
H -31.6820000000 -13.4464550000 2.2398920000
H -31.5260500000 -15.1865110000 1.9544070000
C -30.7284930000 -13.7449950000 -0.8551790000
H -29.6727010000 -13.6775850000 -0.5833610000
C -31.1099770000 -13.5598060000 -2.1923740000
C -30.0757600000 -13.2723230000 -3.2528300000
H -29.3528160000 -12.5212820000 -2.9036230000
H -30.5417940000 -12.8982030000 -4.1743000000
H -29.5068490000 -14.1806620000 -3.5089610000
C -32.4637670000 -13.6702430000 -2.5134560000
H -32.7778720000 -13.5544450000 -3.5539850000
C -33.4461880000 -13.9300030000 -1.5441890000
C -34.8831450000 -14.0824700000 -1.9737440000
H -34.9492280000 -14.7437620000 -2.8499140000
H -35.3087420000 -13.1082150000 -2.2555410000
H -35.5132320000 -14.4951290000 -1.1781360000
N -35.4253860000 -14.3542020000 2.4527570000
C -36.3870640000 -14.0512130000 3.4898550000
C -35.9666460000 -13.9436360000 4.8244090000
C -34.5295980000 -14.1019560000 5.2513170000
H -34.0928950000 -13.1263200000 5.5112800000
H -34.4665970000 -14.7458210000 6.1404750000
H -33.9070930000 -14.5375900000 4.4616280000
C -36.9470680000 -13.6843830000 5.7955730000
H -36.6311020000 -13.5735390000 6.8360310000
C -38.3009240000 -13.5685380000 5.4762840000
C -39.3327300000 -13.2812630000 6.5391240000
H -38.8643820000 -12.9059950000 7.4590100000
H -40.0571460000 -12.5311170000 6.1914220000
H -39.9000450000 -14.1899280000 6.7977820000
C -38.6843940000 -13.7487860000 4.1390270000

H -39.7403530000 -13.6769960000 3.8689250000
C -37.7506570000 -13.9964370000 3.1313370000
C -38.1901900000 -14.1938270000 1.7041200000
H -37.7338390000 -13.4435350000 1.0429250000
H -39.2804520000 -14.1099540000 1.6237330000
H -37.8965090000 -15.1837700000 1.3240110000
S -36.4421980000 -10.8992320000 2.7977020000
C -37.7418860000 -10.5708400000 1.6921510000
C -39.0401930000 -10.1936780000 2.3031860000
C -39.0967250000 -9.2458560000 3.3444930000
H -38.1762910000 -8.7559100000 3.6664640000
C -40.3085130000 -8.9310530000 3.9612460000
H -40.3288360000 -8.1897670000 4.7624730000
C -41.4919790000 -9.5588960000 3.5576750000
H -42.4384020000 -9.3169020000 4.0442430000
C -41.4502230000 -10.5032780000 2.5268450000
H -42.3653340000 -11.0061980000 2.2074870000
C -40.2406910000 -10.8163900000 1.9052020000
H -40.2177100000 -11.5586630000 1.1076180000
C -37.5058570000 -10.7397250000 0.3236010000
C -38.4877490000 -10.4717570000 -0.7574370000
C -39.2291020000 -9.2752480000 -0.7996040000
H -39.0875710000 -8.5305580000 -0.0165000000
C -40.1293410000 -9.0316110000 -1.8379570000
H -40.6891520000 -8.0951790000 -1.8569420000
C -40.3124540000 -9.9757290000 -2.8536490000
H -41.0199120000 -9.7840240000 -3.6622010000
C -39.5782410000 -11.1651410000 -2.8272360000
H -39.7121950000 -11.9096180000 -3.6141330000
C -38.6719140000 -11.4077170000 -1.7939870000
H -38.1008840000 -12.3368030000 -1.7735470000
S -35.9281920000 -11.2381890000 -0.1865530000
C -35.1588840000 -15.6854950000 2.1412120000
C -34.2581910000 -15.6832700000 1.1302040000
H -33.7814600000 -16.4935060000 0.5928490000
H -35.6376390000 -16.4978450000 2.6738340000

Complex 5-BP86 S=1

100

Fe	-34.705096	-11.477428	1.645056
S	-32.970942	-10.665954	0.508144
C	-31.620092	-10.493235	1.621429
C	-30.311198	-10.192522	0.996585
C	-30.220227	-9.262108	-0.057901
H	-31.120345	-8.736276	-0.377902
C	-29.000507	-9.007664	-0.685907
H	-28.953965	-8.277697	-1.495596
C	-27.843299	-9.681310	-0.282590
H	-26.890119	-9.484102	-0.775659
C	-27.918475	-10.610974	0.759741
H	-27.022936	-11.146143	1.080787
C	-29.135782	-10.863222	1.392163
H	-29.185415	-11.592783	2.199594
C	-31.849512	-10.698299	2.969134

C	-30.869932	-10.489581	4.063029
C	-30.094091	-9.315847	4.132156
C	-29.196383	-9.117000	5.181197
H	-28.608007	-8.198575	5.220011
C	-29.054681	-10.081430	6.184594
H	-28.352333	-9.922645	7.004446
C	-29.825407	-11.246608	6.133327
H	-29.724779	-12.004204	6.912515
H	-30.209207	-8.554760	3.360427
C	-30.727652	-11.445384	5.087324
H	-31.330866	-12.353500	5.050820
S	-33.462469	-11.160565	3.472868
C	-34.708520	-13.489384	1.639969
N	-34.014145	-14.341795	0.806716
C	-33.051937	-14.015517	-0.225099
C	-31.693809	-13.943247	0.146532
C	-31.263433	-14.146440	1.575889
H	-30.174090	-14.060179	1.663270
H	-31.724847	-13.399195	2.237346
H	-31.556544	-15.139192	1.949476
C	-30.756640	-13.676212	-0.852506
H	-29.703809	-13.592693	-0.574176
C	-31.132750	-13.494921	-2.191754
C	-30.093968	-13.197360	-3.245159
H	-29.386610	-12.433114	-2.894499
H	-30.557001	-12.837497	-4.173014
H	-29.508466	-14.097650	-3.489724
C	-32.483358	-13.619483	-2.521465
H	-32.793263	-13.501631	-3.562807
C	-33.468198	-13.895593	-1.559117
C	-34.902653	-14.054819	-1.996128
H	-34.960386	-14.698229	-2.886016
H	-35.335131	-13.078092	-2.258169
H	-35.532053	-14.489570	-1.211541
N	-35.410014	-14.342632	2.465952
C	-36.366375	-14.018993	3.503771
C	-35.942374	-13.911734	4.836656
C	-34.505614	-14.078306	5.261943
H	-34.056647	-13.100569	5.492413
H	-34.446819	-14.699317	6.167614
H	-33.890774	-14.541738	4.481707
C	-36.921675	-13.645031	5.807274
H	-36.605927	-13.538824	6.848184
C	-38.274247	-13.516378	5.486353
C	-39.306849	-13.230478	6.549132
H	-38.838718	-12.870803	7.474788
H	-40.022699	-12.470042	6.207464
H	-39.883650	-14.136104	6.795079
C	-38.657801	-13.682925	4.147353
H	-39.712097	-13.595398	3.875661
C	-37.726588	-13.942102	3.140556
C	-38.167054	-14.134178	1.712686
H	-37.709098	-13.382913	1.053447
H	-39.256911	-14.045523	1.633477
H	-37.878271	-15.124636	1.329562
S	-36.440150	-10.667067	2.780526

C	-37.789235	-10.491145	1.665188
C	-39.096830	-10.186164	2.291029
C	-39.183258	-9.258811	3.350060
H	-38.281079	-8.736417	3.671169
C	-40.401411	-9.002956	3.980964
H	-40.445159	-8.274817	4.793419
C	-41.560905	-9.672641	3.576218
H	-42.512871	-9.474623	4.071525
C	-41.490491	-10.597810	2.527814
H	-42.388407	-11.128295	2.203981
C	-40.275148	-10.851188	1.892487
H	-40.229218	-11.577955	1.081419
C	-37.558944	-10.697138	0.317454
C	-38.537474	-10.491075	-0.777975
C	-39.321660	-9.322894	-0.845609
H	-39.212705	-8.562126	-0.072521
C	-40.220716	-9.127929	-1.894648
H	-40.816879	-8.214484	-1.931432
C	-40.354360	-10.090646	-2.900801
H	-41.058153	-9.935847	-3.720457
C	-39.574211	-11.250025	-2.852075
H	-39.668427	-12.006986	-3.632831
C	-38.672052	-11.445721	-1.804935
H	-38.062647	-12.349795	-1.769212
S	-35.945343	-11.161045	-0.183292
C	-35.156126	-15.674930	2.148354
C	-34.281721	-15.674562	1.112481
H	-33.821041	-16.484599	0.560649
H	-35.624318	-16.484803	2.693500

Complex 5-BP86 S=0

100

Fe	-34.720221	-11.564126	1.674115
S	-33.108277	-10.492020	0.472151
C	-31.744363	-10.394004	1.588627
C	-30.433443	-10.101019	0.962578
C	-30.334037	-9.143985	-0.067995
H	-31.229077	-8.600624	-0.373462
C	-29.112071	-8.885794	-0.689658
H	-29.058285	-8.134693	-1.479574
C	-27.962306	-9.583965	-0.305636
H	-27.007538	-9.382841	-0.794286
C	-28.047454	-10.542656	0.709054
H	-27.157181	-11.095367	1.013837
C	-29.266678	-10.797948	1.336477
H	-29.323497	-11.549243	2.123634
C	-31.951074	-10.574256	2.945623
C	-30.936147	-10.363301	4.007786
C	-30.143014	-9.198810	4.034823
C	-29.220285	-8.989984	5.059480
H	-28.620738	-8.077944	5.066688
C	-29.067001	-9.936223	6.078798
H	-28.342456	-9.771284	6.878158
C	-29.856884	-11.089672	6.071666
H	-29.749560	-11.832352	6.864762

H	-30.266483	-8.451468	3.250825
C	-30.786884	-11.297307	5.051630
H	-31.406413	-12.195337	5.050756
S	-33.565099	-10.941956	3.553620
C	-34.655372	-13.767076	1.687808
N	-33.942546	-14.610798	0.869432
C	-32.981012	-14.226565	-0.141317
C	-31.639580	-14.052179	0.245457
C	-31.211617	-14.210026	1.682103
H	-30.119648	-14.155758	1.765714
H	-31.645185	-13.418983	2.311618
H	-31.539265	-15.172982	2.100611
C	-30.713443	-13.720774	-0.747301
H	-29.671774	-13.562582	-0.460058
C	-31.087874	-13.571844	-2.089524
C	-30.063812	-13.195489	-3.131787
H	-29.545013	-12.266913	-2.852826
H	-30.528980	-13.044798	-4.114147
H	-29.296432	-13.977730	-3.235771
C	-32.425841	-13.785898	-2.432718
H	-32.733138	-13.686260	-3.476623
C	-33.396169	-14.123763	-1.478836
C	-34.827072	-14.350267	-1.893463
H	-34.895419	-14.470433	-2.982448
H	-35.457443	-13.494079	-1.602225
H	-35.258223	-15.243517	-1.419663
N	-35.383522	-14.631636	2.470464
C	-36.333132	-14.278579	3.504110
C	-35.881101	-14.137446	4.825175
C	-34.426278	-14.289631	5.185502
H	-33.829101	-13.482874	4.733260
H	-34.294026	-14.246784	6.273477
H	-34.014498	-15.245020	4.828156
C	-36.834702	-13.836128	5.807232
H	-36.499284	-13.708675	6.839026
C	-38.192537	-13.694134	5.505367
C	-39.198667	-13.352941	6.576659
H	-38.716430	-13.229277	7.554751
H	-39.722433	-12.416875	6.335938
H	-39.963386	-14.138344	6.670642
C	-38.600629	-13.869496	4.176307
H	-39.656631	-13.756998	3.919891
C	-37.691304	-14.162225	3.156455
C	-38.151102	-14.319041	1.730331
H	-37.702783	-13.544842	1.089732
H	-39.242296	-14.230547	1.666897
H	-37.862432	-15.294661	1.311813
S	-36.577345	-10.793462	2.817572
C	-37.847511	-10.459936	1.659127
C	-39.148848	-10.074892	2.256209
C	-39.202835	-9.139678	3.308833
H	-38.277796	-8.669461	3.645597
C	-40.417689	-8.809424	3.910580
H	-40.436790	-8.075344	4.718330
C	-41.604969	-9.411500	3.481532
H	-42.554773	-9.154404	3.953785

C	-41.564946	-10.348798	2.443493
H	-42.484924	-10.831819	2.107110
C	-40.352421	-10.678229	1.837608
H	-40.328213	-11.417022	1.036616
C	-37.603684	-10.650823	0.311898
C	-38.547496	-10.345910	-0.789507
C	-39.234694	-9.116747	-0.843102
H	-39.073413	-8.381774	-0.054327
C	-40.101593	-8.830253	-1.898184
H	-40.619891	-7.869731	-1.924745
C	-40.299325	-9.760923	-2.923656
H	-40.977752	-9.534394	-3.748299
C	-39.614514	-10.980452	-2.889088
H	-39.759254	-11.712399	-3.685691
C	-38.743650	-11.267615	-1.837161
H	-38.209631	-12.218956	-1.812472
S	-36.032523	-11.245041	-0.192101
C	-35.128203	-15.960879	2.147718
C	-34.217781	-15.948695	1.138390
H	-33.740321	-16.753788	0.592318
H	-35.616087	-16.779356	2.663260

Complex 5-B3LYP S=0

100

Fe	-34.705578	-11.613408	1.642700
S	-32.919192	-10.980906	0.461072
C	-31.663691	-10.603278	1.609725
C	-30.348693	-10.196971	1.027149
C	-30.281598	-9.235794	0.001321
H	-31.196672	-8.761525	-0.339399
C	-29.059456	-8.889321	-0.578456
H	-29.032258	-8.138886	-1.363921
C	-27.876519	-9.502230	-0.152350
H	-26.925976	-9.234110	-0.605062
C	-27.929497	-10.464058	0.861293
H	-27.018540	-10.950687	1.198177
C	-29.150636	-10.806809	1.444985
H	-29.178257	-11.556666	2.228617
C	-31.919361	-10.723627	2.975341
C	-30.950476	-10.342622	4.047477
C	-30.342775	-9.073870	4.060723
C	-29.458927	-8.716465	5.080170
H	-29.004442	-7.729734	5.074798
C	-29.160342	-9.619865	6.105454
H	-28.468679	-9.341910	6.895860
C	-29.763050	-10.881706	6.108131
H	-29.540690	-11.590889	6.900818
H	-30.571156	-8.365435	3.271146
C	-30.654324	-11.236083	5.092986
H	-31.124577	-12.214849	5.101651
S	-33.482298	-11.255613	3.522524
C	-34.706924	-13.632047	1.639059
N	-34.004046	-14.489131	0.816024
C	-33.051959	-14.182324	-0.232703
C	-31.683309	-14.126840	0.109348

C	-31.221861	-14.310074	1.538192
H	-30.134829	-14.230377	1.599331
H	-31.659723	-13.551464	2.192640
H	-31.511711	-15.289368	1.933311
C	-30.761145	-13.885714	-0.908889
H	-29.706054	-13.818085	-0.654385
C	-31.160008	-13.710093	-2.243875
C	-30.132724	-13.421752	-3.318007
H	-29.567013	-12.514091	-3.080556
H	-30.604186	-13.282825	-4.294071
H	-29.410442	-14.241703	-3.403404
C	-32.517619	-13.813699	-2.545801
H	-32.844601	-13.701224	-3.577263
C	-33.487518	-14.064746	-1.559697
C	-34.935976	-14.212154	-1.976020
H	-35.029721	-14.986802	-2.744315
H	-35.309930	-13.275976	-2.399676
H	-35.584379	-14.475682	-1.141231
N	-35.410826	-14.490717	2.459670
C	-36.360620	-14.186260	3.511168
C	-35.922349	-14.073417	4.837641
C	-34.473183	-14.224639	5.250528
H	-34.100358	-13.294363	5.687949
H	-34.377483	-15.010641	6.006932
H	-33.825136	-14.474690	4.411354
C	-36.890054	-13.824841	5.826631
H	-36.560855	-13.715805	6.857718
C	-38.248325	-13.719819	5.527842
C	-39.273389	-13.435298	6.605124
H	-38.799627	-13.294831	7.579361
H	-39.843382	-12.530380	6.369838
H	-39.991946	-14.257846	6.693065
C	-38.649901	-13.890647	4.193105
H	-39.705492	-13.821777	3.941032
C	-37.729921	-14.128438	3.172059
C	-38.194680	-14.306648	1.743637
H	-37.755087	-13.548564	1.089777
H	-39.281477	-14.222553	1.684790
H	-37.909503	-15.286415	1.346098
S	-36.491146	-10.981466	2.825941
C	-37.745626	-10.599288	1.678038
C	-39.059227	-10.190881	2.262032
C	-39.124341	-9.229188	3.287561
H	-38.208754	-8.754941	3.627209
C	-40.345633	-8.881713	3.868727
H	-40.371804	-8.130506	4.653619
C	-41.529299	-9.494813	3.444973
H	-42.479131	-9.226948	3.899177
C	-41.478287	-10.456520	2.430702
H	-42.390162	-10.942962	2.094901
C	-40.258090	-10.799682	1.845068
H	-40.231251	-11.548834	1.060681
C	-37.491540	-10.719005	0.312010
C	-38.462756	-10.338737	-0.758091
C	-39.073182	-9.071398	-0.769364
H	-38.845093	-8.363154	0.020498

C	-39.959347	-8.714910	-1.787193
H	-40.415792	-7.729053	-1.780509
C	-40.258035	-9.618299	-2.812429
H	-40.951294	-9.340909	-3.601653
C	-39.653561	-10.879307	-2.816396
H	-39.876009	-11.588259	-3.609224
C	-38.759962	-11.232560	-1.803160
H	-38.288219	-12.210582	-1.813034
S	-35.928941	-11.250681	-0.236506
C	-35.148556	-15.822572	2.148069
C	-34.267486	-15.821595	1.123902
H	-33.803202	-16.630963	0.582904
H	-35.613811	-16.632947	2.686621

Complex 5-B3LYP S=1

100

Fe	-34.714209	-11.670655	1.642116
S	-32.899316	-10.959892	0.396854
C	-31.658843	-10.521415	1.563865
C	-30.356012	-10.097725	0.968955
C	-30.311902	-9.153105	-0.073486
H	-31.237665	-8.706134	-0.422730
C	-29.096480	-8.784270	-0.654308
H	-29.084719	-8.043934	-1.450180
C	-27.900301	-9.361486	-0.215796
H	-26.954873	-9.077166	-0.670142
C	-27.931515	-10.310797	0.811416
H	-27.009437	-10.771716	1.156004
C	-29.145083	-10.674408	1.397478
H	-29.159350	-11.413675	2.191541
C	-31.900959	-10.606303	2.923892
C	-30.950012	-10.149510	3.979544
C	-30.372524	-8.866912	3.936993
C	-29.500959	-8.443046	4.941670
H	-29.069256	-7.447066	4.893306
C	-29.186266	-9.291388	6.008674
H	-28.505554	-8.960483	6.788297
C	-29.759716	-10.565236	6.067810
H	-29.525171	-11.231473	6.893705
H	-30.615489	-8.200251	3.116163
C	-30.638294	-10.986409	5.067430
H	-31.086213	-11.974127	5.120261
S	-33.448990	-11.188540	3.526011
C	-34.702900	-13.983864	1.645754
N	-33.966395	-14.830992	0.860719
C	-33.005890	-14.465180	-0.161115
C	-31.655286	-14.311132	0.203555
C	-31.205949	-14.438173	1.642557
H	-30.118992	-14.361104	1.710208
H	-31.644488	-13.645927	2.257218
H	-31.507012	-15.394896	2.080800
C	-30.736683	-14.005554	-0.804357
H	-29.692027	-13.867167	-0.535137
C	-31.127556	-13.851970	-2.141653
C	-30.108548	-13.491085	-3.202059

H	-29.667336	-12.509430	-2.997369
H	-30.561239	-13.458386	-4.195974
H	-29.288896	-14.217594	-3.225909
C	-32.476231	-14.030699	-2.463183
H	-32.796860	-13.922528	-3.496382
C	-33.437107	-14.345901	-1.491254
C	-34.886426	-14.539625	-1.881442
H	-34.996325	-14.503159	-2.968004
H	-35.518447	-13.757155	-1.449010
H	-35.272996	-15.502424	-1.532900
N	-35.427625	-14.833696	2.439005
C	-36.393327	-14.471228	3.457096
C	-35.967977	-14.347980	4.788980
C	-34.519567	-14.534572	5.185885
H	-33.890509	-13.746081	4.759777
H	-34.416472	-14.502685	6.272783
H	-34.124383	-15.493542	4.835543
C	-36.934085	-14.035071	5.756514
H	-36.618234	-13.924088	6.790821
C	-38.282359	-13.863291	5.429415
C	-39.307817	-13.506539	6.485054
H	-38.858634	-13.465725	7.480177
H	-39.756867	-12.529605	6.275329
H	-40.121151	-14.239939	6.509133
C	-38.667006	-14.021143	4.091015
H	-39.711254	-13.888351	3.817417
C	-37.743144	-14.324141	3.087238
C	-38.186197	-14.455411	1.646735
H	-37.764611	-13.650164	1.037092
H	-39.274482	-14.403331	1.576433
H	-37.861274	-15.402398	1.204889
S	-36.532046	-10.964282	2.885989
C	-37.768858	-10.519838	1.717455
C	-39.071384	-10.092405	2.310075
C	-39.114074	-9.150878	3.355600
H	-38.186907	-8.710075	3.708770
C	-40.329289	-8.779102	3.935028
H	-40.339834	-8.042362	4.734033
C	-41.526716	-9.349946	3.491746
H	-42.471800	-9.063481	3.945098
C	-41.497153	-10.295660	2.461348
H	-42.420601	-10.751052	2.112957
C	-40.283697	-10.662352	1.876748
H	-40.271159	-11.399111	1.080282
C	-37.524454	-10.602169	0.357414
C	-38.469814	-10.134812	-0.699190
C	-39.031710	-8.845081	-0.656940
H	-38.783495	-8.182711	0.166019
C	-39.893327	-8.408446	-1.664245
H	-40.311318	-7.406714	-1.616137
C	-40.214777	-9.251320	-2.733533
H	-40.887823	-8.910545	-3.515361
C	-39.657579	-10.532528	-2.792128
H	-39.897373	-11.193944	-3.620356
C	-38.788106	-10.966534	-1.789371
H	-38.352445	-11.959814	-1.842437

S	-35.977902	-11.189237	-0.243347
C	-35.148583	-16.168241	2.152450
C	-34.228051	-16.166680	1.158683
H	-33.737911	-16.976133	0.639852
H	-35.628616	-16.979252	2.678101

Complex 5-B3LYP S=2

100

Fe	-34.704179	-11.518602	1.636956
S	-32.887413	-10.690430	0.408296
C	-31.603681	-10.438597	1.588037
C	-30.259408	-10.157739	1.002906
C	-30.113071	-9.231055	-0.047147
H	-30.985452	-8.690636	-0.401074
C	-28.865542	-8.997900	-0.630161
H	-28.775502	-8.269373	-1.431395
C	-27.737528	-9.694803	-0.186622
H	-26.767391	-9.515638	-0.642050
C	-27.869504	-10.626152	0.849200
H	-27.001166	-11.178097	1.199309
C	-29.114153	-10.853339	1.438202
H	-29.204436	-11.580640	2.238182
C	-31.853071	-10.539946	2.948867
C	-30.854781	-10.216580	4.009610
C	-30.147736	-8.999636	3.992242
C	-29.237187	-8.689107	5.003372
H	-28.706000	-7.741669	4.975508
C	-29.011888	-9.588363	6.051367
H	-28.300287	-9.346753	6.836003
C	-29.715265	-10.796562	6.086421
H	-29.551112	-11.499570	6.898735
H	-30.322539	-8.294170	3.186606
C	-30.633655	-11.103532	5.080613
H	-31.184895	-12.038267	5.115942
S	-33.446072	-10.979222	3.558003
C	-34.707730	-13.818068	1.636665
N	-33.979087	-14.664372	0.844948
C	-33.013543	-14.296873	-0.172858
C	-31.662528	-14.160217	0.196783
C	-31.215246	-14.320382	1.633570
H	-30.126863	-14.269589	1.700430
H	-31.633286	-13.529328	2.263770
H	-31.537042	-15.277477	2.055892
C	-30.739627	-13.849788	-0.805428
H	-29.694817	-13.721670	-0.533018
C	-31.126481	-13.679601	-2.141745
C	-30.101522	-13.317796	-3.195998
H	-29.617609	-12.365628	-2.954582
H	-30.560441	-13.224278	-4.182751
H	-29.313677	-14.076282	-3.258115
C	-32.475245	-13.845918	-2.468690
H	-32.791535	-13.726390	-3.501803
C	-33.441598	-14.162444	-1.502677
C	-34.891800	-14.335839	-1.898124
H	-34.991359	-14.341362	-2.985452

H	-35.503124	-13.517522	-1.504706
H	-35.309309	-15.271240	-1.514380
N	-35.438327	-14.664181	2.426773
C	-36.400424	-14.296785	3.447724
C	-35.969078	-14.166233	4.776851
C	-34.518640	-14.345669	5.168346
H	-33.902938	-13.531677	4.770350
H	-34.416437	-14.348386	6.255904
H	-34.108219	-15.285495	4.786345
C	-36.932425	-13.849188	5.745734
H	-36.613414	-13.731882	6.778371
C	-38.281629	-13.679642	5.422161
C	-39.303448	-13.317013	6.479101
H	-38.842670	-13.226072	7.465381
H	-39.785216	-12.363292	6.239859
H	-40.092904	-14.073632	6.541505
C	-38.671819	-13.846994	4.086406
H	-39.717050	-13.716667	3.816392
C	-37.751877	-14.156938	3.081475
C	-38.202342	-14.314006	1.645222
H	-37.780328	-13.525675	1.014218
H	-39.290494	-14.256951	1.580160
H	-37.886982	-15.273245	1.222523
S	-36.514768	-10.684342	2.870563
C	-37.800908	-10.427724	1.694761
C	-39.141610	-10.144327	2.286499
C	-39.281071	-9.213639	3.333546
H	-38.406881	-8.670187	3.678740
C	-40.524343	-8.981088	3.925582
H	-40.609194	-8.250296	4.725568
C	-41.654617	-9.682183	3.493278
H	-42.621330	-9.503926	3.956261
C	-41.529395	-10.616541	2.459425
H	-42.399432	-11.171331	2.117827
C	-40.288777	-10.843848	1.862371
H	-40.202726	-11.574352	1.065079
C	-37.557227	-10.530362	0.333096
C	-38.561668	-10.208970	-0.723002
C	-39.270974	-8.992891	-0.704274
H	-39.091656	-8.284644	0.097872
C	-40.189599	-8.686408	-1.709389
H	-40.721026	-7.739122	-1.680943
C	-40.423193	-9.590015	-2.751808
H	-41.140958	-9.351834	-3.531773
C	-39.718237	-10.797372	-2.788279
H	-39.887821	-11.503759	-3.596607
C	-38.789784	-11.098891	-1.789831
H	-38.236730	-12.032583	-1.826912
S	-35.966644	-10.972915	-0.281407
C	-35.170194	-15.998050	2.132101
C	-34.250102	-15.998203	1.137236
H	-33.766310	-16.808516	0.613876
H	-35.656247	-16.808363	2.653424

Complex 5-B3LYP* S=0

100

Fe	-34.705657	-11.609571	1.644111
S	-32.937163	-10.976091	0.465536
C	-31.670930	-10.606167	1.603991
C	-30.360379	-10.206218	1.013609
C	-30.296769	-9.257558	-0.024134
H	-31.214505	-8.787455	-0.368168
C	-29.076654	-8.916021	-0.610432
H	-29.052303	-8.173221	-1.404776
C	-27.891766	-9.521039	-0.179094
H	-26.941265	-9.255761	-0.635839
C	-27.941114	-10.470894	0.845863
H	-27.026590	-10.951909	1.187199
C	-29.160088	-10.809053	1.436211
H	-29.185392	-11.550783	2.229324
C	-31.920602	-10.735217	2.970226
C	-30.950301	-10.366028	4.041957
C	-30.325199	-9.105592	4.053829
C	-29.437515	-8.758918	5.073166
H	-28.968020	-7.777787	5.066402
C	-29.152503	-9.664376	6.100269
H	-28.456235	-9.394401	6.890877
C	-29.773190	-10.917033	6.105153
H	-29.561432	-11.628280	6.900567
H	-30.543462	-8.395073	3.261521
C	-30.668003	-11.261353	5.089895
H	-31.152257	-12.234966	5.099115
S	-33.483483	-11.268658	3.512595
C	-34.706869	-13.611085	1.639574
N	-34.000285	-14.469378	0.818260
C	-33.045260	-14.162099	-0.226665
C	-31.678602	-14.103642	0.120746
C	-31.223276	-14.286710	1.549905
H	-30.135881	-14.199831	1.616949
H	-31.670371	-13.532246	2.205248
H	-31.509189	-15.270021	1.941856
C	-30.753481	-13.858779	-0.893682
H	-29.698508	-13.786828	-0.634111
C	-31.147748	-13.681509	-2.229085
C	-30.118467	-13.385269	-3.297263
H	-29.535274	-12.493950	-3.038315
H	-30.589357	-13.212453	-4.269083
H	-29.410669	-14.215989	-3.406251
C	-32.503805	-13.790933	-2.536885
H	-32.827266	-13.678090	-3.570683
C	-33.476473	-14.046156	-1.555260
C	-34.922132	-14.196038	-1.974958
H	-35.006727	-14.937798	-2.777452
H	-35.312821	-13.246748	-2.355754
H	-35.564957	-14.506345	-1.150052
N	-35.415082	-14.470957	2.457455
C	-36.367182	-14.166442	3.505615
C	-35.932403	-14.056917	4.833561
C	-34.485983	-14.211397	5.248821

H	-34.097573	-13.268768	5.647793
H	-34.398588	-14.968497	6.036516
H	-33.843227	-14.503791	4.417573
C	-36.902291	-13.805672	5.818950
H	-36.576001	-13.697552	6.852323
C	-38.259038	-13.695832	5.515139
C	-39.285970	-13.406635	6.587483
H	-38.812445	-13.238126	7.559164
H	-39.871437	-12.514790	6.334718
H	-39.992367	-14.239374	6.694054
C	-38.656786	-13.866723	4.179906
H	-39.712563	-13.794753	3.923686
C	-37.734578	-14.106277	3.161799
C	-38.193947	-14.282736	1.733028
H	-37.746764	-13.526927	1.079293
H	-39.281325	-14.193054	1.669356
H	-37.911565	-15.265312	1.336531
S	-36.472929	-10.974473	2.824390
C	-37.738690	-10.601331	1.686336
C	-39.049425	-10.198929	2.274482
C	-39.113639	-9.246788	3.309007
H	-38.195898	-8.777714	3.653861
C	-40.334460	-8.902583	3.892022
H	-40.359910	-8.159071	4.685534
C	-41.518869	-9.508415	3.460728
H	-42.469559	-9.242544	3.916825
C	-41.469020	-10.460297	2.437712
H	-42.382783	-10.941552	2.095896
C	-40.249590	-10.801566	1.851158
H	-40.223555	-11.545679	1.059795
C	-37.489042	-10.729116	0.320193
C	-38.460536	-10.359541	-0.750010
C	-39.082998	-9.097889	-0.763041
H	-38.860931	-8.385554	0.026735
C	-39.973020	-8.752429	-1.780529
H	-40.439561	-7.769799	-1.775255
C	-40.263894	-9.660897	-2.803650
H	-40.961345	-9.391783	-3.593293
C	-39.646652	-10.915055	-2.806349
H	-39.863159	-11.628831	-3.598365
C	-38.748385	-11.257424	-1.793997
H	-38.266098	-12.231749	-1.801995
S	-35.927352	-11.263358	-0.223654
C	-35.152195	-15.802496	2.145498
C	-34.265857	-15.801470	1.125249
H	-33.798189	-16.611144	0.585349
H	-35.621619	-16.613425	2.681933

Complex 5-B3LYP* S=1

100

Fe	-34.706389	-11.439881	1.644142
S	-32.940356	-10.557532	0.491255
C	-31.602707	-10.451536	1.637613
C	-30.265661	-10.185208	1.037246
C	-30.115383	-9.239217	0.004047

H	-30.981054	-8.668078	-0.320399
C	-28.876193	-9.029669	-0.604411
H	-28.785041	-8.288267	-1.395518
C	-27.757289	-9.764535	-0.199961
H	-26.792374	-9.603029	-0.675213
C	-27.890928	-10.709969	0.822596
H	-27.029035	-11.291484	1.144100
C	-29.128359	-10.917507	1.432657
H	-29.219875	-11.659805	2.219890
C	-31.835047	-10.674729	2.979608
C	-30.838811	-10.464410	4.067591
C	-30.112298	-9.262574	4.154216
C	-29.199192	-9.051799	5.188230
H	-28.652240	-8.112844	5.239752
C	-28.991907	-10.037740	6.158384
H	-28.279926	-9.873996	6.963606
C	-29.715038	-11.232439	6.090595
H	-29.565262	-12.003795	6.843055
H	-30.274911	-8.489451	3.408482
C	-30.634212	-11.440409	5.060716
H	-31.199709	-12.367900	5.016435
S	-33.436975	-11.170368	3.516679
C	-34.703401	-13.550351	1.638384
N	-34.000435	-14.391752	0.814444
C	-33.049022	-14.048026	-0.223910
C	-31.688258	-13.956211	0.134789
C	-31.233244	-14.170966	1.559912
H	-30.147345	-14.073500	1.629921
H	-31.688204	-13.439523	2.235698
H	-31.506523	-15.168304	1.924534
C	-30.767323	-13.657899	-0.869167
H	-29.716873	-13.555844	-0.602590
C	-31.161695	-13.462747	-2.201542
C	-30.136843	-13.120944	-3.260213
H	-29.462402	-12.331708	-2.910882
H	-30.615296	-12.779291	-4.182306
H	-29.518865	-13.994047	-3.506181
C	-32.512486	-13.606839	-2.519804
H	-32.835112	-13.476895	-3.551920
C	-33.481286	-13.914292	-1.550379
C	-34.919231	-14.102636	-1.981881
H	-34.976217	-14.844477	-2.786653
H	-35.331607	-13.163090	-2.362705
H	-35.561262	-14.432333	-1.164082
N	-35.407560	-14.394399	2.458202
C	-36.359049	-14.054195	3.497817
C	-35.926597	-13.926419	4.824958
C	-34.488575	-14.117441	5.255000
H	-34.072515	-13.177645	5.631130
H	-34.432614	-14.856224	6.062580
H	-33.849007	-14.452619	4.437358
C	-36.894942	-13.622551	5.796007
H	-36.571990	-13.497269	6.828565
C	-38.245942	-13.477365	5.478891
C	-39.271016	-13.141312	6.539347
H	-38.792674	-12.803161	7.463171

H	-39.945992	-12.351052	6.193328
H	-39.888277	-14.015980	6.781593
C	-38.640610	-13.666653	4.145805
H	-39.691121	-13.563457	3.880213
C	-37.720053	-13.961048	3.140257
C	-38.176015	-14.171214	1.714799
H	-37.717611	-13.440780	1.040289
H	-39.261545	-14.069063	1.644861
H	-37.906857	-15.169213	1.348513
S	-36.470499	-10.555912	2.799060
C	-37.810487	-10.450972	1.655474
C	-39.146397	-10.183480	2.258070
C	-39.293784	-9.238510	3.292373
H	-38.426597	-8.669537	3.616534
C	-40.531968	-9.027193	3.902038
H	-40.620942	-8.286410	4.694051
C	-41.652803	-9.759078	3.497618
H	-42.617237	-9.594808	3.972618
C	-41.521456	-10.704310	2.475179
H	-42.384838	-11.283286	2.153660
C	-40.285148	-10.913801	1.863903
H	-40.196608	-11.655440	1.075827
C	-37.579705	-10.674944	0.312953
C	-38.576782	-10.464788	-0.774399
C	-39.302003	-9.262189	-0.860800
H	-39.136900	-8.488511	-0.116390
C	-40.217624	-9.051896	-1.892681
H	-40.764555	-8.113028	-1.943469
C	-40.427881	-10.038042	-2.861553
H	-41.143392	-9.874560	-3.664364
C	-39.704592	-11.232725	-2.795688
H	-39.856909	-12.004471	-3.547023
C	-38.783705	-11.441124	-1.766818
H	-38.219022	-12.369115	-1.722658
S	-35.978796	-11.169427	-0.226475
C	-35.144858	-15.725527	2.147899
C	-34.263043	-15.723802	1.119962
H	-33.798044	-16.532741	0.576446
H	-35.610229	-16.536217	2.688445

Complex 5-B3LYP* S=2

100

Fe	-34.704994	-11.535040	1.650000
S	-32.913020	-10.697738	0.418845
C	-31.621516	-10.439850	1.584798
C	-30.285021	-10.158619	0.988323
C	-30.151472	-9.239025	-0.069681
H	-31.030057	-8.702525	-0.418662
C	-28.910770	-9.008580	-0.666876
H	-28.830418	-8.285390	-1.475693
C	-27.777035	-9.700117	-0.229053
H	-26.810791	-9.522342	-0.696180
C	-27.896249	-10.624458	0.814210
H	-27.022198	-11.172879	1.159468
C	-29.134109	-10.849749	1.416843

H	-29.216086	-11.573321	2.222821
C	-31.862365	-10.543837	2.947550
C	-30.860455	-10.218055	4.000721
C	-30.147557	-9.004532	3.971161
C	-29.228728	-8.691897	4.973095
H	-28.693124	-7.745807	4.935289
C	-28.999807	-9.585660	6.024622
H	-28.280914	-9.342092	6.803637
C	-29.709458	-10.789569	6.072800
H	-29.543289	-11.488467	6.889812
H	-30.324910	-8.303027	3.160916
C	-30.637109	-11.098282	5.076522
H	-31.194195	-12.030715	5.121715
S	-33.450671	-10.991133	3.557688
C	-34.705615	-13.810034	1.644320
N	-33.972937	-14.657166	0.856289
C	-33.003524	-14.290808	-0.156565
C	-31.654232	-14.157572	0.218586
C	-31.214952	-14.317031	1.656080
H	-30.126333	-14.255491	1.730050
H	-31.646281	-13.531800	2.287106
H	-31.529942	-15.279745	2.074442
C	-30.727193	-13.851479	-0.780613
H	-29.681791	-13.725741	-0.504030
C	-31.109110	-13.681755	-2.118239
C	-30.080766	-13.323134	-3.168111
H	-29.607638	-12.361978	-2.933941
H	-30.533822	-13.245083	-4.160848
H	-29.283773	-14.075123	-3.215694
C	-32.457180	-13.843541	-2.449747
H	-32.770303	-13.723092	-3.485384
C	-33.427517	-14.155689	-1.487222
C	-34.875931	-14.324657	-1.884571
H	-34.975496	-14.316289	-2.973660
H	-35.490348	-13.511103	-1.479454
H	-35.292171	-15.267529	-1.512534
N	-35.442258	-14.656717	2.429451
C	-36.411651	-14.287978	3.441309
C	-35.989572	-14.151565	4.772456
C	-34.542727	-14.325255	5.173609
H	-33.925049	-13.512990	4.771662
H	-34.445572	-14.318963	6.263034
H	-34.127899	-15.267864	4.800587
C	-36.960745	-13.833061	5.732246
H	-36.649338	-13.711161	6.768249
C	-38.307622	-13.667098	5.397678
C	-39.336984	-13.301483	6.444154
H	-38.886548	-13.223113	7.437484
H	-39.805078	-12.339200	6.206729
H	-40.137377	-14.049325	6.491178
C	-38.687718	-13.839519	4.059993
H	-39.732191	-13.711003	3.780940
C	-37.759882	-14.151705	3.063443
C	-38.196938	-14.314787	1.625536
H	-37.760657	-13.534410	0.992005
H	-39.285082	-14.248968	1.548769

H	-37.885224	-15.280846	1.212187
S	-36.499016	-10.699194	2.879047
C	-37.787683	-10.441204	1.709606
C	-39.126617	-10.164057	2.302414
C	-39.267643	-9.245457	3.360112
H	-38.392584	-8.705708	3.712567
C	-40.511349	-9.020709	3.953580
H	-40.597726	-8.298631	4.762522
C	-41.640602	-9.717153	3.512307
H	-42.609104	-9.544271	3.976382
C	-41.513720	-10.639758	2.468409
H	-42.384176	-11.191303	2.119484
C	-40.273160	-10.859160	1.869587
H	-40.185396	-11.581265	1.062891
C	-37.543466	-10.541807	0.347051
C	-38.541921	-10.212512	-0.708520
C	-39.259753	-9.002049	-0.674163
H	-39.089455	-8.305736	0.142055
C	-40.174027	-8.685765	-1.679308
H	-40.713641	-7.742196	-1.637455
C	-40.393633	-9.572530	-2.738893
H	-41.109254	-9.326263	-3.519935
C	-39.679307	-10.773241	-2.791879
H	-39.838792	-11.467263	-3.614451
C	-38.756188	-11.085435	-1.792278
H	-38.195863	-12.015637	-1.840906
S	-35.953218	-10.987262	-0.259868
C	-35.175441	-15.990328	2.134914
C	-34.247685	-15.990166	1.145025
H	-33.760803	-16.801733	0.624088
H	-35.665961	-16.801404	2.653303

Complex 5-PBE0 S=0

100

Fe	-34.703261	-11.518354	1.642104
S	-32.974085	-10.906902	0.480607
C	-31.665268	-10.591282	1.574531
C	-30.365726	-10.244621	0.953122
C	-30.303875	-9.333538	-0.119020
H	-31.221936	-8.846068	-0.452155
C	-29.092893	-9.054265	-0.752484
H	-29.068929	-8.340959	-1.578224
C	-27.915082	-9.681022	-0.333795
H	-26.967594	-9.465387	-0.831665
C	-27.961864	-10.586999	0.729823
H	-27.049709	-11.085849	1.064253
C	-29.170815	-10.866006	1.366843
H	-29.196493	-11.580567	2.189658
C	-31.898054	-10.748517	2.945073
C	-30.915064	-10.477883	4.022232
C	-30.167761	-9.284703	4.054776
C	-29.268360	-9.037363	5.092147
H	-28.702036	-8.103427	5.102926
C	-29.089892	-9.975629	6.114474
H	-28.381413	-9.781761	6.922179

C	-29.830524	-11.160692	6.097717
H	-29.702411	-11.899123	6.892209
H	-30.303908	-8.545834	3.263791
C	-30.737556	-11.406373	5.066065
H	-31.317024	-12.331754	5.054121
S	-33.475788	-11.229710	3.461847
C	-34.708559	-13.475664	1.641814
N	-33.986330	-14.340264	0.832176
C	-33.015034	-14.028383	-0.191034
C	-31.657021	-13.974251	0.185920
C	-31.238675	-14.194867	1.615024
H	-30.152936	-14.078655	1.720546
H	-31.732707	-13.477985	2.287149
H	-31.508385	-15.204520	1.962443
C	-30.712438	-13.700775	-0.804251
H	-29.660014	-13.623413	-0.519162
C	-31.080994	-13.493199	-2.141355
C	-30.039423	-13.163453	-3.179870
H	-29.350595	-12.388497	-2.811517
H	-30.502541	-12.798611	-4.107307
H	-29.432651	-14.048902	-3.431691
C	-32.429435	-13.613653	-2.480859
H	-32.732697	-13.481761	-3.523486
C	-33.420592	-13.897861	-1.527964
C	-34.851333	-14.051704	-1.973327
H	-34.903357	-14.686879	-2.870404
H	-35.285998	-13.072568	-2.228749
H	-35.484060	-14.495995	-1.195331
N	-35.431699	-14.342590	2.449396
C	-36.403884	-14.034955	3.472944
C	-35.999418	-13.909805	4.810588
C	-34.568604	-14.064807	5.255781
H	-34.126347	-13.084154	5.491616
H	-34.518267	-14.683113	6.164335
H	-33.940915	-14.528115	4.484806
C	-36.990659	-13.624005	5.762771
H	-36.688217	-13.495269	6.805954
C	-38.338265	-13.496027	5.422153
C	-39.378455	-13.163041	6.461205
H	-38.914285	-12.800316	7.388661
H	-40.065362	-12.386334	6.093212
H	-39.987538	-14.046740	6.713162
C	-38.706870	-13.699744	4.084218
H	-39.758581	-13.617067	3.798163
C	-37.762098	-13.975505	3.094597
C	-38.179556	-14.190514	1.664270
H	-37.687105	-13.470159	0.994869
H	-39.265386	-14.075375	1.559960
H	-37.908446	-15.198064	1.312638
S	-36.431036	-10.905569	2.803996
C	-37.740184	-10.587714	1.711207
C	-39.039307	-10.246564	2.336672
C	-39.098215	-9.347407	3.419656
H	-38.179244	-8.863783	3.756441
C	-40.307498	-9.073574	4.059321
H	-40.328876	-8.367438	4.892061

C	-41.487472	-9.693603	3.636226
H	-42.433927	-9.480265	4.137394
C	-41.443846	-10.588093	2.562018
H	-42.357421	-11.082307	2.223901
C	-40.236077	-10.861925	1.919025
H	-40.212649	-11.568732	1.088994
C	-37.507156	-10.741902	0.340100
C	-38.491282	-10.473954	-0.736993
C	-39.244051	-9.284258	-0.767786
H	-39.111281	-8.546029	0.024467
C	-40.144285	-9.039044	-1.804775
H	-40.714768	-8.107837	-1.814247
C	-40.315154	-9.974218	-2.830807
H	-41.021933	-9.780516	-3.639860
C	-39.569369	-11.156512	-2.815495
H	-39.692383	-11.893415	-3.612368
C	-38.664020	-11.401766	-1.782267
H	-38.081745	-12.325442	-1.770952
S	-35.928703	-11.220734	-0.177226
C	-35.162232	-15.672326	2.141843
C	-34.253582	-15.670802	1.136855
H	-33.770382	-16.481779	0.604991
H	-35.645342	-16.485097	2.671731

Complex 5-PBE0 S=1

100

Fe	-34.700473	-11.615015	1.642939
S	-32.915041	-10.954395	0.366789
C	-31.646401	-10.553440	1.500258
C	-30.343146	-10.195552	0.878494
C	-30.289657	-9.321204	-0.219500
H	-31.212451	-8.876444	-0.585920
C	-29.075046	-9.021347	-0.834547
H	-29.054252	-8.333244	-1.677528
C	-27.890668	-9.598901	-0.373166
H	-26.943049	-9.368007	-0.855461
C	-27.932607	-10.478412	0.710683
H	-27.016554	-10.939935	1.074480
C	-29.144811	-10.773109	1.330840
H	-29.170655	-11.461890	2.171744
C	-31.870315	-10.611518	2.864512
C	-30.894128	-10.174200	3.896272
C	-30.219383	-8.946579	3.790484
C	-29.324778	-8.539968	4.777536
H	-28.815331	-7.583148	4.680890
C	-29.084282	-9.350957	5.889021
H	-28.383251	-9.032971	6.657952
C	-29.756478	-10.567905	6.011694
H	-29.581813	-11.205366	6.876159
H	-30.407295	-8.306848	2.931771
C	-30.658167	-10.971612	5.028678
H	-31.188256	-11.916843	5.128148
S	-33.416486	-11.139877	3.491494
C	-34.711380	-13.893628	1.637258
N	-33.961291	-14.738407	0.874668

C	-32.959903	-14.370137	-0.092018
C	-31.634364	-14.211272	0.341064
C	-31.274034	-14.334999	1.797711
H	-30.195536	-14.223973	1.936865
H	-31.781156	-13.560599	2.386082
H	-31.574496	-15.305795	2.208974
C	-30.670647	-13.896761	-0.616956
H	-29.640020	-13.748997	-0.296521
C	-30.997960	-13.738047	-1.968455
C	-29.933808	-13.374345	-2.972371
H	-29.454673	-12.427123	-2.702332
H	-30.351834	-13.270480	-3.976704
H	-29.148995	-14.138316	-3.008634
C	-32.327333	-13.914615	-2.356236
H	-32.598508	-13.794302	-3.404440
C	-33.330524	-14.237794	-1.435427
C	-34.759382	-14.417641	-1.877125
H	-34.835665	-14.349921	-2.965857
H	-35.403238	-13.645868	-1.438217
H	-35.158959	-15.390486	-1.565961
N	-35.476562	-14.737051	2.386163
C	-36.465426	-14.367959	3.365101
C	-36.082294	-14.245559	4.705763
C	-34.650904	-14.429728	5.136920
H	-34.028779	-13.595846	4.786287
H	-34.581562	-14.472441	6.227131
H	-34.219788	-15.351084	4.729273
C	-37.075770	-13.921278	5.636885
H	-36.795003	-13.808814	6.683594
C	-38.406585	-13.731709	5.261903
C	-39.457723	-13.358491	6.275899
H	-39.034175	-13.284373	7.282113
H	-39.909492	-12.392050	6.024264
H	-40.264902	-14.100386	6.299109
C	-38.747050	-13.882423	3.912567
H	-39.779467	-13.726483	3.601737
C	-37.794084	-14.199676	2.945046
C	-38.167482	-14.317499	1.491073
H	-37.649434	-13.554222	0.897314
H	-39.244466	-14.185143	1.360017
H	-37.889826	-15.294962	1.079451
S	-36.483589	-10.953524	2.920396
C	-37.754666	-10.555690	1.787883
C	-39.061977	-10.213935	2.409830
C	-39.126386	-9.353983	3.518052
H	-38.208915	-8.904876	3.891944
C	-40.345195	-9.075925	4.135419
H	-40.374795	-8.399166	4.986908
C	-41.522173	-9.661172	3.665130
H	-42.473146	-9.446579	4.148494
C	-41.469498	-10.527066	2.570119
H	-42.380240	-10.993006	2.198500
C	-40.253294	-10.799341	1.948232
H	-40.217654	-11.477853	1.099462
C	-37.530135	-10.607299	0.424400
C	-38.506394	-10.165478	-0.604528

C	-39.176161	-8.935915	-0.494214
H	-38.984244	-8.299775	0.366330
C	-40.069202	-8.522663	-1.479966
H	-40.575099	-7.564176	-1.380900
C	-40.313511	-9.328665	-2.594009
H	-41.014501	-9.005169	-3.361322
C	-39.648136	-10.548730	-2.719964
H	-39.828181	-11.182987	-3.585869
C	-38.747824	-10.959160	-1.738358
H	-38.223119	-11.907018	-1.840180
S	-35.983311	-11.130476	-0.205090
C	-35.210621	-16.066042	2.097686
C	-34.251070	-16.067050	1.141272
H	-33.749676	-16.877317	0.630513
H	-35.724497	-16.875343	2.597480

Complex 5-PBE0 S=2

100

Fe	-34.711330	-11.465674	1.670098
S	-33.085795	-10.467859	0.431803
C	-31.715825	-10.402846	1.543251
C	-30.389863	-10.223055	0.909012
C	-30.250199	-9.390640	-0.221162
H	-31.123008	-8.850251	-0.592221
C	-29.019350	-9.249458	-0.861250
H	-28.935687	-8.589318	-1.727893
C	-27.896593	-9.941858	-0.395836
H	-26.933746	-9.832222	-0.898666
C	-28.020119	-10.776070	0.720762
H	-27.152450	-11.327089	1.090916
C	-29.248676	-10.914408	1.365908
H	-29.333117	-11.575433	2.229007
C	-31.937663	-10.509447	2.907766
C	-30.920033	-10.298767	3.965588
C	-30.083229	-9.165608	3.953647
C	-29.156142	-8.956434	4.973973
H	-28.521175	-8.068275	4.951464
C	-29.043580	-9.870976	6.026968
H	-28.316658	-9.704591	6.824491
C	-29.877727	-10.992443	6.057984
H	-29.803213	-11.708593	6.879222
H	-30.174991	-8.443202	3.141449
C	-30.811600	-11.200367	5.042109
H	-31.467393	-12.072565	5.070445
S	-33.564477	-10.768787	3.523347
C	-34.640025	-13.680522	1.666422
N	-33.911429	-14.522175	0.861281
C	-32.919721	-14.141192	-0.118518
C	-31.586597	-13.994928	0.305453
C	-31.202839	-14.178843	1.750481
H	-30.115613	-14.100643	1.872774
H	-31.676813	-13.415245	2.385587
H	-31.520487	-15.160698	2.133217
C	-30.630099	-13.665887	-0.658127
H	-29.593154	-13.526362	-0.342928

C	-30.968330	-13.489541	-2.006672
C	-29.914420	-13.101326	-3.011773
H	-29.438163	-12.150254	-2.727043
H	-30.341753	-12.982913	-4.016360
H	-29.117783	-13.859868	-3.066569
C	-32.299748	-13.678349	-2.387585
H	-32.578468	-13.559945	-3.438050
C	-33.299129	-14.014003	-1.463604
C	-34.721929	-14.213370	-1.914435
H	-34.768202	-14.304144	-3.007771
H	-35.352590	-13.360822	-1.613554
H	-35.169939	-15.116094	-1.473910
N	-35.391567	-14.547297	2.422738
C	-36.369391	-14.197859	3.428265
C	-35.952329	-14.031816	4.757335
C	-34.504895	-14.156616	5.152759
H	-33.908831	-13.346487	4.702733
H	-34.397872	-14.094866	6.242831
H	-34.068895	-15.110035	4.816070
C	-36.934582	-13.726744	5.709518
H	-36.628047	-13.579493	6.748537
C	-38.285100	-13.603659	5.369638
C	-39.320777	-13.248846	6.405607
H	-38.871657	-13.145789	7.402440
H	-39.813056	-12.297018	6.153405
H	-40.107808	-14.016768	6.462684
C	-38.657333	-13.804368	4.033553
H	-39.707556	-13.702613	3.747871
C	-37.718574	-14.102199	3.042742
C	-38.133473	-14.277156	1.606017
H	-37.640760	-13.529679	0.965222
H	-39.219359	-14.159680	1.502557
H	-37.858491	-15.269895	1.218050
S	-36.560829	-10.770568	2.843117
C	-37.866469	-10.465571	1.717658
C	-39.170960	-10.161878	2.349273
C	-39.243094	-9.286891	3.451067
H	-38.330958	-8.796699	3.795824
C	-40.457565	-9.043881	4.093548
H	-40.491486	-8.355592	4.940486
C	-41.626384	-9.672546	3.655159
H	-42.576513	-9.482600	4.158431
C	-41.568292	-10.547901	2.565706
H	-42.474224	-11.049156	2.218385
C	-40.356844	-10.791124	1.919895
H	-40.319489	-11.484502	1.078955
C	-37.634001	-10.614960	0.364236
C	-38.610289	-10.344940	-0.716066
C	-39.358190	-9.152348	-0.743339
H	-39.214182	-8.414866	0.047488
C	-40.265332	-8.905388	-1.773872
H	-40.832923	-7.972607	-1.780772
C	-40.444118	-9.839715	-2.799393
H	-41.154588	-9.643702	-3.604982
C	-39.698663	-11.022419	-2.790843
H	-39.827254	-11.757148	-3.588589

C	-38.787484	-11.269797	-1.763778
H	-38.204433	-12.192852	-1.758306
S	-36.044482	-11.123281	-0.169215
C	-35.137781	-15.873764	2.095986
C	-34.200099	-15.858700	1.111617
H	-33.714341	-16.662954	0.570467
H	-35.643977	-16.694157	2.592128

Complex 5-TPSS S=0

100

Fe	-34.705518	-11.553686	1.642776
S	-32.982471	-10.944091	0.492392
C	-31.683215	-10.603224	1.583088
C	-30.388392	-10.218670	0.968585
C	-30.347398	-9.303209	-0.098943
H	-31.272936	-8.849403	-0.440339
C	-29.139720	-8.976939	-0.714593
H	-29.130841	-8.261673	-1.532516
C	-27.946572	-9.562250	-0.283467
H	-27.005923	-9.308835	-0.764486
C	-27.973764	-10.476749	0.772661
H	-27.052928	-10.942287	1.113934
C	-29.179182	-10.801544	1.392918
H	-29.189350	-11.517626	2.207843
C	-31.919635	-10.760383	2.950845
C	-30.950067	-10.458732	4.032573
C	-30.207650	-9.263974	4.036991
C	-29.329381	-8.977293	5.080318
H	-28.771534	-8.045099	5.069772
C	-29.170195	-9.875964	6.138716
H	-28.483517	-9.649924	6.949587
C	-29.905704	-11.063160	6.148935
H	-29.791863	-11.767666	6.968393
H	-30.333493	-8.555089	3.225338
C	-30.789809	-11.349525	5.109666
H	-31.364248	-12.270714	5.120893
S	-33.490236	-11.266107	3.455014
C	-34.706128	-13.504748	1.639569
N	-34.007484	-14.371732	0.811081
C	-33.042012	-14.065356	-0.225585
C	-31.681589	-14.028857	0.138952
C	-31.252057	-14.240556	1.570188
H	-30.168222	-14.142464	1.659299
H	-31.725111	-13.508136	2.231458
H	-31.535525	-15.237109	1.927629
C	-30.741614	-13.785280	-0.860520
H	-29.690289	-13.732821	-0.587077
C	-31.118649	-13.587630	-2.196141
C	-30.076517	-13.293433	-3.250379
H	-29.473385	-12.423461	-2.966760
H	-30.541339	-13.088646	-4.218808
H	-29.391536	-14.141472	-3.372488
C	-32.471450	-13.675606	-2.520967
H	-32.780383	-13.543505	-3.555865
C	-33.457641	-13.932412	-1.555832

C	-34.896145	-14.087697	-1.989967
H	-35.008536	-14.994405	-2.596684
H	-35.203929	-13.235972	-2.602940
H	-35.575175	-14.154312	-1.140306
N	-35.405435	-14.373600	2.465375
C	-36.369898	-14.069195	3.503437
C	-35.953360	-13.939757	4.833777
C	-34.514748	-14.096801	5.266973
H	-34.203762	-13.242594	5.874679
H	-34.404195	-15.000307	5.878574
H	-33.836928	-14.170063	4.416963
C	-36.938701	-13.683885	5.799993
H	-36.629094	-13.554533	6.835031
C	-38.291581	-13.593763	5.476070
C	-39.332847	-13.300733	6.531434
H	-38.867485	-13.098593	7.499752
H	-39.935062	-12.429659	6.250223
H	-40.018619	-14.147908	6.652067
C	-38.669609	-13.788091	4.140227
H	-39.721036	-13.733889	3.867524
C	-37.730474	-14.030455	3.139768
C	-38.160670	-14.238629	1.708269
H	-37.685568	-13.506385	1.048242
H	-39.244242	-14.137391	1.619484
H	-37.879952	-15.235355	1.349115
S	-36.427891	-10.945664	2.795020
C	-37.727471	-10.602091	1.705725
C	-39.020725	-10.216849	2.322966
C	-39.058211	-9.301609	3.390880
H	-38.131479	-8.848605	3.729961
C	-40.264006	-8.974277	4.009578
H	-40.270034	-8.259080	4.827668
C	-41.458862	-9.558075	3.580767
H	-42.398199	-9.303441	4.063655
C	-41.435202	-10.472205	2.524056
H	-42.357476	-10.936464	2.184346
C	-40.231442	-10.798281	1.901191
H	-40.224044	-11.514126	1.086002
C	-37.492362	-10.757068	0.337521
C	-38.463477	-10.455024	-0.742844
C	-39.207221	-9.260857	-0.744988
H	-39.081679	-8.552394	0.067101
C	-40.087161	-8.974069	-1.786972
H	-40.646259	-8.042470	-1.775033
C	-40.246721	-9.872319	-2.845710
H	-40.934742	-9.646553	-3.655506
C	-39.510149	-11.058989	-2.858008
H	-39.624460	-11.763268	-3.677543
C	-38.624217	-11.345191	-1.820460
H	-38.048719	-12.265784	-1.833191
S	-35.921539	-11.260405	-0.168457
C	-35.145415	-15.704673	2.149850
C	-34.268803	-15.703562	1.122327
H	-33.802360	-16.508975	0.578632
H	-35.612617	-16.511373	2.691078

Complex 5-TPSS S=1

100

Fe	-34.703721	-11.491773	1.643047
S	-32.979580	-10.713781	0.507078
C	-31.628283	-10.529856	1.610571
C	-30.319252	-10.225453	0.987007
C	-30.236443	-9.324525	-0.091324
H	-31.138829	-8.826404	-0.431828
C	-29.016915	-9.065785	-0.715782
H	-28.976173	-8.360439	-1.540743
C	-27.852542	-9.705673	-0.284360
H	-26.902655	-9.504944	-0.771906
C	-27.920593	-10.607502	0.781564
H	-27.023173	-11.116623	1.122283
C	-29.137587	-10.865183	1.409990
H	-29.179815	-11.573117	2.230349
C	-31.858579	-10.727898	2.956349
C	-30.882261	-10.512616	4.052277
C	-30.093234	-9.348761	4.105515
C	-29.203519	-9.139916	5.157607
H	-28.608594	-8.231282	5.184447
C	-29.081691	-10.085847	6.179063
H	-28.388218	-9.920412	6.998697
C	-29.865075	-11.241469	6.142183
H	-29.781308	-11.981880	6.932996
H	-30.192014	-8.603599	3.323117
C	-30.759919	-11.450240	5.093337
H	-31.372596	-12.346437	5.070334
S	-33.467780	-11.190844	3.451778
C	-34.705155	-13.491464	1.639985
N	-34.019264	-14.343475	0.801013
C	-33.058238	-14.011825	-0.234296
C	-31.701169	-13.954526	0.136138
C	-31.270022	-14.189937	1.563225
H	-30.187287	-14.085640	1.653619
H	-31.747051	-13.472445	2.237796
H	-31.545134	-15.194880	1.902506
C	-30.765788	-13.666571	-0.855561
H	-29.716917	-13.593769	-0.578938
C	-31.145518	-13.445352	-2.186528
C	-30.108103	-13.112521	-3.234215
H	-29.404030	-12.362633	-2.860018
H	-30.576016	-12.725097	-4.143049
H	-29.527686	-14.002964	-3.506237
C	-32.495346	-13.556485	-2.516573
H	-32.805773	-13.405688	-3.548319
C	-33.477578	-13.857092	-1.560549
C	-34.912572	-14.021372	-2.002558
H	-34.985686	-14.827185	-2.742202
H	-35.274457	-13.101705	-2.472012
H	-35.575666	-14.253240	-1.168417
N	-35.392096	-14.345233	2.476311
C	-36.354577	-14.016874	3.511470
C	-35.937207	-13.865664	4.838799
C	-34.502330	-14.028194	5.281982

H	-34.139948	-13.106422	5.746532
H	-34.430166	-14.830024	6.025805
H	-33.838944	-14.265094	4.449548
C	-36.920820	-13.568717	5.794381
H	-36.611926	-13.420459	6.826967
C	-38.270236	-13.457108	5.462688
C	-39.309043	-13.126787	6.509784
H	-38.842290	-12.740505	7.419565
H	-40.013103	-12.376641	6.136237
H	-39.889154	-14.017961	6.779741
C	-38.647925	-13.675396	4.130546
H	-39.696441	-13.602672	3.852501
C	-37.711194	-13.959996	3.139307
C	-38.140254	-14.192408	1.710967
H	-37.662887	-13.473665	1.038121
H	-39.222956	-14.088924	1.619177
H	-37.863994	-15.196716	1.370425
S	-36.426617	-10.716826	2.781972
C	-37.779052	-10.531158	1.681114
C	-39.086247	-10.224898	2.306671
C	-39.165163	-9.323161	3.384979
H	-38.261080	-8.826553	3.724043
C	-40.383149	-9.060704	4.010732
H	-40.421336	-8.354194	4.835549
C	-41.549525	-9.697298	3.579941
H	-42.498513	-9.492715	4.067737
C	-41.485160	-10.600462	2.514592
H	-42.384639	-11.107134	2.175315
C	-40.269730	-10.862209	1.885360
H	-40.230368	-11.570977	1.065497
C	-37.551340	-10.727980	0.334732
C	-38.529674	-10.512531	-0.759434
C	-39.318678	-9.348555	-0.810605
H	-39.218571	-8.603279	-0.028452
C	-40.210910	-9.140193	-1.860606
H	-40.806339	-8.231851	-1.885972
C	-40.334724	-10.086216	-2.881924
H	-41.030069	-9.920723	-3.699914
C	-39.550911	-11.241649	-2.847612
H	-39.636002	-11.981697	-3.638662
C	-38.653619	-11.449967	-1.800690
H	-38.040609	-12.345976	-1.779232
S	-35.942536	-11.188635	-0.164072
C	-35.136042	-15.676499	2.158417
C	-34.277660	-15.675192	1.113695
H	-33.822533	-16.479715	0.559511
H	-35.593376	-16.482226	2.709350

Complex 5-TPSS S=2

100

Fe	-34.706934	-11.498439	1.674917
S	-33.084698	-10.463145	0.491224
C	-31.719386	-10.411536	1.600317
C	-30.400298	-10.143369	0.980798

C	-30.284330	-9.211651	-0.068699
H	-31.167256	-8.668366	-0.391922
C	-29.056204	-8.980609	-0.686427
H	-28.988876	-8.249651	-1.487747
C	-27.917347	-9.681202	-0.278736
H	-26.960920	-9.502544	-0.762233
C	-28.019646	-10.615440	0.755790
H	-27.142159	-11.171214	1.076685
C	-29.245147	-10.844939	1.378352
H	-29.314251	-11.577623	2.175043
C	-31.932006	-10.606989	2.952220
C	-30.917646	-10.432171	4.020924
C	-30.092376	-9.292665	4.060609
C	-29.178757	-9.113489	5.097015
H	-28.558232	-8.221835	5.115705
C	-29.065241	-10.066072	6.113922
H	-28.351698	-9.923184	6.920553
C	-29.884585	-11.196780	6.090825
H	-29.808932	-11.941143	6.878973
H	-30.184381	-8.541946	3.282827
C	-30.807408	-11.373941	5.060264
H	-31.450682	-12.248678	5.048962
S	-33.546991	-10.961191	3.546734
C	-34.646417	-13.683011	1.685164
N	-33.959851	-14.530744	0.848100
C	-33.013437	-14.147948	-0.182408
C	-31.660364	-14.024716	0.183378
C	-31.209921	-14.248659	1.607346
H	-30.123968	-14.159211	1.678565
H	-31.662870	-13.515501	2.282353
H	-31.495271	-15.244364	1.964731
C	-30.743671	-13.686931	-0.811106
H	-29.697075	-13.570957	-0.540428
C	-31.139333	-13.475676	-2.139435
C	-30.121602	-13.093066	-3.189457
H	-29.526954	-12.234755	-2.859898
H	-30.607411	-12.834018	-4.133399
H	-29.427065	-13.920019	-3.380532
C	-32.486035	-13.634324	-2.462481
H	-32.809425	-13.480403	-3.489890
C	-33.448338	-13.984940	-1.503142
C	-34.882237	-14.194722	-1.931383
H	-34.968866	-15.112723	-2.525763
H	-35.216012	-13.361264	-2.555760
H	-35.558541	-14.269451	-1.079773
N	-35.347396	-14.545719	2.494330
C	-36.303300	-14.183085	3.523618
C	-35.873184	-13.995275	4.841729
C	-34.432260	-14.151423	5.268325
H	-34.108251	-13.272595	5.833085
H	-34.323045	-15.027029	5.919734
H	-33.763225	-14.269775	4.415600
C	-36.844930	-13.662334	5.798297
H	-36.526477	-13.489817	6.824255
C	-38.195390	-13.543899	5.473349
C	-39.223176	-13.173881	6.517828

H	-38.746383	-12.916366	7.467023
H	-39.819747	-12.316544	6.187814
H	-39.915554	-14.004926	6.698253
C	-38.584263	-13.774590	4.146655
H	-39.632530	-13.681607	3.872075
C	-37.658725	-14.092627	3.154848
C	-38.098265	-14.305903	1.726555
H	-37.615719	-13.581884	1.061661
H	-39.180507	-14.186837	1.642549
H	-37.835563	-15.308170	1.369539
S	-36.535341	-10.716448	2.808382
C	-37.834198	-10.463525	1.666514
C	-39.144573	-10.124033	2.271654
C	-39.223287	-9.208373	3.337655
H	-38.317317	-8.713804	3.674808
C	-40.443301	-8.932620	3.954066
H	-40.481791	-8.217081	4.770919
C	-41.610406	-9.569715	3.525896
H	-42.560032	-9.356282	4.008550
C	-41.545442	-10.486884	2.472811
H	-42.445820	-10.994725	2.137390
C	-40.328059	-10.763055	1.853384
H	-40.285494	-11.486521	1.046210
C	-37.594689	-10.672231	0.324372
C	-38.549375	-10.414375	-0.779055
C	-39.303667	-9.227176	-0.827568
H	-39.189915	-8.492952	-0.036691
C	-40.177872	-8.982968	-1.884903
H	-40.747213	-8.057638	-1.907067
C	-40.316941	-9.914441	-2.917598
H	-40.998364	-9.720369	-3.741338
C	-39.565851	-11.092119	-2.887488
H	-39.663978	-11.821275	-3.687288
C	-38.687378	-11.337168	-1.832986
H	-38.102449	-12.252041	-1.812480
S	-36.014307	-11.236472	-0.170917
C	-35.104192	-15.875681	2.165581
C	-34.228223	-15.866708	1.130648
H	-33.772514	-16.669128	0.572856
H	-35.575541	-16.687452	2.696225

Complex 5-BP86 Charge=-1 S=0.5

100

Fe	-34.706301	-11.637654	1.645747
S	-33.003620	-10.883707	0.452012
C	-31.649306	-10.573868	1.543278
C	-30.375752	-10.189942	0.898187
C	-30.365809	-9.361817	-0.247284
H	-31.318510	-8.992902	-0.629639
C	-29.173489	-9.018577	-0.884372
H	-29.201950	-8.370465	-1.763440
C	-27.947077	-9.495209	-0.405363
H	-27.014054	-9.227956	-0.905295
C	-27.937330	-10.326806	0.720388
H	-26.991558	-10.718888	1.101987

C	-29.129430	-10.671369	1.358218
H	-29.105147	-11.330550	2.225667
C	-31.844144	-10.755347	2.903081
C	-30.893411	-10.360995	3.969299
C	-30.250123	-9.105356	3.941047
C	-29.395650	-8.708970	4.969797
H	-28.917301	-7.728028	4.923647
C	-29.160504	-9.552083	6.062256
H	-28.495019	-9.238674	6.869304
C	-29.800371	-10.795508	6.112647
H	-29.633463	-11.461663	6.962207
H	-30.442470	-8.435303	3.102988
C	-30.657302	-11.191992	5.084228
H	-31.165012	-12.156112	5.132093
S	-33.388598	-11.370099	3.469751
C	-34.708156	-13.574101	1.638163
N	-33.951626	-14.450108	0.858040
C	-32.958850	-14.157140	-0.149369
C	-31.610574	-14.066675	0.243455
C	-31.218040	-14.169960	1.692952
H	-30.133688	-14.048678	1.807608
H	-31.722488	-13.395986	2.290321
H	-31.503843	-15.144945	2.117455
C	-30.647984	-13.874587	-0.752472
H	-29.601188	-13.773767	-0.456311
C	-30.993606	-13.784670	-2.106896
C	-29.936640	-13.525275	-3.153513
H	-29.559409	-12.493943	-3.075810
H	-30.335944	-13.662482	-4.167949
H	-29.073424	-14.196769	-3.030277
C	-32.339563	-13.922861	-2.458699
H	-32.626599	-13.873414	-3.512365
C	-33.343419	-14.123423	-1.500086
C	-34.778698	-14.300262	-1.920397
H	-34.859133	-14.309991	-3.015238
H	-35.407810	-13.483796	-1.531297
H	-35.199736	-15.241183	-1.534569
N	-35.469155	-14.453893	2.409099
C	-36.456437	-14.164289	3.422285
C	-36.064055	-14.137931	4.770704
C	-34.627125	-14.324856	5.180971
H	-33.996992	-13.506467	4.797744
H	-34.540426	-14.347517	6.275117
H	-34.212296	-15.262841	4.781731
C	-37.061676	-13.937762	5.735543
H	-36.768910	-13.894806	6.788003
C	-38.409020	-13.793621	5.391421
C	-39.458861	-13.535943	6.445489
H	-39.054190	-13.681458	7.456838
H	-39.831574	-12.502194	6.376347
H	-40.325795	-14.202957	6.322893
C	-38.762775	-13.877395	4.038566
H	-39.810934	-13.772828	3.748531
C	-37.806299	-14.068687	3.036682
C	-38.206514	-14.166668	1.588817
H	-37.699389	-13.395368	0.990310

H	-39.290515	-14.037687	1.479681
H	-37.929797	-15.142957	1.161205
S	-36.407318	-10.882001	2.841024
C	-37.762120	-10.569720	1.750841
C	-39.034088	-10.181105	2.396431
C	-39.041691	-9.349835	3.539607
H	-38.088272	-8.980718	3.919712
C	-40.232949	-9.005458	4.178786
H	-40.202821	-8.356023	5.056835
C	-41.460219	-9.483263	3.703312
H	-42.392417	-9.215544	4.204826
C	-41.472286	-10.316119	2.578360
H	-42.418816	-10.708302	2.198399
C	-40.281576	-10.661932	1.938968
H	-40.307753	-11.322373	1.072561
C	-37.568803	-10.752862	0.391070
C	-38.520977	-10.363110	-0.675562
C	-39.166113	-9.108407	-0.651563
H	-38.974867	-8.434966	0.184119
C	-40.021752	-8.717500	-1.681544
H	-40.501453	-7.736974	-1.639345
C	-40.256355	-9.565494	-2.770409
H	-40.923248	-9.256234	-3.577928
C	-39.614171	-10.807987	-2.816673
H	-39.780090	-11.477919	-3.663567
C	-38.756195	-11.198912	-1.787291
H	-38.246815	-12.162254	-1.831896
S	-36.024237	-11.366042	-0.176968
C	-35.188068	-15.785641	2.109687
C	-34.237568	-15.783487	1.146241
H	-33.732913	-16.594001	0.634885
H	-35.694664	-16.598586	2.615268

Complex 5-BP86 Charge=-1 S=1.5

100

Fe	-34.704968	-11.580380	1.642745
S	-32.934140	-10.830623	0.422188
C	-31.605117	-10.511963	1.552160
C	-30.319954	-10.135140	0.920323
C	-30.292016	-9.272908	-0.197389
H	-31.237092	-8.873671	-0.568056
C	-29.089462	-8.936457	-0.820885
H	-29.099787	-8.260808	-1.679398
C	-27.876792	-9.457386	-0.354688
H	-26.936678	-9.195920	-0.844646
C	-27.887231	-10.326010	0.743171
H	-26.951076	-10.751134	1.112759
C	-29.088940	-10.662833	1.367455
H	-29.086102	-11.349303	2.214167
C	-31.813637	-10.663850	2.904617
C	-30.873900	-10.266830	3.977235
C	-30.178332	-9.039540	3.931557
C	-29.325176	-8.654283	4.965811
H	-28.804889	-7.695759	4.905220
C	-29.144968	-9.478915	6.082605

H	-28.481014	-9.174028	6.894021
C	-29.839691	-10.691512	6.152458
H	-29.717933	-11.341831	7.021755
H	-30.328058	-8.381523	3.075750
C	-30.695095	-11.076346	5.118936
H	-31.245520	-12.015940	5.183138
S	-33.399495	-11.229139	3.470278
C	-34.704483	-13.828280	1.640745
N	-33.970745	-14.692366	0.855303
C	-32.996733	-14.341957	-0.152599
C	-31.654064	-14.189727	0.235837
C	-31.251129	-14.271895	1.683982
H	-30.161177	-14.199562	1.785563
H	-31.709654	-13.448498	2.253669
H	-31.582537	-15.213035	2.147748
C	-30.712796	-13.921071	-0.761925
H	-29.669379	-13.776553	-0.472322
C	-31.077424	-13.801196	-2.109052
C	-30.041939	-13.465381	-3.155194
H	-29.699864	-12.425094	-3.041935
H	-30.447366	-13.578585	-4.169893
H	-29.155015	-14.110681	-3.065373
C	-32.422125	-13.969540	-2.452234
H	-32.725231	-13.875717	-3.498252
C	-33.405333	-14.245976	-1.491400
C	-34.850601	-14.400326	-1.886581
H	-34.953851	-14.390264	-2.979269
H	-35.452756	-13.574287	-1.472638
H	-35.281448	-15.338182	-1.505815
N	-35.433894	-14.693548	2.428889
C	-36.412006	-14.345175	3.433611
C	-36.008904	-14.251962	4.774335
C	-34.565266	-14.407947	5.174981
H	-33.960299	-13.583626	4.761705
H	-34.465882	-14.396188	6.268052
H	-34.134599	-15.347303	4.797564
C	-36.995693	-13.976206	5.731701
H	-36.696794	-13.883765	6.779073
C	-38.338777	-13.806322	5.383344
C	-39.377815	-13.467802	6.425090
H	-38.977210	-13.582290	7.441537
H	-39.716026	-12.426389	6.310286
H	-40.266399	-14.110181	6.331171
C	-38.698167	-13.925066	4.034745
H	-39.740448	-13.779394	3.741032
C	-37.753039	-14.192026	3.040210
C	-38.150446	-14.270976	1.590464
H	-37.690388	-13.445705	1.024813
H	-39.240084	-14.199065	1.484940
H	-37.816282	-15.210573	1.125663
S	-36.475317	-10.833246	2.866292
C	-37.804991	-10.512575	1.737542
C	-39.090671	-10.138384	2.369825
C	-39.118830	-9.279824	3.490286
H	-38.173778	-8.882259	3.862723
C	-40.321362	-8.944612	4.114085

H	-40.311132	-8.271607	4.974688
C	-41.534091	-9.463372	3.645736
H	-42.474182	-9.202999	4.136338
C	-41.523486	-10.328638	2.545293
H	-42.459617	-10.752444	2.174210
C	-40.321623	-10.664029	1.920343
H	-40.324512	-11.347598	1.071321
C	-37.596300	-10.659224	0.384761
C	-38.537553	-10.260340	-0.685932
C	-39.227024	-9.029655	-0.640364
H	-39.071283	-8.370625	0.213797
C	-40.082025	-8.642769	-1.672607
H	-40.597880	-7.681803	-1.612152
C	-40.269729	-9.469156	-2.786941
H	-40.935080	-9.162835	-3.596653
C	-39.581422	-10.685406	-2.856370
H	-39.709898	-11.337376	-3.723534
C	-38.724339	-11.071925	-1.824752
H	-38.178841	-12.014458	-1.888142
S	-36.010036	-11.220039	-0.183633
C	-35.160963	-16.030308	2.141451
C	-34.236216	-16.029548	1.147486
H	-33.743937	-16.841219	0.624667
H	-35.649222	-16.842766	2.666723

Complex 5-BP86 Charge=-1 S=2.5

100

Fe	-34.706094	-11.761414	1.636806
S	-32.940990	-10.649474	0.472961
C	-31.619957	-10.452422	1.621163
C	-30.327030	-10.050519	1.011122
C	-30.275814	-9.109586	-0.039954
H	-31.208905	-8.654338	-0.374707
C	-29.066718	-8.769369	-0.647861
H	-29.059087	-8.031784	-1.453844
C	-27.870113	-9.368418	-0.235884
H	-26.925271	-9.106862	-0.716808
C	-27.903801	-10.315198	0.794554
H	-26.981565	-10.801218	1.121657
C	-29.111897	-10.651290	1.406424
H	-29.127254	-11.396449	2.201753
C	-31.785574	-10.695009	2.977800
C	-30.799394	-10.284721	4.010373
C	-30.202354	-9.006861	3.975569
C	-29.308072	-8.599230	4.966210
H	-28.867937	-7.600710	4.915257
C	-28.985235	-9.454064	6.025818
H	-28.289191	-9.132747	6.803443
C	-29.580333	-10.720345	6.084343
H	-29.345948	-11.395882	6.910580
H	-30.461675	-8.327601	3.163301
C	-30.479566	-11.125170	5.097004
H	-30.958436	-12.103587	5.155492
S	-33.266912	-11.401114	3.608080

C	-34.704644	-13.947104	1.638210
N	-33.969386	-14.806039	0.853140
C	-33.000253	-14.426321	-0.149161
C	-31.666496	-14.222387	0.248807
C	-31.263326	-14.310082	1.696606
H	-30.178145	-14.188501	1.801282
H	-31.760180	-13.521026	2.284002
H	-31.549656	-15.274975	2.141550
C	-30.733402	-13.903644	-0.742369
H	-29.697932	-13.719226	-0.446518
C	-31.096656	-13.785444	-2.089807
C	-30.070153	-13.398914	-3.127155
H	-29.782499	-12.342513	-3.011940
H	-30.459453	-13.533686	-4.145393
H	-29.152919	-13.998431	-3.026844
C	-32.431830	-14.005191	-2.441896
H	-32.733613	-13.912393	-3.488220
C	-33.407606	-14.331187	-1.489381
C	-34.842708	-14.542451	-1.896125
H	-34.936184	-14.538836	-2.989684
H	-35.484560	-13.740508	-1.494171
H	-35.239934	-15.495656	-1.516987
N	-35.434008	-14.804158	2.430560
C	-36.407309	-14.422741	3.428160
C	-36.006420	-14.328456	4.770439
C	-34.573474	-14.541053	5.184210
H	-33.928800	-13.741351	4.782468
H	-34.484819	-14.534054	6.278162
H	-34.176011	-15.496071	4.810005
C	-36.986268	-14.000907	5.717926
H	-36.689543	-13.908584	6.765734
C	-38.319276	-13.778069	5.359192
C	-39.349613	-13.388271	6.391525
H	-38.965731	-13.524131	7.411620
H	-39.633348	-12.331082	6.274798
H	-40.268267	-13.984666	6.286828
C	-38.676153	-13.895768	4.010081
H	-39.709782	-13.709043	3.708999
C	-37.738733	-14.217024	3.023608
C	-38.135270	-14.306902	1.574257
H	-37.639558	-13.515889	0.988409
H	-39.220516	-14.190403	1.464852
H	-37.842586	-15.270664	1.131063
S	-36.464856	-10.649151	2.808229
C	-37.790695	-10.453649	1.665080
C	-39.082604	-10.055738	2.280127
C	-39.132279	-9.120747	3.336323
H	-38.199214	-8.664250	3.669379
C	-40.339860	-8.787958	3.951476
H	-40.346484	-8.055019	4.761545
C	-41.536477	-9.387646	3.541015
H	-42.479865	-9.132219	4.028105
C	-41.504420	-10.327287	2.504293
H	-42.426437	-10.814328	2.178416
C	-40.297803	-10.656754	1.885940
H	-40.283416	-11.397887	1.086862

C	-37.629165	-10.692942	0.307478
C	-38.617475	-10.278147	-0.721140
C	-39.208293	-8.997644	-0.682275
H	-38.943257	-8.321295	0.130672
C	-40.103080	-8.583855	-1.669893
H	-40.537820	-7.583159	-1.616211
C	-40.433491	-9.435778	-2.729686
H	-41.130325	-9.109795	-3.504717
C	-39.844774	-10.704952	-2.791884
H	-40.084849	-11.378223	-3.618365
C	-38.944356	-11.115471	-1.808020
H	-38.470218	-12.095962	-1.869705
S	-36.149493	-11.396449	-0.330268
C	-35.159693	-16.140643	2.145233
C	-34.234064	-16.141858	1.150406
H	-33.741485	-16.954609	0.630052
H	-35.648081	-16.952151	2.671387

Complex 5-BP86 Charge=-2 S=0

100

Fe	-34.704922	-11.630543	1.643036
S	-32.932570	-10.890629	0.445765
C	-31.591981	-10.580801	1.560842
C	-30.310271	-10.233356	0.920388
C	-30.281172	-9.433587	-0.250045
H	-31.232016	-9.071393	-0.643368
C	-29.084127	-9.117944	-0.891533
H	-29.105549	-8.489628	-1.786445
C	-27.859744	-9.599283	-0.404026
H	-26.922541	-9.357536	-0.911400
C	-27.866358	-10.405794	0.742062
H	-26.926257	-10.803902	1.134538
C	-29.063199	-10.716142	1.389967
H	-29.048018	-11.353564	2.273893
C	-31.797414	-10.745759	2.925083
C	-30.859614	-10.357786	3.990508
C	-30.098222	-9.163701	3.922425
C	-29.252368	-8.776846	4.960760
H	-28.688741	-7.843537	4.872790
C	-29.134143	-9.558919	6.119702
H	-28.476083	-9.250285	6.935838
C	-29.894720	-10.733483	6.216830
H	-29.827231	-11.354720	7.114818
H	-30.198666	-8.530115	3.041076
C	-30.742878	-11.120589	5.179606
H	-31.342762	-12.027699	5.266065
S	-33.386323	-11.308559	3.485639
C	-34.706123	-13.500400	1.638668
N	-34.005413	-14.405801	0.803740
C	-33.013277	-14.123804	-0.199867
C	-31.664081	-14.040364	0.194734
C	-31.285502	-14.125047	1.648099
H	-30.200158	-14.016847	1.771679
H	-31.786131	-13.330928	2.224055
H	-31.595628	-15.087069	2.086342

C	-30.693941	-13.867194	-0.797387
H	-29.648398	-13.765103	-0.495442
C	-31.033577	-13.782907	-2.153615
C	-29.969184	-13.530212	-3.195851
H	-29.594429	-12.497163	-3.125191
H	-30.361665	-13.677748	-4.212281
H	-29.103968	-14.198430	-3.061654
C	-32.379279	-13.907788	-2.510515
H	-32.662557	-13.855760	-3.565956
C	-33.388832	-14.090546	-1.552894
C	-34.828204	-14.234869	-1.969465
H	-34.913858	-14.239138	-3.065090
H	-35.433486	-13.403320	-1.567842
H	-35.269697	-15.165549	-1.580638
N	-35.409069	-14.409209	2.468084
C	-36.398835	-14.130820	3.475075
C	-36.020665	-14.103291	4.827563
C	-34.580737	-14.251533	5.240866
H	-33.975545	-13.417551	4.843981
H	-34.493326	-14.263329	6.336315
H	-34.140428	-15.179743	4.844991
C	-37.027891	-13.920930	5.787790
H	-36.742345	-13.872321	6.842878
C	-38.373890	-13.790737	5.433728
C	-39.435117	-13.535670	6.478577
H	-39.041450	-13.688585	7.493917
H	-39.804063	-12.500107	6.411798
H	-40.304400	-14.198552	6.343887
C	-38.716349	-13.871031	4.078022
H	-39.762246	-13.765152	3.778428
C	-37.748641	-14.043792	3.083513
C	-38.130500	-14.123544	1.630687
H	-37.629641	-13.328682	1.056032
H	-39.215917	-14.012961	1.509831
H	-37.823212	-15.084820	1.188833
S	-36.475288	-10.892162	2.843126
C	-37.816758	-10.579459	1.730188
C	-39.097004	-10.230462	2.372537
C	-39.123180	-9.428540	3.541626
H	-38.171286	-9.066372	3.932477
C	-40.318789	-9.110473	4.184536
H	-40.295238	-8.480767	5.078578
C	-41.544455	-9.591193	3.699325
H	-42.480550	-9.347466	4.207666
C	-41.540626	-10.399816	2.554777
H	-42.481823	-10.797942	2.164753
C	-40.345175	-10.712922	1.905665
H	-40.362377	-11.351999	1.022891
C	-37.613170	-10.743109	0.365695
C	-38.554381	-10.357526	-0.697665
C	-39.316769	-9.164176	-0.629833
H	-39.214186	-8.528766	0.249818
C	-40.166985	-8.781020	-1.666045
H	-40.731344	-7.848259	-1.578399
C	-40.288838	-9.566213	-2.822492
H	-40.950047	-9.260709	-3.637111

C	-39.527702	-10.740183	-2.919059
H	-39.598291	-11.363834	-3.814922
C	-38.675180	-11.123463	-1.883980
H	-38.074944	-12.030204	-1.970060
S	-36.024370	-11.303005	-0.197487
C	-35.147131	-15.740501	2.147453
C	-34.271012	-15.738344	1.115701
H	-33.802383	-16.553565	0.576480
H	-35.617645	-16.557850	2.681868

Complex 5-BP86 Charge=-2 S=1

100

Fe	-34.706875	-11.579997	1.642895
S	-32.986675	-10.729786	0.431568
C	-31.610739	-10.482793	1.529359
C	-30.339495	-10.132653	0.876021
C	-30.311059	-9.301922	-0.274270
H	-31.260156	-8.907213	-0.640021
C	-29.118796	-9.000051	-0.931026
H	-29.142296	-8.348717	-1.809764
C	-27.895999	-9.522544	-0.480754
H	-26.962833	-9.291451	-1.000640
C	-27.902587	-10.360808	0.644178
H	-26.966326	-10.795711	1.006344
C	-29.093545	-10.660826	1.304889
H	-29.077815	-11.327259	2.167323
C	-31.778643	-10.721641	2.890272
C	-30.830302	-10.351691	3.953256
C	-30.041497	-9.174883	3.889457
C	-29.180566	-8.813828	4.924865
H	-28.594379	-7.894643	4.836687
C	-29.074311	-9.602898	6.080275
H	-28.404614	-9.314429	6.894240
C	-29.861447	-10.759099	6.174727
H	-29.806435	-11.384464	7.070596
H	-30.130282	-8.533492	3.012828
C	-30.720616	-11.123541	5.138319
H	-31.338244	-12.018601	5.223614
S	-33.327682	-11.384327	3.455466
C	-34.705654	-13.734036	1.639850
N	-33.935729	-14.612088	0.885635
C	-32.945349	-14.264919	-0.103646
C	-31.608464	-14.104131	0.303479
C	-31.231342	-14.177718	1.757825
H	-30.149487	-14.040208	1.882559
H	-31.753215	-13.391636	2.329681
H	-31.516438	-15.144267	2.201966
C	-30.650397	-13.839368	-0.681286
H	-29.614917	-13.674491	-0.373373
C	-30.992439	-13.734675	-2.034985
C	-29.944475	-13.382332	-3.064658
H	-29.641807	-12.328344	-2.962435
H	-30.323827	-13.527880	-4.086388
H	-29.036627	-13.993847	-2.944468
C	-32.329261	-13.921953	-2.400824

H	-32.615811	-13.839116	-3.453193
C	-33.327147	-14.191694	-1.453038
C	-34.763693	-14.361219	-1.869975
H	-34.850998	-14.352596	-2.965100
H	-35.383033	-13.542852	-1.461790
H	-35.189427	-15.303353	-1.492139
N	-35.476032	-14.615342	2.389637
C	-36.464758	-14.271776	3.381771
C	-36.080795	-14.201642	4.730744
C	-34.643504	-14.371180	5.144892
H	-34.025695	-13.550763	4.738503
H	-34.554469	-14.366081	6.239887
H	-34.217514	-15.311618	4.763285
C	-37.077270	-13.935024	5.680828
H	-36.789123	-13.854980	6.732927
C	-38.414681	-13.746930	5.317452
C	-39.461090	-13.396884	6.349536
H	-39.081932	-13.549679	7.370274
H	-39.760045	-12.341154	6.253687
H	-40.371156	-14.004473	6.226005
C	-38.758809	-13.848317	3.964073
H	-39.794757	-13.682795	3.658195
C	-37.802290	-14.110355	2.977115
C	-38.181466	-14.180158	1.523137
H	-37.658955	-13.393667	0.952354
H	-39.263243	-14.040708	1.400136
H	-37.898414	-15.146124	1.076453
S	-36.426461	-10.731497	2.855916
C	-37.802647	-10.481427	1.759232
C	-39.072070	-10.127294	2.414439
C	-39.096052	-9.295954	3.564372
H	-38.145580	-8.902909	3.927970
C	-40.285922	-8.992194	4.224450
H	-40.258930	-8.340831	5.102974
C	-41.510555	-9.513224	3.778039
H	-42.441365	-9.281483	4.301476
C	-41.508748	-10.350625	2.652779
H	-42.446754	-10.783387	2.293156
C	-40.320091	-10.652639	1.988554
H	-40.339287	-11.318840	1.125895
C	-37.636610	-10.721208	0.398345
C	-38.586061	-10.351520	-0.663737
C	-39.371093	-9.172149	-0.601302
H	-39.278842	-8.529091	0.273791
C	-40.232428	-8.810651	-1.636229
H	-40.815113	-7.889176	-1.549593
C	-40.343384	-9.602354	-2.789341
H	-41.013321	-9.313592	-3.602909
C	-39.560826	-10.761749	-2.882114
H	-39.620201	-11.389413	-3.776038
C	-38.700737	-11.126358	-1.846439
H	-38.086462	-12.023789	-1.930412
S	-36.088394	-11.384376	-0.168635
C	-35.193997	-15.952310	2.106929
C	-34.219845	-15.950230	1.160977
H	-33.706326	-16.764327	0.661450

H	-35.708620	-16.768509	2.602054

Complex 5-BP86 Charge=-2 S=2

100

Fe	-34.773894	-11.713978	1.716342
S	-32.972403	-10.632128	0.523608
C	-31.612291	-10.441527	1.637650
C	-30.331210	-10.089008	0.984145
C	-30.291679	-9.228034	-0.140720
H	-31.234949	-8.805061	-0.489506
C	-29.097923	-8.938278	-0.800591
H	-29.111163	-8.262509	-1.660981
C	-27.887357	-9.508989	-0.379845
H	-26.954321	-9.293883	-0.906764
C	-27.905019	-10.378281	0.719427
H	-26.978633	-10.851516	1.057172
C	-29.098419	-10.662589	1.383935
H	-29.092776	-11.355300	2.225313
C	-31.730045	-10.705263	3.004634
C	-30.707772	-10.316877	4.005318
C	-30.043049	-9.068661	3.947567
C	-29.119518	-8.686733	4.922393
H	-28.634924	-7.709385	4.848109
C	-28.821524	-9.534322	5.997187
H	-28.103575	-9.231587	6.763818
C	-29.480191	-10.770573	6.080940
H	-29.271815	-11.444404	6.917119
H	-30.277383	-8.391237	3.126345
C	-30.410193	-11.146984	5.112247
H	-30.945849	-12.093855	5.194394
S	-33.191957	-11.399775	3.689764
C	-34.701596	-13.861008	1.669590
N	-33.914525	-14.712889	0.908765
C	-32.942646	-14.326507	-0.084519
C	-31.613475	-14.106239	0.319660
C	-31.230031	-14.160170	1.773181
H	-30.150597	-14.002432	1.893035
H	-31.762988	-13.379245	2.343206
H	-31.496199	-15.127736	2.226378
C	-30.670403	-13.803620	-0.669251
H	-29.641928	-13.593665	-0.365262
C	-31.020925	-13.720272	-2.022256
C	-29.990877	-13.334744	-3.057861
H	-29.738509	-12.266226	-2.972769
H	-30.362651	-13.514351	-4.076867
H	-29.055415	-13.900485	-2.927816
C	-32.350761	-13.959755	-2.383348
H	-32.643978	-13.890618	-3.434810
C	-33.334709	-14.265034	-1.431843
C	-34.765827	-14.485695	-1.844485
H	-34.852142	-14.504875	-2.939422
H	-35.412527	-13.677322	-1.460088
H	-35.165509	-15.430111	-1.445272
N	-35.447046	-14.759942	2.421210

C	-36.428253	-14.422462	3.422387
C	-36.025861	-14.338828	4.766053
C	-34.583479	-14.505684	5.165160
H	-33.969447	-13.675505	4.771373
H	-34.485434	-14.516199	6.259204
H	-34.153731	-15.436608	4.765715
C	-37.009366	-14.053550	5.724036
H	-36.708470	-13.962349	6.771516
C	-38.348341	-13.855351	5.372747
C	-39.376601	-13.477090	6.412535
H	-39.009243	-13.675517	7.429709
H	-39.616102	-12.404221	6.343752
H	-40.317783	-14.030154	6.270871
C	-38.708807	-13.962950	4.024469
H	-39.745830	-13.786147	3.728319
C	-37.767016	-14.244799	3.028856
C	-38.160608	-14.307748	1.579270
H	-37.656951	-13.505241	1.009892
H	-39.245871	-14.187483	1.468141
H	-37.862481	-15.262182	1.118723
S	-36.633334	-10.743159	2.853065
C	-37.922871	-10.463449	1.675025
C	-39.209118	-10.039583	2.270317
C	-39.256174	-9.131567	3.356522
H	-38.312184	-8.718837	3.715474
C	-40.460779	-8.785313	3.967928
H	-40.454945	-8.075935	4.800880
C	-41.672839	-9.342796	3.533099
H	-42.614606	-9.082004	4.022480
C	-41.647143	-10.255940	2.470114
H	-42.576242	-10.717446	2.123330
C	-40.443018	-10.597115	1.853194
H	-40.439304	-11.320736	1.037532
C	-37.744706	-10.724148	0.318273
C	-38.694046	-10.292091	-0.730311
C	-39.334276	-9.029492	-0.688586
H	-39.130129	-8.367793	0.153513
C	-40.197819	-8.614177	-1.703118
H	-40.667037	-7.628539	-1.636996
C	-40.457412	-9.439931	-2.805775
H	-41.130814	-9.112320	-3.601820
C	-39.818554	-10.686588	-2.876025
H	-39.996454	-11.343424	-3.732685
C	-38.948985	-11.098149	-1.866203
H	-38.431025	-12.056122	-1.934383
S	-36.289912	-11.545604	-0.260525
C	-35.133108	-16.087867	2.133442
C	-34.164203	-16.057532	1.181544
H	-33.634620	-16.855655	0.673973
H	-35.626034	-16.917694	2.627165

Complex 5-B3LYP* Charge=-1 S=0.5

100

Fe	-34.706667	-11.627015	1.639990
S	-32.998784	-10.790111	0.438748

C	-31.637483	-10.551067	1.562293
C	-30.345332	-10.173877	0.931297
C	-30.303707	-9.284273	-0.164162
H	-31.235884	-8.854038	-0.520459
C	-29.099901	-8.960043	-0.791937
H	-29.103794	-8.266171	-1.631197
C	-27.894675	-9.518053	-0.350501
H	-26.956254	-9.267619	-0.841455
C	-27.916469	-10.410098	0.727492
H	-26.991038	-10.863066	1.079224
C	-29.120618	-10.734758	1.353769
H	-29.120144	-11.439483	2.180371
C	-31.825457	-10.757550	2.910728
C	-30.844772	-10.378015	3.967136
C	-30.250139	-9.100627	3.970288
C	-29.363061	-8.718556	4.977369
H	-28.924222	-7.722454	4.956296
C	-29.047327	-9.602522	6.015112
H	-28.357972	-9.303667	6.802476
C	-29.640332	-10.869736	6.035243
H	-29.411877	-11.565459	6.841246
H	-30.501009	-8.403996	3.175080
C	-30.531613	-11.248937	5.029095
H	-31.003518	-12.227779	5.057493
S	-33.357181	-11.400136	3.518220
C	-34.704638	-13.635439	1.639009
N	-33.949023	-14.496682	0.864066
C	-32.954845	-14.186609	-0.141462
C	-31.611073	-14.066182	0.257553
C	-31.211316	-14.189414	1.708773
H	-30.134980	-14.033846	1.821237
H	-31.736318	-13.451775	2.325392
H	-31.456928	-15.182049	2.107285
C	-30.651962	-13.826050	-0.730592
H	-29.613194	-13.697196	-0.430457
C	-30.996912	-13.716340	-2.083507
C	-29.943515	-13.392843	-3.121203
H	-29.608270	-12.353320	-3.018773
H	-30.331162	-13.523078	-4.136726
H	-29.059901	-14.031996	-3.006899
C	-32.335745	-13.893498	-2.443361
H	-32.620371	-13.831773	-3.492999
C	-33.335424	-14.143072	-1.492104
C	-34.765436	-14.362829	-1.928313
H	-34.834900	-14.352959	-3.019917
H	-35.425642	-13.581888	-1.533535
H	-35.150924	-15.325273	-1.570230
N	-35.455711	-14.497042	2.418011
C	-36.452926	-14.186513	3.420600
C	-36.075922	-14.144153	4.772212
C	-34.647646	-14.368260	5.212005
H	-33.984129	-13.589776	4.817649
H	-34.580670	-14.357685	6.303817
H	-34.264579	-15.332421	4.855757
C	-37.077083	-13.891184	5.720906
H	-36.794996	-13.830114	6.771240

C	-38.414422	-13.710727	5.357625
C	-39.469531	-13.384331	6.392508
H	-39.083890	-13.512493	7.409047
H	-39.803889	-12.345010	6.286963
H	-40.353127	-14.023227	6.277940
C	-38.756184	-13.820235	4.003993
H	-39.793829	-13.688969	3.701486
C	-37.795307	-14.062892	3.018144
C	-38.192152	-14.185861	1.566117
H	-37.666490	-13.447877	0.950466
H	-39.268327	-14.030732	1.451702
H	-37.945355	-15.178313	1.167821
S	-36.411704	-10.787757	2.843705
C	-37.774546	-10.546388	1.722564
C	-39.065508	-10.173457	2.358704
C	-39.105218	-9.287906	3.457427
H	-38.172963	-8.856140	3.811578
C	-40.307296	-8.970329	4.091810
H	-40.302027	-8.279387	4.933456
C	-41.512359	-9.531805	3.654297
H	-42.449466	-9.286926	4.150166
C	-41.492111	-10.419943	2.573167
H	-42.417449	-10.875382	2.224105
C	-40.289991	-10.737307	1.939863
H	-40.291625	-11.438993	1.110641
C	-37.588617	-10.749848	0.373327
C	-38.571712	-10.368215	-0.680105
C	-39.170535	-9.092482	-0.676878
H	-38.920657	-8.398372	0.120811
C	-40.060475	-8.708908	-1.680783
H	-40.502675	-7.714419	-1.654544
C	-40.375055	-9.589282	-2.722128
H	-41.066595	-9.289263	-3.507046
C	-39.777916	-10.854494	-2.748732
H	-40.005094	-11.547463	-3.557482
C	-38.884103	-11.235443	-1.745316
H	-38.409376	-12.212785	-1.778806
S	-36.057598	-11.392614	-0.236634
C	-35.169651	-15.829521	2.128949
C	-34.225513	-15.829304	1.161940
H	-33.722378	-16.639531	0.655511
H	-35.668387	-16.640055	2.639277

Complex 5-B3LYP* Charge=-1 S=1.5

100

Fe	-34.703962	-11.513653	1.641546
S	-32.903207	-10.751251	0.396321
C	-31.573607	-10.488704	1.560483
C	-30.265559	-10.134508	0.943675
C	-30.193986	-9.223084	-0.130411
H	-31.113388	-8.764645	-0.485047
C	-28.975131	-8.912456	-0.736571
H	-28.951795	-8.198779	-1.558656
C	-27.789631	-9.511483	-0.295290
H	-26.839917	-9.272474	-0.770321

C	-27.843693	-10.428999	0.760006
H	-26.932527	-10.912154	1.109900
C	-29.062508	-10.737949	1.365905
H	-29.091925	-11.460424	2.176967
C	-31.780875	-10.646360	2.904868
C	-30.810495	-10.265257	3.968007
C	-30.165645	-9.012055	3.950057
C	-29.281476	-8.638427	4.963132
H	-28.803131	-7.661278	4.924853
C	-29.020501	-9.505380	6.030366
H	-28.335323	-9.212358	6.823494
C	-29.664342	-10.746964	6.072892
H	-29.479347	-11.428242	6.901980
H	-30.375108	-8.326578	3.133495
C	-30.551599	-11.117773	5.060025
H	-31.061897	-12.076657	5.106351
S	-33.363895	-11.207252	3.516991
C	-34.704888	-13.849099	1.638716
N	-33.964318	-14.705276	0.860657
C	-32.983909	-14.348860	-0.141935
C	-31.643938	-14.187692	0.252442
C	-31.238001	-14.284512	1.703990
H	-30.151090	-14.215128	1.802018
H	-31.690025	-13.470421	2.282529
H	-31.565505	-15.228026	2.156037
C	-30.701236	-13.895311	-0.736982
H	-29.664418	-13.739681	-0.442338
C	-31.061151	-13.760237	-2.083578
C	-30.022898	-13.388417	-3.120530
H	-29.695878	-12.350129	-2.983537
H	-30.420537	-13.485065	-4.135718
H	-29.132208	-14.023054	-3.039784
C	-32.401143	-13.944862	-2.435556
H	-32.699453	-13.842200	-3.477987
C	-33.384836	-14.243999	-1.482001
C	-34.828804	-14.415283	-1.893417
H	-34.919210	-14.402048	-2.983607
H	-35.445664	-13.603637	-1.486490
H	-35.247452	-15.359376	-1.525419
N	-35.443818	-14.705572	2.418041
C	-36.425977	-14.349072	3.418977
C	-36.028766	-14.245633	4.760335
C	-34.586315	-14.419183	5.176170
H	-33.967105	-13.608300	4.771342
H	-34.499247	-14.406321	6.266694
H	-34.167771	-15.363748	4.809311
C	-37.014707	-13.945181	5.711193
H	-36.719330	-13.843450	6.754539
C	-38.353187	-13.758012	5.355476
C	-39.393881	-13.384894	6.389486
H	-38.998522	-13.479288	7.405774
H	-39.721305	-12.347251	6.249618
H	-40.283916	-14.020224	6.308028
C	-38.709466	-13.891565	4.007765
H	-39.745050	-13.733566	3.710296
C	-37.764526	-14.185543	3.021015

C	-38.166454	-14.282550	1.568442
H	-37.710986	-13.470082	0.990439
H	-39.252941	-14.211064	1.467314
H	-37.839604	-15.227251	1.118380
S	-36.501717	-10.750476	2.890082
C	-37.833465	-10.487196	1.728350
C	-39.140975	-10.135675	2.347911
C	-39.211487	-9.226480	3.423924
H	-38.291951	-8.767216	3.777426
C	-40.429487	-8.918901	4.033649
H	-40.451836	-8.206612	4.857143
C	-41.615087	-9.519096	3.594184
H	-42.564119	-9.282604	4.071894
C	-41.561899	-10.434715	2.537148
H	-42.473076	-10.918715	2.188770
C	-40.344155	-10.739918	1.927091
H	-40.315750	-11.460177	1.114034
C	-37.627688	-10.641447	0.383351
C	-38.600985	-10.259467	-0.676586
C	-39.250386	-9.008823	-0.652066
H	-39.041203	-8.325591	0.166355
C	-40.140201	-8.635495	-1.660427
H	-40.622964	-7.660813	-1.616439
C	-40.402557	-9.500334	-2.728901
H	-41.093645	-9.208334	-3.517328
C	-39.753450	-10.738955	-2.778352
H	-39.940497	-11.419259	-3.607805
C	-38.860278	-11.109219	-1.770602
H	-38.347667	-12.066633	-1.821152
S	-36.044872	-11.198665	-0.232260
C	-35.170127	-16.042067	2.130939
C	-34.235951	-16.041907	1.149141
H	-33.741815	-16.852207	0.632880
H	-35.663273	-16.852545	2.647839

Complex 5-B3LYP* Charge=-1 S=2.5

100

Fe	-34.705504	-11.687432	1.642002
S	-32.891883	-10.665825	0.429644
C	-31.581511	-10.469770	1.617057
C	-30.270680	-10.085305	1.013900
C	-30.190530	-9.119731	-0.010355
H	-31.104323	-8.629465	-0.335368
C	-28.971382	-8.798045	-0.609822
H	-28.942427	-8.041198	-1.392113
C	-27.792805	-9.441580	-0.214712
H	-26.843184	-9.195261	-0.686525
C	-27.855010	-10.412897	0.790227
H	-26.950139	-10.931047	1.104381
C	-29.074133	-10.729692	1.391980
H	-29.109485	-11.491578	2.165615
C	-31.757987	-10.688841	2.966855
C	-30.755580	-10.280448	3.995900
C	-30.185191	-8.991806	3.974270

C	-29.275378	-8.585393	4.951574
H	-28.857169	-7.581064	4.910341
C	-28.910873	-9.455047	5.984434
H	-28.205065	-9.136918	6.748970
C	-29.479810	-10.733374	6.030970
H	-29.214840	-11.418005	6.835018
H	-30.472725	-8.304740	3.183386
C	-30.395089	-11.135402	5.056385
H	-30.852081	-12.120232	5.109954
S	-33.255137	-11.366495	3.640001
C	-34.703985	-13.944522	1.638973
N	-33.961391	-14.793221	0.859449
C	-32.984846	-14.413104	-0.138895
C	-31.651674	-14.215199	0.263062
C	-31.244027	-14.324014	1.713164
H	-30.159965	-14.221769	1.812586
H	-31.721349	-13.536840	2.309673
H	-31.540064	-15.286659	2.146986
C	-30.716798	-13.880029	-0.720289
H	-29.686339	-13.695842	-0.420804
C	-31.077825	-13.738537	-2.065672
C	-30.049505	-13.321369	-3.094777
H	-29.752867	-12.276567	-2.940816
H	-30.442606	-13.413917	-4.112030
H	-29.141223	-13.931311	-3.021400
C	-32.410158	-13.961914	-2.424660
H	-32.708518	-13.854815	-3.466439
C	-33.386573	-14.305352	-1.479160
C	-34.821073	-14.524325	-1.900802
H	-34.903736	-14.510133	-2.991293
H	-35.472058	-13.737094	-1.499419
H	-35.209307	-15.483693	-1.539846
N	-35.443698	-14.794496	2.420094
C	-36.423166	-14.416049	3.416427
C	-36.025563	-14.311247	4.758243
C	-34.592434	-14.531958	5.183798
H	-33.939329	-13.745959	4.783307
H	-34.512537	-14.516805	6.274554
H	-34.204659	-15.492380	4.824780
C	-37.004354	-13.968180	5.701352
H	-36.709009	-13.863488	6.744217
C	-38.334904	-13.741107	5.338660
C	-39.364821	-13.320656	6.364722
H	-38.974315	-13.412248	7.383080
H	-39.658781	-12.275613	6.208223
H	-40.274211	-13.928557	6.290096
C	-38.692297	-13.880862	3.992126
H	-39.721728	-13.694821	3.689975
C	-37.755089	-14.216292	3.011151
C	-38.159973	-14.324160	1.560097
H	-37.681334	-13.537057	0.964430
H	-39.243840	-14.221513	1.458722
H	-37.863580	-15.286904	1.126752
S	-36.515885	-10.664339	2.858351
C	-37.828194	-10.465387	1.673614
C	-39.138152	-10.082251	2.279523

C	-39.216772	-9.121927	3.309112
H	-38.301918	-8.635523	3.636912
C	-40.435604	-8.801095	3.910140
H	-40.463384	-8.049208	4.697048
C	-41.615332	-9.439480	3.510049
H	-42.564775	-9.193367	3.981915
C	-41.554709	-10.404896	2.499463
H	-42.460296	-10.918818	2.181311
C	-40.335863	-10.722257	1.897721
H	-40.302015	-11.480478	1.120475
C	-37.653903	-10.681867	0.323188
C	-38.657830	-10.272665	-0.703951
C	-39.230937	-8.985463	-0.679797
H	-38.943127	-8.298462	0.110780
C	-40.145702	-8.580970	-1.653271
H	-40.567394	-7.578265	-1.609434
C	-40.511456	-9.450833	-2.685639
H	-41.221850	-9.134690	-3.446917
C	-39.938294	-10.727017	-2.735633
H	-40.204552	-11.411997	-3.539120
C	-39.018851	-11.127214	-1.764523
H	-38.560106	-12.111082	-1.819986
S	-36.158291	-11.360865	-0.353018
C	-35.166724	-16.129428	2.132806
C	-34.232545	-16.128679	1.149936
H	-33.738024	-16.938710	0.633992
H	-35.658560	-16.940347	2.649928

Complex 5-B3LYP* Charge=-2 S=0

100

Fe	-34.703266	-11.652853	1.640653
S	-32.888347	-10.870081	0.392623
C	-31.564904	-10.571252	1.550549
C	-30.267690	-10.194224	0.935175
C	-30.225189	-9.346738	-0.198746
H	-31.167209	-8.967776	-0.585541
C	-29.021567	-9.009840	-0.818287
H	-29.033712	-8.347439	-1.683975
C	-27.804555	-9.518929	-0.343142
H	-26.865486	-9.263593	-0.832472
C	-27.824299	-10.373858	0.766127
H	-26.893166	-10.794608	1.146038
C	-29.029050	-10.704378	1.390103
H	-29.021395	-11.378881	2.241594
C	-31.767094	-10.742541	2.908267
C	-30.809748	-10.334149	3.965298
C	-30.141746	-9.088299	3.923386
C	-29.282602	-8.683884	4.945792
H	-28.792962	-7.712416	4.879695
C	-29.060151	-9.506170	6.058496
H	-28.394781	-9.187605	6.859826
C	-29.726501	-10.737120	6.129255
H	-29.577508	-11.387813	6.991129
H	-30.321169	-8.430662	3.077410
C	-30.589179	-11.138006	5.108094

H	-31.122368	-12.082617	5.178532
S	-33.327210	-11.346720	3.522123
C	-34.706219	-13.588324	1.638260
N	-33.972872	-14.481961	0.840680
C	-32.982028	-14.195457	-0.167195
C	-31.633662	-14.092753	0.222551
C	-31.242971	-14.169966	1.678071
H	-30.161730	-14.046110	1.791345
H	-31.748154	-13.386479	2.255128
H	-31.530802	-15.133886	2.117340
C	-30.670146	-13.898904	-0.771576
H	-29.629375	-13.776037	-0.474461
C	-31.015971	-13.810707	-2.125683
C	-29.959337	-13.521076	-3.171200
H	-29.602761	-12.486830	-3.083182
H	-30.354947	-13.655338	-4.184200
H	-29.086830	-14.176785	-3.055176
C	-32.359510	-13.959517	-2.478810
H	-32.647301	-13.901903	-3.528608
C	-33.361811	-14.163987	-1.518372
C	-34.802933	-14.329544	-1.938575
H	-34.883777	-14.337552	-3.030715
H	-35.420967	-13.510620	-1.547029
H	-35.228980	-15.264373	-1.553582
N	-35.442096	-14.481330	2.434239
C	-36.432427	-14.193682	3.442338
C	-36.052410	-14.166183	4.793428
C	-34.611891	-14.339084	5.212548
H	-33.990770	-13.520878	4.824555
H	-34.530722	-14.352529	6.304587
H	-34.189983	-15.273821	4.822980
C	-37.053827	-13.960178	5.754580
H	-36.765863	-13.905923	6.804506
C	-38.396879	-13.806162	5.401788
C	-39.452507	-13.514387	6.447823
H	-39.055936	-13.647287	7.460656
H	-39.808755	-12.480064	6.358423
H	-40.325547	-14.169946	6.333762
C	-38.743398	-13.891866	4.047710
H	-39.783981	-13.765496	3.751221
C	-37.780833	-14.087013	3.053029
C	-38.172906	-14.161623	1.597692
H	-37.665314	-13.379699	1.020633
H	-39.253796	-14.033423	1.485512
H	-37.889476	-15.126414	1.157476
S	-36.514465	-10.867916	2.891241
C	-37.840558	-10.568372	1.736996
C	-39.136228	-10.195696	2.358522
C	-39.175730	-9.350679	3.494512
H	-38.233112	-8.968994	3.877369
C	-40.377308	-9.019280	4.121036
H	-40.362914	-8.358158	4.987636
C	-41.595024	-9.531421	3.650735
H	-42.532406	-9.280011	4.145068
C	-41.578070	-10.384049	2.539576
H	-42.509588	-10.807328	2.163613

C	-40.375275	-10.709361	1.908983
H	-40.384602	-11.382619	1.056590
C	-37.641271	-10.737009	0.378375
C	-38.602228	-10.330487	-0.676148
C	-39.280852	-9.090683	-0.628879
H	-39.106451	-8.434681	0.219276
C	-40.144470	-8.689388	-1.648964
H	-40.641875	-7.722311	-1.578651
C	-40.360955	-9.508524	-2.765099
H	-41.029477	-9.192261	-3.564674
C	-39.683593	-10.733110	-2.841596
H	-39.826837	-11.381120	-3.706440
C	-38.816702	-11.130760	-1.822762
H	-38.274786	-12.070023	-1.897832
S	-36.080892	-11.338985	-0.238418
C	-35.167305	-15.813894	2.132907
C	-34.249624	-15.814375	1.141695
H	-33.764218	-16.628457	0.622911
H	-35.654400	-16.627246	2.651268

Complex 5-B3LYP* Charge=-2 S=1

100

Fe	-34.708126	-11.671454	1.644615
S	-32.970929	-10.706162	0.395842
C	-31.609714	-10.481327	1.535226
C	-30.324305	-10.092505	0.907986
C	-30.290980	-9.230724	-0.216037
H	-31.235278	-8.833573	-0.578744
C	-29.096038	-8.908096	-0.858957
H	-29.116167	-8.235395	-1.717131
C	-27.877042	-9.442180	-0.417499
H	-26.945158	-9.198954	-0.926166
C	-27.886800	-10.308458	0.684145
H	-26.954868	-10.749452	1.038070
C	-29.082208	-10.628001	1.329264
H	-29.068205	-11.317579	2.168490
C	-31.768486	-10.744383	2.885712
C	-30.805489	-10.340151	3.938461
C	-30.174996	-9.074045	3.920749
C	-29.306224	-8.673581	4.936212
H	-28.847208	-7.686335	4.888841
C	-29.033522	-9.521028	6.018312
H	-28.358964	-9.206830	6.813405
C	-29.660597	-10.773255	6.065313
H	-29.471376	-11.445046	6.902782
H	-30.392470	-8.398256	3.098453
C	-30.534337	-11.170240	5.051724
H	-31.034673	-12.133627	5.104489
S	-33.269020	-11.486970	3.499965
C	-34.704032	-13.873293	1.641149
N	-33.930341	-14.740068	0.891035
C	-32.940247	-14.370835	-0.092860
C	-31.610658	-14.172287	0.320532
C	-31.225362	-14.267083	1.776274
H	-30.149150	-14.111779	1.897396

H	-31.756772	-13.506925	2.365168
H	-31.485474	-15.245809	2.199234
C	-30.661007	-13.846270	-0.653357
H	-29.637531	-13.646891	-0.339098
C	-31.003443	-13.717099	-2.004024
C	-29.966959	-13.285486	-3.020268
H	-29.714902	-12.226067	-2.884334
H	-30.334212	-13.416535	-4.044116
H	-29.036100	-13.856752	-2.914203
C	-32.330050	-13.949212	-2.379409
H	-32.616642	-13.846827	-3.425729
C	-33.318981	-14.278414	-1.441598
C	-34.750533	-14.487040	-1.875552
H	-34.824620	-14.471902	-2.967813
H	-35.396660	-13.694441	-1.473924
H	-35.149671	-15.442613	-1.514461
N	-35.476059	-14.744169	2.388829
C	-36.467088	-14.379051	3.372948
C	-36.087142	-14.288999	4.721379
C	-34.655161	-14.498728	5.153473
H	-34.009589	-13.704600	4.753963
H	-34.580098	-14.487461	6.245725
H	-34.256023	-15.452798	4.788546
C	-37.075331	-13.961260	5.660452
H	-36.787726	-13.860238	6.706636
C	-38.402333	-13.729298	5.286445
C	-39.437785	-13.300442	6.304570
H	-39.070516	-13.436028	7.327724
H	-39.688467	-12.240205	6.173052
H	-40.369137	-13.870113	6.195950
C	-38.746001	-13.856480	3.935916
H	-39.769772	-13.657324	3.622887
C	-37.796953	-14.180357	2.960734
C	-38.182959	-14.271876	1.504843
H	-37.653647	-13.508573	0.918085
H	-39.259616	-14.118616	1.384819
H	-37.920610	-15.248573	1.078763
S	-36.446777	-10.708890	2.896156
C	-37.804928	-10.477125	1.755104
C	-39.089898	-10.085129	2.380795
C	-39.123734	-9.219639	3.501800
H	-38.179453	-8.823165	3.865198
C	-40.319681	-8.892737	4.140854
H	-40.300341	-8.217816	4.997278
C	-41.538729	-9.426307	3.698633
H	-42.471425	-9.179916	4.204242
C	-41.528189	-10.296875	2.600520
H	-42.460219	-10.737559	2.246123
C	-40.331845	-10.620477	1.959077
H	-40.345092	-11.312599	1.122004
C	-37.645852	-10.738280	0.404313
C	-38.609309	-10.331968	-0.647235
C	-39.239468	-9.065764	-0.626412
H	-39.019738	-8.390692	0.195921
C	-40.112725	-8.664902	-1.637819
H	-40.573056	-7.678165	-1.586267

C	-40.388017	-9.510554	-2.720666
H	-41.065551	-9.195756	-3.513088
C	-39.758927	-10.761626	-2.772388
H	-39.948497	-11.431532	-3.611364
C	-38.882491	-11.160041	-1.761290
H	-38.381684	-12.123157	-1.817070
S	-36.146310	-11.483715	-0.210900
C	-35.188153	-16.080530	2.109946
C	-34.211783	-16.077926	1.169607
H	-33.696592	-16.890025	0.676467
H	-35.699465	-16.895463	2.602505

Complex 5-B3LYP* Charge=-2 S=2

100

Fe	-34.702605	-11.637475	1.641389
S	-32.810931	-10.666775	0.437420
C	-31.494936	-10.468395	1.625453
C	-30.185119	-10.093493	1.022738
C	-30.105659	-9.158442	-0.035789
H	-31.029882	-8.701177	-0.378825
C	-28.889849	-8.838604	-0.640910
H	-28.870600	-8.105116	-1.447297
C	-27.699695	-9.454259	-0.227084
H	-26.751865	-9.211994	-0.706311
C	-27.758083	-10.399465	0.804075
H	-26.849459	-10.903565	1.133548
C	-28.975330	-10.713502	1.412491
H	-29.002432	-11.458189	2.203065
C	-31.654748	-10.719335	2.979112
C	-30.651732	-10.310631	4.000223
C	-30.041829	-9.035754	3.967286
C	-29.135523	-8.631165	4.949326
H	-28.693667	-7.636437	4.892485
C	-28.803640	-9.485287	6.007945
H	-28.101437	-9.167979	6.777831
C	-29.410819	-10.748145	6.069644
H	-29.177047	-11.423830	6.892751
H	-30.302724	-8.356187	3.160646
C	-30.324648	-11.145604	5.093075
H	-30.821233	-12.110072	5.162801
S	-33.151261	-11.411314	3.658033
C	-34.706478	-13.946037	1.637929
N	-33.966899	-14.800941	0.858778
C	-32.988202	-14.417166	-0.134201
C	-31.659842	-14.202401	0.274468
C	-31.266420	-14.282837	1.728900
H	-30.184977	-14.160129	1.838907
H	-31.765381	-13.491299	2.305928
H	-31.555264	-15.242526	2.175296
C	-30.722129	-13.861078	-0.705222
H	-29.698737	-13.650739	-0.397798
C	-31.078434	-13.724277	-2.051567
C	-30.053794	-13.275871	-3.072384
H	-29.801206	-12.218626	-2.920723
H	-30.432725	-13.389259	-4.093852

H	-29.121870	-13.848822	-2.985782
C	-32.406897	-13.958892	-2.417806
H	-32.704302	-13.842374	-3.459478
C	-33.385229	-14.307366	-1.475777
C	-34.822241	-14.507550	-1.895710
H	-34.905313	-14.502464	-2.987234
H	-35.458442	-13.702646	-1.499685
H	-35.228634	-15.455082	-1.522336
N	-35.449015	-14.801273	2.413813
C	-36.425884	-14.417688	3.408577
C	-36.027710	-14.312822	4.750169
C	-34.591116	-14.518199	5.169030
H	-33.953085	-13.713056	4.776397
H	-34.508030	-14.517909	6.260545
H	-34.186819	-15.465051	4.791596
C	-37.004407	-13.963439	5.693561
H	-36.705900	-13.850338	6.735236
C	-38.332239	-13.723336	5.328622
C	-39.354683	-13.273431	6.350959
H	-38.974804	-13.387860	7.371889
H	-39.605683	-12.215932	6.200062
H	-40.287470	-13.844661	6.265356
C	-38.689898	-13.856228	3.982185
H	-39.712777	-13.641865	3.675817
C	-37.753764	-14.198040	3.001284
C	-38.147664	-14.274435	1.546757
H	-37.646127	-13.483518	0.971196
H	-39.228692	-14.148129	1.436964
H	-37.861873	-15.234298	1.098713
S	-36.591343	-10.662513	2.848833
C	-37.909573	-10.464918	1.663316
C	-39.218776	-10.093396	2.269377
C	-39.297907	-9.157396	3.326999
H	-38.374205	-8.696191	3.666235
C	-40.512615	-8.842074	3.936557
H	-40.531733	-8.107835	4.742343
C	-41.701491	-9.464053	3.528779
H	-42.648231	-9.226230	4.012305
C	-41.643469	-10.409340	2.497679
H	-42.551306	-10.917958	2.172515
C	-40.427605	-10.718076	1.884143
H	-40.400628	-11.463174	1.093904
C	-37.752715	-10.714594	0.308967
C	-38.760427	-10.307898	-0.708539
C	-39.373689	-9.034720	-0.672638
H	-39.110585	-8.354554	0.132733
C	-40.286491	-8.632731	-1.649931
H	-40.731139	-7.639455	-1.590619
C	-40.620601	-9.487359	-2.707263
H	-41.327309	-9.171865	-3.473737
C	-40.009371	-10.748170	-2.772534
H	-40.244737	-11.424177	-3.594884
C	-39.089816	-11.143333	-1.800291
H	-38.590776	-12.106366	-1.872621
S	-36.256133	-11.400543	-0.375132
C	-35.179591	-16.137926	2.123813

C	-34.241847	-16.137674	1.143007
H	-33.748299	-16.948853	0.627199
H	-35.676255	-16.949291	2.636324

Complex 5-TPSS Charge=-1 S=0.5

100

Fe	-34.704080	-11.540319	1.643858
S	-32.990239	-10.798448	0.497992
C	-31.637280	-10.558311	1.598261
C	-30.345877	-10.208945	0.967380
C	-30.300327	-9.345674	-0.148392
H	-31.230203	-8.917492	-0.510114
C	-29.096872	-9.047488	-0.785426
H	-29.096826	-8.374412	-1.640318
C	-27.895731	-9.604944	-0.334723
H	-26.957577	-9.374628	-0.833842
C	-27.921943	-10.468314	0.765569
H	-27.000039	-10.920664	1.125025
C	-29.124972	-10.767087	1.403430
H	-29.128531	-11.449701	2.247104
C	-31.851554	-10.769499	2.947818
C	-30.884905	-10.477790	4.032483
C	-30.130101	-9.287751	4.042257
C	-29.258033	-8.996690	5.089547
H	-28.692786	-8.067648	5.072262
C	-29.117315	-9.881489	6.163692
H	-28.440115	-9.650804	6.982173
C	-29.870175	-11.059193	6.176915
H	-29.779413	-11.753943	7.009019
H	-30.245224	-8.585235	3.223170
C	-30.743910	-11.350439	5.129906
H	-31.337942	-12.259368	5.149258
S	-33.421431	-11.332878	3.477616
C	-34.705160	-13.472499	1.641490
N	-34.009703	-14.349718	0.811354
C	-33.043186	-14.047140	-0.222125
C	-31.688170	-13.971225	0.153815
C	-31.280452	-14.118402	1.598076
H	-30.200854	-13.988721	1.702977
H	-31.787053	-13.372410	2.219376
H	-31.549289	-15.108815	1.985245
C	-30.739587	-13.751976	-0.843116
H	-29.693634	-13.661744	-0.558627
C	-31.105564	-13.613242	-2.188728
C	-30.058742	-13.330617	-3.242891
H	-29.533999	-12.393198	-3.025081
H	-30.512386	-13.246262	-4.235002
H	-29.305337	-14.127449	-3.277634
C	-32.452548	-13.733609	-2.524309
H	-32.753295	-13.639344	-3.566409
C	-33.445668	-13.967074	-1.559533
C	-34.880268	-14.141545	-1.999780
H	-34.988200	-15.067570	-2.579439
H	-35.184676	-13.306547	-2.637153
H	-35.564053	-14.173605	-1.152575

N	-35.401802	-14.350404	2.469841
C	-36.369448	-14.048178	3.502476
C	-35.968889	-13.969743	4.840548
C	-34.535113	-14.145764	5.282774
H	-34.227493	-13.306269	5.912660
H	-34.431095	-15.067000	5.870635
H	-33.851308	-14.188117	4.436012
C	-36.963079	-13.735832	5.804135
H	-36.663720	-13.642935	6.846793
C	-38.309382	-13.613053	5.466670
C	-39.357209	-13.328957	6.519482
H	-38.904656	-13.245573	7.512206
H	-39.880008	-12.390531	6.301170
H	-40.112135	-14.124471	6.553143
C	-38.673574	-13.750597	4.120428
H	-39.718986	-13.658666	3.834481
C	-37.723897	-13.970465	3.124705
C	-38.129907	-14.116185	1.679819
H	-37.621412	-13.370525	1.059676
H	-39.209165	-13.984948	1.573209
H	-37.861985	-15.106730	1.292403
S	-36.417305	-10.799950	2.791793
C	-37.771644	-10.561140	1.692352
C	-39.063446	-10.215912	2.324563
C	-39.109320	-9.357125	3.443742
H	-38.179335	-8.931518	3.808136
C	-40.313162	-9.059393	4.080110
H	-40.313349	-8.389215	4.937132
C	-41.514355	-9.613493	3.625650
H	-42.453005	-9.383017	4.123655
C	-41.487543	-10.473847	2.523144
H	-42.409697	-10.923610	2.160964
C	-40.284145	-10.772632	1.885970
H	-40.280552	-11.452895	1.040505
C	-37.557259	-10.767835	0.342143
C	-38.524040	-10.472491	-0.741555
C	-39.278677	-9.282169	-0.747932
H	-39.163627	-8.582300	0.073398
C	-40.150394	-8.987402	-1.794479
H	-40.715508	-8.058370	-1.774592
C	-40.291382	-9.869077	-2.871106
H	-40.968774	-9.635953	-3.688768
C	-39.539006	-11.047015	-2.887734
H	-39.630303	-11.739495	-3.721665
C	-38.665021	-11.341445	-1.841847
H	-38.071446	-12.250592	-1.863858
S	-35.987105	-11.328716	-0.189266
C	-35.144157	-15.682454	2.153864
C	-34.268939	-15.682037	1.124916
H	-33.801676	-16.488013	0.582494
H	-35.612813	-16.488833	2.694495

Complex 5- TPSS Charge=-1 S=1.5

100

Fe	-34.703619	-11.470209	1.642107
S	-32.930916	-10.755335	0.441011
C	-31.589904	-10.497766	1.565016
C	-30.289428	-10.179290	0.930829
C	-30.229554	-9.332015	-0.194552
H	-31.152759	-8.894435	-0.562428
C	-29.018345	-9.060973	-0.830010
H	-29.002556	-8.397231	-1.691686
C	-27.830340	-9.636072	-0.368945
H	-26.886838	-9.427999	-0.867629
C	-27.873780	-10.490200	0.737643
H	-26.960820	-10.955892	1.102296
C	-29.083701	-10.759824	1.375307
H	-29.105158	-11.433870	2.225355
C	-31.804627	-10.655299	2.911953
C	-30.838617	-10.343665	3.990048
C	-30.051784	-9.174528	3.965094
C	-29.168425	-8.878063	5.001711
H	-28.578531	-7.965460	4.957890
C	-29.049065	-9.735895	6.100009
H	-28.363666	-9.500737	6.910559
C	-29.835230	-10.890561	6.149413
H	-29.762261	-11.562386	7.001747
H	-30.150493	-8.492339	3.127026
C	-30.720462	-11.186428	5.113386
H	-31.339484	-12.077175	5.162018
S	-33.409554	-11.157600	3.463237
C	-34.703665	-13.706055	1.647575
N	-33.978880	-14.575324	0.858610
C	-33.009883	-14.228280	-0.159079
C	-31.667048	-14.086137	0.221497
C	-31.254686	-14.202044	1.667824
H	-30.172996	-14.083866	1.765041
H	-31.747335	-13.426551	2.264338
H	-31.538038	-15.173462	2.089361
C	-30.732843	-13.797983	-0.775646
H	-29.692119	-13.658246	-0.492116
C	-31.108234	-13.650888	-2.115246
C	-30.085782	-13.266879	-3.161112
H	-29.883670	-12.189740	-3.117219
H	-30.440839	-13.502600	-4.168969
H	-29.134864	-13.784914	-2.997657
C	-32.452259	-13.826342	-2.453978
H	-32.760724	-13.722403	-3.492526
C	-33.425707	-14.124007	-1.492561
C	-34.872307	-14.298730	-1.885018
H	-35.278812	-15.245734	-1.510226
H	-34.973554	-14.284229	-2.973752
H	-35.482672	-13.488416	-1.465000
N	-35.418633	-14.570380	2.451554
C	-36.400043	-14.217794	3.455753
C	-36.000126	-14.102680	4.793154
C	-34.558838	-14.280907	5.204207
H	-34.451890	-14.129012	6.281204
H	-34.194764	-15.286587	4.958992
H	-33.917523	-13.558954	4.685148

C	-36.984959	-13.798146	5.740695
H	-36.687931	-13.682736	6.781404
C	-38.325094	-13.626701	5.385436
C	-39.358316	-13.230579	6.415982
H	-39.014941	-13.457174	7.430210
H	-39.556832	-12.153025	6.359443
H	-40.309041	-13.747539	6.246591
C	-38.684689	-13.785728	4.043050
H	-39.721979	-13.648559	3.746218
C	-37.738512	-14.080066	3.058913
C	-38.134655	-14.206381	1.609019
H	-37.638575	-13.432752	1.012918
H	-39.215689	-14.093001	1.499575
H	-37.843219	-15.179454	1.196888
S	-36.477942	-10.760647	2.844085
C	-37.818131	-10.500044	1.719081
C	-39.121554	-10.192937	2.352644
C	-39.189230	-9.355932	3.485172
H	-38.269583	-8.916390	3.859399
C	-40.403586	-9.097826	4.120181
H	-40.425484	-8.441469	4.987290
C	-41.587040	-9.676057	3.651545
H	-42.532997	-9.477892	4.149614
C	-41.535822	-10.520052	2.537636
H	-42.445210	-10.987726	2.166645
C	-40.322898	-10.776700	1.900476
H	-40.295396	-11.443093	1.044625
C	-37.600377	-10.646993	0.371272
C	-38.563631	-10.327137	-0.707029
C	-39.354698	-9.160969	-0.672076
H	-39.262369	-8.488208	0.174414
C	-40.233907	-8.855106	-1.709460
H	-40.826944	-7.944825	-1.657595
C	-40.344662	-9.699693	-2.819061
H	-41.026418	-9.456750	-3.630355
C	-39.554219	-10.851168	-2.878485
H	-39.620560	-11.513097	-3.739272
C	-38.673597	-11.156718	-1.841237
H	-38.051772	-12.045194	-1.897201
S	-35.992910	-11.141448	-0.179496
C	-35.144948	-15.907108	2.168413
C	-34.236007	-15.910366	1.164618
H	-33.748821	-16.718725	0.642493
H	-35.622669	-16.712253	2.704100

Complex 5- TPSS Charge=-1 S=2.5

100

Fe	-34.707343	-11.625301	1.645404
S	-32.932033	-10.537892	0.523231
C	-31.594003	-10.425784	1.659436
C	-30.291962	-10.058692	1.044988
C	-30.221398	-9.092840	0.021050
H	-31.136817	-8.596232	-0.285843
C	-29.010110	-8.780897	-0.594966
H	-28.986207	-8.025099	-1.376932

C	-27.832217	-9.433109	-0.217251
H	-26.889116	-9.193607	-0.702322
C	-27.886701	-10.405780	0.785494
H	-26.982924	-10.932976	1.083221
C	-29.097098	-10.715051	1.404653
H	-29.127047	-11.478852	2.174786
C	-31.762304	-10.703254	3.004021
C	-30.738673	-10.426950	4.045456
C	-30.007580	-9.222249	4.056297
C	-29.076806	-8.951226	5.058450
H	-28.533757	-8.009069	5.043976
C	-28.850457	-9.873432	6.084827
H	-28.128234	-9.659523	6.868936
C	-29.579705	-11.066459	6.098584
H	-29.424217	-11.789785	6.896191
H	-30.187409	-8.491143	3.274876
C	-30.514181	-11.334698	5.099250
H	-31.094407	-12.252166	5.124168
S	-33.284627	-11.329177	3.614661
C	-34.704630	-13.813654	1.645707
N	-33.979066	-14.675040	0.854368
C	-33.021003	-14.295573	-0.162914
C	-31.688967	-14.082183	0.222975
C	-31.269671	-14.195735	1.667327
H	-30.192452	-14.042331	1.762518
H	-31.785608	-13.444398	2.276191
H	-31.517895	-15.180896	2.078949
C	-30.770715	-13.736239	-0.771164
H	-29.739881	-13.540974	-0.484929
C	-31.150825	-13.604797	-2.110656
C	-30.150650	-13.157267	-3.152351
H	-30.048617	-12.065320	-3.135372
H	-30.466285	-13.449736	-4.158035
H	-29.159720	-13.581473	-2.960830
C	-32.481448	-13.856867	-2.454843
H	-32.792407	-13.767063	-3.493895
C	-33.440105	-14.209641	-1.497675
C	-34.873205	-14.463574	-1.897243
H	-35.232654	-15.426479	-1.516291
H	-34.966705	-14.464782	-2.986625
H	-35.530748	-13.682480	-1.493812
N	-35.418987	-14.671146	2.451532
C	-36.387765	-14.285207	3.455986
C	-35.982357	-14.191457	4.794293
C	-34.554846	-14.453306	5.209509
H	-34.443799	-14.311945	6.288092
H	-34.247661	-15.476475	4.962179
H	-33.869620	-13.766322	4.700110
C	-36.949841	-13.829839	5.739161
H	-36.648824	-13.731140	6.780269
C	-38.276485	-13.579057	5.379800
C	-39.287404	-13.124619	6.408134
H	-38.957510	-13.365811	7.422713
H	-39.428000	-12.039183	6.347439
H	-40.263254	-13.590899	6.240033
C	-38.642687	-13.718500	4.037378

H	-39.669982	-13.522931	3.739106
C	-37.715100	-14.071730	3.054769
C	-38.120258	-14.193662	1.607162
H	-37.605028	-13.440429	0.999964
H	-39.197847	-14.049437	1.501848
H	-37.860176	-15.178246	1.201650
S	-36.480195	-10.534432	2.763592
C	-37.817216	-10.425649	1.625511
C	-39.121793	-10.068694	2.240739
C	-39.198893	-9.105606	3.266671
H	-38.287076	-8.602273	3.573323
C	-40.411723	-8.805362	3.885448
H	-40.440964	-8.051162	4.668785
C	-41.584535	-9.467145	3.508460
H	-42.528820	-9.236358	3.995535
C	-41.523653	-10.436700	2.503117
H	-42.423881	-10.969910	2.205532
C	-40.311879	-10.733951	1.880876
H	-40.276517	-11.494708	1.108032
C	-37.645761	-10.697142	0.279857
C	-38.667734	-10.416007	-0.761719
C	-39.401947	-9.213133	-0.764265
H	-39.227366	-8.489015	0.024780
C	-40.327964	-8.934254	-1.768578
H	-40.873112	-7.993408	-1.747751
C	-40.546405	-9.846471	-2.805495
H	-41.264495	-9.625956	-3.591540
C	-39.814671	-11.037994	-2.826920
H	-39.964460	-11.753588	-3.632494
C	-38.885221	-11.314147	-1.825145
H	-38.302651	-12.229931	-1.856066
S	-36.120072	-11.316098	-0.329166
C	-35.144077	-16.006713	2.168031
C	-34.235241	-16.009200	1.162323
H	-33.748778	-16.817873	0.640252
H	-35.621347	-16.812787	2.702444

Complex 5- TPSS Charge=-2 S=0

100

Fe	-34.704624	-11.508309	1.643471
S	-32.917396	-10.801046	0.481564
C	-31.573438	-10.563332	1.605911
C	-30.274588	-10.257440	0.980600
C	-30.211944	-9.460360	-0.188857
H	-31.142850	-9.069032	-0.588418
C	-29.002133	-9.186428	-0.822646
H	-28.997433	-8.563177	-1.715956
C	-27.798601	-9.705443	-0.326777
H	-26.854539	-9.496334	-0.826164
C	-27.839661	-10.509567	0.818420
H	-26.920363	-10.938454	1.214658
C	-29.048973	-10.781511	1.457103
H	-29.057228	-11.419561	2.334690
C	-31.803041	-10.745404	2.961453
C	-30.847125	-10.460631	4.046275

C	-30.010243	-9.319785	4.033540
C	-29.147130	-9.037724	5.090292
H	-28.525697	-8.144583	5.047614
C	-29.086455	-9.878060	6.209765
H	-28.416725	-9.652953	7.037342
C	-29.920240	-11.002730	6.250301
H	-29.897221	-11.664788	7.114978
H	-30.060621	-8.645891	3.184371
C	-30.786643	-11.283953	5.195583
H	-31.443218	-12.148167	5.238153
S	-33.417173	-11.231472	3.492116
C	-34.706081	-13.367505	1.640894
N	-34.071062	-14.276800	0.756717
C	-33.098458	-13.998337	-0.270940
C	-31.742169	-13.942242	0.111242
C	-31.356173	-14.057495	1.563516
H	-30.274672	-13.949812	1.680637
H	-31.855356	-13.278841	2.151847
H	-31.659512	-15.028595	1.975283
C	-30.778115	-13.768650	-0.879991
H	-29.733422	-13.688590	-0.585477
C	-31.129203	-13.644997	-2.231231
C	-30.066711	-13.390075	-3.278197
H	-29.547931	-12.444784	-3.078934
H	-30.507005	-13.332960	-4.279283
H	-29.308718	-14.184470	-3.282494
C	-32.475936	-13.736804	-2.576365
H	-32.766265	-13.646727	-3.622865
C	-33.482409	-13.930643	-1.614842
C	-34.919468	-14.064173	-2.060272
H	-35.049520	-14.974700	-2.662053
H	-35.206152	-13.205430	-2.674668
H	-35.599289	-14.095236	-1.209784
N	-35.342640	-14.278382	2.522309
C	-36.314803	-14.001742	3.550789
C	-35.930606	-13.938378	4.894811
C	-34.493618	-14.073970	5.339649
H	-34.200613	-13.207996	5.940785
H	-34.368046	-14.976530	5.954123
H	-33.815469	-14.121266	4.488595
C	-36.936670	-13.745861	5.856991
H	-36.646007	-13.659264	6.903709
C	-38.283334	-13.651275	5.512208
C	-39.345451	-13.397717	6.559925
H	-38.905085	-13.344601	7.561302
H	-39.862391	-12.450765	6.363558
H	-40.105050	-14.190700	6.561663
C	-38.634782	-13.770908	4.160624
H	-39.679426	-13.688882	3.866479
C	-37.671099	-13.943280	3.168916
C	-38.057525	-14.055103	1.716527
H	-37.557795	-13.275724	1.129814
H	-39.138948	-13.946120	1.599959
H	-37.755252	-15.025594	1.302600
S	-36.491261	-10.803193	2.807380
C	-37.835221	-10.562604	1.683705

C	-39.133819	-10.257172	2.309825
C	-39.196363	-9.460276	3.479298
H	-38.265411	-9.068973	3.878655
C	-40.405963	-9.186620	4.113473
H	-40.410536	-8.563759	5.007036
C	-41.609488	-9.705608	3.617783
H	-42.553430	-9.496703	4.117468
C	-41.568680	-10.509030	2.472073
H	-42.488146	-10.937446	2.075779
C	-40.359476	-10.780888	1.833266
H	-40.351172	-11.418547	0.955390
C	-37.605853	-10.741578	0.327683
C	-38.562463	-10.455477	-0.756071
C	-39.400229	-9.315508	-0.741208
H	-39.349756	-8.642631	0.108628
C	-40.265387	-9.033626	-1.796392
H	-40.888248	-8.141686	-1.751835
C	-40.326517	-9.872473	-2.916789
H	-40.997497	-9.647118	-3.743290
C	-39.491231	-10.995791	-2.959694
H	-39.514190	-11.656492	-3.825275
C	-38.623318	-11.277261	-1.906289
H	-37.965851	-12.140454	-1.950549
S	-35.991732	-11.226343	-0.204424
C	-35.105816	-15.609831	2.182692
C	-34.309366	-15.608884	1.092717
H	-33.880051	-16.419382	0.524494
H	-35.536456	-16.421345	2.748353

Complex 5- TPSS Charge=-2 S=1

100

Fe	-34.709076	-11.580344	1.636694
S	-32.998655	-10.750094	0.424327
C	-31.619626	-10.506749	1.510665
C	-30.350529	-10.151666	0.854761
C	-30.334448	-9.352372	-0.315257
H	-31.284505	-8.984576	-0.691442
C	-29.147024	-9.049799	-0.977795
H	-29.178838	-8.425245	-1.869623
C	-27.918612	-9.539525	-0.512297
H	-26.992147	-9.307295	-1.033712
C	-27.913104	-10.346318	0.633074
H	-26.974512	-10.754216	1.006166
C	-29.099526	-10.649113	1.298254
H	-29.072533	-11.291961	2.171832
C	-31.784584	-10.746503	2.868226
C	-30.829131	-10.392447	3.931531
C	-30.051867	-9.210471	3.884865
C	-29.191851	-8.860619	4.923327
H	-28.618015	-7.938012	4.852494
C	-29.072885	-9.670723	6.060589
H	-28.404946	-9.392944	6.873586
C	-29.846118	-10.835485	6.135163
H	-29.779789	-11.475555	7.013869
H	-30.148443	-8.557499	3.023691

C	-30.707998	-11.186327	5.097591
H	-31.316428	-12.082841	5.169322
S	-33.329008	-11.400033	3.434554
C	-34.706314	-13.722112	1.642215
N	-33.936189	-14.605369	0.893270
C	-32.943518	-14.258794	-0.096949
C	-31.610262	-14.101441	0.313325
C	-31.236977	-14.196609	1.770380
H	-30.162189	-14.043640	1.898856
H	-31.774432	-13.434194	2.348801
H	-31.504781	-15.175154	2.187744
C	-30.653067	-13.815043	-0.663600
H	-29.623294	-13.651027	-0.353589
C	-30.996364	-13.686189	-2.013388
C	-29.954176	-13.290473	-3.036232
H	-29.715908	-12.224345	-2.942144
H	-30.311858	-13.469530	-4.055889
H	-29.020981	-13.847424	-2.894057
C	-32.328999	-13.881522	-2.384552
H	-32.613766	-13.785582	-3.431418
C	-33.323608	-14.174741	-1.443371
C	-34.759604	-14.357924	-1.865877
H	-35.168215	-15.304250	-1.493588
H	-34.841129	-14.346546	-2.957345
H	-35.383916	-13.552013	-1.457299
N	-35.465636	-14.603457	2.404876
C	-36.462304	-14.253877	3.389886
C	-36.087491	-14.167962	4.737659
C	-34.653620	-14.356870	5.166149
H	-34.564600	-14.247153	6.251193
H	-34.279777	-15.349312	4.884069
H	-34.006314	-13.611978	4.684112
C	-37.085240	-13.871326	5.674357
H	-36.804119	-13.772524	6.721977
C	-38.416084	-13.674255	5.297556
C	-39.460633	-13.271904	6.315512
H	-39.113086	-13.464056	7.336454
H	-39.682950	-12.201398	6.228118
H	-40.400875	-13.814240	6.161527
C	-38.754047	-13.804866	3.946649
H	-39.782142	-13.638674	3.632107
C	-37.793263	-14.094028	2.973913
C	-38.160175	-14.189577	1.515372
H	-37.620782	-13.426882	0.939030
H	-39.234441	-14.037382	1.382220
H	-37.889703	-15.168177	1.099795
S	-36.416512	-10.753486	2.853163
C	-37.795200	-10.502624	1.767364
C	-39.065467	-10.152093	2.423604
C	-39.084772	-9.357708	3.596772
H	-38.135858	-8.990623	3.976545
C	-40.273766	-9.058283	4.257470
H	-40.244535	-8.437548	5.152019
C	-41.500816	-9.547177	3.787260
H	-42.428479	-9.318213	4.307940
C	-41.503163	-10.349422	2.639006

H	-42.440518	-10.756729	2.262160
C	-40.315172	-10.648717	1.975347
H	-40.339570	-11.287952	1.099084
C	-37.629654	-10.732188	0.407989
C	-38.583793	-10.364883	-0.651752
C	-39.361352	-9.183407	-0.591148
H	-39.264272	-8.540133	0.277126
C	-40.222841	-8.822391	-1.624275
H	-40.797699	-7.901315	-1.541243
C	-40.342697	-9.619301	-2.770771
H	-41.012461	-9.333136	-3.579292
C	-39.567719	-10.781807	-2.860168
H	-39.633969	-11.411278	-3.746472
C	-38.704549	-11.144242	-1.827545
H	-38.095399	-12.039343	-1.910370
S	-36.086377	-11.386098	-0.161659
C	-35.175561	-15.939991	2.134193
C	-34.208891	-15.941258	1.185125
H	-33.692680	-16.751651	0.693227
H	-35.681696	-16.749204	2.638359

Complex 5- TPSS Charge=-2 S=2

100

Fe	-34.749247	-11.735253	1.685193
S	-32.966236	-10.664756	0.514185
C	-31.601128	-10.459879	1.611244
C	-30.337519	-10.073515	0.941884
C	-30.334748	-9.192086	-0.164655
H	-31.284557	-8.771493	-0.481355
C	-29.160505	-8.880935	-0.847654
H	-29.200295	-8.193414	-1.691498
C	-27.936945	-9.448409	-0.466636
H	-27.022576	-9.214693	-1.008516
C	-27.919511	-10.335201	0.616288
H	-26.984797	-10.803611	0.921762
C	-29.093527	-10.642894	1.302847
H	-29.061722	-11.348475	2.126724
C	-31.699534	-10.743350	2.970806
C	-30.665663	-10.368368	3.963644
C	-29.970855	-9.138719	3.893774
C	-29.035977	-8.772346	4.861051
H	-28.528778	-7.812519	4.776628
C	-28.757378	-9.616603	5.942395
H	-28.032573	-9.326833	6.700795
C	-29.448529	-10.831232	6.039975
H	-29.257709	-11.498474	6.879557
H	-30.189428	-8.462889	3.073428
C	-30.388462	-11.193663	5.077161
H	-30.945412	-12.121350	5.170019
S	-33.138994	-11.488615	3.643002
C	-34.709042	-13.865367	1.674892
N	-33.922358	-14.731022	0.926794
C	-32.931532	-14.343974	-0.050759
C	-31.609518	-14.139065	0.374292

C	-31.240582	-14.246583	1.831105
H	-30.168071	-14.083100	1.964872
H	-31.788021	-13.496519	2.419230
H	-31.498286	-15.232588	2.236806
C	-30.659784	-13.789979	-0.589644
H	-29.640121	-13.589076	-0.268581
C	-30.999581	-13.643303	-1.937900
C	-29.969098	-13.175128	-2.941593
H	-29.768961	-12.105062	-2.807735
H	-30.318154	-13.329733	-3.968341
H	-29.017167	-13.704089	-2.815623
C	-32.319791	-13.887545	-2.324271
H	-32.601984	-13.777190	-3.370185
C	-33.307127	-14.244445	-1.397698
C	-34.729899	-14.484250	-1.838069
H	-35.081232	-15.476567	-1.532366
H	-34.806208	-14.408668	-2.927016
H	-35.408371	-13.744884	-1.391442
N	-35.469488	-14.755013	2.422902
C	-36.460820	-14.395637	3.410480
C	-36.072262	-14.288577	4.753514
C	-34.637956	-14.490890	5.175710
H	-34.549864	-14.418015	6.263434
H	-34.261913	-15.471332	4.860208
H	-33.986557	-13.730900	4.724301
C	-37.056689	-13.955417	5.692213
H	-36.765455	-13.842317	6.735360
C	-38.385671	-13.738503	5.320856
C	-39.414953	-13.298042	6.338529
H	-39.067668	-13.485796	7.359447
H	-39.610991	-12.223762	6.239421
H	-40.368062	-13.818960	6.195549
C	-38.736404	-13.885773	3.975372
H	-39.763231	-13.703590	3.665421
C	-37.790798	-14.213877	3.000086
C	-38.173463	-14.319378	1.547027
H	-37.643638	-13.556060	0.958677
H	-39.250020	-14.172930	1.425620
H	-37.902635	-15.298074	1.132290
S	-36.580421	-10.731984	2.820172
C	-37.898347	-10.482219	1.674154
C	-39.175076	-10.062667	2.294049
C	-39.200789	-9.173732	3.393978
H	-38.255129	-8.769012	3.742287
C	-40.393520	-8.836164	4.030978
H	-40.372630	-8.144489	4.872017
C	-41.612427	-9.383405	3.608393
H	-42.541502	-9.128820	4.114841
C	-41.607095	-10.278893	2.532188
H	-42.538835	-10.732230	2.196648
C	-40.415025	-10.612697	1.890843
H	-40.427836	-11.323076	1.070358
C	-37.749502	-10.764386	0.320947
C	-38.721943	-10.354420	-0.717384
C	-39.388500	-9.108265	-0.668959
H	-39.195670	-8.446274	0.168995

C	-40.261380	-8.707206	-1.679257
H	-40.747238	-7.735198	-1.609599
C	-40.503558	-9.531771	-2.784416
H	-41.179800	-9.214789	-3.576052
C	-39.840189	-10.763208	-2.859662
H	-40.003667	-11.416289	-3.715924
C	-38.962566	-11.161244	-1.853124
H	-38.426941	-12.102966	-1.927390
S	-36.310060	-11.585420	-0.270216
C	-35.164270	-16.086306	2.144784
C	-34.187464	-16.070585	1.205050
H	-33.661079	-16.872354	0.710746
H	-35.667974	-16.904127	2.636664