Supplementary Information

Alternate Heme Ligation Steers Activity and Selectivity in Engineered Cytochrome P450-Catalyzed Carbene Transfer Reactions

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I. General Procedures

General. Unless otherwise noted, all chemicals and reagents were obtained from commercial suppliers (Sigma-Aldrich, VWR, Alfa Aesar) and used without further purification. Silica gel chromatography was carried out using AMD Silica Gel 60, 230-400 mesh. ^{1}H and ^{13}C NMR spectra were taken using a Bruker Prodigy 400 MHz instrument and are internally referenced to the residual solvent peak (chloroform). Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets), coupling constant (Hz), integration. Sonication was performed using a Qsonica Q500 sonicator. High-resolution mass spectra were obtained at the California Institute of Technology Mass Spectral Facility. Synthetic reactions were monitored using thin layer chromatography (Merck 60 gel plates) using a UV-lamp for visualization.

Chromatography. Analytical reversed-phase high-performance liquid chromatography (HPLC) was carried out using an Agilent 1200 series instrument and a poroshell C18 column (4.6 × 50 mm, 5 µm) with water and acetonitrile as the mobile phase and visualization at 210 nm for library screening. Analytical normal-phase HPLC was carried out using an Agilent 1200 series instrument and chiral columns Chiralpak IC (4.6 mm × 25 cm), IA (4.6 mm × 25 cm), AS-H (4.6 mm × 25 cm) and OJ-H (4.6 mm × 25 cm) with *n*-hexane and isopropanol as the mobile phase and visualization at 210 nm for chiral separation. Gas chromatography (GC) analyses were carried out using an Agilent 7820A or Shimadzu GC-17A gas chromatograph, FID detector, and a J&W HP-5 column (30 m × 0.32 mm, 0.25 µm film). Gas chromatography-mass spectrometry (GC-MS) analyses were carried out using a Shimadzu GCMS-QP2010SE system and J&W HP-5m column.

Cloning and site-saturation mutagenesis. pET22b(+) containing a *C*-terminal 6x-His tag was used as a cloning and expression vector for all enzymes described in this study. Site-saturation mutagenesis was performed using a modified QuikChange™ mutagenesis protocol (*1*). Primer sequences are available upon request. The PCR products were digested with DpnI, gel purified, and fragments were assembled using Gibson Mix (*2*). The ligation mixture was used to directly transform *E. coli* strain BL21 *E. cloni*® (Lucigen). Cells were grown using Luria-Bertani medium (LB) or Hyperbroth (AthenaES) (HB) with 0.1 mg/mL ampicillin (LB_{amp} or HB_{amp}). Electrocompetent *E. coli* cells were prepared following the protocol of Sambrook *et al*. (*3*). T5 exonuclease, Phusion polymerase, and Taq ligase were purchased from New England Biolabs (NEB, Ipswich, MA). M9-N minimal medium (abbreviated as M9-N buffer; pH 7.4) was used as a buffering system for whole cells, lysates, and purified proteins, unless otherwise specified. M9-N buffer was used without a carbon source; it contains 47.7 mM Na_2HPO_4, 22.0 mM KH_2PO_4, 8.6 mM NaCl, 2.0 mM $MgSO_4$, and 0.1 mM $CaCl_2$.

Determination of hemeprotein concentration. A solution of sodium dithionite (10 mg/mL) was prepared in M9-N buffer. Separately, a solution of 1 M NaOH (0.4 mL) was mixed with pyridine (1 mL), followed by centrifugation (14,000 rpm, 30 s) to separate the excess aqueous layer, yielding a pyridine-NaOH solution. To a cuvette containing 700 µL

protein solution (purified protein or cell lysate) in M9-N buffer, 50 μL of dithionite solution (0.1 M in M9-N) and 250 μL pyridine-NaOH solution were added. The cuvette was sealed with Parafilm, and the UV-Vis spectrum of the reduced Fe^{II} state was recorded immediately. To another cuvette containing 700 μL protein solution (purified protein or lysate) in M9-N buffer, 50 μL of potassium ferricyanide (0.1 M in M9-N) and 250 μL pyridine-NaOH solution were added. The cuvette was sealed with Parafilm, and the UV-Vis spectrum of the oxidized Fe^{III} state was recorded immediately. Hemeprotein concentration was determined using $\varepsilon_{557[Re]-540[Ox]} = 23.98\ mM^{-1}cm^{-1}$ (*4*).

Expression of P450 and P411 proteins. *E. coli* BL21 *E. cloni*® cells carrying a plasmid encoding a P450 or P411 variant were grown overnight in 5 mL LB_{amp} (37 ºC, 250 rpm). The pre-culture was used to inoculate 45 mL of HB_{amp} in a 125 mL Erlenmeyer flask; this culture was incubated at 37 ºC, 220 rpm for 2 h and 15 min. Cultures were then cooled on ice (20 min), and expression was induced with 0.5 mM IPTG and 1.0 mM 5-aminolevulinic acid (final concentrations). Expression was conducted at room temperature (24 ºC), at 140 rpm, for 18 – 21 h. Cultures were then centrifuged (4,500 × g, 5 min, 4 ºC), and the pellets were resuspended to an OD_{600} of 30 in M9-N buffer. Aliquots of the cell suspension (4 mL) were used to determine the P450 and P411 expression level after lysis by sonication. The expression level in OD_{600} = 30 lysates is typically in the range of 8 – 12 μM for the P450-G8S variant, and 1.2 – 3 μM for the P411-G8S variant.

Biotransformations. The cell suspension in M9-N (with a certain OD_{600}) was degassed by sparging with argon in sealed vials or flasks for 30 min. Separately, a glucose solution (250 mM in M9-N) was degassed by sparging with argon for 30 minutes. All solutions were uncapped and transferred into an anaerobic chamber. Resuspended cells (340 μL) were added to 2 mL vials, followed by *D*-glucose (40 μL, 250 mM in M9-N), olefin or thiol (10 μL of an EtOH stock), and **LAD** (10 μL of an EtOH stock). Final concentrations were typically 5.0 – 10.0 mM olefin or thiol, 5.0 – 10.0 mM **LAD** (olefin or thiol: **LAD** = 1 : 1, unless indicated otherwise), and 25 mM *D*-glucose; final reaction volume was 400 μL. The vials were sealed, removed from the anaerobic chamber, and shaken at room temperature and 600 rpm for 12 h for cyclopropanation and 40 min for S–H insertion. After the reaction was completed, internal standard 1,3,5-trimethoxybenzene (20 μL of 20 mM stock solution in toluene) was added to the reaction vial followed by mixed solvent (hexane / ethyl acetate = 1 : 1, 1.0 mL). The mixture was transferred to a 1.5 mL microcentrifuge tube, and then subjected to vortexing (15 s × 3) and centrifugation (14,000 rpm, 5 min) to completely separate the organic and aqueous layers. A sample of the organic layer (0.8 mL) was transferred to a vial for GC analysis. The procedure for preparative-scale enzymatic reactions is outlined in detail (See **Section V and VI**).

Reaction screening in 96-well plate format. Libraries (single-site-saturation libraries generated employing the "22c-trick" method (*1*) or collection libraries of various hemeprotein variants) were screened in 96-well plates.

E. coli libraries for P411 or P450 variants were cultured in LB_{amp} (300 μL/well) at 37 ºC, 250 rpm and 80% relative humidity overnight. HB_{amp} (950 μL/well) was inoculated with the pre-culture (50 μL/well) and incubated at 37 ºC, 250 rpm, 80% humidity for 2 h and 45 min. The plates were cooled on ice for 30 minutes, and expression was induced

with 0.5 mM IPTG and 1.0 mM 5-aminolevulinic acid (final concentrations). Expression was conducted at 24 ºC and 200 rpm for 20 – 24 h.

Expression of *Rma* cytochrome *c* variants in 96-well plates employed a different protocol. *E. coli* libraries for *Rma* cytochrome *c* variants were cultured in $LB_{amp/chlor}$ (400 µL/well) at 37 ºC, 250 rpm and 80% relative humidity overnight. $HB_{amp/chlor}$ (950 µL/well) was inoculated with the pre-culture (30 µL/well) and incubated at 37 ºC, 250 rpm, 80% humidity for 2 h and 45 min. The plates were cooled on ice for 30 minutes, and expression was induced with 20 µM IPTG and 0.2 mM 5-aminolevulinic acid (final concentrations). Expression was conducted at 24 ºC and 200 rpm for 20 – 24 h.

The cells were pelleted (4,500 × g, 5 min, 4 ºC) and resuspended with M9-N buffer (340 µL/well) and *D*-glucose solution (40 µL/well, in M9-N). The 96-well plate was then transferred to an anaerobic chamber. In the anaerobic chamber, olefin or thiol (10 µL/well, 400 mM in EtOH) and **LAD** (10 µL/well, 400 mM in EtOH). The plate was sealed with an aluminum foil, removed from the anaerobic chamber, and shaken at 600 rpm. See below for the reaction workup protocol:

Cyclopropanation screening. After 12 h, the seal was removed and acetonitrile (580 µL/well) and internal standard ethyl phenylacetate (PhEA, 20 mM in acetonitrile, 20 µL/well) were added. The plate was tightly sealed with a reusable silicone mat, vortexed (15 s × 3) and centrifuged (4,500 × g, 5 min). The supernatant (200 µL/well) was filtered through an AcroPrep 96-well filter plate (0.2 µm) into a shallow-well plate for reversed-phase HPLC analysis (C18 poroshell column, MeCN : H_2O = 50 : 50, 1.2 mL/min flow, 2.95 min, 210 nm).

S–H insertion screening. After 8 h, the seal was removed and mixed solvent (hexane / ethyl acetate = 1 : 1, 600 µL/well) was added. The plate was tightly sealed with a reusable silicone mat, vortexed (15 s × 3) and centrifuged (4,500 × g, 5 min) to completely separate the organic and aqueous layers. The organic layers (200 µL/well) were transferred to 300 µL vial inserts, which were then placed in 2 mL vials for normal-phase chiral HPLC analysis (OJ-H chiral column, hexane : ^{i}PrOH = 60 : 40, 1.35 mL/min flow, 12.5 min, 220 nm).

Purification of P411-G8S and P450-G8S. To obtain purified protein of P411-G8S and P450-G8S, single colonies of *E. coli* BL21(DE3) freshly transformed with plasmid encoding either of the two variants were used to inoculate 30 mL LB_{amp} broth and cultures were grown at 37 ºC, 250 rpm for 14h. Subsequently, 950 mL of HB_{amp} broth in a 2.8 L flask were inoculated with 15 mL of the precultures and incubated at 37 ºC, 180 rpm for 2.5 h (to OD_{600} ~1.5). Cultures were then cooled in an ice-water bath for 20 min and induced with 0.5 mM IPTG and 1.0 mM 5-aminolevulinic acid (final concentrations). Expression was conducted at 24 ºC, 150 rpm, for 18 h. Cultures were then centrifuged (5,000 × g, 5 min, 4 ºC), the supernatant was discarded, and the cell pellets were frozen on dry ice and stored at -20 ºC. For protein purification, frozen cells were thawed on ice and resuspended in buffer A (25 mM tris, 20 mM imidazole, 100 mM NaCl, pH 7.5; 4 mL buffer per g of wet cell weight). The cell suspension was supplemented with 1 mg/mL lysozyme, 0.1 mg/mL DNAse I, and one protease inhibitor tablet (Pierce Protease Inhibitor Tablets, Thermo Scientific). The cell suspension was lysed by sonication (QSonica sonicator, 1 min total time, 1 s on / off cycles, 40% output). To pellet insoluble material, lysates were centrifuged (20,000 × g, 20 min, 4 ºC), and the cleared lysate was filtered

through a 0.45 µm filter unit. His-tagged P411 or P450 proteins were purified from the lysate using a nickel NTA column (1 mL HisTrap HP, GE Healthcare) using an AKTAxpress purifier FPLC system (GE healthcare). Proteins were eluted on a stepwise gradient from 100% buffer A to 100% buffer B (25 mM tris, 300 mM imidazole, 100 mM NaCl, pH 7.5): 0 to 35 % buffer B over 5 column volumes (CV), hold at 35% buffer B for 5 CV, and 35 to 100 % buffer B over 3 CV. Both P411-G8S and P450-G8S eluted at 30-35 % buffer B. Fractions containing eluted protein were pooled and subjected to three rounds of buffer exchange to storage buffer (25 mM Tris-HCl, 100 mM NaCl, pH 7.5) using centrifugal spin filters (30 kDa molecular weight cut-off, Amicon Ultra, Merck Millipore). Subsequently, the concentrated protein was aliquoted, flash-frozen on powdered dry ice, and stored at –20 ºC. Protein concentrations were determined via the pyridine/hemochrome assay specified above prior to setting up biocatalytic reactions.

II. Screening of Different Hemeproteins for *spiro*[2.4]-Lactone Formation

Figure S1. Summary of different hemeproteins tested for *spiro*[2.4]-lactone formation. P/I value refers to the peak area ratio of cyclopropane products to internal standard based on the absorbance at wavelength of 210 nm by HPLC screening. Protein identities are listed in Table S1.

Table S1. Information of hemeprotein variants (corresponding to individual well positions in the summary chart of **Figure S1**).

location	name	Mutations
A1	P450-WT ($P450_{BM3}$-wild type, CYP102A1)	-
A2	P450-C400S	C400S (relative to P450-WT)
A3	P411-CIS	V78A F87V P142S T175I A184V S226R H236Q E252G T268A A290V L353V I366V C400S E442K (relative to $P450_{BM3}$-wild type, CYP102A1)
A4	P450-CIS	S400C (relative to P411-CIS)
A5	P450-CIS H*	C400H (relative to P450-CIS)
A6	P411-"**A10**"	T438S I263F A328V L437V (relative to P411-CIS)
A7	P450-"**A10**"	S400C (relative to P411-"**A10**")
A8	P450-"**A10**" C400H	C400H (relative to P450-"**A10**")
A9	P450-"**A10**" C400A	C400A (relative to P450-"**A10**")
A10	P411-CIS T438S	T438S (relative to P411-CIS)

B1	P411-CIS T268A	T268A (relative to P411-CIS)
B2	P411-CIS T268A F87V	T268A F87V (relative to P411-CIS)
B3	P411-CIS T268A F87A	T268A F87A (relative to P411-CIS)
B4	P411-“I263F”	I263F T438S (relative to P411-CIS)
B5	P411-“I263F” F263Y	I263Y T438S (relative to P411-CIS)
B6	P411-“I263F” F263M	I263M T438S (relative to P411-CIS)
B7	P411-CIS L75A L181A	L75A L181A (relative to P411-CIS)
B8	P411-CIS L75A I263A L437A	L75A I263A L437A (relative to P411-CIS)
B9	P411-“**P2**”	A328V (relative to P411-“I263F”)
B10	P411-“**P3**”	A328V V87A (relative to P411-“I263F”)
C1	P411-“**P4**”	V87A A268G A328V (relative to P411-“I263F”)
C2	P11-“A82L”	V87A A268G A328V A82L (relative to P411-“I263F”)
C3	P11-“A82I”	V87A A268G A328V A82I (relative to P411-“I263F”)
C4	P411-“**E10**”	A78V F263L (relative to P411-“A82L”)
C5	P411-“**E10**” E267D	E267D (relative to P411-“**E10**”)
C6	P411-“**E10**” S438A	S438A (relative to P411-“**E10**”)
C7	P411-“**E10**” V78F	V78F (relative to P411-“**E10**”)
C8	P411-“**E10**” V78Y	V78Y (relative to P411-“**E10**”)
C9	P411-“**E10**” V78F S438A	V78F S438A (relative to P411-“**E10**”)
C10	P411-“**E10**” V78Y S438A	V78Y S438A (relative to P411-“**E10**”)
D1	P411-“**K1**”	A87F (relative to P411-“**P4**”)
D2	P411-“**C1**”	A87W (relative to P411-“**P4**”)
D3	P411-“**P4**” A87I	A87I (relative to P411-“**P4**”)
D4	P411-“**C2**”	L437G (relative to P411-“**C1**”)
D5	P411-“**C3**”	V328Y (relative to P411-“**C2**”)
D6	P411-“**C4**”	T328V (relative to P411-“**C3**”)
D7	P411-“**C6**”	F261M T436H (relative to P411-“**C4**”)
D8	P411-“**K3**”	F261G T327P (relative to P411-“**K1**”)
D9	P411-“**K5**”	S72W L437F (relative to P411-

		"**K3**")
D10	P411-"**K6**"	T269L (relative to P411-"**K5**")
E1	P411-"**K8**"	A78S A330V (relative to P411-"**K6**")
E2	P411-"**K10**"	L188C T436M (relative to P411-"**K8**")
E3	P411-"**P4**" F261M	F261M (relative to P411-"**P4**")
E4	P411-"**P4**" F261M T269L	F261M T269L (relative to P411-"**P4**")
E5	P411-"**P4**" A87F F261C	A87F F261C (relative to P411-"**P4**")
E6	P411-"**P4**" F81V	F81V (relative to P411-"**P4**")
E7	P411-"A82L" F263Y A78L T327L	F263Y A78L T327L (relative to P411-"A82L")
E8	P411-"M177L" H266V N70E A330Y ΔFAD	N70E A74G A78L A82L M177L F263Y H266V T327I A330Y T436L L437Q S438T (relative to P411-"**P4**") with FAD domain truncated
E9	P411-"L437Q" S438T T436L V178E ΔFAD	A74G A78L A82L V178E F263Y T327I T436L L437Q S438T (relative to P411-"**P4**") with FAD domain truncated
E10	P411-"A82L" F263Y A78L T327I	F263Y A78L T327I (relative to P411-"**A82L**")
F1	P411-"**G8**"	L437F T438Q (relative to P411-CIS)
F2	P411-"**G8**" L75Y	L75Y (relative to P411-"**G8**")
F3	P411-"**G8S**" (or P411-**VAC**$_{cis}$)	L75Y L181I (relative to P411-"**G8**")
F4	P411-"**G8**" L181V	L181V (relative to P411-"**G8**")
F5	P411-"**E12**"	I263G L437F (relative to P411-CIS)
F6	P411-"**E12**" V87L	V87L (relative to P411-"**E12**")
F7	P411-"**E12**" V87L L181R	V87L L181R (relative to P411-"**E12**")
F8	P411-"**F3**"	V87T T438C (relative to P411-CIS)
F9	P411-"**H9**"	I263G L437F (relative to P411-"**F3**")
F10	P411-"**6C9**"	V87T L181G I263M V281L T438C (relative to P411-CIS) with FAD domain truncated
G1	*Rma* cyt *c*-wild type	-
G2	*Rma* cyt *c*-M100D	M100D (relative to *Rma* cyt *c*-wild type)

G3	*Rma* cyt *c*-V75K M100D	V75K M100D (relative to *Rma* cyt *c*-wild type)
G4	*Rma* cyt *c*-V75P M100D	V75P M100D (relative to *Rma* cyt *c*-wild type)
G5	*Rma* cyt *c*-V75G M100D	V75G M100D (relative to *Rma* cyt *c*-wild type)
G6	*Rma* cyt *c*-V75C M100D	V75C M100D (relative to *Rma* cyt *c*-wild type)
G7	*Rma* cyt *c*-V75T M100D M103E	V75T M100D M103E (relative to *Rma* cyt *c*-wild type)
G8	*Rma* cyt *c*-V75T M100D M103D	V75T M100D M103D (relative to *Rma* cyt *c*-wild type)
G9	*Rma* cyt *c*-V75T M100D M103N	V75T M100D M103N (relative to *Rma* cyt *c*-wild type)
G10	*Rma* cyt *c*-V75T M100D M103A	V75T M100D M103A (relative to *Rma* cyt *c*-wild type)
H1	*Rma* cyt *c*-R66Y V75G M100D	R66Y V75G M100D (relative to *Rma* cyt *c*-wild type)
H2	*Rma* cyt *c*-V75G M89H M100D	V75G M89H M100D (relative to *Rma* cyt *c*-wild type)
H3	*Rma* cyt *c*-V75K M100D M103V	V75K M100D M103V (relative to *Rma* cyt *c*-wild type)
H4	*Rma* cyt *c*-V75K M100D T101C M103A	V75K M100D T101C M103A (relative to *Rma* cyt *c*-wild type)
H5	*Rma* cyt *c*-V75R M99C M100D M103D	V75R M99C M100D M103D (relative to *Rma* cyt *c*-wild type)
H6	*Rma* cyt *c*-V75R M100D T101Q M103D	V75R M100D T101Q M103D (relative to *Rma* cyt *c*-wild type)
H7	*Rma* cyt *c*-V75P M99Y M100D	V75P M99Y M100D (relative to *Rma* cyt *c*-wild type)
H8	*Rma* cyt *c*-V75P M99Y M100D T101W	V75P M99Y M100D T101W (relative to *Rma* cyt *c*-wild type)
H9	*Rma* cyt *c*-R67W V75G M100D	R67W V75G M100D (relative to *Rma* cyt *c*-wild type)
H10	*Rma* cyt *c*-R67P V75G M100D	R67P V75G M100D (relative to *Rma* cyt *c*-wild type)

III. Comparison of P450-G8S and P411-G8S for Cyclopropanation and S–H Insertion

G8S variants	TTN	*de*	*ee*
P411-G8S	3090 ± 120	>99%	>98%
P450-G8S	380 ± 20	>99%	99%

Figure S2. G8S variant catalytic performance for *spiro*[2.4]-lactone formation.

G8S variants	TTN	*ee*
P411-G8S	1610 ± 120	84 ± 1%
P450-G8S	300 ± 30	15 ± 2%

Figure S3. G8S variant catalytic performance for S–H insertion.

Note: Analytical reactions were set up in quadruplicate according to the procedure described in **biotransformations** (**Section I**) using whole-cell catalyst and were analyzed by GC using the standard calibration curve of **2a** and **4a** (see **Section IX**). The TTNs for *spiro*[2.4]-lactone formation were obtained using cell suspensions at OD_{600} = 30 for both variants; the TTNs for S–H insertion were obtained using cell suspensions at OD_{600} = 30 for P411-G8S variant and OD_{600} = 15 for P450-G8S. TTNs reported are the average of biological duplicates. Each biological set contains four reactions. The errors in all tables are standard deviations. Diastereomeric excess (*de*) and enantiomeric excess (*ee*) were determined by chiral HPLC.

Note for S–H insertion: Oxidation product disulfide was observed in S–H insertion reactions (very small amount with P450-G8S; significant amount with P411-G8S). In the case of P411-G8S, the disulfide formation may also result from cage-escaped thiyl radical homo-coupling.

Heme controls. Reaction conditions: hemin (0.5, 2.0 or 5.0 mol %), $Na_2S_2O_4$ (10 mM), with or without BSA (bovine serum albumin), alkene or thiol (**1a**, **1j** or **3a**, 10 mM), **LAD** (10 mM), 5 vol% EtOH in M9-N buffer (pH 7.4) at room temperature under anaerobic conditions for 6 hours. Reactions were analyzed by GC-MS. No desired products were detected, suggesting free heme does not catalyze the cyclopropanation or S–H insertion reaction.

G8S variants	**Relative efficiency**	***de***	***ee***
P411-G8S whole cell	1.000 ± 0.013	99.2%	98.6%
P411-G8S lysate	0.0063 ± 0.0003	n.d.	n.d.

P411-G8S purified protein	0.0077 ± 0.0007	n.d.	n.d.
P450-G8S whole cell	0.183 ± 0.010	>99.5%	99.2%
P450-G8S lysate	0.028 ± 0.001	>99.5%	99.0%
P450-G8S purified protein	0.037 ± 0.001	>99.5%	99.0%

G8S variants	**Relative efficiency**	***ee***
P450-G8S whole cell	1.000 ± 0.019	85%
P450-G8S lysate	0.481 ± 0.019	80%
P450-G8S purified protein	0.571 ± 0.010	78%
P411-G8S whole cell	0.167 ± 0.006	13%
P411-G8S lysate	0.022 ± 0.001	n.d.
P411-G8S purified protein	0.035 ± 0.001	n.d.

Figure S4. Catalytic performance of **G8S** variants in different forms.

Note: Analytical reactions were set up in triplicate according to the procedure described in **biotransformations** (**Section I**) using protein catalysts in the form of whole cell, lysate and purified protein, and were analyzed by GC. Protein concentration of P450-G8S catalyst was adjusted to 4.25 μM, and that of P411-G8S catalyst was adjusted to 1.70 μM in the analytical reactions. Relative catalytic efficiency represents relative product formation over total amount of catalyst. The errors in all tables are standard deviations. Diastereomeric excess (*de*) and enantiomeric excess (*ee*) were determined by chiral HPLC. n.d. = not determined.

For reactions catalyzed by cell lysate or purified protein, protein denaturation was observed

(rapid aggregation of P411-G8S variant occurred within 5 minutes upon addition of diazo reagent; aggregation of P450-G8S variant was slower). Analysis of the reaction mixture showed that no **LAD** was left over, which indicates rapid backbone modification with carbene might be the major process of protein denaturation (*5*).

G8S variants	TTN for S–H insertion	TTN for cyclopropanation	S–H insertion: cyclopropanation
P450-G8S	1330 ± 10	84 ± 16	16 : 1
P411-G8S	1100 ± 80	2200 ± 40	1 : 2

Figure S5. Competition reactions in presence of both olefin and thiol substrates.

Note: Analytical reactions were set up in triplicate according to the procedure described in **biotransformations** (**Section I**) using whole-cell catalyst (P411-G8S variant at OD_{600} = 30 and P450-G8S variant at OD_{600} = 15) and were analyzed by GC using the standard calibration curve of **2c** and **4b** (see **Section IX**). The errors in the table are standard deviations.

Table S2. Mutational information of **G8S** variants

Name	**Mutations relative to P450$_{BM3}$-wild type**
P411-G8S	L75Y V78A F87V P142S T175I L181I A184V S226R H236Q E252G T268A A290V L353V I366V C400S L437F T438Q E442K
P450-G8S	L75Y V78A F87V P142S T175I L181I A184V S226R H236Q E252G T268A A290V L353V I366V L437F T438Q E442K

Nucleotide sequence of cytochrome P411-G8S

ATGACAATTAAAGAAATGCCTCAGCCAAAAACGTTTGGAGAGCTTAAAAATTTACCGTTATTAAA
CACAGATAAACCGGTTCAAGCTTTGATGAAAATTGCGGATGAATTAGGAGAAATCTTTAAATTCG
AGGCGCCTGGTCGTGTAACGCGCTACTTATCAAGTCAGCGTCTAATTAAAGAAGCATGCGATGAA
TCACGCTTTGATAAAAACTTAAGTCAAGCGTATAAATTTGCACGTGATTTTGCAGGAGACGGGTT
AGTGACAAGCTGGACGCATGAAAAAAATTGGAAAAAAGCGCATAATATCTTACTTCCAAGCTTTA
GTCAGCAGGCAATGAAAGGCTATCATGCGATGATGGTCGATATCGCCGTGCAGCTTGTTCAAAAG
TGGGAGCGTCTAAATGCAGATGAGCATATTGAAGTATCGGAAGACATGACACGTTTAACGCTTGA
TACAATTGGTCTTTGCGGCTTTAACTATCGCTTTAACAGCTTTTACCGAGATCAGCCTCATCCAT
TTATTATAAGTATGGTCCGTGCAATTGATGAAGTAATGAACAAGCTGCAGCGAGCAAATCCAGAC
GACCCAGCTTATGATGAAAACAAGCGCCAGTTTCAAGAAGATATCAAGGTGATGAACGACCTAGT
AGATAAAATTATTGCAGATCGCAAAGCAAGGGGTGAACAAAGCGATGATTTATTAACGCAGATGC
TAAACGGAAAAGATCCAGAAACGGGTGAGCCGCTTGATGACGGGAACATTCGCTATCAAATTATT
ACATTCTTAATTGCGGGACACGAAGCAACAAGTGGTCTTTTATCATTTGCGCTGTATTTCTTAGT
GAAAAATCCACATGTATTACAAAAAGTAGCAGAAGAAGCAGCACGAGTTCTAGTAGATCCTGTTC
CAAGCTACAAACAAGTCAAACAGCTTAAATATGTCGGCATGGTCTTAAACGAAGCGCTGCGCTTA
TGGCCAACTGCTCCTGCGTTTTCCCTATATGCAAAAGAAGATACGGTGCTTGGAGGAGAATATCC
TTTAGAAAAAGGCGACGAAGTAATGGTTCTGATTCCTCAGCTTCACCGTGATAAAACAGTTTGGG
GAGACGATGTGGAGGAGTTCCGTCCAGAGCGTTTTGAAAATCCAAGTGCGATTCCGCAGCATGCG
TTTAAACCGTTTGGAAACGGTCAGCGTGCG**TCT**ATCGGTCAGCAGTTCGCTCTTCATGAAGCAAC
GCTGGTACTTGGTATGATGCTAAAACACTTTGACTTTGAAGATCATACAAACTACGAGCTCGATA
TTAAAGAAACTTTTCAGTTAAAACCTAAAGGCTTTGTGGTAAAAGCAAAATCGAAAAAAATTCCG
CTTGGCGGTATTCCTTCACCTAGCACTGAACAGTCTGCTAAAAAAGTACGCAAAAAGGCAGAAAA
CGCTCATAATACGCCGCTGCTTGTGCTATACGGTTCAAATATGGGTACCGCTGAAGGAACGGCGC
GTGATTTAGCAGATATTGCAATGAGCAAAGGATTTGCACCGCAGGTCGCAACGCTTGATTCACAC
GCCGGAAATCTTCCGCGCGAAGGAGCTGTATTAATTGTAACGGCGTCTTATAACGGTCATCCGCC
TGATAACGCAAAGCAATTTGTCGACTGGTTAGACCAAGCGTCTGCTGATGAAGTAAAAGGCGTTC
GCTACTCCGTATTTGGATGCGGCGATAAAAACTGGGCTACTACGTATCAAAAAGTGCCTGCTTTT
ATCGATGAAACGCTTGCCGCTAAAGGGGCAGAAAACATCGCTGACCGCGGTGAAGCAGATGCAAG
CGACGACTTTGAAGGCACATATGAAGAATGGCGTGAACATATGTGGAGTGACGTAGCAGCCTACT
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GCCGCGGATATGCCGCTTGCGAAAATGCACGGTGCGTTTTCAACGAACGTCGTAGCAAGCAAAGA
ACTTCAACAGCCAGGCAGTGCACGAAGCACGCGACATCTTGAAATTGAACTTCCAAAAGAAGCTT
CTTATCAAGAAGGAGATCATTTAGGTGTTATTCCTCGCAACTATGAAGGAATAGTAAACCGTGTA
ACAGCAAGGTTCGGCCTAGATGCATCACAGCAAATCCGTCTGGAAGCAGAAGAAGAAAAATTAGC
TCATTTGCCACTCGCTAAAACAGTATCCGTAGAAGAGCTTCTGCAATACGTGGAGCTTCAAGATC
CTGTTACGCGCACGCAGCTTCGCGCAATGGCTGCTAAAACGGTCTGCCCGCCGCATAAAGTAGAG
CTTGAAGCCTTGCTTGAAAAGCAAGCCTACAAAGAACAAGTGCTGGCAAAACGTTTAACAATGCT
TGAACTGCTTGAAAAATACCCGGCGTGTGAAATGAAATTCAGCGAATTTATCGCCCTTCTGCCAA
GCATACGCCCGCGCTATTACTCGATTTCTTCATCACCTCGTGTCGATGAAAAACAAGCAAGCATC
ACGGTCAGCGTTGTCTCAGGAGAAGCGTGGAGCGGATATGGAGAATATAAAGGAATTGCGTCGAA
CTATCTTGCCGAGCTGCAAGAAGGAGATACGATTACGTGCTTTATTTCCACACCGCAGTCAGAAT
TTACGCTGCCAAAAGACCCTGAAACGCCGCTTATCATGGTCGGACCGGGAACAGGCGTCGCGCCG
TTTAGAGGCTTTGTGCAGGCGCGCAAACAGCTAAAAGAACAAGGACAGTCACTTGGAGAAGCACA
TTTATACTTCGGCTGCCGTTCACCTCATGAAGACTATCTGTATCAAGAAGAGCTTGAAAACGCCC
AAAGCGAAGGCATCATTACGCTTCATACCGCTTTTTCTCGCATGCCAAATCAGCCGAAAACATAC
GTTCAGCACGTAATGGAACAAGACGGCAAGAAATTGATTGAACTTCTTGATCAAGGAGCGCACTT
CTATATTTGCGGAGACGGAAGCCAAATGGCACCTGCCGTTGAAGCAACGCTTATGAAAAGCTATG
CTGACGTTCACCAAGTGAGTGAAGCAGACGCTCGCTTATGGCTGCAGCAGCTAGAAGAAAAAGGC
CGATACGCAAAAGACGTGTGGGCTGGGCTCGAGCACCACCACCACCACCACTGA

Amino acid sequence of cytochrome P411-G8S

MTIKEMPQPKTFGELKNLPLLNTDKPVQALMKIADELGEIFKFEAPGRVTRYLSSQRLIKEACDE
SRFDKNLSQAYKFARDFAGDGLVTSWTHEKNWKKAHNILLPSFSQQAMKGYHAMMVDIAVQLVQK
WERLNADEHIEVSEDMTRLTLDTIGLCGFNYRFNSFYRDQPHPFIISMVRAIDEVMNKLQRANPD
DPAYDENKRQFQEDIKVMNDLVDKIIADRKARGEQSDDLLTQMLNGKDPETGEPLDDGNIRYQII
TFLIAGHEATSGLLSFALYFLVKNPHVLQKVAEEAARVLVDPVPSYKQVKQLKYVGMVLNEALRL
WPTAPAFSLYAKEDTVLGGEYPLEKGDEVMVLIPQLHRDKTVWGDDVEEFRPERFENPSAIPQHA
FKPFGNGQRA**S**IGQQFALHEATLVLGMMLKHFDFEDHTNYELDIKETFQLKPKGFVVKAKSKKIP
LGGIPSPSTEQSAKKVRKKAENAHNTPLLVLYGSNMGTAEGTARDLADIAMSKGFAPQVATLDSH
AGNLPREGAVLIVTASYNGHPPDNAKQFVDWLDQASADEVKGVRYSVFGCGDKNWATTYQKVPAF
IDETLAAKGAENIADRGEADASDDFEGTYEEWREHMWSDVAAYFNLDIENSEDNKSTLSLQFVDS
AADMPLAKMHGAFSTNVVASKELQQPGSARSTRHLEIELPKEASYQEGDHLGVIPRNYEGIVNRV
TARFGLDASQQIRLEAEEEKLAHLPLAKTVSVEELLQYVELQDPVTRTQLRAMAAKTVCPPHKVE
LEALLEKQAYKEQVLAKRLTMLELLEKYPACEMKFSEFIALLPSIRPRYYSISSSPRVDEKQASI
TVSVVSGEAWSGYGEYKGIASNYLAELQEGDTITCFISTPQSEFTLPKDPETPLIMVGPGTGVAP
FRGFVQARKQLKEQGQSLGEAHLYFGCRSPHEDYLYQEELENAQSEGIITLHTAFSRMPNQPKTY
VQHVMEQDGKKLIELLDQGAHFYICGDGSQMAPAVEATLMKSYADVHQVSEADARLWLQQLEEKG
RYAKDVWAGLEHHHHHH

Nucleotide sequence of cytochrome P450-G8S

ATGACAATTAAAGAAATGCCTCAGCCAAAAACGTTTGGAGAGCTTAAAAATTTACCGTTATTAAA
CACAGATAAACCGGTTCAAGCTTTGATGAAAATTGCGGATGAATTAGGAGAAATCTTTAAATTCG
AGGCGCCTGGTCGTGTAACGCGCTACTTATCAAGTCAGCGTCTAATTAAAGAAGCATGCGATGAA
TCACGCTTTGATAAAAACTTAAGTCAAGCGTATAAATTTGCACGTGATTTTGCAGGAGACGGGTT
AGTGACAAGCTGGACGCATGAAAAAAATTGGAAAAAAGCGCATAATATCTTACTTCCAAGCTTTA
GTCAGCAGGCAATGAAAGGCTATCATGCGATGATGGTCGATATCGCCGTGCAGCTTGTTCAAAAG
TGGGAGCGTCTAAATGCAGATGAGCATATTGAAGTATCGGAAGACATGACACGTTTAACGCTTGA
TACAATTGGTCTTTGCGGCTTTAACTATCGCTTTAACAGCTTTTACCGAGATCAGCCTCATCCAT
TTATTATAAGTATGGTCCGTGCAATTGATGAAGTAATGAACAAGCTGCAGCGAGCAAATCCAGAC
GACCCAGCTTATGATGAAAACAAGCGCCAGTTTCAAGAAGATATCAAGGTGATGAACGACCTAGT
AGATAAAATTATTGCAGATCGCAAAGCAAGGGGTGAACAAAGCGATGATTTATTAACGCAGATGC
TAAACGGAAAAGATCCAGAAACGGGTGAGCCGCTTGATGACGGGAACATTCGCTATCAAATTATT
ACATTCTTAATTGCGGGACACGAAGCAACAAGTGGTCTTTTATCATTTGCGCTGTATTTCTTAGT
GAAAAATCCACATGTATTACAAAAAGTAGCAGAAGAAGCAGCACGAGTTCTAGTAGATCCTGTTC
CAAGCTACAAACAAGTCAAACAGCTTAAATATGTCGGCATGGTCTTAAACGAAGCGCTGCGCTTA
TGGCCAACTGCTCCTGCGTTTTCCCTATATGCAAAAGAAGATACGGTGCTTGGAGGAGAATATCC
TTTAGAAAAAGGCGACGAAGTAATGGTTCTGATTCCTCAGCTTCACCGTGATAAAACAGTTTGGG
GAGACGATGTGGAGGAGTTCCGTCCAGAGCGTTTTGAAAATCCAAGTGCGATTCCGCAGCATGCG
TTTAAACCGTTTGGAAACGGTCAGCGTGCG**TGT**ATCGGTCAGCAGTTCGCTCTTCATGAAGCAAC
GCTGGTACTTGGTATGATGCTAAAACACTTTGACTTTGAAGATCATACAAACTACGAGCTCGATA
TTAAAGAAACTTTTCAGTTAAAACCTAAAGGCTTTGTGGTAAAAGCAAAATCGAAAAAAATTCCG
CTTGGCGGTATTCCTTCACCTAGCACTGAACAGTCTGCTAAAAAAGTACGCAAAAAGGCAGAAAA
CGCTCATAATACGCCGCTGCTTGTGCTATACGGTTCAAATATGGGTACCGCTGAAGGAACGGCGC
GTGATTTAGCAGATATTGCAATGAGCAAAGGATTTGCACCGCAGGTCGCAACGCTTGATTCACAC
GCCGGAAATCTTCCGCGCGAAGGAGCTGTATTAATTGTAACGGCGTCTTATAACGGTCATCCGCC
TGATAACGCAAAGCAATTTGTCGACTGGTTAGACCAAGCGTCTGCTGATGAAGTAAAAGGCGTTC
GCTACTCCGTATTTGGATGCGGCGATAAAAACTGGGCTACTACGTATCAAAAAGTGCCTGCTTTT
ATCGATGAAACGCTTGCCGCTAAAGGGGCAGAAAACATCGCTGACCGCGGTGAAGCAGATGCAAG
CGACGACTTTGAAGGCACATATGAAGAATGGCGTGAACATATGTGGAGTGACGTAGCAGCCTACT

TTAACCTCGACATTGAAAACAGTGAAGATAATAAATCTACTCTTTCACTTCAATTTGTCGACAGC
GCCGCGGATATGCCGCTTGCGAAAATGCACGGTGCGTTTTCAACGAACGTCGTAGCAAGCAAAGA
ACTTCAACAGCCAGGCAGTGCACGAAGCACGCGACATCTTGAAATTGAACTTCCAAAAGAAGCTT
CTTATCAAGAAGGAGATCATTTAGGTGTTATTCCTCGCAACTATGAAGGAATAGTAAACCGTGTA
ACAGCAAGGTTCGGCCTAGATGCATCACAGCAAATCCGTCTGGAAGCAGAAGAAGAAAAATTAGC
TCATTTGCCACTCGCTAAAACAGTATCCGTAGAAGAGCTTCTGCAATACGTGGAGCTTCAAGATC
CTGTTACGCGCACGCAGCTTCGCGCAATGGCTGCTAAAACGGTCTGCCCGCCGCATAAAGTAGAG
CTTGAAGCCTTGCTTGAAAAGCAAGCCTACAAAGAACAAGTGCTGGCAAAACGTTTAACAATGCT
TGAACTGCTTGAAAAATACCCGGCGTGTGAAATGAAATTCAGCGAATTTATCGCCCTTCTGCCAA
GCATACGCCCGCGCTATTACTCGATTTCTTCATCACCTCGTGTCGATGAAAAACAAGCAAGCATC
ACGGTCAGCGTTGTCTCAGGAGAAGCGTGGAGCGGATATGGAGAATATAAAGGAATTGCGTCGAA
CTATCTTGCCGAGCTGCAAGAAGGAGATACGATTACGTGCTTTATTTCCACACCGCAGTCAGAAT
TTACGCTGCCAAAAGACCCTGAAACGCCGCTTATCATGGTCGGACCGGGAACAGGCGTCGCGCCG
TTTAGAGGCTTTGTGCAGGCGCGCAAACAGCTAAAAGAACAAGGACAGTCACTTGGAGAAGCACA
TTTATACTTCGGCTGCCGTTCACCTCATGAAGACTATCTGTATCAAGAAGAGCTTGAAAACGCCC
AAAGCGAAGGCATCATTACGCTTCATACCGCTTTTTCTCGCATGCCAAATCAGCCGAAAACATAC
GTTCAGCACGTAATGGAACAAGACGGCAAGAAATTGATTGAACTTCTTGATCAAGGAGCGCACTT
CTATATTTGCGGAGACGGAAGCCAAATGGCACCTGCCGTTGAAGCAACGCTTATGAAAAGCTATG
CTGACGTTCACCAAGTGAGTGAAGCAGACGCTCGCTTATGGCTGCAGCAGCTAGAAGAAAAAGGC
CGATACGCAAAAGACGTGTGGGCTGGGCTCGAGCACCACCACCACCACCACTGA

Amino acid sequence of cytochrome P450-G8S

MTIKEMPQPKTFGELKNLPLLNTDKPVQALMKIADELGEIFKFEAPGRVTRYLSSQRLIKEACDE
SRFDKNLSQAYKFARDFAGDGLVTSWTHEKNWKKAHNILLPSFSQQAMKGYHAMMVDIAVQLVQK
WERLNADEHIEVSEDMTRLTLDTIGLCGFNYRFNSFYRDQPHPFIISMVRAIDEVMNKLQRANPD
DPAYDENKRQFQEDIKVMNDLVDKIIADRKARGEQSDDLLTQMLNGKDPETGEPLDDGNIRYQII
TFLIAGHEATSGLLSFALYFLVKNPHVLQKVAEEAARVLVDPVPSYKQVKQLKYVGMVLNEALRL
WPTAPAFSLYAKEDTVLGGEYPLEKGDEVMVLIPQLHRDKTVWGDDVEEFRPERFENPSAIPQHA
FKPFGNGQRA**C**IGQQFALHEATLVLGMMLKHFDFEDHTNYELDIKETFQLKPKGFVVKAKSKKIP
LGGIPSPSTEQSAKKVRKKAENAHNTPLLVLYGSNMGTAEGTARDLADIAMSKGFAPQVATLDSH
AGNLPREGAVLIVTASYNGHPPDNAKQFVDWLDQASADEVKGVRYSVFGCGDKNWATTYQKVPAF
IDETLAAKGAENIADRGEADASDDFEGTYEEWREHMWSDVAAYFNLDIENSEDNKSTLSLQFVDS
AADMPLAKMHGAFSTNVVASKELQQPGSARSTRHLEIELPKEASYQEGDHLGVIPRNYEGIVNRV
TARFGLDASQQIRLEAEEEKLAHLPLAKTVSVEELLQYVELQDPVTRTQLRAMAAKTVCPPHKVE
LEALLEKQAYKEQVLAKRLTMLELLEKYPACEMKFSEFIALLPSIRPRYYSISSSPRVDEKQASI
TVSVVSGEAWSGYGEYKGIASNYLAELQEGDTITCFISTPQSEFTLPKDPETPLIMVGPGTGVAP
FRGFVQARKQLKEQGQSLGEAHLYFGCRSPHEDYLYQEELENAQSEGIITLHTAFSRMPNQPKTY
VQHVMEQDGKKLIELLDQGAHFYICGDGSQMAPAVEATLMKSYADVHQVSEADARLWLQQLEEKG
RYAKDVWAGLEHHHHHH

Figure S6. Heme-domain structures of P450-BM3 (top, PDB: 1bvy) and P411-CIS (bottom, PDB: 4h23). Amino acid residues that were mutated in the evolution of P450-BM3 to P411-CIS and P411-CIS to P411-G8S are highlighted.

IV. Synthesis and Characterization of Substrate LAD and Standard Products

3-Diazodihydrofuran-2(3*H*)-one (LAD)

The preparation of the title compound **LAD** followed a modified procedure reported by Sattely *et al.* (*6*). Sodium azide (4.83 g, 74.3 mmol, 4 equiv.), sodium hydroxide (80 mL of 2 M in water, 160 mmol), tetrabutylammonium bromide (60.0 mg, 0.190 mmol, 0.01 equiv.), and hexane (80 mL) were combined in a 500-mL flask with magnetic stir bar open to the air and cooled to 0 °C. With vigorous stirring, triflic anhydride (6.20 mL, 37.1 mmol, 2 equiv.) was added dropwise. After 15 min, a solution of 2-acetyl-butyrolactone (2.00 mL, 18.6 mmol) in acetonitrile (70 mL) was poured into the vessel through a funnel, followed by an additional 10 mL of acetonitrile to complete the transfer. The initially colorless reaction mixture immediately turned yellow. After stirring for 20 min at 0 °C, the mixture was diluted with ice water (50 mL) and chilled EtOAc (50 mL) and transferred to a separatory funnel. After phase separation and removal of the organic fraction, the aqueous layer was washed with chilled EtOAc (50 mL × 5). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified through a silica column using hexane: ethyl acetate (3:1 to 2:1) as eluents. The yellow-colored fractions were concentrated to afford the product as a bright yellow crystalline solid (1.2 – 1.6 g, 60 – 75% yield).

General procedure for the synthesis of *spiro*[2.4]-lactone standard products:
To a 20 mL vial was added olefin (1.0 mmol, 2.0 equiv.), $Rh_2(OAc)_4$ (2.2 mg, 1 mol%) and DCM (5 mL). The mixture was cooled to –78 °C, and a solution of **LAD** (0.5 mmol, 1.0 equiv.) in DCM (3 mL) was added dropwise to the reaction mixture over 2 hours through a syringe pump. The reaction was allowed to slowly warm up to room temperature over 8 hours and stirred at room temperature for another 8 hours. Evaporation of the organic solvent and purification by silica column chromatography using hexane and ethyl acetate as eluents afforded racemic cyclopropane products in 20 – 60% yields (diastereomers can be separated).

(*E*)-1-Phenyl-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.30 (m, 2H), 7.30 – 7.23 (m, 1H), 7.18 – 7.08 (m, 2H), 4.40 (td, *J* = 8.9, 5.6 Hz, 1H), 4.27 (td, *J* = 8.9, 6.7 Hz, 1H), 2.76 (dd, *J* = 9.4, 7.1 Hz, 1H), 2.15 (ddd, *J* = 13.1, 8.9, 6.8 Hz, 1H), 1.90 (ddd, *J* = 13.0, 8.8, 5.6 Hz, 1H), 1.80 (dd, *J* = 9.4, 5.1 Hz, 1H), 1.47 (dd, *J* = 7.1, 5.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.50, 136.11, 128.74, 128.17, 127.24, 66.01, 31.10, 27.53, 25.51, 18.53.

(*Z*)-1-Phenyl-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.19 (m, 5H), 4.51 – 4.36 (m, 2H), 2.74 – 2.54 (m, 2H), 2.27 (ddd, *J* = 12.7, 7.2, 2.9 Hz, 1H), 1.93 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.54 (dd, *J* = 8.9, 5.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.97, 135.38, 129.02, 128.24, 127.19, 65.66, 34.76, 32.10,

27.83, 17.33.
HRMS (TOF) m/z: 189.0917 (M + H^+); calc. for $C_{12}H_{13}O_2$: 189.0916.

(*E*)-1-(4-Methoxyphenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 4.40 (td, *J* = 9.0, 5.5 Hz, 1H), 4.26 (td, *J* = 8.9, 6.9 Hz, 1H), 3.80 (s, 3H), 2.71 (dd, *J* = 9.4, 7.1 Hz, 1H), 2.12 (ddd, *J* = 13.0, 8.9, 6.9 Hz, 1H), 1.88 (ddd, *J* = 13.0, 8.7, 5.5 Hz, 1H), 1.77 (dd, *J* = 9.4, 5.1 Hz, 1H), 1.40 (dd, *J* = 7.1, 5.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.66, 158.84, 129.31, 127.99, 114.18, 66.02, 55.44, 30.64, 27.29, 25.56, 18.52.

(*Z*)-1-(4-Methoxyphenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, *J* = 8.3 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.46 (td, *J* = 9.0, 2.9 Hz, 1H), 4.40 (ddd, *J* = 9.8, 9.0, 7.3 Hz, 1H), 3.77 (s, 3H), 2.61 (dt, *J* = 12.1, 9.1 Hz, 2H), 2.25 (ddd, *J* = 12.7, 7.1, 2.8 Hz, 1H), 1.87 (dd, *J* = 7.6, 5.2 Hz, 1H), 1.51 (dd, *J* = 8.9, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.15, 158.69, 130.04, 127.42, 113.70, 65.67, 55.34, 34.27, 32.05, 27.66, 17.47.
HRMS (TOF) m/z: 219.1024 (M + H^+); calc. for $C_{13}H_{15}O_3$: 219.1021.

(*E*)-1-(3-Methoxyphenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.15 (m, 1H), 6.74 (ddd, *J* = 8.3, 2.6, 0.9 Hz, 1H), 6.64 (dp, *J* = 7.7, 0.8 Hz, 1H), 6.62 – 6.57 (m, 1H), 4.34 (td, *J* = 8.9, 5.7 Hz, 1H), 4.21 (td, *J* = 8.9, 6.7 Hz, 1H), 3.74 (s, 3H), 2.66 (dd, *J* = 9.3, 7.1 Hz, 1H), 2.09 (ddd, *J* = 13.1, 8.9, 6.8 Hz, 1H), 1.86 (ddd, *J* = 13.0, 8.8, 5.7 Hz, 1H), 1.71 (dd, *J* = 9.3, 5.1 Hz, 1H), 1.38 (dd, *J* = 7.1, 5.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.38, 159.80, 137.67, 129.64, 120.28, 114.14, 112.24, 65.96, 55.25, 31.01, 27.44, 25.46, 18.47.

(*Z*)-1-(3-Methoxyphenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (t, *J* = 7.9 Hz, 1H), 6.77 (ddd, *J* = 6.9, 1.5, 0.8 Hz, 1H), 6.73 (t, *J* = 2.1 Hz, 1H), 6.69 (dd, *J* = 8.2, 2.5 Hz, 1H), 4.43 – 4.30 (m, 2H), 3.72 (s, 3H), 2.63 – 2.48 (m, 2H), 2.19 (ddd, *J* = 12.9, 7.1, 2.9 Hz, 1H), 1.84 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.46 (dd, *J* = 8.8, 5.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.79, 159.33, 136.89, 129.08, 121.31, 114.89, 112.34, 65.53, 55.17, 34.63, 32.02, 27.77, 17.33.
HRMS (TOF) m/z: 219.1021 (M + H^+); calc. for $C_{13}H_{15}O_3$: 219.1021.

(*E*)-1-(4-Tolyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 7.9 Hz, 2H), 7.01 (d, *J* = 8.1 Hz, 2H), 4.40 (td, *J* = 8.9, 5.6 Hz, 1H), 4.26 (td, *J* = 8.9, 6.8 Hz, 1H), 2.72 (dd, *J* = 9.4, 7.1 Hz, 1H), 2.34 (s, 3H), 2.14 (ddd, *J* = 13.0, 8.9, 6.8 Hz, 1H), 1.89 (ddd, *J* = 12.9, 8.7, 5.5 Hz, 1H), 1.78

(dd, J = 9.3, 5.1 Hz, 1H), 1.43 (dd, J = 7.1, 5.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.63, 136.96, 132.99, 129.44, 128.09, 66.03, 30.94, 27.40, 25.54, 21.19, 18.47.

(*Z*)-1-(4-Tolyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (q, J = 8.1 Hz, 4H), 4.49 – 4.37 (m, 2H), 2.69 – 2.54 (m, 2H), 2.30 (s, 3H), 2.24 (dd, J = 7.1, 2.9 Hz, 1H), 1.90 (dd, J = 7.7, 5.2 Hz, 1H), 1.51 (dd, J = 8.9, 5.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.09, 136.79, 132.33, 129.01, 128.88, 65.66, 34.57, 32.12, 27.73, 21.27, 17.34.

HRMS (TOF) m/z: 203.1074 (M + H$^+$); calc. for $C_{13}H_{15}O_2$: 203.1072

(*E*)-1-(4-Chlorophenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, J = 8.5 Hz, 2H), 7.06 (d, J = 8.1 Hz, 2H), 4.41 (td, J = 9.0, 5.8 Hz, 1H), 4.28 (td, J = 8.9, 6.5 Hz, 1H), 2.72 (dd, J = 9.3, 7.1 Hz, 1H), 2.14 (ddd, J = 13.1, 8.9, 6.5 Hz, 1H), 1.88 (ddd, J = 13.0, 8.8, 5.8 Hz, 1H), 1.80 (dd, J = 9.3, 5.2 Hz, 1H), 1.42 (dd, J = 7.1, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.19, 134.71, 133.12, 129.50, 128.96, 65.98, 30.34, 27.61, 25.49, 18.70.

(*Z*)-1-(4-Chlorophenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, J = 8.5 Hz, 2H), 7.18 (d, J = 8.3 Hz, 2H), 4.47 (td, J = 9.0, 3.0 Hz, 1H), 4.40 (ddd, J = 9.6, 9.0, 7.4 Hz, 1H), 2.68 – 2.54 (m, 2H), 2.28 (ddd, J = 12.7, 7.3, 2.9 Hz, 1H), 1.89 (dd, J = 7.7, 5.3 Hz, 1H), 1.55 (dd, J = 8.9, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.85, 133.89, 133.00, 130.37, 128.41, 65.69, 33.93, 31.91, 27.92, 17.61.

HRMS (TOF) m/z: 223.0542 (M + H$^+$); calc. for $C_{12}H_{12}O_2Cl$: 223.0526.

(*E*)-1-(4-Bromophenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J = 8.4 Hz, 2H), 7.00 (d, J = 8.5 Hz, 2H), 4.41 (td, J = 9.0, 5.8 Hz, 1H), 4.28 (td, J = 8.9, 6.6 Hz, 1H), 2.77 – 2.63 (m, 1H), 2.14 (ddd, J = 13.1, 8.9, 6.5 Hz, 1H), 1.88 (ddd, J = 13.2, 8.8, 5.8 Hz, 1H), 1.80 (dd, J = 9.3, 5.2 Hz, 1H), 1.42 (dd, J = 7.1, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.15, 135.25, 131.90, 129.85, 121.17, 65.98, 30.40, 27.61, 25.48, 18.66.

(*Z*)-1-(4-Bromophenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 8.4 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 4.47 (td, J = 9.0, 3.0 Hz, 1H), 4.40 (ddd, J = 9.6, 9.0, 7.4 Hz, 1H), 2.66 – 2.54 (m, 2H), 2.28 (ddd, J = 13.0, 7.5, 3.2 Hz, 1H), 1.88 (dd, J = 7.7, 5.4 Hz, 1H), 1.55 (dd, J = 8.8, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.84, 134.43, 131.33, 130.73, 121.14, 65.69, 33.97, 31.89, 27.91, 17.56.

HRMS (TOF) m/z: 267.0044 (M + H$^+$); calc. for $C_{12}H_{12}O_2Br$: 267.0021.

(*E*)-1-((4-(Trifluoromethyl)phenyl))-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.9 Hz, 2H), 7.24 (d, *J* = 8.7 Hz, 2H), 4.43 (td, *J* = 9.0, 5.9 Hz, 1H), 4.29 (td, *J* = 9.0, 6.4 Hz, 1H), 2.80 (dd, *J* = 9.3, 7.1 Hz, 1H), 2.17 (ddd, *J* = 13.1, 8.9, 6.4 Hz, 1H), 1.94 – 1.82 (m, 2H), 1.51 (dd, *J* = 7.1, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.94, 140.47, 129.54 (130.02, 129.70, 129.37, 129.05, q, *J* = 32.5 Hz), 128.45, 125.73 (125.79, 125.75, 125.71, 125.67, q, *J* =3.8 Hz), 124.16 (128.21, 125.51, 122.81, 120.11, q, *J* = 271.8 Hz), 65.98, 30.48, 28.00, 25.46, 18.91.

(*Z*)-1-((4-(Trifluoromethyl)phenyl))-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.1 Hz, 2H), 7.37 (d, *J* = 8.6 Hz, 2H), 4.49 (td, *J* = 9.0, 3.1 Hz, 1H), 4.42 (td, *J* = 9.3, 7.4 Hz, 1H), 2.74 – 2.57 (m, 2H), 2.32 (ddd, *J* = 12.8, 7.3, 3.1 Hz, 1H), 1.96 (dd, *J* = 7.7, 5.4 Hz, 1H), 1.61 (dd, *J* = 8.8, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.69, 139.45, 129.39, 129.33 (129.81, 129.49, 129.16, 128.84, q, *J* = 32.5 Hz), 125.19 (125.24, 125.21, 125.17, 125.13, q, *J* = 3.8 Hz), 124.29 (128.34, 125.64, 122.94, 120.22, q, *J* = 271.9 Hz), 65.73, 34.06, 31.89, 28.23, 17.69.

HRMS (TOF) m/z: 257.0796 (M + H$^+$); calc. for $C_{13}H_{12}O_2F_3$: 257.0789.

(*E*)-1-(2-Fluorophenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.23 (m, 1H), 7.12 (td, *J* = 7.5, 1.1 Hz, 1H), 7.10 – 7.02 (m, 2H), 4.41 (dtd, *J* = 8.9, 4.9, 0.3 Hz, 1H), 4.34 (td, *J* = 8.6, 7.5 Hz, 1H), 2.84 – 2.70 (m, 1H), 2.15 (ddd, *J* = 13.0, 9.0, 7.4 Hz, 1H), 1.84 – 1.74 (m, 2H), 1.45 (dd, *J* = 7.2, 5.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.32, 162.49 (163.72, 161.27, d, *J* = 248.2 Hz), 129.39 (129.41, 129.38, d, *J* = 3.7 Hz), 129.18 (129.22, 129.14, d, *J* = 8.2 Hz), 124.39 (124.40, 124.37, d, *J* = 3.7 Hz), 123.73 (123.80, 123.66, d, *J* = 14.7 Hz), 115.62 (115.73, 115.51, d, *J* = 21.5 Hz), 66.15, 26.49, 25.89, 25.50 (25.52, 25.48, d, *J* = 3.7 Hz), 17.43 (17.43, 17.42, d, *J* = 1.5 Hz).

(*Z*)-1-(2-Fluorophenyl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.17 (m, 2H), 7.09 (td, *J* = 7.5, 1.1 Hz, 1H), 6.99 (ddd, *J* = 9.6, 8.3, 1.2 Hz, 1H), 4.52 – 4.44 (m, 2H), 2.68 – 2.54 (m, 2H), 2.33 (ddd, *J* = 12.7, 6.3, 4.0 Hz, 1H), 1.86 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.54 (dd, *J* = 8.7, 5.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.26, 162.33 (163.54, 161.11, d, J = 245.9 Hz), 130.43 (130.45, 130.41, d, J = 3.7 Hz), 128.97 (129.01, 128.93, d, J = 8.3 Hz), 123.90 (123.92, 123.88, d, J = 3.5 Hz), 123.15 (123.22, 123.07, d, J = 14.8 Hz), 114.94 (115.04, 114.83, d, J = 21.4 Hz), 65.92, 31.56, 28.11 (28.13, 28.09, d, J = 3.8 Hz), 26.95, 16.51.

HRMS (TOF) m/z: 207.0842 (M + H$^+$); calc. for $C_{12}H_{12}O_2F$: 207.0821.

(*E*)-1-(Naphthalen-2-yl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.76 (m, 3H), 7.60 – 7.55 (m, 1H), 7.53 – 7.44 (m, 2H), 7.26 (dd, *J* = 8.4, 1.8 Hz, 1H), 4.40 (td, *J* = 9.0, 5.5 Hz, 1H), 4.26 (td, *J* = 8.9, 6.8 Hz, 1H), 2.92 (dd, *J* = 9.2, 7.2 Hz, 1H), 2.18 (ddd, *J* = 13.1, 8.9, 6.8 Hz, 1H), 1.95 – 1.82 (m, 2H), 1.63 (dd, *J* = 7.2, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.48, 133.70, 133.47, 132.64, 128.47, 127.82, 127.70, 126.70, 126.58, 126.50, 126.11, 66.07, 31.36, 27.80, 25.61, 18.53.

(*Z*)-1-(Naphthalen-2-yl)-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.74 (m, 3H), 7.71 (dd, *J* = 1.9, 1.0 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.37 (dd, *J* = 8.5, 1.8 Hz, 1H), 4.52 – 4.42 (m, 2H), 2.80 (t, *J* = 8.3 Hz, 1H), 2.67 (dt, *J* = 12.5, 9.3 Hz, 1H), 2.34 (ddd, *J* = 12.7, 6.9, 3.3 Hz, 1H), 2.07 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.62 (dd, *J* = 8.8, 5.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.97, 133.31, 132.89, 132.72, 127.91, 127.87, 127.85, 127.75, 127.14, 126.13, 125.81, 65.71, 34.97, 32.15, 17.60.

HRMS (TOF) m/z: 239.1079 (M + H$^+$); calc. for $C_{16}H_{15}O_2$: 239.1072.

(*E*)-1-Phenethyl-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 2H), 7.23 – 7.13 (m, 3H), 4.36 (td, *J* = 9.0, 3.5 Hz, 1H), 4.18 (q, *J* = 8.6 Hz, 1H), 2.79 – 2.54 (m, 2H), 2.39 (dt, *J* = 12.5, 9.0 Hz, 1H), 2.09 – 1.83 (m, 3H), 1.30 (p, *J* = 7.4 Hz, 1H), 1.23 – 1.10 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.51, 141.60, 128.71, 128.48, 126.02, 65.79, 35.82, 31.87, 30.36, 28.56, 24.18, 20.22.

(*Z*)-1-Phenethyl-5-oxaspiro[2.4]heptan-4-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 2H), 7.24 – 7.15 (m, 3H), 4.37 (td, *J* = 8.6, 6.7 Hz, 1H), 4.20 (td, *J* = 8.7, 6.4 Hz, 1H), 2.83 – 2.68 (m, 2H), 2.17 – 2.05 (m, 2H), 1.74 – 1.59 (m, 2H), 1.51 (dq, *J* = 9.1, 6.8 Hz, 1H), 1.40 (dd, *J* = 9.1, 4.2 Hz, 1H), 0.60 (dd, *J* = 6.7, 4.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 180.22, 141.31, 128.51, 128.48, 126.13, 65.92, 35.64, 31.89, 25.59, 25.52, 24.17, 21.13.

HRMS (TOF) m/z: 217.1233 (M + H$^+$); calc. for $C_{14}H_{17}O_2$: 217.1229.

General procedure for the synthesis of α-thio-γ-lactone standard products:

To a 100 mL round-bottom flask was added (substituted) thiophenol (2.0 mmol, 1.0 equiv.), NaOMe (162 mg, 3.0 mmol, 1.5 equiv.) and dry MeOH (30 mL). The mixture was stirred at room temperature for 1 hour before 3-bromodihydrofuran-2(3*H*)-one (214 μL, 1.3 equiv.) was added in one portion. The reaction was stirred at room temperature for another 24 hours. Methanol was evaporated under reduced pressure. The crude mixture was then dissolved in DCM and washed with water. The aqueous phase was extracted by DCM (30 mL × 3). The combined organic layer was dried over Na_2SO_4, filtered, and

concentrated under reduced pressure. Purification by silica column chromatography using hexane and ethyl acetate as eluents afforded racemic α-thio-γ-lactones in 50 – 80% yields.

3-(Phenylthio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.50 (m, 2H), 7.39 – 7.29 (m, 3H), 4.31 – 4.17 (m, 2H), 3.86 (dd, *J* = 8.6, 6.2 Hz, 1H), 2.67 (dddd, *J* = 13.4, 8.7, 7.7, 6.6 Hz, 1H), 2.27 (ddt, *J* = 13.5, 7.4, 6.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.10, 133.73, 131.81, 129.40, 128.86, 66.62, 44.54, 30.10. HRMS (TOF) m/z: 195.0468 (M + H$^+$); calc. for $C_{10}H_{11}O_2S$: 195.0480.

3-((3-Methoxyphenyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.21 (m, 1H), 7.12 (dt, *J* = 7.4, 1.6 Hz, 2H), 6.87 (ddd, *J* = 8.4, 2.3, 1.3 Hz, 1H), 4.31 – 4.20 (m, 2H), 3.88 (dd, *J* = 8.7, 6.4 Hz, 1H), 3.80 (s, 3H), 2.68 (dddd, *J* = 13.5, 8.7, 7.5, 6.6 Hz, 1H), 2.28 (ddt, *J* = 13.6, 7.4, 6.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.12, 160.00, 133.04, 130.17, 125.53, 118.46, 114.82, 66.65, 55.51, 44.53, 30.17. HRMS (TOF) m/z: 225.0564 (M + H$^+$); calc. for $C_{11}H_{13}O_3S$: 225.0585.

3-((4-Fluorophenyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.9, 5.3 Hz, 2H), 7.05 (dd, *J* = 8.9, 8.5 Hz, 2H), 4.31 – 4.17 (m, 2H), 3.77 (dd, *J* = 8.7, 6.2 Hz, 1H), 2.66 (dddd, *J* = 13.5, 8.7, 7.7, 6.6 Hz, 1H), 2.25 (ddt, *J* = 13.5, 7.4, 6.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.80, 163.41 (164.66, 162.17, d, *J* = 150.8 Hz), 136.72 (136.76, 136.67, d, *J* = 8.5 Hz), 126.49 (126.51, 126.48, d, *J* = 3.6 Hz), 116.49 (116.60, 116.39, d, *J* = 22.1 Hz), 66.43, 44.82 (44.83, 44.81, d, *J* = 1.4 Hz), 29.73. HRMS (FAB) m/z: 213.0386 (M + H$^+$); calc. for $C_{10}H_{10}O_2SF$: 213.0396.

3-((4-Chlorophenyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.6 Hz, 2H), 7.31 (d, *J* = 8.5 Hz, 2H), 4.27 (t, *J* = 6.9 Hz, 2H), 3.82 (dd, *J* = 8.7, 6.3 Hz, 1H), 2.74 – 2.62 (m, 1H), 2.25 (td, *J* = 13.4, 6.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.83, 135.31, 135.12, 130.26, 129.59, 66.59, 44.55, 29.93. HRMS (TOF) m/z: 229.0080 (M + H$^+$); calc. for $C_{10}H_{10}O_2SCl$: 229.0090.

3-((4-Bromophenyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.36 (m, 4H), 4.28 (td, *J* = 7.0, 1.0 Hz, 2H), 3.83 (dd, *J* = 8.7, 6.4 Hz, 1H), 2.68 (ddtd, *J* = 14.1, 8.7, 7.0, 0.6 Hz, 1H), 2.25 (dqd, *J* = 13.4, 6.7, 1.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.81, 135.20, 132.54, 130.98, 123.40, 66.60, 44.43, 29.95. HRMS (TOF) m/z: 271.9518 (M + H$^+$); calc. for $C_{10}H_9O_2SBr$: 271.9507.

3-((4-Tolyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 4.27 – 4.15 (m, 2H), 3.78 (dd, *J* = 8.7, 6.0 Hz, 1H), 2.64 (dddd, *J* = 13.5, 8.7, 7.8, 6.7 Hz, 1H), 2.35 (s, 3H), 2.31 – 2.21 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.19, 139.44, 134.52, 130.22, 127.85, 66.62, 44.82, 29.99, 21.38. HRMS (TOF) m/z: 209.0631 (M + H^+); calc. for $C_{11}H_{13}O_2S$: 209.0636.

3-((4-Isopropylphenyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 4.28 – 4.14 (m, 2H), 3.80 (dd, *J* = 8.7, 6.1 Hz, 1H), 2.90 (hept, *J* = 7.0 Hz, 1H), 2.65 (dddd, *J* = 13.5, 8.7, 7.7, 6.6 Hz, 1H), 2.27 (ddt, *J* = 13.5, 7.4, 6.0 Hz, 1H), 1.24 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.25, 150.17, 134.42, 128.26, 127.60, 66.61, 44.80, 33.97, 30.10, 23.95. HRMS (TOF) m/z: 237.0931 (M + H^+); calc. for $C_{13}H_{17}O_2S$: 237.0949.

3-((4-(Trifluoromethyl)phenyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 8.3 Hz, 2H), 4.36 (qdd, *J* = 9.1, 7.5, 6.2 Hz, 2H), 3.98 (dd, *J* = 8.7, 6.5 Hz, 1H), 2.75 (dddd, *J* = 13.7, 8.7, 7.5, 6.4 Hz, 1H), 2.29 (ddt, *J* = 13.7, 7.5, 6.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.48, 137.51, 131.68, 130.02 (130.51, 130.18, 129.86, 129.53, q, *J* = 32.3 Hz), 126.04 (126.09, 126.06, 126.02, 125.98, q, *J* = 3.8 Hz), 123.85 (127.90, 125.20, 122.49, 119.79, q, *J* = 273.1 Hz), 66.53, 43.48, 29.98. HRMS (FAB) m/z: 263.0347 (M + H^+); calc. for $C_{11}H_{10}O_2SF_3$: 263.0354.

3-((3,4-Dimethoxyphenyl)thio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.15 (d, *J* = 2.1 Hz, 1H), 6.85 (d, *J* = 8.3 Hz, 1H), 4.24 (ddd, *J* = 8.9, 7.8, 5.8 Hz, 1H), 4.15 (ddd, *J* = 8.9, 7.6, 6.5 Hz, 1H), 3.90 (s, 6H), 3.75 (dd, *J* = 8.8, 6.2 Hz, 1H), 2.66 (dddd, *J* = 13.4, 8.7, 7.8, 6.5 Hz, 1H), 2.28 (ddt, *J* = 13.5, 7.6, 6.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.41, 150.38, 149.20, 128.46, 121.81, 117.98, 111.50, 66.57, 56.16, 56.03, 45.26, 29.73. HRMS (TOF) m/z: 255.0707 (M + H^+); calc. for $C_{12}H_{15}O_4S$: 255.0691.

3-(Naphthalen-2-ylthio)dihydrofuran-2(3*H*)-one

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 1.7 Hz, 1H), 7.85 – 7.78 (m, 3H), 7.60 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.55 – 7.47 (m, 2H), 4.30 – 4.21 (m, 2H), 3.96 (dd, *J* = 8.7, 6.3 Hz, 1H), 2.74 – 2.64 (m, 1H), 2.36 – 2.27 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.10, 133.67, 133.16,

133.07, 130.24, 129.13, 129.08, 127.86, 127.02, 126.89, 66.67, 44.58, 30.11. HRMS (TOF) m/z: 245.0619 ($M + H^+$); calc. for $C_{14}H_{13}O_2S$: 245.0636.

V. Enzymatic Synthesis of *spiro*[2.4]-Lactones in Analytical and Preparative Scale

All enzymatic reactions for *spiro*[2.4]-lactone formation in analytical scale were conducted following the general procedure described below and analyzed with gas chromatography (GC). All TTNs for the different products were determined using the GC standard curve of the corresponding racemic standard product made with $Rh_2(OAc)_4$ (see **Section IV**).

General procedure for analytical-scale reactions:
To a 2 mL vial were added degassed suspension of *E. coli* expressing the P411-**G8S** variant in M9-N buffer (OD_{600} = 15 or 30, 340 μL), olefin (10 μL of 400 or 200 mM stock solution in EtOH, 10 or 5 mM), **LAD** (10 μL of 400 or 200 mM stock solution in EtOH, 10 or 5 mM, 1.0 equiv.), *D*-glucose (40 μL of 250 mM stock solution in M9-N buffer, 25 mM) under anaerobic conditions. The vial was capped and shaken at 600 rpm at room temperature for 12 h. After the reaction was completed, internal standard 1,3,5-trimethoxybenzene (20 μL of 20 mM stock solution in toluene) was added to the reaction vial followed by mixed solvent (hexane / ethyl acetate = 1 : 1, 1.0 mL). The mixture was transferred to a 1.5 mL microcentrifuge tube, and then vortexed (15 seconds × 3) and centrifuged (14,000 rpm, 5 min) to completely separate the organic and aqueous layers. 0.8 mL of organic layer was taken for GC analysis. TTN was calculated based on measured protein concentration. Diastereomeric excess (*de*) and enantiomeric excess (*ee*) were measured by chiral HPLC. Reactions for every substrate were set up in quadruplicate.

GC standard curve:
All data points represent the average of duplicate runs. The calibration curves depict product concentration in mM (y-axis) against the ratio of product area to internal standard area on the GC (x-axis).

All enzymatic reactions for *spiro*[2.4]-lactone formation in preparative scale were conducted following the general procedure described below and the corresponding *spiro*[2.4]-lactone products were isolated. Detailed conditions for preparative-scale reactions of different substrates are indicated separately.

General procedure for preparative-scale reactions:
To a 40 mL vial or 250 mL flask were added degassed suspension of *E. coli* expressing P411-**G8S** variant (OD_{600} = 20 – 30), olefin (0.25 – 2.0 mmol), **LAD** (1.0 equiv.), *D*-glucose (10 – 15 mM, 250 mM stock in M9-N), 1 – 5 vol% EtOH, M9-N buffer (pH 7.4) under anaerobic conditions. The vial or flask was capped and shaken (420 rpm for vials and 250 rpm for flasks) at room temperature for 12 h.
After the reaction was completed, 35 mL portions of preparative-scale reaction mixture were transferred to 50 mL centrifuge tubes. The reaction container was washed with water (2 mL × 2) followed by mixed organic solvent (hexane / ethyl acetate = 1 : 1, 2 mL × 3). The washing solution was combined with the reaction mixture in the centrifuge tubes. An additional 12 mL of hexane / ethyl acetate solvent was added to every tube. After the tube (with ~48 mL mixture in total) was capped, it was vortexed (1 min × 3) and shaken vigorously, and centrifuged (12,000 × g, 5 min). The organic layer was separated and the aqueous layer was subjected to three more rounds of extraction. The organic layers were

combined, dried over Na_2SO_4 and concentrated under reduced pressure. Purification by silica column chromatography with hexane / ethyl acetate as eluent afforded the desired *spiro*[2.4]-lactones. Diastereomeric excess (*de*) and enantiomeric excess (*ee*) were measured by chiral HPLC. TTNs were calculated based on measured protein concentration and isolated product yield.

(1*S*, 2*S*)-1-Phenyl-5-oxaspiro[2.4]heptan-4-one (2a)

GC calibration curve:

Analysis data (10 mM **1a**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2a-(1)	6096.9	679.8	8.969	4.54	1.32	3445	
2a-(2)	5411.4	645.4	8.384	4.25	1.32	3230	
2a-(3)	5192.7	627.3	8.278	4.20	1.32	3191	
2a-(4)	5137.1	619.8	8.288	4.21	1.32	3194	3265
2a-(5)	31945	3196	9.995	5.03	1.62	3103	
2a-(6)	29685	3210	9.248	4.67	1.62	2882	
2a-(7)	28300	3177	8.908	4.51	1.62	2781	
2a-(8)	28124	3037	9.260	4.68	1.62	2886	2913

Chiral HPLC trace:

Chiralpak OJ-H, 20% *i*-PrOH in hexane, 1.0 mL/min, 24 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2a**:

***rac-Z*- and *E*-2a**			**(1*S*, 2*S*)-2a**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
15.315 (*E*)	33379.8	41.30	15.431	1901.6	98.60
16.539 (*E*)	34416.7	42.58	16.713	16.7	0.86
22.940 (*Z*)	6497.4	8.04	23.159	4.6	0.24
24.044 (*Z*)	6536.8	8.08	24.299	5.8	0.30
Total	80830.7	100.00	Total	1928.7	100.00

(1*S*, 2*S*)-1-(4-Methoxyphenyl)-5-oxaspiro[2.4]heptan-4-one (2b)

GC calibration curve:

Analysis data (10 mM **1b**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2b-(1)	46399	2981	15.565	8.53	0.81	10524	
2b-(2)	48120	2993	16.078	8.78	0.81	10838	
2b-(3)	46572	3013	15.457	8.47	0.81	10457	
2b-(4)	46397	3128	14.833	8.16	0.81	10072	10473

Preparative-scale reaction:

***E. coli* suspension expressing P411-G8S in M9-N**	***D*-glucose in M9-N**

OD_{600}	volume/mL	[PC]/μM	n_pro/μmol	volume/mL	[Glu]/mM
28	32.0	2.618	0.0877	2.0	~15
olefin (1b) stock in EtOH			**LAD stock in EtOH**		
stock/M	volume/μL	n_1/mmol	stock/M	volume/μL	n_2/mmol
2.0	400	0.80	1.0	800	0.80
purification eluent		**Product**			
Ethyl acetate in hexanes (0% to 25% gradient)		m[Pdt]/mg	n[Pdt]/mmol	yield	TTN
		124.3	0.600	71%	6500

Note: [PC] = protein concentration in original cell suspension, n_pro = amount of protein in the reaction, [Glu] = *D*-glucose concentration in reaction mixture, n_1 = amount of alkyne in the reaction, n_2 = amount of EDA in the reaction, m[Pdt] = mass of product isolated, n[Pdt] = amount of product. The same for the following tables.

Optical rotation: $[\alpha]^{23}_{D} = -159.9 \pm 0.3°$ (*c* 0.6, ethyl acetate).

Chiral HPLC trace:
Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2b**:

***rac-Z*- and *E*-2b**			**(1*S*, 2*S*)-2b**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
13.219 (*E*)	1862.5	32.97	13.262	43.5	0.20
14.333 (*E*)	1819.7	32.22	14.116	20914.3	99.80
22.285 (*Z*)	836.6	14.81	-	-	-
23.845 (*Z*)	1129.5	20.00	-	-	-
Total	5648.3	100.00	Total	20957.8	100.00

(1*S*, 2*S*)-1-(3-Methoxyphenyl)-5-oxaspiro[2.4]heptan-4-one (2c)
GC calibration curve:

Analysis data (10 mM **1c**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2c-(1)	50973	3011	16.929	9.60	0.81	11854	
2c-(2)	50742	2986	16.993	9.64	0.81	11895	
2c-(3)	48424	3070	15.773	9.00	0.81	11112	
2c-(4)	41983	3068	13.684	7.90	0.81	9746	11152

Preparative-scale reaction:

***E. coli* suspension expressing P411-G8S in M9-N**				***D*-glucose in M9-N**	
OD_{600}	volume/mL	[PC]/μM	n_pro/μmol	volume/mL	[Glu]/mM
27	85.0	3.218	0.2734	5	~13
olefin (1c) stock in EtOH			**LAD stock in EtOH**		
stock/M	volume/μL	n_1/mmol	stock/M	volume/μL	n_2/mmol
2.0	1000	2.0	1.0	2000	2.0
purification eluent		**Product**			
Ethyl acetate in hexanes (0% to 25% gradient)		m[Pdt]/mg	n[Pdt]/mmol	yield	TTN
		415.8	1.91	95%	6970

Optical rotation: $[\alpha]^{23}_{D} = -138.0 \pm 0.3°$ (*c* 0.8, ethyl acetate).

Chiral HPLC trace:
Chiralpak OD-H, 12% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2c**:

***rac-Z*- and *E*-2c**			**(1*S*, 2*S*)-2c**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
14.561 (*E*)	3572.1	26.00	14.370	18512.0	99.89
15.510 (*E*)	3653.2	26.59	15.508	20.0	0.11
32.441 (*Z*)	3295.4	23.99	-	-	-
43.220 (*Z*)	3217.4	23.42	-	-	-
Total	13738.1	100.00	Total	18532.0	100.00

(1*S*, 2*S*)-1-(4-Tolyl)-5-oxaspiro[2.4]heptan-4-one (2d)

GC calibration curve:

Analysis data (10 mM **1d**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2d-(1)	37022	3016	12.275	6.83	1.62	4216	
2d-(2)	31892	3006	10.609	5.98	1.62	3693	
2d-(3)	39781	3192	12.463	6.93	1.62	4274	
2d-(4)	33482	3047	10.989	6.18	1.62	3814	3999

Chiral HPLC trace:
Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2d**:

***rac-Z*- and *E*-2d**			**(1*S*, 2*S*)-2d**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
8.345 (*E*)	3711.6	33.33	8.380	17.6	0.20
9.018 (*E*)	3734.9	33.54	8.994	8588.6	99.80
11.533 (*Z*)	1812.1	16.27	-	-	-
13.369 (*Z*)	1878.4	16.87	-	-	-
Total	11137.0	100.00	Total	8606.2	100.00

(1*S*, 2*S*)-1-(4-Chlorophenyl)-5-oxaspiro[2.4]heptan-4-one (2e)
GC calibration curve:

Analysis data (10 mM **1e**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2e-(1)	36851	3058	12.051	6.73	1.62	4153	
2e-(2)	32339	3091	10.462	5.87	1.62	3623	
2e-(3)	29981	3095	9.687	5.45	1.62	3362	
2e-(4)	30644	3032	10.107	5.68	1.62	3504	3660

Chiral HPLC trace:
Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2e**:

***rac-Z*- and *E*-2e**	**(1*S*, 2*S*)-2e**

Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
11.666 (*E*)	13836.6	30.27	11.776	19.1	0.14
12.234 (*E*)	15269.7	33.40	12.157	13271.6	99.86
15.066 (*Z*)	7751.6	16.96	-	-	-
15.918 (*Z*)	8858.9	19.38	-	-	-
Total	45716.8	100.00	Total	13290.7	100.00

(1*S*, 2*S*)-1-(4-Bromophenyl)-5-oxaspiro[2.4]heptan-4-one (2f)

GC calibration curve:

Analysis data (10 mM **1f**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2f-(1)	27512	3015	9.125	5.20	1.62	3207	
2f-(2)	28599	3090	9.255	5.27	1.62	3251	
2f-(3)	28701	2984	9.618	5.47	1.62	3374	
2f-(4)	24259	2994	8.103	4.63	1.62	2860	3173

Preparative-scale reaction:

***E. coli* suspension expressing P411-G8S in M9-N**				***D*-glucose in M9-N**	
OD_{600}	volume/mL	[PC]/μM	n_pro/μmol	volume/mL	[Glu]/mM
28	32.0	2.618	0.0877	2	~15
olefin (1f) stock in EtOH			**LAD stock in EtOH**		
stock/M	volume/μL	n_1/mmol	stock/M	volume/μL	n_2/mmol
1.0	250	0.25	1.0	250	0.25
purification eluent		**Product**			
Ethyl acetate in hexanes (0% to 25% gradient)		m[Pdt]/mg	n[Pdt]/mmol	yield	TTN
		42.4	0.159	64%	1810

Optical rotation: $[\alpha]^{23}_{D} = -139.7 \pm 0.5°$ (*c* 0.3, ethyl acetate).

Chiral HPLC trace:
Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2f**:

***rac*-*Z*- and *E*-2f**			**(1*S*, 2*S*)-2f**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
13.069 (*E*)	5457.4	46.93	13.003	10229.1	100.00
16.245 (*Z*)	3026.5	26.02	-	-	-
17.461 (*Z*)	3145.8	27.05	-	-	-
Total	11629.4	100.00	Total	10229.1	100.00

Chiralpak OD-H, 10% *i*-PrOH in hexane, 1.2 mL/min, 40 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2f**:

***rac-Z*- and *E*-2f**			**(1*S*, 2*S*)-2f**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
12.126 (*E*)	4399.4	20.03	12.474	43.6	0.28
12.764 (*E*)	3765.8	17.14	12.822	15758.5	99.72
13.229 (*Z*)	13800.5	62.83	-	-	-
Total	21965.7	100.00	Total	15802.1	100.00

(1*S*, 2*S*)-1-((4-(Trifluoromethyl)phenyl))-5-oxaspiro[2.4]heptan-4-one (2g)

GC calibration curve:

Analysis data (10 mM **1g**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2g-(1)	12126	3113	3.895	2.60	1.62	1605	
2g-(2)	12245	2903	4.218	2.81	1.62	1734	
2g-(3)	10252	2928	3.501	2.35	1.62	1448	
2g-(4)	11080	2887	3.838	2.56	1.62	1583	1592

Chiral HPLC trace:

Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2g**:

***rac*-*Z*- and *E*-2g**			**(1*S*, 2*S*)-2g**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
10.229 (*E*)	9090.3	32.72	10.366	12.6	0.12
10.716 (*E*)	10145.7	36.51	10.835	10408.0	99.53
11.768 (*Z*)	4309.0	15.51	12.085	36.8	0.35
12.954 (*Z*)	4240.2	15.26	-	-	-
Total	27785.2	100.00	Total	10457.4	100.00

(1*S*, 2*S*)-1-(2-Fluorophenyl)-5-oxaspiro[2.4]heptan-4-one (2h)

GC calibration curve:

Analysis data (5 mM **1h**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2h-(1)	9723	3063	3.174	1.92	1.16	1651	
2h-(2)	9766	3134	3.116	1.89	1.16	1621	
2h-(3)	9697	3044	3.186	1.93	1.16	1657	
2h-(4)	9879	3059	3.229	1.96	1.16	1679	1652

Chiral HPLC trace:
Chiralpak OD-H, 10% *i*-PrOH in hexane, 1.2 mL/min, 40 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2h**:

***rac-Z*- and *E*-2h**	**(1*S*, 2*S*)-2h**

Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
9.479 (*E*)	2041.9	29.79	9.410	2641.7	98.50
10.035 (*E*)	2113.2	30.83	9.984	21.6	0.81
11.311 (*Z*)	1328.8	19.38	11.324	18.6	0.69
12.029 (*Z*)	1370.7	20.00	-	-	-
Total	6854.6	100.00	Total	2681.9	100.00

(1*S*, 2*S*)-1-(Naphthalen-2-yl)-5-oxaspiro[2.4]heptan-4-one (2i)

GC calibration curve:

Analysis data (10 mM **1i**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2i-(1)	27834	3149	8.839	4.73	1.62	2916	
2i-(2)	28556	3193	8.943	4.78	1.62	2949	
2i-(3)	23350	3223	7.245	3.90	1.62	2410	
2i-(4)	25288	3386	7.468	4.02	1.62	2481	2613

Chiral HPLC trace:

Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and **(1*S*, 2*S*)-2i**:

***rac-Z* and *E*-2i**			**(1*S*, 2*S*)-2i**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
10.968 (*E*)	22742.3	41.91	11.072	114.4	0.44
12.455 (*E*)	22947.4	42.28	12.503	25881.0	99.56
19.082 (*Z*)	3991.7	7.36	-	-	-
20.099 (*Z*)	4583.7	8.45	-	-	-
Total	54265.1	100.00	Total	25995.4	100.00

(–)-(*Z*)-1-Phenethyl-5-oxaspiro[2.4]heptan-4-one (2j)

GC calibration curve:

Analysis data (5 mM **1j**):

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
2j-(1)	11942	2840	4.205	2.14	1.16	1835	
2j-(2)	12393	3173	3.906	1.99	1.16	1707	
2j-(3)	12453	3189	3.905	1.99	1.16	1706	
2j-(4)	11944	3062	3.901	1.99	1.16	1704	
2j-(5)	12213	3030	4.031	2.05	1.16	1760	1743

Preparative-scale reaction:

***E. coli* suspension expressing P411-G8S in M9-N**				***D*-glucose in M9-N**	
OD_{600}	volume/mL	[PC]/μM	n_pro/μmol	volume/mL	[Glu]/mM
24	98	1.37	0.1343	5	~12
olefin (1j) stock in EtOH			**LAD stock in EtOH**		
stock/M	volume/μL	n_1/mmol	stock/M	volume/μL	n_2/mmol
1.0	250	0.25	1.0	250	0.25
purification eluent		**Product**			
Ethyl acetate in hexanes (0% to 25% gradient)		m[Pdt]/mg	n[Pdt]/mmol	yield	TTN
		35.8	0.166	66%	1230

Optical rotation: $[\alpha]^{23}_{D} = -55.0 \pm 0.6°$ (*c* 0.2, ethyl acetate).

Chiral HPLC trace:
Chiralpak OD-H, 10% *i*-PrOH in hexane, 1.2 mL/min, 40 °C, 220 nm

Area% report for ***rac***- and **(–)-*Z*-2j**:

***rac*-*Z*- and *E*-2j**			**(–)-*Z*-2j**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
9.125 (*E*)	1904.2	36.06	9.135	56.8	1.94
10.072 (*E*)	1977.2	37.44	-	-	-
12.654 (*Z*)	689.4	13.06	-	-	-
13.362 (*Z*)	709.8	13.44	13.270	2868.3	98.06
Total	5280.6	100.00	Total	2925.1	100.00

VI. Enzymatic Synthesis of *α*-Thio-*γ*-Lactones in Analytical and Preparative Scale

All enzymatic reactions for *α*-thio-*γ*-lactone synthesis in analytical scale were conducted following the general procedure described below and analyzed with gas chromatography (GC). All TTNs for the different products were determined using the GC standard curve of the corresponding racemic standard product (see **Section IV**).

General procedure for analytical-scale reactions:
To a 2 mL vial were added degassed suspension of *E. coli* expressing the P450-**G8S** variant in M9-N buffer (OD_{600} = 15, 340 μL), thiol (10 μL of 400 mM stock solution in EtOH, 10 mM), **LAD** (10 μL of 400 mM stock solution in EtOH, 10 mM, 1.0 equiv.), *D*-glucose (40 μL of 250 mM stock solution in M9-N buffer, 25 mM) under anaerobic conditions. The vial was capped and shaken at 600 rpm at room temperature for 12 h. After the reaction was completed, internal standard 1,3,5-trimethoxybenzene (20 μL of 20 mM stock solution in toluene) was added to the reaction vial followed by mixed solvent (hexane / ethyl acetate = 1 : 1, 1.0 mL). The mixture was transferred to a 1.5 mL microcentrifuge tube, and then vortexed (15 seconds × 3) and centrifuged (14,000 rpm, 5 min) to completely separate the organic and aqueous layers. 0.8 mL of organic layer was taken for GC analysis. TTN was calculated based on measured protein concentration. Enantiomeric excess was measured by chiral HPLC. Reactions for every substrate were set up in quadruplicate.

GC standard curve:
All data points represent the average of duplicate runs. The standard curves plot product concentration in mM (y-axis) against the ratio of product area to internal standard area on the GC (x-axis).

All enzymatic reactions for *α*-thio-*γ*-lactone synthesis in preparative scale were conducted following the general procedure described below and the corresponding *α*-thio-*γ*-lactone products were isolated. Detailed conditions for preparative-scale reactions of different substrates are indicated separately.

General procedure for preparative-scale reactions:
To a 40 mL vial or 250 mL flask were added degassed suspension of *E. coli* expressing P450-**G8S** variant (OD_{600} = 15 – 20), thiol (1.5 equiv.), **LAD** (1.5 or 2.4 mmol.), *D*-glucose (10 – 15 mM, 250 mM stock in M9-N), 1 – 5 vol% EtOH, M9-N buffer (pH 7.4) under anaerobic conditions. The flask was capped and shaken (250 rpm) at room temperature for 2 h.
After the reaction was completed, 35 mL portions of preparative-scale reaction mixture were transferred to 50 mL centrifuge tubes. The reaction container was washed with water (2 mL × 2) followed by mixed organic solvent (hexane / ethyl acetate = 1 : 1, 2 mL × 3). The washing solution was combined with the reaction mixture in the centrifuge tubes. An additional 12 mL of hexane / ethyl acetate solvent was added to every tube. After the tube (with ~48 mL mixture in total) was capped, it was vortexed (1 min × 3) and shaken vigorously, and centrifuged (12,000 × g, 5 min). The organic layer was separated and the aqueous layer was subjected to three more rounds of extraction. The organic layers were combined, dried over Na_2SO_4 and concentrated under reduced pressure. Purification by

silica column chromatography with hexane / ethyl acetate as eluent afforded the desired α-thio-γ-lactones. Enantiomeric excess (*ee*) was measured by chiral HPLC. TTNs were calculated based on measured protein concentration and isolated product yield.

(*R*)-3-(Phenylthio)dihydrofuran-2(3*H*)-one (4a)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4a-(1)	25062	3496	7.169	6.54	4.21	1552	
4a-(2)	27038	3413	7.922	7.22	4.21	1715	
4a-(3)	28412	3453	8.228	7.50	4.21	1782	
4a-(4)	26034	3429	7.592	6.92	4.21	1644	1673
4a-(5)	24779	3388	7.314	6.67	4.28	1558	
4a-(6)	23497	3388	6.935	6.32	4.28	1478	
4a-(7)	24733	3275	7.552	6.89	4.28	1609	
4a-(8)	24427	3373	7.242	6.60	4.28	1543	1547

Chiral HPLC trace:

Chiralpak OJ-H, 24% *i*-PrOH in hexane, 1.2 mL/min, 24 °C, 235 nm

Area% report for ***rac***- and ***R*-4a**:

***rac*-4a**			***R*-4a**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
17.778	3476.6	49.99	17.759	546.8	8.08
21.927	3477.0	50.01	21.779	6223.7	91.92
Total	6953.6	100.00	Total	6770.5	100.00

(*R*)-3-((3-Methoxyphenyl)thio)dihydrofuran-2(3*H*)-one (4b)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4b-(1)	33529	3364	9.967	7.91	4.28	1849	
4b-(2)	33478	3418	9.795	7.78	4.28	1818	
4b-(3)	32920	3379	9.743	7.74	4.28	1809	
4b-(4)	33936	3458	9.814	7.79	4.28	1822	1824

Chiral HPLC trace:

Chiralpak OD-H, 12% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and ***R*-4b**:

***rac*-4b**			***R*-4b**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
20.566	7657.0	47.61	20.687	22518.9	94.44
21.435	8426.2	52.39	21.669	1325.7	5.56
Total	16083.2	100.00	Total	23844.6	100.00

(*R*)-3-((4-Fluorophenyl)thio)dihydrofuran-2(3*H*)-one (4c)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4c-(1)	44068	5404	8.155	8.09	4.43	1826	
4c-(2)	42946	5518	7.782	7.73	4.43	1745	
4c-(3)	42540	5443	7.816	7.76	4.43	1752	
4c-(4)	42676	5503	7.755	7.70	4.43	1739	1765

Chiral HPLC trace:
Chiralpak OD-H, 10% *i*-PrOH in hexane, 1.2 mL/min, 40 °C, 235 nm

Area% report for ***rac***- and ***R*-4c**:

***rac*-4c**			***R*-4c**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
14.082	4962.6	50.35	14.008	3532.1	93.21
15.822	4892.7	49.65	15.769	257.2	6.79
Total	9855.3	100.00	Total	3789.3	100.00

(*R*)-3-((4-Chlorophenyl)thio)dihydrofuran-2(3*H*)-one (4d)
GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4d-(1)	35908	3306	10.861	8.18	4.28	1913	
4d-(2)	37309	3237	11.526	8.65	4.28	2023	
4d-(3)	37284	3289	11.336	8.52	4.28	1991	
4d-(4)	36890	3390	10.882	8.20	4.28	1916	1961

Preparative-scale reaction:

***E. coli* suspension expressing P450-G8S in M9-N**				***D*-glucose in M9-N**	
OD_{600}	volume/mL	[PC]/μM	n_pro/μmol	volume/mL	[Glu]/mM
20	150	4.506	0.8757	10	~15
thiol (3d) stock in EtOH			**LAD stock in EtOH**		
stock/M	volume/μL	n_1/mmol	stock/M	volume/μL	n_2/mmol
2.0	1800	3.60	1.0	2400	2.40
purification eluent		**Product**			
Ethyl acetate in hexanes (0% to 25% gradient)		m[Pdt]/mg	n[Pdt]/mmol	yield	TTN
		438.3	1.92	80%	2190

Optical rotation: $[\alpha]^{23}_{D} = -45.6 \pm 0.2°$ (*c* 0.8, ethyl acetate).

Chiral HPLC trace:
Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and ***R*-4d**:

***rac*-4d**			***R*-4d**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
16.171	1834.6	49.77	16.222	338.2	6.98
17.370	1850.1	50.23	17.320	4510.2	93.02
Total	3684.7	100.00	Total	4848.4	100.00

***R*-4d_scale-up**		
Retention Time (min)	Area (mAU*s)	Area %
17.149	496.7	6.11
18.332	7628.2	93.89
Total	8124.9	100.00

(*R*)-3-((4-Bromophenyl)thio)dihydrofuran-2(3*H*)-one (4e)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4e-(1)	36496	3382	10.791	7.98	4.28	1866	
4e-(2)	34803	3354	10.377	7.70	4.28	1799	
4e-(3)	34274	3318	10.330	7.67	4.28	1792	
4e-(4)	35519	3357	10.581	7.84	4.28	1832	1822

Preparative-scale reaction:

***E. coli* suspension expressing P450-G8S in M9-N**				***D*-glucose in M9-N**	
OD_{600}	volume/mL	[PC]/μM	n_pro/μmol	volume/mL	[Glu]/mM
15	160	3.320	0.7149	10	~15
thiol (3e) stock in EtOH			**LAD stock in EtOH**		
stock/M	volume/μL	n_1/mmol	stock/M	volume/μL	n_2/mmol
1.0	2250	2.25	1.0	1500	1.50
purification eluent		**Product**			
Ethyl acetate in hexanes (0% to 25% gradient)		m[Pdt]/mg	n[Pdt]/mmol	yield	TTN
		386.5	1.42	94%	1980

Optical rotation: $[\alpha]^{23}_{D} = -41.7 \pm 0.2°$ (*c* 0.8, ethyl acetate).

Chiral HPLC trace:
Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and ***R***-**4e**:

***rac*-4e**			***R*-4e**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
17.405	2136.7	50.02	17.530	560.1	8.24
19.056	2133.6	49.98	19.039	6235.9	91.76
Total	4270.3	100.00	Total	6796.6	100.00

***R*-4e_scale-up**		
Retention Time (min)	Area (mAU*s)	Area %
16.934	661.0	6.86
18.412	8979.1	93.14
Total	9640.1	100.00

(*R*)-3-((4-Tolyl)thio)dihydrofuran-2(3*H*)-one (4f)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4f-(1)	23458	3376	6.948	4.61	4.28	1077	
4f-(2)	22953	3235	7.095	4.70	4.28	1099	
4f-(3)	23421	3341	7.010	4.65	4.28	1086	
4f-(4)	23731	3351	7.082	4.69	4.28	1097	1089

Chiral HPLC trace:
Chiralpak OJ-H, 24% *i*-PrOH in hexane, 1.2 mL/min, 28 °C, 220 nm

Area% report for ***rac***- and ***R*-4f**:

***rac*-4f**			***R*-4f**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
16.373	1840.0	49.97	16.306	2647.7	12.44

17.622	1842.5	50.03	17.412	18639.0	87.56
Total	3682.5	100.00	Total	21286.7	100.00

(*R*)-3-((4-Isopropylphenyl)thio)dihydrofuran-2(3*H*)-one (4g)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4g-(1)	9404	3133	3.002	1.80	4.28	422	
4g-(2)	9015	2968	3.037	1.83	4.28	427	
4g-(3)	9040	3255	2.777	1.67	4.28	391	
4g-(4)	9319	2983	3.124	1.88	4.28	439	420

Chiral HPLC trace:

Chiralpak OD-H, 10% *i*-PrOH in hexane, 1.2 mL/min, 40 °C, 235 nm

Area% report for ***rac***- and ***R*-4g**:

***rac*-4g**			***R*-4g**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
9.760	7857.7	50.00	10.072	1790.6	27.36
10.398	7857.3	50.00	10.687	4754.7	72.64
Total	15715.0	100.00	Total	6545.3	100.00

(*R*)-3-((4-Trifluoromethylphenyl)thio)dihydrofuran-2(3*H*)-one (4h)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4h-(1)	1062	678.8	1.565	1.32	4.81	275	
4h-(2)	1124.1	681.5	1.649	1.39	4.81	290	
4h-(3)	1211.8	678.9	1.785	1.51	4.81	314	
4h-(4)	1236.2	674.1	1.834	1.55	4.81	322	300

Chiral HPLC trace:

Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and ***R*-4h**:

***rac*-4h**			***R*-4h**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
15.352	11827.4	50.11	15.469	436.1	20.03
18.400	11774.0	49.89	18.514	1741.5	79.97
Total	23601.4	100.00	Total	2177.6	100.00

(*R*)-3-((3,4-Dimethoxyphenyl)thio)dihydrofuran-2(3*H*)-one (4i)

GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4i-(1)	9814	3203	3.064	2.64	4.28	617	

4i-(2)	9941	4040	2.461	2.13	4.28	499	
4i-(3)	10085	4349	2.319	2.01	4.28	471	
4i-(4)	10000	3671	2.724	2.36	4.28	551	534

Chiral HPLC trace:
Chiralpak OD-H, 12% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and ***R***-**4i**:

***rac*-4i**			***R*-4i**		
Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
28.834	15965.9	50.10	29.384	4271.0	92.17
36.512	15901.9	49.90	37.577	362.7	7.82
Total	31867.8	100.00	Total	4633.7	100.00

(*R*)-3-(Naphthalen-2-ylthio)dihydrofuran-2 (3*H*)-one (4j)
GC calibration curve:

Analysis data:

Pdt-Entries	Pdt	Std	Pdt/Std	[Pdt]/mM	[PC]/μM	TTN	Avg. TTN
4j-(1)	6820	3552	1.920	1.17	4.28	273	
4j-(2)	6843	3267	2.095	1.27	4.28	298	
4j-(3)	8152	3195	2.551	1.55	4.28	361	
4j-(4)	7779	3394	2.292	1.39	4.28	325	328

Chiral HPLC trace:
Chiralpak IA, 8% *i*-PrOH in hexane, 1.2 mL/min, 32 °C, 235 nm

Area% report for ***rac***- and ***R*-4j**:

***rac*-4j**	***R*-4j**

Retention Time (min)	Area (mAU*s)	Area %	Retention Time (min)	Area (mAU*s)	Area %
20.286	7644.6	49.75	20.338	1139.1	14.33
21.838	7721.4	50.25	21.847	6810.3	85.67
Total	15366.0	100.00	Total	7949.4	100.00

VII. Crystal Structure Information

Identification code	v18081	
Empirical formula	C13 H14 O3	
Formula weight	218.24	
Temperature	175 K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.2610(7) Å	α = 90°
	b = 7.4076(8) Å	β = 90°
	c = 24.242(2) Å	γ = 90°
Volume	1124.3(2) $Å^3$	
Z	4	
Density (calculated)	1.289 g/cm^3	
Absorption coefficient	0.744 mm^{-1}	
F(000)	464	
Crystal size	0.26 x 0.21 x 0.15 mm^3	
Theta range for data collection	3.646 to 80.268°.	
Index ranges	-7 □ h □ 7, -9 □ k □ 9, -30 □ l □ 30	
Reflections collected	28343	
Independent reflections	2423 [R(int) = 0.0298]	
Completeness to theta = 67.679°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.9262	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2423 / 0 / 147	
Goodness-of-fit on F^2	1.092	
Final R indices [I>2sigma(I)]	R1 = 0.0261, wR2 = 0.0678	
R indices (all data)	R1 = 0.0261, wR2 = 0.0679	
Absolute structure parameter [Flack]	0.03(3)	
Absolute structure parameter [Hooft]	0.05(3)	
Extinction coefficient	0.0083(9)	
Largest diff. peak and hole	0.179 and -0.132 e.$Å^{-3}$	

Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	46890(20)	48359(19)	46362(4)	473(3)
O(2)	46989(19)	21596(15)	50615(5)	409(3)
O(3)	83281(17)	57607(14)	80518(4)	323(2)
C(1)	44980(20)	39700(20)	50554(6)	332(3)
C(2)	45630(30)	15030(20)	56281(7)	416(4)
C(3)	34740(20)	29870(20)	59523(6)	321(3)
C(4)	40430(20)	46280(18)	56196(5)	276(3)
C(5)	31550(30)	64840(20)	57013(7)	374(4)
C(6)	54540(30)	61597(19)	58396(6)	308(3)
C(7)	62170(20)	60527(18)	64219(5)	267(3)
C(8)	51820(20)	69434(19)	68530(6)	311(3)
C(9)	59200(20)	68050(20)	73903(6)	306(3)
C(10)	77270(20)	57844(18)	75100(5)	258(3)
C(11)	87870(20)	48833(18)	70873(6)	278(3)
C(12)	80130(20)	50259(19)	65503(5)	292(3)
C(13)	102960(30)	49040(20)	81913(6)	358(3)

Bond lengths [Å] and angles [°]

O(1)-C(1)	1.2079(19)
O(2)-C(1)	1.347(2)
O(2)-C(2)	1.460(2)
O(3)-C(10)	1.3664(16)
O(3)-C(13)	1.4266(18)
C(1)-C(4)	1.4798(18)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.514(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.5016(19)
C(4)-C(5)	1.496(2)
C(4)-C(6)	1.5338(19)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(5)-C(6)	1.497(2)
C(6)-H(6)	1.0000
C(6)-C(7)	1.4923(18)
C(7)-C(8)	1.3954(19)
C(7)-C(12)	1.393(2)
C(8)-H(8)	0.9500
C(8)-C(9)	1.386(2)
C(9)-H(9)	0.9500

C(9)-C(10)	1.391(2)
C(10)-C(11)	1.3912(18)
C(11)-H(11)	0.9500
C(11)-C(12)	1.3930(19)
C(12)-H(12)	0.9500
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(1)-O(2)-C(2)	109.68(12)
C(10)-O(3)-C(13)	118.13(11)
O(1)-C(1)-O(2)	121.94(15)
O(1)-C(1)-C(4)	128.43(15)
O(2)-C(1)-C(4)	109.63(13)
O(2)-C(2)-H(2A)	110.6
O(2)-C(2)-H(2B)	110.6
O(2)-C(2)-C(3)	105.82(12)
H(2A)-C(2)-H(2B)	108.7
C(3)-C(2)-H(2A)	110.6
C(3)-C(2)-H(2B)	110.6
C(2)-C(3)-H(3A)	111.4
C(2)-C(3)-H(3B)	111.4
H(3A)-C(3)-H(3B)	109.3
C(4)-C(3)-C(2)	101.67(12)
C(4)-C(3)-H(3A)	111.4
C(4)-C(3)-H(3B)	111.4
C(1)-C(4)-C(3)	105.98(12)
C(1)-C(4)-C(5)	119.79(12)
C(1)-C(4)-C(6)	117.03(12)
C(3)-C(4)-C(6)	123.27(12)
C(5)-C(4)-C(3)	125.77(13)
C(5)-C(4)-C(6)	59.22(10)
C(4)-C(5)-H(5A)	117.6
C(4)-C(5)-H(5B)	117.6
C(4)-C(5)-C(6)	61.64(10)
H(5A)-C(5)-H(5B)	114.7
C(6)-C(5)-H(5A)	117.6
C(6)-C(5)-H(5B)	117.6
C(4)-C(6)-H(6)	115.3
C(5)-C(6)-C(4)	59.15(9)
C(5)-C(6)-H(6)	115.3
C(7)-C(6)-C(4)	118.30(11)
C(7)-C(6)-C(5)	121.87(13)
C(7)-C(6)-H(6)	115.3
C(8)-C(7)-C(6)	122.32(13)

C(12)-C(7)-C(6)	119.92(12)
C(12)-C(7)-C(8)	117.76(12)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-C(7)	120.91(13)
C(9)-C(8)-H(8)	119.5
C(8)-C(9)-H(9)	119.7
C(8)-C(9)-C(10)	120.51(12)
C(10)-C(9)-H(9)	119.7
O(3)-C(10)-C(9)	115.56(12)
O(3)-C(10)-C(11)	124.78(13)
C(9)-C(10)-C(11)	119.66(12)
C(10)-C(11)-H(11)	120.5
C(10)-C(11)-C(12)	119.08(13)
C(12)-C(11)-H(11)	120.5
C(7)-C(12)-H(12)	119.0
C(11)-C(12)-C(7)	122.07(12)
C(11)-C(12)-H(12)	119.0
O(3)-C(13)-H(13A)	109.5
O(3)-C(13)-H(13B)	109.5
O(3)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

Anisotropic displacement parameters ($Å^2 x 10^4$) for v18081. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	460(6)	716(8)	243(5)	68(5)	17(4)	-69(6)
O(2)	385(6)	434(6)	409(6)	-133(5)	24(5)	11(5)
O(3)	358(5)	344(5)	265(5)	-53(4)	-19(4)	60(4)
C(1)	276(7)	454(8)	265(7)	-33(6)	-11(5)	-46(6)
C(2)	377(8)	334(7)	536(10)	30(7)	-7(7)	25(6)
C(3)	355(7)	317(7)	290(7)	29(6)	4(6)	-78(6)
C(4)	301(6)	300(7)	227(6)	9(5)	2(5)	-28(5)
C(5)	435(8)	326(7)	361(8)	2(6)	-87(7)	51(6)
C(6)	366(7)	281(6)	276(7)	27(5)	-2(5)	-57(6)
C(7)	294(7)	238(6)	270(6)	-10(5)	-1(5)	-42(5)
C(8)	281(7)	301(6)	352(7)	-37(6)	-16(5)	51(6)
C(9)	290(6)	323(7)	306(7)	-79(6)	34(5)	49(6)
C(10)	287(6)	219(5)	268(6)	-24(5)	5(5)	-21(5)
C(11)	275(6)	245(6)	314(7)	-34(5)	8(5)	34(5)
C(12)	313(7)	279(6)	282(6)	-55(5)	53(5)	13(6)
C(13)	402(8)	349(7)	322(7)	-21(6)	-65(6)	54(7)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3})

	x	y	z	U(eq)
H(2A)	6007	1263	5778	50
H(2B)	3719	374	5645	50
H(3A)	1909	2804	5967	38
H(3B)	4043	3069	6332	38
H(5A)	2149	6668	6011	45
H(5B)	2836	7207	5368	45
H(6)	6506	6662	5570	37
H(8)	3954	7655	6777	37
H(9)	5187	7411	7679	37
H(11)	10021	4180	7164	33
H(12)	8733	4403	6263	35
H(13A)	11463	5467	7984	54
H(13B)	10216	3619	8098	54
H(13C)	10561	5038	8588	54

Torsion angles [°]

O(1)-C(1)-C(4)-C(3)	167.20(16)
O(1)-C(1)-C(4)-C(5)	17.4(2)
O(1)-C(1)-C(4)-C(6)	-50.9(2)
O(2)-C(1)-C(4)-C(3)	-13.05(16)
O(2)-C(1)-C(4)-C(5)	-162.88(14)
O(2)-C(1)-C(4)-C(6)	128.84(14)
O(2)-C(2)-C(3)-C(4)	-26.37(15)
O(3)-C(10)-C(11)-C(12)	-179.66(13)
C(1)-O(2)-C(2)-C(3)	20.00(16)
C(1)-C(4)-C(5)-C(6)	-105.57(14)
C(1)-C(4)-C(6)-C(5)	110.20(15)
C(1)-C(4)-C(6)-C(7)	-137.66(14)
C(2)-O(2)-C(1)-O(1)	175.36(15)
C(2)-O(2)-C(1)-C(4)	-4.41(16)
C(2)-C(3)-C(4)-C(1)	23.77(15)
C(2)-C(3)-C(4)-C(5)	171.26(14)
C(2)-C(3)-C(4)-C(6)	-115.10(15)
C(3)-C(4)-C(5)-C(6)	110.97(15)
C(3)-C(4)-C(6)-C(5)	-115.02(15)
C(3)-C(4)-C(6)-C(7)	-2.9(2)
C(4)-C(5)-C(6)-C(7)	-106.19(14)
C(4)-C(6)-C(7)-C(8)	-96.89(17)
C(4)-C(6)-C(7)-C(12)	82.66(17)
C(5)-C(4)-C(6)-C(7)	112.14(16)
C(5)-C(6)-C(7)-C(8)	-27.4(2)
C(5)-C(6)-C(7)-C(12)	152.10(14)

C(6)-C(7)-C(8)-C(9)	179.45(13)
C(6)-C(7)-C(12)-C(11)	-179.98(13)
C(7)-C(8)-C(9)-C(10)	0.6(2)
C(8)-C(7)-C(12)-C(11)	-0.4(2)
C(8)-C(9)-C(10)-O(3)	179.17(13)
C(8)-C(9)-C(10)-C(11)	-0.6(2)
C(9)-C(10)-C(11)-C(12)	0.1(2)
C(10)-C(11)-C(12)-C(7)	0.4(2)
C(12)-C(7)-C(8)-C(9)	-0.1(2)
C(13)-O(3)-C(10)-C(9)	-173.24(13)
C(13)-O(3)-C(10)-C(11)	6.5(2)

Identification code	v18091	
Empirical formula	C12 H11 Br O2	
Formula weight	267.12	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.3854(18) Å	α = 90°
	b = 6.702(2) Å	β = 90°
	c = 25.222(5) Å	γ = 90°
Volume	1079.4(5) $Å^3$	
Z	4	
Density (calculated)	1.644 g/cm^3	
Absorption coefficient	3.783 mm^{-1}	
F(000)	536	
Crystal size	0.30 x 0.26 x 0.14 mm^3	
Theta range for data collection	3.145 to 45.297°.	
Index ranges	-12 □ h □ 10, -13 □ k □ 13, -50 □ l □ 50	
Reflections collected	65957	
Independent reflections	8908 [R(int) = 0.0351]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8289	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8908 / 0 / 137	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0210, wR2 = 0.0533	
R indices (all data)	R1 = 0.0262, wR2 = 0.0542	
Absolute structure parameter [Flack]	0.028(4)	
Absolute structure parameter [Hooft]	0.046(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.633 and -0.799 e.$Å^{-3}$	

Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	17392(2)	65892(2)	53213(2)	250(1)
O(1)	123245(11)	14711(12)	73083(3)	224(1)
O(2)	92242(11)	13810(11)	77193(3)	186(1)
C(1)	104376(13)	13435(11)	72814(4)	159(1)
C(2)	70111(14)	13354(13)	75687(3)	173(1)
C(3)	69584(13)	5628(12)	69992(3)	153(1)
C(4)	91030(13)	11410(12)	68032(3)	143(1)
C(5)	100885(16)	5508(14)	62885(4)	208(2)
C(6)	94655(14)	26924(13)	63602(3)	168(1)
C(7)	75983(14)	35770(12)	60993(3)	156(1)
C(8)	63565(17)	25409(13)	57389(3)	212(2)
C(9)	45957(18)	34156(15)	55100(3)	226(2)
C(10)	40902(15)	53621(14)	56440(3)	178(1)
C(11)	52868(16)	64299(14)	60056(3)	204(1)
C(12)	70361(16)	55330(13)	62312(4)	194(1)

Bond lengths [Å] and angles [°].

Br(1)-C(10)	1.8954(10)
O(1)-C(1)	1.2098(11)
O(2)-C(1)	1.3494(11)
O(2)-C(2)	1.4636(11)
C(1)-C(4)	1.4831(12)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.5273(12)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.5066(12)
C(4)-C(5)	1.4958(12)
C(4)-C(6)	1.5437(12)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(5)-C(6)	1.5004(14)
C(6)-H(6)	1.0000
C(6)-C(7)	1.4854(13)
C(7)-C(8)	1.3918(12)
C(7)-C(12)	1.3994(13)
C(8)-H(8)	0.9500
C(8)-C(9)	1.3933(15)
C(9)-H(9)	0.9500
C(9)-C(10)	1.3859(14)
C(10)-C(11)	1.3884(13)
C(11)-H(11)	0.9500

C(11)-C(12)	1.3903(14)
C(12)-H(12)	0.9500
C(1)-O(2)-C(2)	109.97(7)
O(1)-C(1)-O(2)	121.65(8)
O(1)-C(1)-C(4)	128.63(9)
O(2)-C(1)-C(4)	109.72(7)
O(2)-C(2)-H(2A)	110.6
O(2)-C(2)-H(2B)	110.6
O(2)-C(2)-C(3)	105.81(7)
H(2A)-C(2)-H(2B)	108.7
C(3)-C(2)-H(2A)	110.6
C(3)-C(2)-H(2B)	110.6
C(2)-C(3)-H(3A)	111.4
C(2)-C(3)-H(3B)	111.4
H(3A)-C(3)-H(3B)	109.3
C(4)-C(3)-C(2)	101.61(7)
C(4)-C(3)-H(3A)	111.4
C(4)-C(3)-H(3B)	111.4
C(1)-C(4)-C(3)	106.20(7)
C(1)-C(4)-C(5)	119.22(8)
C(1)-C(4)-C(6)	116.15(7)
C(3)-C(4)-C(6)	123.16(7)
C(5)-C(4)-C(3)	126.80(8)
C(5)-C(4)-C(6)	59.14(6)
C(4)-C(5)-H(5A)	117.6
C(4)-C(5)-H(5B)	117.6
C(4)-C(5)-C(6)	62.02(5)
H(5A)-C(5)-H(5B)	114.7
C(6)-C(5)-H(5A)	117.6
C(6)-C(5)-H(5B)	117.6
C(4)-C(6)-H(6)	115.2
C(5)-C(6)-C(4)	58.84(6)
C(5)-C(6)-H(6)	115.2
C(7)-C(6)-C(4)	117.98(7)
C(7)-C(6)-C(5)	122.77(8)
C(7)-C(6)-H(6)	115.2
C(8)-C(7)-C(6)	123.20(8)
C(8)-C(7)-C(12)	118.46(8)
C(12)-C(7)-C(6)	118.32(8)
C(7)-C(8)-H(8)	119.3
C(7)-C(8)-C(9)	121.36(8)
C(9)-C(8)-H(8)	119.3
C(8)-C(9)-H(9)	120.6
C(10)-C(9)-C(8)	118.88(8)

C(10)-C(9)-H(9)	120.6
C(9)-C(10)-Br(1)	119.22(7)
C(9)-C(10)-C(11)	121.16(9)
C(11)-C(10)-Br(1)	119.62(7)
C(10)-C(11)-H(11)	120.4
C(10)-C(11)-C(12)	119.21(8)
C(12)-C(11)-H(11)	120.4
C(7)-C(12)-H(12)	119.5
C(11)-C(12)-C(7)	120.92(8)
C(11)-C(12)-H(12)	119.5

Anisotropic displacement parameters ($Å^2 x\ 10^4$).The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	266(1)	293(1)	192(1)	-60(1)	-45(1)	80(1)
O(1)	99(2)	206(3)	368(3)	-24(3)	-25(2)	10(2)
O(2)	135(2)	225(3)	197(2)	-7(2)	-21(2)	8(2)
C(1)	108(3)	128(3)	240(3)	-10(2)	-9(2)	15(2)
C(2)	119(3)	200(3)	199(3)	-11(2)	15(2)	4(2)
C(3)	112(3)	163(3)	184(3)	4(2)	0(2)	-17(2)
C(4)	106(3)	133(2)	190(3)	-20(2)	17(2)	4(2)
C(5)	193(4)	189(3)	243(3)	-64(3)	61(3)	31(3)
C(6)	158(3)	155(3)	191(3)	-16(2)	44(2)	-10(2)
C(7)	185(3)	139(3)	144(2)	-13(2)	26(2)	-17(2)
C(8)	288(5)	165(3)	183(3)	-48(2)	-29(3)	10(3)
C(9)	292(4)	201(3)	185(3)	-56(3)	-53(3)	10(3)
C(10)	210(4)	191(3)	132(2)	-14(2)	4(2)	4(3)
C(11)	240(4)	172(3)	199(3)	-44(3)	-20(3)	20(3)
C(12)	223(4)	152(3)	208(3)	-46(2)	-27(3)	-2(3)

Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^{\ 3}$)

	x	y	z	U(eq)
H(2A)	6394	2688	7589	21
H(2B)	6215	437	7806	21
H(3A)	6754	-901	6988	18
H(3B)	5842	1220	6790	18
H(5A)	9244	-270	6042	25
H(5B)	11603	235	6291	25
H(6)	10651	3638	6423	20
H(8)	6717	1210	5647	25
H(9)	3756	2690	5266	27
H(11)	4914	7758	6098	24
H(12)	7861	6258	6478	23

Torsion angles [°].

Br(1)-C(10)-C(11)-C(12)	-178.54(7)
O(1)-C(1)-C(4)-C(3)	166.97(9)
O(1)-C(1)-C(4)-C(5)	15.64(14)
O(1)-C(1)-C(4)-C(6)	-52.01(12)
O(2)-C(1)-C(4)-C(3)	-13.27(8)
O(2)-C(1)-C(4)-C(5)	-164.60(7)
O(2)-C(1)-C(4)-C(6)	127.74(8)
O(2)-C(2)-C(3)-C(4)	-25.22(8)
C(1)-O(2)-C(2)-C(3)	18.71(9)
C(1)-C(4)-C(5)-C(6)	-104.72(9)
C(1)-C(4)-C(6)-C(5)	109.89(9)
C(1)-C(4)-C(6)-C(7)	-136.85(8)
C(2)-O(2)-C(1)-O(1)	176.24(8)
C(2)-O(2)-C(1)-C(4)	-3.54(9)
C(2)-C(3)-C(4)-C(1)	23.17(8)
C(2)-C(3)-C(4)-C(5)	171.64(8)
C(2)-C(3)-C(4)-C(6)	-114.41(8)
C(3)-C(4)-C(5)-C(6)	110.41(9)
C(3)-C(4)-C(6)-C(5)	-116.31(9)
C(3)-C(4)-C(6)-C(7)	-3.04(11)
C(4)-C(5)-C(6)-C(7)	-105.24(9)
C(4)-C(6)-C(7)-C(8)	-73.84(11)
C(4)-C(6)-C(7)-C(12)	104.74(9)
C(5)-C(4)-C(6)-C(7)	113.27(9)
C(5)-C(6)-C(7)-C(8)	-4.62(13)
C(5)-C(6)-C(7)-C(12)	173.96(8)
C(6)-C(7)-C(8)-C(9)	178.86(8)
C(6)-C(7)-C(12)-C(11)	-179.07(8)
C(7)-C(8)-C(9)-C(10)	0.39(15)
C(8)-C(7)-C(12)-C(11)	-0.42(13)
C(8)-C(9)-C(10)-Br(1)	178.41(7)
C(8)-C(9)-C(10)-C(11)	-0.94(15)
C(9)-C(10)-C(11)-C(12)	0.80(14)
C(10)-C(11)-C(12)-C(7)	-0.11(14)
C(12)-C(7)-C(8)-C(9)	0.28(14)

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Identification code	V18160	
Empirical formula	C10 H9 Br O2 S	
Formula weight	273.14	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 5.7304(6) Å	α = 90°.
	b = 8.3275(7) Å	β = 92.034(3)°.
	c = 10.4712(8) Å	γ = 90°.
Volume	499.37(8) $Å^3$	
Z	2	
Density (calculated)	1.817 Mg/m^3	
Absorption coefficient	4.292 mm^{-1}	
F(000)	272	
Crystal size	0.250 x 0.150 x 0.150 mm^3	
Theta range for data collection	3.126 to 36.330°.	
Index ranges	-9 □□h □□9, -13 □□k □□13, -17 □□l □□17	
Reflections collected	13036	
Independent reflections	4669 [R(int) = 0.0244]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7471 and 0.6420	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4669 / 1 / 127	
Goodness-of-fit on F^2	0.859	
Final R indices [I>2sigma(I)]	R1 = 0.0163, wR2 = 0.0408	
R indices (all data)	R1 = 0.0175, wR2 = 0.0412	
Absolute structure parameter	0.030(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.388 and -0.336 e.$Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-410(1)	7451(1)	5386(1)	15(1)

C(1)	1597(3)	5952(2)	6234(1)	11(1)
C(2)	943(3)	5327(2)	7400(1)	11(1)
C(3)	2405(3)	4226(2)	8025(1)	12(1)
C(4)	4479(3)	3732(2)	7481(1)	11(1)
C(7)	4757(3)	763(2)	8778(1)	12(1)
C(8)	3062(3)	1156(2)	9829(1)	13(1)
O(1)	1071(2)	323(1)	9628(1)	16(1)
O(2)	3351(2)	2043(1)	10722(1)	17(1)
C(9)	1301(3)	-792(2)	8561(1)	18(1)
C(10)	3228(3)	-91(2)	7767(1)	15(1)
S(1)	6517(1)	2424(1)	8263(1)	14(1)
C(5)	5095(3)	4377(2)	6309(1)	13(1)
C(6)	3667(3)	5505(2)	5686(1)	13(1)

Bond lengths [Å] and angles [°].

Br(1)-C(1)	1.8960(14)
C(1)-C(6)	1.387(2)
C(1)-C(2)	1.3914(18)
C(2)-C(3)	1.390(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.398(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3965(18)
C(4)-S(1)	1.7759(14)
C(7)-C(10)	1.526(2)
C(7)-C(8)	1.5290(19)
C(7)-S(1)	1.8053(14)
C(7)-H(7)	1.0000
C(8)-O(2)	1.1990(17)
C(8)-O(1)	1.3454(19)
O(1)-C(9)	1.4619(18)
C(9)-C(10)	1.522(2)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(5)-C(6)	1.393(2)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(6)-C(1)-C(2)	121.55(13)
C(6)-C(1)-Br(1)	119.79(10)
C(2)-C(1)-Br(1)	118.67(10)
C(3)-C(2)-C(1)	118.93(13)
C(3)-C(2)-H(2)	120.5

C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	120.62(12)
C(2)-C(3)-H(3)	119.7
C(4)-C(3)-H(3)	119.7
C(5)-C(4)-C(3)	119.36(12)
C(5)-C(4)-S(1)	117.27(11)
C(3)-C(4)-S(1)	123.19(10)
C(10)-C(7)-C(8)	103.61(12)
C(10)-C(7)-S(1)	117.60(9)
C(8)-C(7)-S(1)	115.28(9)
C(10)-C(7)-H(7)	106.5
C(8)-C(7)-H(7)	106.5
S(1)-C(7)-H(7)	106.5
O(2)-C(8)-O(1)	122.22(13)
O(2)-C(8)-C(7)	128.28(15)
O(1)-C(8)-C(7)	109.50(12)
C(8)-O(1)-C(9)	110.37(11)
O(1)-C(9)-C(10)	105.12(12)
O(1)-C(9)-H(9A)	110.7
C(10)-C(9)-H(9A)	110.7
O(1)-C(9)-H(9B)	110.7
C(10)-C(9)-H(9B)	110.7
H(9A)-C(9)-H(9B)	108.8
C(9)-C(10)-C(7)	102.09(11)
C(9)-C(10)-H(10A)	111.4
C(7)-C(10)-H(10A)	111.4
C(9)-C(10)-H(10B)	111.4
C(7)-C(10)-H(10B)	111.4
H(10A)-C(10)-H(10B)	109.2
C(4)-S(1)-C(7)	104.02(7)
C(6)-C(5)-C(4)	120.52(13)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(1)-C(6)-C(5)	118.99(12)
C(1)-C(6)-H(6)	120.5
C(5)-C(6)-H(6)	120.5

Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	14(1)	15(1)	15(1)	5(1)	-1(1)	1(1)
C(1)	12(1)	9(1)	12(1)	1(1)	-1(1)	-1(1)
C(2)	11(1)	11(1)	12(1)	1(1)	1(1)	0(1)
C(3)	13(1)	12(1)	12(1)	1(1)	2(1)	1(1)
C(4)	11(1)	9(1)	13(1)	1(1)	0(1)	-1(1)

C(7)	13(1)	11(1)	14(1)	1(1)	2(1)	1(1)
C(8)	14(1)	10(1)	14(1)	3(1)	1(1)	2(1)
O(1)	15(1)	15(1)	17(1)	-1(1)	4(1)	-2(1)
O(2)	22(1)	15(1)	14(1)	-2(1)	2(1)	0(1)
C(9)	18(1)	16(1)	19(1)	-2(1)	2(1)	-4(1)
C(10)	18(1)	14(1)	14(1)	-1(1)	2(1)	-2(1)
S(1)	10(1)	13(1)	19(1)	3(1)	0(1)	0(1)
C(5)	11(1)	13(1)	14(1)	0(1)	3(1)	0(1)
C(6)	14(1)	14(1)	12(1)	1(1)	2(1)	-1(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}).

	x	y	z	U(eq)
H(2)	-480	5647	7763	14
H(3)	1991	3806	8830	14
H(7)	5865	-60	9140	15
H(9A)	-182	-867	8050	21
H(9B)	1734	-1877	8876	21
H(10A)	2591	673	7119	18
H(10B)	4105	-946	7335	18
H(5)	6500	4043	5934	15
H(6)	4104	5962	4899	16

Torsion angles [°].

C(6)-C(1)-C(2)-C(3)	-0.1(2)
Br(1)-C(1)-C(2)-C(3)	179.91(10)
C(1)-C(2)-C(3)-C(4)	-1.2(2)
C(2)-C(3)-C(4)-C(5)	1.1(2)
C(2)-C(3)-C(4)-S(1)	176.16(11)
C(10)-C(7)-C(8)-O(2)	-166.83(14)
S(1)-C(7)-C(8)-O(2)	-36.93(19)
C(10)-C(7)-C(8)-O(1)	13.60(15)
S(1)-C(7)-C(8)-O(1)	143.51(10)
O(2)-C(8)-O(1)-C(9)	-173.56(13)
C(7)-C(8)-O(1)-C(9)	6.04(15)
C(8)-O(1)-C(9)-C(10)	-23.45(16)
O(1)-C(9)-C(10)-C(7)	30.25(15)
C(8)-C(7)-C(10)-C(9)	-26.25(14)
S(1)-C(7)-C(10)-C(9)	-154.73(11)
C(5)-C(4)-S(1)-C(7)	-134.75(11)
C(3)-C(4)-S(1)-C(7)	50.10(13)
C(10)-C(7)-S(1)-C(4)	54.59(12)
C(8)-C(7)-S(1)-C(4)	-68.13(12)
C(3)-C(4)-C(5)-C(6)	0.2(2)
S(1)-C(4)-C(5)-C(6)	-175.13(11)

C(2)-C(1)-C(6)-C(5)	1.4(2)
Br(1)-C(1)-C(6)-C(5)	-178.62(11)
C(4)-C(5)-C(6)-C(1)	-1.4(2)

VIII. Computational Study

All DFT calculations were performed with the Gaussian 09 software package (*7*). Geometry optimizations of all the minima and transition states were carried out at the B3LYP (*8*) level of theory with the LANL2DZ basis set (*9*) for Fe and the 6-31G(d) basis set for the other atoms. Vibrational frequencies were computed at the same level to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K, and to check whether each optimized structure is a transition state or not. The single-point energies were computed at the same level of theory combined with def2-TZVP (*9*) basis set using the optimized structures. The 3D diagrams of molecules were generated using CYLView (*10*). For clarity, all the C–H bonds are omitted in the 3D diagrams of molecules. In addition, to correct the Gibbs free energies under pressure of 1 atm to the standard state in solution (1 mol/L), a correction of $R\mathrm{T}\ln(c_s/c_g)$ (about 1.9 kcal/mol) is added to energies of all species except carbon dioxide. c_s is the standard molar concentration in solution (1 mol/L), c_g is the standard molar concentration in gas phase (0.0446 mol/L), and R is the gas constant. However, no solvation energies were introduced. In addition, the stabilities of the wavefunctions for each structure were all confirmed. Some spin states that are difficult to converge were subjected to a higher numerical accuracy for the integral of DFT. For some high energy transition states that are difficult to locate were subjected to a loose convergence threshold.

Figure S7. The Gibbs free energy changes of the deprotonation at B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ level.

The deprotonation of neutral species **cat3** and **cat4** are even more exothermic than the deprotonation of AcOH by 16.1 kcal/mol and 13.3 kcal/mol, respectively. Both the S–H bond and the O–H bond should be deprotonated under the reaction conditions. Thus, only the anionic species were considered in the calculations.

Table S3. Free energies for **cat1**, **cat2**, **cat3** and **cat4** at B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ level with all the located spin states given in parentheses. The free energies of the most stable spin states are given in crimson and bold. CSS is closed-shell singlet and OSS is open-shell singlet.

Structure	$\Delta\Delta G$ (kcal/mol)
cat1(*CSS*)	16.4
cat1(*OSS*)	14.1

cat1(*triplet*)	8.9
cat1(*quintet*)	**0.0**
cat2(*CSS*)	23.2
cat2(*OSS*)	20.6
cat2(*triplet*)	12.5
cat2(*quintet*)	**0.0**
cat3(CSS)	17.5
cat3(OSS)	15.5
cat3(triplet)	**0.0**
cat3(quintet)	8.6
cat4(CSS)	19.5
cat4(OSS)	10.8
cat4(triplet)	**0.0**
cat4(quintet)	1.7

Figure S8. Scheme of orbital changes for alpha and beta electrons in radical recombination processes.

Since the free doublet species could have very fast spin flips, the recombination would give either triplet or OSS states without any system cross-over. This accounts for the changes of spin states from **TS2** to **int3**, **int3** to **TS4**, **TS9** to **int10** and **int10** to **TS11**, where PhS• is generated and then recombined with **int3** or **int10**.

Table S4. Relative free energies for the most favorable reaction pathway of S–H bond insertion at B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ level with all the located

spin states given in parentheses. The free energies of the most stable spin states are given in crimson and bold. CSS is closed-shell singlet and OSS is open-shell singlet.

Structure	ΔG (kcal/mol)
cat1(*CSS*)	16.4
cat1(*OSS*)	14.1
cat1(*triplet*)	8.9
cat1(*quintet*)	**0.0**
cat2(*CSS*)	23.2
cat2(*OSS*)	20.6
cat2(*triplet*)	12.5
cat2(*quintet*)	**0.0**
int1(*CSS*)	8.2
int1(*OSS*)	**0.0**
int1(*triplet*)	1.9
int1(*quintet*)	30.1
TS2(*CSS*)	28.7
TS2(*OSS*)	19.7
TS2(*triplet*)	**19.4**
TS2(*quintet*)	59.3
int3(*doublet*)	**−6.1**
int3(*quartet*)	8.7
int3(*sextet*)	2.7
TS4(*CSS*)	*nonexistent*
TS4(*OSS*)	**0.3**
TS4(*triplet*)	1.7
TS4(*quintet*)	9.8
int5(*CSS*)	
TS6(*doublet*)	8.8
TS6(*quartet*)	5.2
TS6(*sextet*)	**4.0**
int7(*doublet*)	
int8(*CSS*)	9.1
int8(*OSS*)	**0.0**
int8(*triplet*)	1.8
int8(*quintet*)	11.8
TS9(*CSS*)	31.5
TS9(*OSS*)	19.1
TS9(*triplet*)	**18.5**
TS9(*quintet*)	34.9
int10(*doublet*)	**−5.4**
int10(*quartet*)	3.1

int10(*sextet*)	10.6
TS11(*CSS*)*	23.5
TS11(*OSS*)	4.7
TS11(*triplet*)	**1.7**
TS11(*quintet*)	*nonexistent*
TS12(*doublet*)*	3.5
TS12(*quartet*)	4.2
TS12(*sextet*)	**0.6**

*This species is a saddle point only with loose convergence threshold.

Alternative reaction pathways

For some alternative reaction pathways, we have also considered direct C–S bond formation processes. The pathway featuring attack of neutral PhSH on carbenoid carbon is shown in Table S5. The pathway featuring attack of anionic PhS^- on carbenoid carbon is shown in Table S6. The proton transfer between **cat1**/**cat2** and PhSH is unfavorable as shown below in **Figure S9**. Thus, the C–S bond formation with **cat3** and **cat4** are unfavorable.

Figure S9. Free energy changes for proton transfer between PhSH and **cat1** or **cat2**.

Table S5. Free energy for the alternative pathway of S–H bond insertion featuring attack of neutral PhSH on carbenoid carbon at B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ level. Spin states are given in parentheses. CSS is closed-shell singlet and OSS is open-shell singlet.

Structure	$\Delta G^{\ddagger}$ (kcal/mol)
TS-S1(*CSS*)	37.1
TS-S1(*OSS*)	**35.3**
TS-S1(*triplet*)	38.4
TS-S1(*quintet*)	38.6
TS-S2(*CSS*)	39.6
TS-S2(*OSS*)	**36.0**
TS-S2(*triplet*)	39.0
TS-S2(*quintet*)	44.8

Table S6. Free energy for the alternative pathway of S–H bond insertion attack of anionic PhS^{-} on carbenoid on carbenoid carbon at B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ level. Spin states are given in parentheses. CSS is closed-shell singlet and OSS is open-shell singlet.

Structure	$\Delta G^{\ddagger}$ (kcal/mol)
TS-S3(*CSS*)	66.9
TS-S3(*OSS*)	**66.0**
TS-S3(*triplet*)	76.5
TS-S3(*quintet*)	102.6
TS-S5(*CSS*)	71.8
TS-S5(*OSS*)	**70.8**
TS-S5(*triplet*)	78.0
TS-S5(*quintet*)	74.4

Figure S10. Free energy for the most favorable reaction pathway of C=C bond insertion at B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ. The most stable spin states are shown in parentheses.

Figure S11. Comparison between open-chain carbenoid species (**intS5**) and **int1** (**int8**). The geometries of **intS5** were taken from ref (*11*). CSS is closed-shell singlet and OSS is open-shell singlet.

As shown above, from the highlighted dihedral angle $d_{(\text{Fe-C-C-O})}$, we could deduct that $d_{(\text{Fe-C-C-O})}$ for CSS and OSS should be ~90 degrees and $d_{(\text{Fe-C-C-O})}$ for triplet should be ~0 degree if there were no ring (**intS5**). However, in **int1** and **int8**, the 5-membered ring system locks the $d_{(\text{Fe-C-C-O})}$ to less than 20 degrees. The near-planar geometry featuring small $d_{(\text{Fe-C-C-O})}$ makes the CSS state much less stable due to strong repulsion between fully occupied orbitals. Since the OSS ground states are distorted from the open chain structure, the triplet states are much less unstable compared to OSS states.

Table S7. Free energy for the alternative pathway of C=C bond insertion at B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ level. Spin states are given in parentheses. The free energies of the most stable spin states are given in crimson and bold. CSS is closed-shell singlet and OSS is open-shell singlet.

Structure	$\Delta G^{\ddagger}$ (kcal/mol)
TS-S6(*CSS*)	38.6
TS-S6(*OSS*)	**27.5**
TS-S6(*triplet*)	28.1
TS-S6(*quintet*)	36.9
TS-S8(*CSS*)	32.4
TS-S8(*OSS*)	**28.5**
TS-S8(*triplet*)	28.6
TS-S8(*quintet*)	37.4

Figure S12. Fast rotation around the Fe–C bond in **int3** and **int10**. However, this has no effect on the outcome of the reaction.

Table S8. Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the B3LYP/def2-TZVP//B3LYP/6-31G(d)-LANL2DZ level of theory. Spin states are shown in parentheses. CSS is closed-shell singlet and OSS is open-shell singlet.

Structures	*ZPE*	*TCH*	*TCG*	*E*	*H*	*G*	Imaginary Frequency	Wavefunction Stability
PhSH	0.099565	0.106841	0.068779	-630.555739	-630.448898	-630.486960		YES
PhS$^{\bullet}$	0.090881	0.09738	0.060411	-629.924107	-629.826727	-629.863696		YES
PhS^{-}	0.089769	0.096258	0.060647	-630.001929	-629.905671	-629.941282		YES
styrene	0.133748	0.141462	0.102269	-309.7652918	-309.6238298	-309.6630228		YES
cat1(*CSS*)	0.312832	0.335171	0.263437	-2690.768900	-2690.433729	-2690.505463		NO
cat1(*OSS*)	0.312288	0.334919	0.262209	-2690.771256	-2690.436337	-2690.509047		YES
cat1(*triplet*)	0.311635	0.334641	0.259023	-2690.776470	-2690.441829	-2690.517447		YES
cat1(*quintet*)	0.310109	0.333639	0.256437	-2690.788008	-2690.454369	-2690.531571		YES
cat2(*CSS*)	0.314599	0.336273	0.266394	-2367.775535	-2367.439262	-2367.509141		NO
cat2(*OSS*)	0.313874	0.335844	0.265271	-2367.778552	-2367.442708	-2367.513281		YES
cat2(*triplet*)	0.312866	0.335253	0.261854	-2367.788142	-2367.452889	-2367.526288		YES
cat2(*quintet*)	0.311539	0.334670	0.258026	-2367.804157	-2367.469487	-2367.546131		YES
cat3(*CSS*)	0.324797	0.347238	0.275488	-2691.307313	-2690.960075	-2691.031825		NO
cat3(*OSS*)	0.324852	0.347289	0.275529	-2691.310548	-2690.963259	-2691.035019		YES
cat3(*triplet*)	0.323129	0.346732	0.267883	-2691.327576	-2690.980844	-2691.059693		YES
cat3(*quintet*)	0.321413	0.345223	0.267378	-2691.313396	-2690.968173	-2691.046018		YES
cat4(*CSS*)	0.330261	0.352278	0.281629	-2368.329256	-2367.976978	-2368.047627		NO
cat4(*OSS*)	0.329114	0.351700	0.279402	-2368.340924	-2367.989224	-2368.061522		YES
cat4(*triplet*)	0.328745	0.351628	0.277027	-2368.355793	-2368.004165	-2368.078766		YES
cat4(*quintet*)	0.326950	0.350190	0.274416	-2368.350463	-2368.000273	-2368.076047		YES
water	0.021139	0.024918	0.003473	-76.462904	-76.437986	-76.459431		YES
OH^{-}	0.007696	0.011001	-0.008602	-75.810759	-75.799758	-75.819361		YES
AcOH	0.062048	0.067548	0.034855	-229.189174	-229.121626	-229.154319		YES
AcO^{-}	0.048296	0.053696	0.020653	-228.621085	-228.567389	-228.600432		YES
int1(*CSS*)	0.389208	0.417377	0.333216	-2996.112258	-2995.694881	-2995.779042		NO
int1(*OSS*)	0.388726	0.417064	0.332431	-2996.124541	-2995.707477	-2995.792110		YES
int1(*triplet*)	0.388490	0.416950	0.331036	-2996.120050	-2995.703100	-2995.789014		YES

int1(*quintet*)	0.384672	0.413769	0.325539	-2996.069716	-2995.655947	-2995.744177		YES
TS2(*CSS*)	0.487418	0.522582	0.421274	-3626.651588	-3626.129006	-3626.230314	859.9*i*	NO
TS2(*OSS*)	0.487053	0.522412	0.420763	-3626.665478	-3626.143066	-3626.244715	846.4*i*	YES
TS2(*triplet*)	0.486811	0.522325	0.419128	-3626.664221	-3626.141896	-3626.245093	750.6*i*	YES
TS2(*quintet*)	0.482982	0.519081	0.414520	-3626.596057	-3626.076976	-3626.181537	937.0*i*	YES
int3(*doublet*)	0.401757	0.430060	0.344878	-2996.770402	-2996.340342	-2996.425524		YES
int3(*quartet*)	0.398325	0.427092	0.340666	-2996.742233	-2996.315141	-2996.401567		YES
int3(*sextet*)	0.397719	0.427494	0.336072	-2996.747131	-2996.319637	-2996.411059		YES
TS4(*CSS*)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
TS4(*OSS*)	0.491967	0.528196	0.420370	-3626.695906	-3626.167710	-3626.275536	31.5*i*	YES
TS4(*triplet*)	0.492603	0.528424	0.422647	-3626.695940	-3626.167516	-3626.273293	133.4*i*	YES
TS4(*quintet*)	0.489739	0.526263	0.417219	-3626.677687	-3626.151424	-3626.260468	130.6*i*	YES
int5(*CSS*)	0.181549	0.193751	0.142653	-935.963945	-935.770194	-935.821292		YES
TS6(*doublet*)	0.397396	0.427014	0.332654	-2996.734011	-2996.306997	-2996.401357	12.5*i*	YES
TS6(*quartet*)	0.398155	0.427253	0.337555	-2996.744658	-2996.317405	-2996.407103	84.7*i*	YES
TS6(*sextet*)	0.397579	0.426545	0.337813	-2996.746801	-2996.320256	-2996.408988	55.1*i*	YES
int7(*doublet*)	0.084727	0.091054	0.054648	-305.960902	-305.869848	-305.906254		YES
int8(*CSS*)	0.391169	0.418605	0.336572	-2673.126866	-2672.708261	-2672.790294		NO
int8(*OSS*)	0.390703	0.418368	0.335533	-2673.140278	-2672.721910	-2672.804745		YES
int8(*triplet*)	0.390603	0.418385	0.334095	-2673.136020	-2672.717635	-2672.801925		YES
int8(*quintet*)	0.388598	0.416853	0.331060	-2673.117061	-2672.700208	-2672.786001		YES
TS9(*CSS*)	0.489764	0.524072	0.425536	-3303.664052	-3303.139980	-3303.238516	882.2*i*	NO
TS9(*OSS*)	0.489050	0.523822	0.422790	-3303.681015	-3303.157193	-3303.258225	882.8*i*	YES
TS9(*triplet*)	0.488931	0.523792	0.421449	-3303.680704	-3303.156912	-3303.259255	775.1*i*	YES
TS9(*quintet*)	0.486802	0.522164	0.418498	-3303.651605	-3303.129441	-3303.233107	834.0*i*	YES
int10(*doublet*)	0.403946	0.431540	0.348208	-2673.785102	-2673.353562	-2673.436894		YES
int10(*quartet*)	0.401198	0.429599	0.343652	-2673.766797	-2673.337198	-2673.423145		YES
int10(*sextet*)	0.397274	0.426154	0.339085	-2673.750250	-2673.324096	-2673.411165		YES
TS11(*CSS*)	0.495026	0.529421	0.429492	-3303.680701	-3303.151280	-3303.251209		YES
TS11(*OSS*)	0.495129	0.530277	0.426793	-3303.708000	-3303.177723	-3303.281207	24.3*i*	YES
TS11(*triplet*)	0.494616	0.530081	0.423382	-3303.709307	-3303.179226	-3303.285925	83.2*i*	YES
TS11(*quintet*)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
TS12(*doublet*)	0.398567	0.427634	0.335442	-2673.757876	-2673.330242	-2673.422434	30.0*i*	YES
TS12(*quartet*)	0.398968	0.427535	0.339974	-2673.761357	-2673.333822	-2673.421383	138.8*i*	YES
TS12(*sextet*)	0.398982	0.427468	0.339813	-2673.766929	-2673.339461	-2673.427116	103.7*i*	YES
TS[PhS$^{\cdot}$+ **int7**](*OSS*)	0.176457	0.189643	0.133617	-935.888802	-935.699159	-935.755185	26.2*i*	YES
TS-S1(*CSS*)	0.491204	0.525873	0.427356	-3626.644277	-3626.118404	-3626.216921	218.5*i*	NO
TS-S1(*OSS*)	0.490983	0.525675	0.426958	-3626.646686	-3626.121011	-3626.219728	353.3*i*	YES
TS-S1(*triplet*)	0.489178	0.524216	0.423270	-3626.638109	-3626.113893	-3626.214839	306.1*i*	YES
TS-S1(*quintet*)	0.486723	0.523018	0.416632	-3626.631152	-3626.108134	-3626.214520	243.4*i*	YES
TS-S2(*CSS*)	0.493081	0.527030	0.430061	-3303.655686	-3303.128656	-3303.225625	227.1*i*	NO
TS-S2(*OSS*)	0.492880	0.526833	0.429930	-3303.661332	-3303.134499	-3303.231402	254.3*i*	YES
TS-S2(*triplet*)	0.491678	0.525938	0.426974	-3303.653521	-3303.127583	-3303.226547	291.0*i*	YES
TS-S2(*quintet*)	0.487138	0.523500	0.415582	-3303.632896	-3303.109396	-3303.217314	285.5*i*	YES
TS-S3(*CSS*)	0.478411	0.513413	0.411693	-3626.035405	-3625.521992	-3625.623712	57.9*i*	NO
TS-S3(*OSS*)	0.478086	0.513157	0.411130	-3626.036010	-3625.522853	-3625.624880	159.9*i*	YES
TS-S3(*triplet*)	0.475902	0.511450	0.407151	-3626.015576	-3625.504126	-3625.608425	257.0*i*	YES
TS-S3(*quintet*)	0.474107	0.510747	0.401227	-3625.968140	-3625.457393	-3625.566913	53.4*i*	YES
TS-S5(*CSS*)	0.479840	0.514047	0.415237	-3303.043882	-3302.529835	-3302.628645	76.5*i*	NO
TS-S5(*OSS*)	0.479365	0.513674	0.414670	-3303.044918	-3302.531244	-3302.630248	188.1*i*	YES
TS-S5(*triplet*)	0.478050	0.512821	0.410782	-3303.029503	-3302.516682	-3302.618721	240.9*i*	YES
TS-S5(*quintet*)	0.475331	0.511149	0.405002	-3303.029376	-3302.518227	-3302.624374	97.2*i*	YES
TS-S6(*CSS*)	0.525279	0.560523	0.460120	-3305.850697	-3305.290174	-3305.390577	328.4*i*	NO
TS-S6(*OSS*)	0.523964	0.559632	0.457423	-3305.865724	-3305.306092	-3305.408301	455.4*i*	YES
TS-S6(*triplet*)	0.524047	0.559805	0.455873	-3305.863279	-3305.303474	-3305.407406	351.6*i*	YES
TS-S6(*quintet*)	0.521335	0.557789	0.451977	-3305.845370	-3305.287581	-3305.393393	385.4*i*	YES

S7	0.214343	0.226765	0.174989	-615.169188	-614.942423	-614.994199		YES
TS-S8(*CSS*)	0.526924	0.561371	0.463459	-2982.876588	-2982.315217	-2982.413129	341.3*i*	NO
TS-S8(*OSS*)	0.526529	0.561318	0.462104	-2982.881381	-2982.320063	-2982.419277	452.2*i*	YES
TS-S8(*triplet*)	0.526373	0.561284	0.460797	-2982.880001	-2982.318717	-2982.419204	421.0*i*	YES
TS-S8(*quintet*)	0.524074	0.559590	0.456520	-2982.861668	-2982.302078	-2982.405148	379.9*i*	YES
TS-S9(*doublet*)	0.401707	0.429089	0.347159	-2996.768472	-2996.339383	-2996.421313	25.4*i*	YES
S10(*doublet*)	0.401811	0.430059	0.345209	-2996.770366	-2996.340307	-2996.425157		YES
TS-S11(*doublet*)	0.403884	0.430571	0.350378	-2673.783058	-2673.352487	-2673.432680	25.6*i*	YES
S12(*doublet*)	0.403963	0.431498	0.348632	-2673.785232	-2673.353734	-2673.436600		YES

Coordinates of all the calculated structures

PhSH

S	2.29361100	-0.08358800	0.00001400
C	0.50739500	0.00001100	0.00000500
C	-0.19593500	1.21136000	-0.00000200
C	-0.20121200	-1.20961900	-0.00001200
C	-1.59154500	1.20804000	0.00000000
H	0.34053900	2.15649300	-0.00001000
C	-1.59541700	-1.20214200	-0.00000600
H	0.33642100	-2.15405500	-0.00007500
C	-2.29833500	0.00466400	0.00001100
H	-2.12514900	2.15489800	-0.00003000
H	-2.13310700	-2.14658200	0.00000300
H	-3.38446400	0.00677500	0.00004100
H	2.51826400	1.24598500	-0.00012900

$PhS^{\bullet}$

S	-2.30558500	-0.00002800	0.00001300
C	-0.57855800	-0.00042400	0.00000900
C	0.14939200	1.22010300	-0.00000100
C	0.15031800	-1.22066000	0.00000100
C	1.53796000	1.21581600	-0.00001000
H	-0.40391500	2.15370400	0.00000000
C	1.53863400	-1.21541600	-0.00001000
H	-0.40279200	-2.15437800	0.00000400
C	2.23624900	0.00049700	-0.00001500
H	2.08393000	2.15512700	-0.00001500
H	2.08528900	-2.15434100	-0.00001600
H	3.32286600	0.00083700	-0.00002500

PhS^{-}

C	0.00000000	0.00000000	0.59897200
C	0.00000000	1.20120600	-0.16468600
C	0.00000000	-1.20120600	-0.16468600
C	0.00000000	1.20043300	-1.55750300
H	0.00000000	2.14464200	0.37674400
S	0.00000000	0.00000000	2.34689000
C	0.00000000	-1.20043300	-1.55750300
H	0.00000000	-2.14464200	0.37674400
C	0.00000000	0.00000000	-2.27999200
H	0.00000000	2.15235700	-2.09131200
H	0.00000000	-2.15235700	-2.09131200
H	0.00000000	0.00000000	-3.36873700

styrene

C	2.97789300	0.33506800	0.00001800
C	1.95506100	-0.52953600	-0.00001100
H	2.84076600	1.41308800	0.00005000
H	4.00494300	-0.01702500	0.00002000
H	2.18661300	-1.59490600	-0.00003200

C	0.51535000	-0.22048300	-0.00000600
C	-0.40651100	-1.28161900	-0.00000300
C	0.00898300	1.09280900	-0.00001500
C	-1.78126600	-1.04646700	0.00000700
H	-0.03503400	-2.30403200	-0.00000700
C	-1.36244600	1.32990500	-0.00000300
H	0.69406500	1.93567200	-0.00004100
C	-2.26578300	0.26186000	0.00001100
H	-2.47243400	-1.88523300	0.00000800
H	-1.73072500	2.35257800	-0.00000500
H	-3.33587500	0.45063500	0.00002400

cat1(*CSS*)

Fe	-0.06626600	-0.00007700	-0.15252000
N	-1.85284200	-0.92766400	-0.24804200
N	-1.00537000	1.78211600	-0.28608900
N	0.86354500	-1.77914900	-0.35169000
N	1.70874900	0.93014900	-0.38299200
C	-2.07882700	-2.28219600	-0.23373200
C	-0.42063500	3.02380200	-0.30146500
C	-3.09684700	-0.34492900	-0.23892800
C	-2.35897000	2.01186500	-0.26679700
C	0.27753600	-3.02065100	-0.32473400
C	1.93540400	2.28580000	-0.39541100
C	2.21371900	-2.01038200	-0.46000300
C	2.94921100	0.34749100	-0.49600400
C	-3.49865200	-2.56068400	-0.22072400
C	-1.42887400	4.06235500	-0.29763900
C	-4.13195300	-1.35584600	-0.22595000
C	-2.63506100	3.43258400	-0.27804600
C	1.28074900	-4.05931300	-0.41580300
C	3.35029200	2.56363100	-0.51074800
C	2.48532100	-3.43100900	-0.50277200
C	3.98030700	1.35821000	-0.57738300
C	-1.08986800	-3.25802900	-0.25282100
C	0.94789900	3.26229400	-0.33745500
C	3.18877100	-1.02145700	-0.52571600
C	-3.33626700	1.02410300	-0.24288800
H	-1.41461200	-4.29582900	-0.23750300
H	1.27281100	4.30010200	-0.34987600
H	4.22342300	-1.34513800	-0.61224000
H	-4.37396700	1.34903000	-0.22816200
S	-0.13194200	-0.03873800	2.17696000
C	1.60630800	0.04019900	2.76545700
H	2.21288300	-0.77185400	2.35013400
H	2.08471000	0.99306700	2.51252300
H	1.60181600	-0.06186900	3.85835900
H	5.04059400	1.15403300	-0.67378900
H	3.78489700	3.55618300	-0.54428500

H	-1.22134400	5.12626300	-0.31169400
H	-3.62679200	3.87025700	-0.27102000
H	-5.19644000	-1.15115800	-0.22042900
H	-3.93400400	-3.55337800	-0.21142800
H	1.07138200	-5.12294000	-0.41796600
H	3.47267800	-3.87014900	-0.58939700

cat1(*OSS*)

Fe	-0.06869100	0.01935700	-0.13145900
N	-1.85809700	-0.91409500	-0.23455600
N	-1.02148000	1.80437200	-0.30906600
N	0.87030700	-1.76614500	-0.35099400
N	1.70699400	0.95292500	-0.38363000
C	-2.07642200	-2.26890700	-0.21732200
C	-0.43690800	3.04433400	-0.33895000
C	-3.10214500	-0.33448000	-0.23329200
C	-2.37467100	2.02788000	-0.29563900
C	0.28423900	-3.00604700	-0.32286200
C	1.92509400	2.30832700	-0.41182600
C	2.22006800	-1.99113100	-0.45724600
C	2.94777200	0.37233700	-0.49146700
C	-3.49620800	-2.55206700	-0.20086100
C	-1.44790700	4.07998900	-0.34910000
C	-4.13399000	-1.34984700	-0.21244300
C	-2.65359000	3.44768800	-0.32379900
C	1.28996700	-4.04203500	-0.41170000
C	3.33993900	2.59042900	-0.52724200
C	2.49436800	-3.41111600	-0.49726600
C	3.97544500	1.38730500	-0.57946300
C	-1.08451500	-3.24283900	-0.24539700
C	0.93296600	3.28266400	-0.37368600
C	3.19150900	-0.99648300	-0.52002500
C	-3.34731200	1.03431000	-0.25743600
H	-1.40826400	-4.28089700	-0.22932300
H	1.25615200	4.32072200	-0.39917800
H	4.22757900	-1.31617800	-0.60339700
H	-4.38654900	1.35424000	-0.24781800
S	-0.10974200	0.01681900	2.26112900
C	1.63602700	-0.10631900	2.82333400
H	2.12727500	-1.00050700	2.42282100
H	2.22422600	0.76919600	2.52494500
H	1.65318900	-0.17123400	3.91891700
H	5.03675500	1.18720400	-0.67242900
H	3.77102700	3.58413400	-0.57009100
H	-1.24396600	5.14438300	-0.37354400
H	-3.64571300	3.88438600	-0.32231900
H	-5.19928800	-1.14963900	-0.20888100
H	-3.92854000	-3.54600400	-0.18659400
H	1.08431400	-5.10638200	-0.41098600
H	3.48225800	-3.84955500	-0.58056800

cat1(*triplet*)

Fe	-0.07571300	-0.00003400	-0.11974100
N	-1.52085600	-1.42284700	-0.26535300
N	-1.52059600	1.42312900	-0.26562700
N	1.34575200	-1.42356900	-0.41147100
N	1.34604100	1.42313700	-0.41128700
C	-1.32531900	-2.78016100	-0.28708300
C	-1.32477800	2.78040300	-0.28742400
C	-2.87942600	-1.23571600	-0.24299000
C	-2.87920300	1.23628500	-0.24325100
C	1.14815900	-2.78092400	-0.41816000
C	1.14872700	2.78054300	-0.41808600
C	2.70024700	-1.23659400	-0.53333800
C	2.70049900	1.23589100	-0.53324200
C	-2.59688500	-3.46998900	-0.26970100
C	-2.59618600	3.47048800	-0.27017900
C	-3.56310100	-2.51054700	-0.24315800
C	-3.56261000	2.51124000	-0.24356500
C	2.41351300	-3.47073400	-0.53888000
C	2.41423400	3.47008800	-0.53879900
C	3.37862300	-2.51175900	-0.61061000
C	3.37913800	2.51091600	-0.61053300
C	-0.08890500	-3.41491200	-0.34886400
C	-0.08818800	3.41484100	-0.34902200
C	3.33654100	-0.00041300	-0.58643900
C	-3.51752700	0.00033900	-0.22758300
H	-0.09002000	-4.50207500	-0.36375000
H	-0.08901600	4.50200400	-0.36395100
H	4.41959100	-0.00051800	-0.68101900
H	-4.60443600	0.00043600	-0.20555200
S	-0.03009800	0.00002300	2.39393600
C	1.74300400	0.00065300	2.88307500
H	2.26478700	-0.88478300	2.49891000
H	2.26413500	0.88653700	2.49905700
H	1.83621400	0.00059500	3.97682700
H	4.45097000	2.63688600	-0.71064700
H	2.53117100	4.54739300	-0.56619400
H	-2.71511100	4.54784800	-0.27972600
H	-4.63902000	2.63667900	-0.22742600
H	-4.63954200	-2.63572100	-0.22696900
H	-2.71601300	-4.54732600	-0.27917100
H	2.53024800	-4.54806200	-0.56623600
H	4.45043000	-2.63797100	-0.71067900

cat1(*quintet*)

Fe	-0.06020400	-0.00000600	0.27462400
N	-1.56271700	-1.45511300	-0.29128000
N	-1.55854600	1.45937100	-0.29168400
N	1.35438200	-1.46271300	-0.46340900
N	1.35851200	1.45863000	-0.46360800
C	-1.36202900	-2.80366000	-0.37121000

C	-1.35404500	2.80732700	-0.37176300
C	-2.91242800	-1.24951400	-0.27797400
C	-2.90883800	1.25760500	-0.27824300
C	1.14113500	-2.81015200	-0.52742900
C	1.14912500	2.80667100	-0.52775800
C	2.69533200	-1.25851100	-0.62736300
C	2.69889500	1.25058500	-0.62746000
C	-2.64187300	-3.49003700	-0.39321200
C	-2.63193100	3.49733500	-0.39377600
C	-3.60461400	-2.52495800	-0.33528800
C	-3.59741400	2.53502100	-0.33566100
C	2.40503300	-3.49824600	-0.72014200
C	2.41499100	3.49113100	-0.72047200
C	3.37016800	-2.53494200	-0.78208200
C	3.37738600	2.52507000	-0.78217000
C	-0.11295300	-3.43077400	-0.46197800
C	-0.10319100	3.43088800	-0.46252000
C	3.31909900	-0.00484800	-0.68113700
C	-3.53530700	0.00494600	-0.25177100
H	-0.11990800	-4.51700900	-0.52462400
H	-0.10703700	4.51713000	-0.52527700
H	4.39864200	-0.00638300	-0.81734300
H	-4.62331100	0.00650600	-0.24351200
S	0.05873800	-0.00051200	2.68655100
C	1.87835100	0.00006100	2.99750900
H	2.35773100	-0.88714300	2.57007200
H	2.35717600	0.88759200	2.57013600
H	2.05763300	0.00007600	4.07909200
H	4.44395400	2.65247900	-0.93061000
H	2.53897300	4.56472800	-0.80867500
H	-2.76169700	4.57203100	-0.45617900
H	-4.67374800	2.66621900	-0.34141100
H	-4.68131400	-2.65312500	-0.34106800
H	-2.77467000	-4.56436600	-0.45552500
H	2.52594700	-4.57220400	-0.80820300
H	4.43635000	-2.66540600	-0.93063900

cat2(*CSS*)

Fe	0.04163600	-0.00010100	-0.03255700
N	1.96585300	-0.60580300	-0.17915700
N	-0.56804600	-1.91659700	-0.20697000
N	0.64833100	1.92149300	-0.18987600
N	-1.87811200	0.60775300	-0.23627200
C	3.08480300	0.18707200	-0.17965400
C	-1.85953300	-2.37984200	-0.28561800
C	2.42417900	-1.89760900	-0.16662000
C	0.22785300	-3.03553500	-0.19833700
C	1.94212600	2.38060100	-0.19063500
C	-2.99809800	-0.18545100	-0.31455800
C	-0.14368500	3.04211800	-0.21457000
C	-2.33764400	1.90282500	-0.26508900

C	4.28288900	-0.62517600	-0.18184200
C	-1.87870500	-3.82645500	-0.32665700
C	3.87162800	-1.92352300	-0.17230800
C	-0.58105100	-4.23432400	-0.26931900
C	1.96734600	3.82791800	-0.22140700
C	-4.19128400	0.62800000	-0.38940500
C	0.66993100	4.23986000	-0.23522900
C	-3.78103500	1.92661800	-0.35556100
C	3.07720700	1.57800200	-0.17822400
C	-2.99333500	-1.57674500	-0.32988600
C	-1.53398800	3.03781800	-0.23745400
C	1.61757100	-3.03111600	-0.16114500
H	4.04169800	2.08094700	-0.17768500
H	-3.95703100	-2.07718100	-0.39199300
H	-2.03512000	4.00288100	-0.25992100
H	2.11729300	-3.99723500	-0.15409000
O	0.19453000	-0.02609000	1.84821500
C	-0.94844400	-0.00842200	2.61914500
H	-1.53920500	0.93180000	2.54493100
H	-1.65759600	-0.83757300	2.40544300
H	-0.66807600	-0.11226400	3.68816200
H	-5.20127100	0.24040900	-0.46120500
H	-4.38389200	2.82677800	-0.39627200
H	0.28203300	5.25194400	-0.26122700
H	2.86803400	4.43138800	-0.23246200
H	5.29515000	-0.23686800	-0.18717900
H	4.47555400	-2.82392000	-0.16988800
H	-0.18944800	-5.24523800	-0.28147900
H	-2.77546200	-4.43227000	-0.39220600

cat2(*OSS*)

Fe	0.03958100	0.02566700	-0.01439700
N	2.01665000	-0.37898900	-0.15702800
N	-0.37229300	-1.95679800	-0.20505400
N	0.45498600	2.00934600	-0.22772800
N	-1.93039400	0.43018700	-0.23570600
C	3.04818600	0.52398900	-0.17345100
C	-1.60864800	-2.54643300	-0.27974100
C	2.60220400	-1.61852400	-0.13884000
C	0.53525900	-2.98430300	-0.18764700
C	1.69347700	2.59548400	-0.23437400
C	-2.96242700	-0.47394600	-0.31054100
C	-0.44952600	3.03792300	-0.26251300
C	-2.51613300	1.67178600	-0.28111200
C	4.32361900	-0.16401200	-0.16754000
C	-1.47988900	-3.98711800	-0.31208000
C	4.04612700	-1.49625600	-0.14483200
C	-0.14572200	-4.25938000	-0.25235600
C	1.57002900	4.03709400	-0.28268000
C	-4.23300200	0.21499100	-0.39318300
C	0.23571200	4.31256300	-0.29924900

C	-3.95575900	1.54784700	-0.37255400
C	2.90321800	1.90725100	-0.20325500
C	-2.81797400	-1.85753700	-0.32304300
C	-1.83337900	2.88409100	-0.27509500
C	1.91834700	-2.83006000	-0.13956600
H	3.81381800	2.50205900	-0.21135900
H	-3.72728000	-2.45135300	-0.38209500
H	-2.43354400	3.79058100	-0.30922300
H	2.51785100	-3.73759400	-0.12773200
O	0.15472100	0.05846600	1.90077200
C	-0.94820200	-0.22660500	2.67417000
H	-1.76699500	0.52543300	2.60283000
H	-1.41840400	-1.21113200	2.45437800
H	-0.66212100	-0.26172400	3.74784400
H	-5.19853100	-0.27305700	-0.46305400
H	-4.64662500	2.38183900	-0.42322600
H	-0.25340000	5.27956100	-0.33373000
H	2.40274200	4.73114200	-0.30042900
H	5.29136000	0.32452500	-0.18090900
H	4.73863000	-2.33041300	-0.13602500
H	0.34607700	-5.22561100	-0.25563400
H	-2.30883900	-4.68322900	-0.37238600

cat2(*triplet*)

Fe	0.01758500	0.04000900	0.04517400
N	2.01100300	-0.42117900	-0.27989700
N	-0.43587300	-1.90254000	-0.19436200
N	0.47363600	1.98432400	-0.10856500
N	-1.97283200	0.50619000	-0.30257400
C	3.05901900	0.45859600	-0.26720800
C	-1.69389600	-2.46033400	-0.28208600
C	2.56276900	-1.67352700	-0.32168900
C	0.44705000	-2.95924800	-0.26964600
C	1.73075800	2.54301100	-0.12470700
C	-3.02191400	-0.37168500	-0.35140600
C	-0.40844600	3.04064000	-0.13318600
C	-2.52217000	1.75951300	-0.29610200
C	4.31028500	-0.25328800	-0.32895900
C	-1.59872900	-3.90422100	-0.36922200
C	4.00005600	-1.58578300	-0.36340900
C	-0.27551300	-4.21227100	-0.36174300
C	1.63729500	3.99118000	-0.12420600
C	-4.27130600	0.34393300	-0.40533800
C	0.31457800	4.29857600	-0.12933400
C	-3.95838600	1.67594400	-0.37072700
C	2.92868200	1.84751200	-0.18720000
C	-2.89104000	-1.76280300	-0.33595400
C	-1.78962000	2.94631300	-0.20869300
C	1.82970500	-2.86261600	-0.30956100
H	3.84422800	2.43421200	-0.19034600
H	-3.80490200	-2.34947400	-0.39239700

H	-2.35038400	3.87801600	-0.21804600
H	2.39038700	-3.79310700	-0.35883900
O	0.01455900	0.13308200	1.98815400
C	-0.36917700	-0.89108700	2.82573100
H	-1.43575300	-1.18741300	2.70900000
H	0.22096200	-1.82516500	2.69578400
H	-0.25103600	-0.60416900	3.89410800
H	-5.25147100	-0.11671300	-0.45363400
H	-4.63140400	2.52578300	-0.38524300
H	-0.15218600	5.27691200	-0.14422800
H	2.48792100	4.66310600	-0.13420300
H	5.29028000	0.21021800	-0.33676100
H	4.67472700	-2.43345100	-0.40358500
H	0.19168300	-5.18811100	-0.43008000
H	-2.44827400	-4.57322200	-0.44560500

cat2(*quintet*)

Fe	0.03512500	-0.00012400	0.42195800
N	1.54419500	-1.43773600	-0.20649400
N	-1.38004400	-1.48576600	-0.31190600
N	1.49800200	1.48403500	-0.20857800
N	-1.42590700	1.43974900	-0.31408800
C	2.88906700	-1.21078900	-0.23021700
C	-2.72626300	-1.30005500	-0.43778000
C	1.36050900	-2.78735000	-0.28528000
C	-1.14885100	-2.82892700	-0.37860100
C	2.84940800	1.29948900	-0.23176100
C	-2.76566700	1.21152500	-0.43933300
C	1.27202900	2.82709500	-0.28868800
C	-1.23727200	2.78947900	-0.38218000
C	3.59963000	-2.47626800	-0.31043900
C	-3.38828800	-2.58668900	-0.57335100
C	2.64997500	-3.45572700	-0.34470800
C	-2.40841300	-3.53635200	-0.53680900
C	3.51982500	2.58666200	-0.31306300
C	-3.46799100	2.47653100	-0.57602300
C	2.53988500	3.53571500	-0.34844800
C	-2.51857700	3.45665300	-0.54072800
C	3.49312200	0.05424400	-0.22113500
C	-3.36842400	-0.05400600	-0.47443400
C	0.00850600	3.43156800	-0.34832200
C	0.11658100	-3.43129200	-0.34408700
H	4.58104500	0.07141600	-0.24466900
H	-4.45139900	-0.07103900	-0.58097500
H	-0.00522000	4.51783700	-0.41391900
H	0.13708000	-4.51752500	-0.40863800
O	-0.01331800	-0.00307900	2.31095000
C	-1.09867800	0.00138400	3.16196500
H	-1.72743200	0.91347100	3.07148500
H	-1.78395000	-0.86025500	3.00991800
H	-0.77945200	-0.04550500	4.22493500

H	-4.54008200	2.58870100	-0.69552900
H	-2.66114800	4.52842000	-0.62570800
H	2.65368500	4.61186500	-0.42021200
H	4.59380000	2.73293200	-0.35013800
H	4.67765100	-2.58885700	-0.34772300
H	2.79777300	-4.52780200	-0.41547600
H	-2.51719400	-4.61214500	-0.62090400
H	-4.45624700	-2.73296400	-0.69295900

cat3(*CSS*)

Fe	-0.00572593	-0.12001467	-0.16562310
N	-1.81194219	-1.01357157	-0.23370942
N	-0.90919959	1.68176170	-0.13690792
N	0.87901899	-1.90400121	-0.47625169
N	1.77874123	0.79023253	-0.38305117
C	-2.06869451	-2.36227297	-0.32944564
C	-0.30427572	2.91806368	-0.15206098
C	-3.04341275	-0.40879695	-0.12151290
C	-2.25889583	1.93228679	-0.03572736
C	0.26774845	-3.13476688	-0.53450150
C	2.03072756	2.14355974	-0.37494048
C	2.22623269	-2.15462745	-0.59169299
C	3.00823654	0.18619260	-0.51922443
C	-3.49085393	-2.60974323	-0.28047175
C	-1.29349673	3.96654848	-0.05561978
C	-4.09587378	-1.39776572	-0.14919075
C	-2.50676508	3.35446042	0.01887730
C	1.25155726	-4.18136401	-0.69362464
C	3.44709277	2.39501422	-0.50514407
C	2.46776122	-3.57307951	-0.72748818
C	4.05421083	1.17992989	-0.59199849
C	-1.10235435	-3.35218511	-0.45970418
C	1.06508791	3.13611721	-0.25476858
C	3.22143319	-1.18495192	-0.59660057
C	-3.25289893	0.96069796	-0.01013936
H	-1.44777920	-4.38019004	-0.52070458
H	1.40672885	4.16732711	-0.25975863
H	4.24815437	-1.52463546	-0.69876424
H	-4.28074435	1.30203413	0.07378485
S	0.03480525	-0.36981849	2.12517601
C	1.14005580	0.89770723	2.85769554
H	2.16130624	0.58564938	2.63365087
H	0.95418627	1.87349013	2.40808745
H	0.99485684	0.92733115	3.94001134
H	5.10807508	0.95958114	-0.70865694
H	3.89966898	3.37845919	-0.53418935
H	-1.07203874	5.02663625	-0.05661947
H	-3.48749131	3.80808954	0.09086861
H	-5.15384141	-1.17550005	-0.08588679
H	-3.94945323	-3.58855529	-0.34565419
H	1.02256426	-5.23672398	-0.77381490

H	3.44521310	-4.02485521	-0.84227774
H	-1.12962438	0.23299795	2.45185569

cat3(*OSS*)

Fe	0.07262140	0.13384946	-0.17614507
N	-1.68262873	-0.84768194	-0.04200655
N	-0.92567254	1.87662181	-0.35212632
N	1.03816049	-1.63154380	-0.28705064
N	1.79769138	1.09100096	-0.58929978
C	-1.87309923	-2.20809440	0.04507972
C	-0.38640578	3.12719808	-0.55036760
C	-2.93924391	-0.29258808	0.04472098
C	-2.28232402	2.07348541	-0.22699081
C	0.49057875	-2.88980474	-0.17726702
C	1.97824073	2.44490621	-0.75077933
C	2.39247516	-1.82930779	-0.43417159
C	3.05220784	0.53642724	-0.68837624
C	-3.27734228	-2.51393172	0.19279184
C	-1.42598272	4.12993112	-0.55445095
C	-3.93895760	-1.32461615	0.19474386
C	-2.60240842	3.47653279	-0.35133616
C	1.52161659	-3.89839230	-0.25437583
C	3.37593829	2.74776562	-0.95903490
C	2.70256758	-3.24005783	-0.41109950
C	4.04311912	1.56306581	-0.91843442
C	-0.86233822	-3.16124389	-0.01007919
C	0.96548982	3.39555562	-0.72655957
C	3.33454161	-0.82123926	-0.60087789
C	-3.21925814	1.06738495	-0.02284993
H	-1.15599248	-4.20438554	0.06597097
H	1.25257635	4.43330501	-0.86968552
H	4.37358209	-1.12212019	-0.70041971
H	-4.26035428	1.36622221	0.06029687
S	0.29279942	0.48240085	2.09204961
C	0.50963884	-1.12806757	2.94293745
H	1.52282960	-1.46413291	2.71704102
H	0.40142614	-0.98864964	4.02101037
H	-0.20562633	-1.85999886	2.56667089
H	5.10369999	1.38141733	-1.04040134
H	3.77485643	3.74150480	-1.12029799
H	-1.26008611	5.18996832	-0.70099566
H	-3.60239093	3.88876064	-0.29819211
H	-5.00397020	-1.14571387	0.27562571
H	-3.68678716	-3.51336244	0.27241558
H	1.34639803	-4.96587304	-0.20295713
H	3.69719502	-3.65532631	-0.51634174
H	-1.00127987	0.66557675	2.43589658

cat3(*triplet*)

Fe	-0.07467764	-0.08520489	-0.27060426
N	-1.84117192	-1.04425459	-0.17582510

N	-1.03609783	1.67805766	-0.12040109
N	0.87001120	-1.83804244	-0.56087503
N	1.67480906	0.88448941	-0.50304011
C	-2.04451534	-2.40311758	-0.22195166
C	-0.46911860	2.93135592	-0.11991741
C	-3.08909116	-0.48474628	-0.01747413
C	-2.39026847	1.88046672	0.02893849
C	0.30340006	-3.09024900	-0.55432242
C	1.87951437	2.24427930	-0.45359353
C	2.21613439	-2.03783861	-0.76746029
C	2.91531526	0.32738192	-0.72174593
C	-3.44970488	-2.70483614	-0.08715161
C	-1.48706267	3.94206083	0.03845365
C	-4.09830531	-1.51442654	0.03814791
C	-2.67930536	3.29016646	0.12929517
C	1.31489534	-4.09968712	-0.75938920
C	3.27834515	2.54735872	-0.63957914
C	2.50189750	-3.44663698	-0.89329086
C	3.92062036	1.35810874	-0.80755349
C	-1.04980534	-3.35894994	-0.38811435
C	0.88716762	3.19930180	-0.26373618
C	3.17239105	-1.03285954	-0.84100088
C	-3.34908120	0.87634352	0.08083278
H	-1.35696432	-4.40040357	-0.40475254
H	1.19421779	4.24089482	-0.24669149
H	4.20203346	-1.33381225	-1.01023091
H	-4.38441323	1.17989058	0.20428987
S	0.20249528	-0.29348016	2.71740801
C	1.77008684	0.58642499	3.08592516
H	2.57350428	-0.12268243	2.87474013
H	1.89112429	1.45580721	2.43733940
H	1.81928433	0.87883040	4.13725570
H	4.97473532	1.17972477	-0.97913168
H	3.69762527	3.54580965	-0.64585791
H	-1.29864496	5.00807084	0.06726486
H	-3.67008191	3.71018300	0.24898285
H	-5.15925232	-1.33341523	0.15615978
H	-3.86926206	-3.70307387	-0.09355255
H	1.12410875	-5.16492029	-0.79731386
H	3.48622416	-3.86429208	-1.06361480
H	-0.63155764	0.73908428	2.96093266

cat3(*quintet*)

Fe	0.01134116	-0.14973322	-0.11307922
N	-1.87410334	-1.06218870	-0.22227326
N	-0.90869679	1.70677927	-0.13517584
N	0.89113075	-1.96386139	-0.56028350
N	1.86087845	0.79899501	-0.39134981
C	-2.11757802	-2.40157322	-0.35973813
C	-0.27934811	2.92822665	-0.14323265
C	-3.08514728	-0.43171204	-0.12837988

C	-2.25982453	1.93930630	-0.03973919
C	0.25437390	-3.17855839	-0.62757346
C	2.09485522	2.14784346	-0.38471196
C	2.23620577	-2.19357757	-0.71248585
C	3.06248036	0.17484206	-0.59484747
C	-3.55017830	-2.63600079	-0.32971803
C	-1.27122348	3.97417991	-0.04173356
C	-4.14805074	-1.41927900	-0.18611045
C	-2.49289551	3.36397626	0.02283319
C	1.23696565	-4.21914394	-0.82985057
C	3.51443371	2.39139469	-0.56533861
C	2.45987878	-3.61153333	-0.88177813
C	4.11217909	1.17268159	-0.69417712
C	-1.12952322	-3.37804475	-0.52842887
C	1.10512899	3.12813584	-0.24857404
C	3.23360280	-1.20841703	-0.71951384
C	-3.25689416	0.95336383	-0.02280942
H	-1.47315287	-4.40547035	-0.61403666
H	1.44177532	4.16152527	-0.25329889
H	4.25177129	-1.55861009	-0.86729951
H	-4.28105729	1.30990952	0.04932237
S	0.07274510	-0.38075850	2.60814046
C	1.09516989	1.03456745	3.17527947
H	2.13510361	0.73810444	3.02468459
H	0.89040484	1.92377993	2.57729018
H	0.92521497	1.22958629	4.23613406
H	5.16126103	0.95892848	-0.85823491
H	3.97929456	3.36901988	-0.60272809
H	-1.05704576	5.03588389	-0.03128739
H	-3.46682363	3.83224754	0.09592032
H	-5.20729596	-1.19856971	-0.13698797
H	-4.02483362	-3.60533321	-0.42023754
H	1.01429378	-5.27487406	-0.92395184
H	3.42762962	-4.07561152	-1.02707162
H	-1.13634430	0.18632193	2.80071358

cat4(*CSS*)

Fe	-0.03323803	-0.09300462	-0.10277522
N	1.90608351	-0.66756613	-0.11092046
N	-0.59272485	-2.01211696	-0.34338991
N	0.55006928	1.84000095	-0.11200025
N	-1.94942595	0.49127938	-0.28331661
C	3.01600581	0.14637891	-0.03374901
C	-1.87673584	-2.49151909	-0.43524287
C	2.39210402	-1.95565686	-0.17491429
C	0.22046843	-3.12021666	-0.36793033
C	1.83783040	2.32049980	-0.03430606
C	-3.05461663	-0.32023644	-0.38834777
C	-0.26002329	2.95164149	-0.14928938
C	-2.43145454	1.78022334	-0.29401495
C	4.22137724	-0.64742128	-0.03800346

C	-1.87247194	-3.93454566	-0.52931068
C	3.83445359	-1.95064025	-0.12658406
C	-0.57031350	-4.32495092	-0.48855591
C	1.83645048	3.76534842	-0.02167895
C	-4.25933705	0.47485578	-0.45694860
C	0.53473466	4.15685676	-0.09476957
C	-3.87276218	1.77845869	-0.39964910
C	2.98458578	1.53575320	0.01738681
C	-3.02500791	-1.70860088	-0.44560095
C	-1.64834295	2.92683923	-0.22330779
C	1.60782375	-3.09877763	-0.28447718
H	3.93832514	2.05240972	0.07682010
H	-3.97800158	-2.22364444	-0.52636484
H	-2.16294691	3.88333702	-0.24324623
H	2.12369421	-4.05407408	-0.31995521
O	-0.04083719	-0.29524042	1.90674801
C	-0.42743245	0.79061607	2.76899123
H	0.21960278	1.66089601	2.62854680
H	-1.44932996	1.04821556	2.49494016
H	-0.39673761	0.45010645	3.80941876
H	-5.26049702	0.07223902	-0.54809823
H	-4.49077954	2.66709848	-0.43368499
H	0.13403986	5.16271192	-0.11771658
H	2.72431342	4.38354729	0.02679437
H	5.22580214	-0.24537805	0.00980750
H	4.45666025	-2.83613509	-0.16547465
H	-0.16471342	-5.32786782	-0.53726614
H	-2.75876306	-4.55030203	-0.61902437
H	0.89117285	-0.52329321	2.06676794

cat4(*OSS*)

Fe	0.07103653	-0.01502246	-0.12108423
N	1.99140892	-0.62565780	-0.21543142
N	-0.55081042	-1.92622592	-0.23351601
N	0.69611720	1.90979051	-0.18378978
N	-1.84749961	0.60705114	-0.27558227
C	3.11846715	0.16161764	-0.22558910
C	-1.84797430	-2.37993083	-0.30168275
C	2.44032798	-1.92346331	-0.21022067
C	0.23943556	-3.05037378	-0.22842859
C	1.99643991	2.36397797	-0.20824290
C	-2.97393842	-0.17997485	-0.34238221
C	-0.09533748	3.03659691	-0.20727220
C	-2.29637396	1.90724175	-0.28225623
C	4.30591722	-0.66082322	-0.23463741
C	-1.87437685	-3.82456051	-0.32852269
C	3.88475987	-1.95530458	-0.22316819
C	-0.57929985	-4.24027227	-0.28146121
C	2.02257941	3.80714585	-0.23166920
C	-4.15857482	0.64301834	-0.39392431
C	0.72583718	4.22421348	-0.22908773

C	-3.73824663	1.93838558	-0.35453631
C	3.12541699	1.55229411	-0.21950622
C	-2.97788460	-1.57101167	-0.34778058
C	-1.48602901	3.03767546	-0.23607530
C	1.62952420	-3.05343293	-0.20455685
H	4.09296079	2.04572918	-0.23323244
H	-3.94313086	-2.06624657	-0.40210251
H	-1.98150711	4.00424928	-0.25185932
H	2.12464335	-4.02022817	-0.20369192
O	0.10681819	0.10705187	2.06411413
C	-1.05910078	-0.15025560	2.85786322
H	-1.87807998	0.53091187	2.60322238
H	-1.36228470	-1.17292387	2.63260961
H	-0.81706451	-0.06845395	3.92409706
H	-5.17169121	0.26558414	-0.45605471
H	-4.33653902	2.84080181	-0.37906303
H	0.34525109	5.23787225	-0.25193818
H	2.92287940	4.40843261	-0.25580126
H	5.32028341	-0.28205130	-0.24916210
H	4.48290398	-2.85805923	-0.22688030
H	-0.19639871	-5.25321853	-0.29095148
H	-2.77366213	-4.42525491	-0.38436437
H	0.38190078	1.03122944	2.17990668

cat4(*triplet*)

Fe	0.07285023	-0.03736747	-0.17470124
N	1.99244710	-0.63822174	-0.24716269
N	-0.54383576	-1.94614951	-0.29514152
N	0.69291238	1.88841533	-0.19453785
N	-1.84566795	0.57864838	-0.28967698
C	3.11865680	0.15229010	-0.24805120
C	-1.84007726	-2.40411449	-0.36477231
C	2.44541173	-1.93501794	-0.25099134
C	0.25026302	-3.06760699	-0.29504818
C	1.99198414	2.34853837	-0.21532851
C	-2.97112232	-0.21022898	-0.36426914
C	-0.10288398	3.01224723	-0.19420098
C	-2.29858248	1.87735492	-0.27126693
C	4.30749270	-0.66674565	-0.25631400
C	-1.86129997	-3.84706103	-0.40231059
C	3.88939021	-1.96213879	-0.25565190
C	-0.56435395	-4.25848088	-0.35690066
C	2.01239089	3.79067984	-0.21432363
C	-4.15793322	0.60974988	-0.39325753
C	0.71348199	4.20209983	-0.19884713
C	-3.74072244	1.90501018	-0.33338417
C	3.12379805	1.54200272	-0.23428697
C	-2.97290208	-1.59990188	-0.39621945
C	-1.49338032	3.00997532	-0.21361170
C	1.63982366	-3.06775486	-0.26320769
H	4.08999138	2.03782023	-0.24184667

H	-3.93683522	-2.09692119	-0.45368846
H	-1.99213155	3.97481795	-0.20990017
H	2.13783020	-4.03286281	-0.26754473
O	0.10835602	0.12567408	2.20192236
C	-1.07405851	0.00478203	2.99516169
H	-1.85306512	0.70788479	2.67689129
H	-1.43942260	-1.01317859	2.84990597
H	-0.85126243	0.15606818	4.05942788
H	-5.17009826	0.23001745	-0.45493539
H	-4.34118720	2.80626288	-0.33705462
H	0.32873310	5.21441120	-0.20092670
H	2.91025622	4.39570816	-0.22979645
H	5.32067155	-0.28488628	-0.26187576
H	4.48951044	-2.86351394	-0.26126516
H	-0.17803615	-5.27004348	-0.37008863
H	-2.75860048	-4.45033108	-0.46014690
H	0.43031166	1.04019350	2.24553182

cat4(*quintet*)

Fe	-0.04640056	-0.10858270	-0.00664900
N	1.97319643	-0.69841883	-0.07801228
N	-0.61579701	-2.05799738	-0.38544978
N	0.57132187	1.87246425	-0.11800776
N	-2.02326972	0.50645440	-0.28862395
C	3.06809411	0.12474488	-0.04312037
C	-1.90318189	-2.51282851	-0.51479488
C	2.42971236	-1.98615707	-0.18073677
C	0.21406412	-3.15123042	-0.40841813
C	1.86467798	2.33016761	-0.05227363
C	-3.10784458	-0.31061712	-0.46058627
C	-0.25401613	2.96950350	-0.15771773
C	-2.47220551	1.79987118	-0.32348125
C	4.27510166	-0.67940901	-0.09135185
C	-1.88890987	-3.95468316	-0.62826143
C	3.88076091	-1.98265496	-0.17642541
C	-0.58243276	-4.34864858	-0.56261153
C	1.85696597	3.77587179	-0.04778235
C	-4.30629057	0.50039560	-0.57917524
C	0.54974890	4.17034006	-0.11241506
C	-3.91408647	1.80339070	-0.49421135
C	3.01123193	1.52353537	-0.00678702
C	-3.05000910	-1.70635182	-0.54391387
C	-1.65384853	2.93224089	-0.24209196
C	1.61210732	-3.11546715	-0.30928251
H	3.96372292	2.04591809	0.02833722
H	-3.99742432	-2.22375458	-0.66979583
H	-2.15657866	3.89524968	-0.27720171
H	2.11991037	-4.07480771	-0.36515092
O	0.08340638	-0.22750449	2.22215233
C	-0.46957447	0.77555866	3.08483045
H	-0.00213393	1.75188099	2.91491983

H	-1.52951556	0.83952094	2.83680913
H	-0.35845776	0.48214955	4.13514914
H	-5.30784512	0.11429874	-0.72417538
H	-4.53197702	2.69081421	-0.55656196
H	0.16067762	5.18091794	-0.13634116
H	2.73929906	4.40288975	-0.00748324
H	5.28538443	-0.28892187	-0.07925644
H	4.50621313	-2.86409646	-0.24776532
H	-0.18772002	-5.35579459	-0.61672890
H	-2.76653485	-4.57832063	-0.74641797
H	1.03956115	-0.30380678	2.37316918

water

O	0.00000000	-0.13952200	0.00000000
H	0.76260700	0.45760300	0.00000000
H	-0.76260700	0.45760300	0.00000000

OH^-

O	0.00000000	0.00000000	0.12090100
H	0.00000000	0.00000000	-0.86756800

AcOH

O	0.10707700	-0.11350600	-0.00007200
H	-0.70802700	0.42321400	0.00169900
C	1.13600900	0.77344200	0.00005000
O	0.96110400	1.97097000	0.00205800
C	2.46965000	0.06820100	-0.00258400
H	2.55459300	-0.57661000	0.87840200
H	2.55247000	-0.57405100	-0.88563700
H	3.27183600	0.80639800	-0.00247400

AcO^-

O	0.09919800	-0.11004000	0.00065400
C	1.04363800	0.72053500	0.00015700
O	1.01225600	1.97675600	0.00167700
C	2.47841800	0.06942900	-0.00265700
H	2.59919100	-0.58083500	0.87650300
H	2.59720000	-0.57756400	-0.88450300
H	3.27741600	0.82217600	-0.00221300

int1(*CSS*)

Fe	0.07220400	0.03587000	-0.19160300
N	1.50216200	-1.39311700	-0.41498300
N	1.54157200	1.44429400	-0.24682800
N	-1.38543500	-1.35989300	-0.28076300
N	-1.34889400	1.47067900	-0.12051100
C	1.27986100	-2.74179200	-0.46466600
C	1.35391700	2.79453900	-0.13490800
C	2.85144600	-1.21684900	-0.55536400
C	2.88524100	1.25141700	-0.40965300
C	-1.19779000	-2.71241600	-0.34116200

C	-1.12456400	2.81504800	-0.01962200
C	-2.73758100	-1.15680800	-0.28945100
C	-2.70499100	1.30544800	-0.15087000
C	2.53402400	-3.44732700	-0.63148800
C	2.62617500	3.48204300	-0.21559400
C	3.50952800	-2.49966400	-0.69305900
C	3.57686200	2.52320200	-0.39291600
C	-2.47671100	-3.39287800	-0.37925900
C	-2.38538400	3.52904500	0.02222800
C	-3.43291400	-2.42496900	-0.35523400
C	-3.36664800	2.59116400	-0.06770800
C	0.03459300	-3.35946000	-0.40030300
C	0.12390800	3.43176700	0.00149200
C	-3.36200800	0.08410900	-0.24276200
C	3.50560800	0.01300500	-0.55658700
H	0.01911100	-4.44537400	-0.45069200
H	0.13628900	4.51601900	0.08061200
H	-4.44847500	0.09918800	-0.25535700
H	4.58527400	0.00539200	-0.68194800
S	0.10805200	0.21677600	-2.63075100
C	-1.58657000	0.12288500	-3.32325100
H	-2.08051300	-0.81849400	-3.05615300
H	-2.21384700	0.94654900	-2.96303900
H	-1.53377100	0.18570500	-4.41715800
C	0.20727900	-0.04582900	1.61414100
C	1.47503000	0.02921300	2.42366700
C	1.12443700	-0.69146600	3.73344300
H	1.58902400	-0.25919500	4.62651800
H	1.38581800	-1.75759800	3.68597700
H	1.70318800	1.08966400	2.62043000
H	2.34305300	-0.39489700	1.91540700
O	-0.29617500	-0.56796300	3.86890900
C	-0.86512300	-0.22604000	2.64295800
O	-2.06815700	-0.10994900	2.56901200
H	-4.51043600	-2.53813400	-0.37490600
H	-2.60331200	-4.46805800	-0.42899300
H	2.63239800	-4.52418200	-0.70450800
H	4.57665200	-2.63588900	-0.82534200
H	4.64740200	2.64670700	-0.50918900
H	2.75293100	4.55693500	-0.15933100
H	-2.48310100	4.60563100	0.09923900
H	-4.44077400	2.73422600	-0.07409500

int1(*OSS*)

Fe	0.06833600	0.02994400	-0.26798300
N	1.50183800	-1.40085500	-0.44620200
N	1.53902800	1.43538500	-0.27473300
N	-1.38529700	-1.36845600	-0.32522700
N	-1.34963100	1.45990000	-0.14794000
C	1.28010100	-2.74968900	-0.49611500
C	1.35132000	2.78474400	-0.15373800

C	2.85353100	-1.22452000	-0.56881900
C	2.88529600	1.24178400	-0.41946300
C	-1.19628500	-2.72106600	-0.38201300
C	-1.12543500	2.80375700	-0.03437900
C	-2.73817200	-1.16713900	-0.31288500
C	-2.70686500	1.29249700	-0.15757300
C	2.53580800	-3.45427800	-0.64637900
C	2.62469600	3.47084300	-0.21592900
C	3.51237900	-2.50647500	-0.69675100
C	3.57689800	2.51212600	-0.38712300
C	-2.47455200	-3.40207100	-0.40385600
C	-2.38599800	3.51387400	0.03309200
C	-3.43188300	-2.43552000	-0.36869800
C	-3.36776100	2.57523900	-0.05132700
C	0.03511400	-3.36854800	-0.44128300
C	0.12184200	3.42213600	-0.01571600
C	-3.36406500	0.07160800	-0.24914200
C	3.50760400	0.00454300	-0.56228800
H	0.02024000	-4.45442600	-0.48813700
H	0.13414800	4.50531800	0.07463900
H	-4.45040400	0.08509100	-0.24252300
H	4.58878900	-0.00286800	-0.67256200
S	0.10789600	0.19623800	-2.66923800
C	-1.60052800	0.17030800	-3.33252500
H	-2.12377900	-0.75464200	-3.06507200
H	-2.19065900	1.01456800	-2.95833700
H	-1.55752800	0.23832100	-4.42633800
C	0.20149600	-0.07556600	1.66190300
C	1.48271300	0.00887200	2.44746800
C	1.12281400	-0.60300700	3.81169300
H	1.58880800	-0.10051400	4.66726900
H	1.38550200	-1.67029900	3.85372100
H	1.77211900	1.06672100	2.56154500
H	2.32439400	-0.49448900	1.96442400
O	-0.29544800	-0.47008400	3.93404900
C	-0.85962000	-0.23839900	2.67096300
O	-2.07086400	-0.18623600	2.58271400
H	-4.50930600	-2.55013900	-0.36997600
H	-2.60026900	-4.47756200	-0.44695000
H	2.63542100	-4.53126000	-0.71444600
H	4.58126600	-2.64301000	-0.81265800
H	4.64913900	2.63495800	-0.48622500
H	2.75189000	4.54494500	-0.14823800
H	-2.48430300	4.58911500	0.12558400
H	-4.44190900	2.71656000	-0.03625400

int1(*triplet*)

Fe	0.04380000	-0.00561100	-0.29157400
N	1.25115500	-1.63568100	-0.42834700
N	1.65928700	1.19200400	-0.04283100
N	-1.55489200	-1.20548800	-0.55426900

N	-1.14689500	1.61104200	-0.16584300
C	0.87032300	-2.94281600	-0.54852000
C	1.66233500	2.53494300	0.22260600
C	2.61947600	-1.62622900	-0.44138600
C	2.97048200	0.80344500	-0.10248400
C	-1.56763400	-2.56872300	-0.65516600
C	-0.77818900	2.89773000	0.12182800
C	-2.85049400	-0.79456600	-0.69030000
C	-2.50122100	1.62675600	-0.34598500
C	2.03592400	-3.79568400	-0.63366000
C	3.02126100	3.01550400	0.33575100
C	3.12279700	-2.97705000	-0.57596400
C	3.83363600	1.94160300	0.12420400
C	-2.92151200	-3.04086300	-0.85707600
C	-1.94115900	3.75928100	0.12535300
C	-3.71611900	-1.93755700	-0.89061700
C	-3.00892400	2.97138400	-0.17707900
C	-0.44545100	-3.38978900	-0.62728100
C	0.52637700	3.33298400	0.33040200
C	-3.29544000	0.51924300	-0.62000600
C	3.42336600	-0.49815100	-0.30372300
H	-0.60592200	-4.46012400	-0.72511600
H	0.67403800	4.38793500	0.54564500
H	-4.36207700	0.68970500	-0.73627600
H	4.49937400	-0.65003700	-0.32681700
S	0.20480400	0.18163400	-2.65626700
C	0.43059200	1.94981800	-3.08279700
H	-0.40801400	2.55736900	-2.72534500
H	1.35293400	2.35055200	-2.64768300
H	0.49051900	2.04821400	-4.17313800
C	-0.03597700	-0.26247700	1.67978200
C	1.17033500	-0.39215400	2.56936100
C	0.59015900	-0.94575800	3.88408000
H	1.04958200	-0.52456700	4.78667300
H	0.68600000	-2.04176500	3.93029800
H	1.62928400	0.59798600	2.73162300
H	1.95588800	-1.03217900	2.15487400
O	-0.79305400	-0.59852200	3.87833300
C	-1.19343300	-0.29967600	2.55584900
O	-2.38159000	-0.10722800	2.35172800
H	-4.78985600	-1.88127900	-1.02376600
H	-3.20256700	-4.08169200	-0.96559200
H	2.00673300	-4.87410200	-0.73604300
H	4.17237400	-3.24403600	-0.61598900
H	4.91677800	1.90481000	0.12405200
H	3.29905400	4.04291300	0.53980900
H	-1.92080400	4.82372900	0.32714800
H	-4.05148700	3.25198800	-0.26765500

int1(*quintet*)

Fe	0.04456300	-0.01034400	-0.27834100

N	1.09765200	-1.73819600	-0.47832400
N	1.75996200	1.03021300	-0.04546000
N	-1.65741200	-1.04584700	-0.55292400
N	-0.99810200	1.71354600	-0.10769800
C	0.60259600	-3.01687400	-0.60440100
C	1.89465500	2.37164600	0.25608900
C	2.46748200	-1.86622800	-0.50947900
C	3.04142100	0.53017100	-0.14275000
C	-1.80349400	-2.41085700	-0.67513200
C	-0.51436600	2.96721000	0.21262700
C	-2.91880900	-0.51409200	-0.68402600
C	-2.34675800	1.87202600	-0.28732700
C	1.66166200	-3.95728700	-0.70915800
C	3.29661800	2.72012100	0.34907100
C	2.83879400	-3.23139200	-0.65485000
C	4.00344400	1.58863800	0.09050200
C	-3.20034500	-2.74523000	-0.87603700
C	-1.56985400	3.91771100	0.23774000
C	-3.88476100	-1.57490100	-0.89781300
C	-2.72409900	3.23018700	-0.08802200
C	-0.77383100	-3.32573800	-0.67293600
C	0.84931800	3.25972400	0.40636500
C	-3.24107100	0.82209500	-0.59647300
C	3.37288600	-0.79005800	-0.37255600
H	-1.03717600	-4.37476200	-0.78266500
H	1.10161700	4.28999700	0.64566800
H	-4.28723600	1.09075200	-0.71552300
H	4.43131400	-1.03465700	-0.41620700
S	0.21388800	0.27184800	-2.66412600
C	0.44028600	2.05242500	-3.02116700
H	-0.43344400	2.63845900	-2.72044500
H	1.32329500	2.45513300	-2.51491700
H	0.58198100	2.16174600	-4.10322200
C	-0.03830000	-0.30097500	1.67509300
C	1.17055400	-0.50961200	2.54034300
C	0.57085000	-1.06919100	3.84346800
H	1.05471100	-0.69288000	4.75228100
H	0.61167200	-2.16854800	3.86003600
H	1.67633300	0.45334000	2.72236600
H	1.91800500	-1.17633300	2.09943100
O	-0.79607300	-0.65464200	3.85791500
C	-1.19667000	-0.30596600	2.55273200
O	-2.37287200	-0.05555000	2.35760900
H	-4.94847800	-1.41614800	-1.02884600
H	-3.57844900	-3.75359000	-0.99586600
H	1.53507200	-5.02726900	-0.82409300
H	3.85771300	-3.59659700	-0.70702300
H	5.07873500	1.45641500	0.06334700
H	3.66920600	3.71312900	0.57180700
H	-1.45292400	4.97214000	0.45832600
H	-3.73519000	3.61125400	-0.16630700

TS2(*CSS*)

Fe	-0.96039800	0.06047900	0.40184800
N	-1.86367100	-1.73433700	0.18343800
N	-2.19901300	0.84225600	-1.04517500
N	0.12779000	-0.65159300	1.89708100
N	-0.22109400	1.92931900	0.74163800
C	-1.58647500	-2.87837000	0.87157400
C	-2.25415100	2.14369500	-1.46631100
C	-2.90035600	-2.03953300	-0.65514100
C	-3.16670000	0.16862100	-1.74145100
C	0.14112600	-1.94233000	2.36548700
C	-0.56015400	3.08639800	0.08954700
C	0.99627000	0.04769300	2.70016900
C	0.69207800	2.28635000	1.69446400
C	-2.46151900	-3.95237500	0.44801800
C	-3.26801200	2.29379700	-2.48919200
C	-3.28398800	-3.42637500	-0.49725100
C	-3.83515500	1.06733200	-2.65725600
C	1.05746100	-2.06469000	3.47751600
C	0.17576000	4.20461800	0.63483000
C	1.58593400	-0.83068800	3.68732300
C	0.95601600	3.70674600	1.63566300
C	-0.63268200	-2.98633100	1.87862200
C	-1.48421300	3.18549700	-0.94982200
C	1.26932000	1.40615100	2.60746200
C	-3.49667100	-1.16907600	-1.55879300
H	-0.50941800	-3.95777400	2.34957500
H	-1.64430800	4.17365100	-1.37433200
H	1.97748700	1.82001200	3.32102600
H	-4.29889000	-1.56859900	-2.17333100
C	-3.00168000	2.25081000	2.22959200
H	-2.09929600	2.66000600	2.69479800
H	-3.23020600	2.84104800	1.33465000
H	-3.83764700	2.36214900	2.93105100
C	0.20234100	-0.15395400	-1.13695200
C	0.97815500	0.99617400	-1.75095900
C	1.57282100	0.43523600	-3.05008300
H	2.59481900	0.06481600	-2.90935500
H	1.56866500	1.14898600	-3.88135700
H	1.73464800	1.41344600	-1.08094100
H	0.28532000	1.81276900	-1.99297700
S	2.49997600	-1.93242900	-0.25273700
C	3.89001800	-0.85164200	-0.50761200
C	4.06415200	0.33905500	0.22280200
C	4.88731500	-1.21902900	-1.43107900
C	5.18890800	1.13921100	0.01932800
H	3.31487400	0.62755100	0.95307300
C	6.02205800	-0.42742700	-1.61198000
H	4.75800400	-2.13056900	-2.00771300
C	6.17748100	0.76038200	-0.89306800

H	5.29714900	2.06040200	0.58803600
H	6.78109000	-0.73430000	-2.32881200
H	7.05685200	1.38259900	-1.04189000
H	1.29739900	-0.98339000	-0.41023300
S	-2.83553000	0.47052000	1.83398400
O	0.73136300	-0.66506200	-3.40774100
C	-0.02045600	-1.07806800	-2.32256000
O	-0.69047900	-2.07908300	-2.43206700
H	-4.07634100	-3.91379000	-1.05249600
H	-2.43866800	-4.96112700	0.84248700
H	1.25321900	-2.98485300	4.01457700
H	2.30715700	-0.52145900	4.43442900
H	1.64067800	4.23794400	2.28636200
H	0.08877100	5.22938100	0.29311000
H	-3.50965200	3.22446700	-2.98896500
H	-4.63765900	0.78107600	-3.32650700

TS2(*OSS*)

Fe	-1.05497800	0.10046700	0.39475600
N	-2.10006100	-1.57742700	-0.02518000
N	-2.10741600	1.14248700	-0.99766700
N	-0.06166400	-0.90471800	1.82853100
N	-0.08980400	1.81636600	0.89256100
C	-1.95217000	-2.81103300	0.53387200
C	-2.00264700	2.47215900	-1.30655600
C	-3.10323300	-1.69109700	-0.94460700
C	-3.10283300	0.63597200	-1.79162200
C	-0.18836600	-2.22879300	2.15571200
C	-0.25063600	3.06065600	0.33572500
C	0.83519300	-0.37463500	2.71589000
C	0.82369600	1.96364400	1.90040500
C	-2.89724500	-3.74381300	-0.04463100
C	-2.94873400	2.81674700	-2.34388800
C	-3.61654300	-3.04573100	-0.96079800
C	-3.63188900	1.67637700	-2.64375400
C	0.66478600	-2.54906700	3.27827400
C	0.60576600	4.01777100	0.99793900
C	1.29590400	-1.39730400	3.62992100
C	1.27246000	3.33688400	1.97209900
C	-1.04837100	-3.12995400	1.54155700
C	-1.12771700	3.37118200	-0.69783500
C	1.25792300	0.94917400	2.75125300
C	-3.56562600	-0.67557600	-1.77209900
H	-1.03850700	-4.15501500	1.90109200
H	-1.15269800	4.40215700	-1.04066900
H	1.98058700	1.21869200	3.51689500
H	-4.36530000	-0.92642300	-2.46366100
C	-3.04929500	2.31554600	2.14212200
H	-2.14112200	2.81685400	2.49201300
H	-3.36218500	2.78193600	1.20148100
H	-3.84097600	2.47233200	2.88445900

C	0.27314500	-0.27610700	-1.14768900
C	1.02200900	0.86398000	-1.80825000
C	1.58264700	0.27236600	-3.11188400
H	2.62601100	-0.04957800	-3.00171200
H	1.51538900	0.95097800	-3.96976200
H	1.80162600	1.29629300	-1.17355000
H	0.32221800	1.67757600	-2.03636400
S	2.63298500	-1.94378700	-0.11947700
C	3.97721700	-0.81461900	-0.42301000
C	4.07939200	0.42666400	0.23166100
C	5.00878900	-1.19566500	-1.30034700
C	5.17021300	1.26420900	-0.00322100
H	3.30084100	0.72718000	0.92576400
C	6.11032500	-0.36489000	-1.51124500
H	4.93355600	-2.14736600	-1.81859300
C	6.19472200	0.87291700	-0.86961000
H	5.22253300	2.22506600	0.50416200
H	6.89797800	-0.68125700	-2.19201600
H	7.04734800	1.52520300	-1.04319200
H	1.43932300	-1.06358600	-0.37828300
S	-2.80228800	0.51013800	1.94681700
O	0.77694600	-0.87659800	-3.39068100
C	0.09450800	-1.27845500	-2.24831600
O	-0.49934300	-2.33520500	-2.27287800
H	-4.41439100	-3.39510600	-1.60487400
H	-2.98015700	-4.78840300	0.23009400
H	0.75180300	-3.53207600	3.72489800
H	2.01404100	-1.23492900	4.42460700
H	1.99602100	3.71414500	2.68512600
H	0.66859000	5.06962600	0.74511100
H	-3.06680500	3.80666800	-2.76849600
H	-4.42597900	1.53569200	-3.36727400

TS2(*triplet*)

Fe	-1.05528900	0.08313000	0.42079500
N	-1.14640500	-1.89417600	0.80108000
N	-2.55353200	-0.06767500	-0.92169000
N	0.40568400	0.25653000	1.82179400
N	-1.02010300	2.08891200	0.10669900
C	-0.38821200	-2.61111700	1.68677500
C	-3.07942900	0.92574800	-1.70616800
C	-2.05444600	-2.76908100	0.27444100
C	-3.25487100	-1.20451400	-1.21459500
C	0.94137600	-0.73989900	2.58995300
C	-1.75774900	2.80330700	-0.80023700
C	0.97157300	1.42542000	2.25525600
C	-0.23056600	2.99514200	0.76342800
C	-0.81082300	-3.99493100	1.69876100
C	-4.14030500	0.39519100	-2.53406100
C	-1.85073700	-4.09070300	0.82773200
C	-4.25557200	-0.92429700	-2.22044900

C	1.89331200	-0.19081000	3.52813400
C	-1.42519700	4.20701000	-0.71608000
C	1.91034400	1.15595900	3.32352200
C	-0.48000600	4.32628500	0.25881000
C	0.59600000	-2.08512400	2.51388000
C	-2.69827300	2.26250400	-1.67342700
C	0.69410600	2.69534500	1.75903400
C	-3.04210900	-2.45623400	-0.65038800
H	1.11427600	-2.77273200	3.17557200
H	-3.20672900	2.94549300	-2.34842700
H	1.23877500	3.52827000	2.19571000
H	-3.68365700	-3.26649200	-0.98476800
C	-3.91870300	1.52571300	1.65606100
H	-3.51525700	2.50675300	1.38375300
H	-4.47005200	1.12799200	0.79754500
H	-4.62020600	1.65721900	2.48818100
C	0.29834200	-0.15787700	-1.15525400
C	1.03290500	1.01783600	-1.77147800
C	1.59829200	0.46911400	-3.09202400
H	2.62930200	0.11093300	-2.97983900
H	1.56483200	1.18758100	-3.91898000
H	1.80508500	1.44411900	-1.12316700
H	0.31896600	1.82385800	-1.98462200
S	2.72510900	-1.91429600	-0.38768700
C	4.04905300	-0.73027600	-0.53298500
C	4.11399100	0.42766500	0.26299700
C	5.10029600	-0.98587300	-1.43211600
C	5.19021000	1.30773800	0.14461200
H	3.32394000	0.62903400	0.97831000
C	6.18565400	-0.11366400	-1.52847000
H	5.05354600	-1.87245900	-2.05810200
C	6.23417000	1.04207800	-0.74578300
H	5.21641800	2.20202200	0.76354700
H	6.98891800	-0.33244600	-2.22910500
H	7.07448200	1.72739900	-0.82852800
H	1.52425300	-1.02433400	-0.51423900
S	-2.59240700	0.38413700	2.19494800
O	0.76003900	-0.63977600	-3.43209900
C	0.06977000	-1.07888400	-2.30496900
O	-0.56469400	-2.11097500	-2.37882100
H	-2.43502500	-4.96441800	0.56552500
H	-0.36288300	-4.77075100	2.30773900
H	2.46026800	-0.77316100	4.24417500
H	2.49189200	1.91052500	3.83989200
H	0.01252000	5.22342000	0.61486000
H	-1.87040300	4.98538400	-1.32438300
H	-4.71523200	0.97431300	-3.24677700
H	-4.94041000	-1.65809900	-2.62799200

TS2(*quintet*)

Fe	-1.02289700	0.09737700	0.40496700

N	-0.97684000	-1.86025300	0.90073700
N	-2.57867400	-0.23040100	-0.85522500
N	0.44328600	0.45694200	1.77089400
N	-1.15158200	2.07445200	0.00237700
C	-0.14953500	-2.47626900	1.81140900
C	-3.20590000	0.67801300	-1.68219200
C	-1.84003700	-2.83178600	0.45370500
C	-3.22467100	-1.42176500	-1.05893500
C	1.06848700	-0.45494300	2.59062800
C	-1.97097300	2.69387800	-0.92537400
C	0.96838400	1.68383700	2.11329500
C	-0.39388000	3.08025400	0.56972600
C	-0.47032500	-3.88690300	1.90280500
C	-4.24877100	0.05244800	-2.41446700
C	-1.51961800	-4.10400400	1.07116900
C	-4.26778900	-1.27126000	-2.01374700
C	1.99727100	0.19279200	3.44709600
C	-1.71977400	4.11949700	-0.93516300
C	1.93538400	1.54337500	3.14503900
C	-0.75302000	4.35760100	-0.01130900
C	0.79828800	-1.84161900	2.58507100
C	-2.89490600	2.05287200	-1.72291600
C	0.58157300	2.90839400	1.52847100
C	-2.88384400	-2.63831700	-0.42489000
H	1.37649900	-2.45577600	3.26953100
H	-3.46547400	2.66577100	-2.41625400
H	1.09212800	3.80086400	1.88136400
H	-3.48429300	-3.50660000	-0.68203800
C	-4.10240700	1.18393900	1.57771800
H	-3.92351100	2.11235900	1.02575700
H	-4.60918600	0.47562200	0.91590000
H	-4.75769900	1.40967300	2.42747300
C	0.30191200	-0.17094900	-1.13079700
C	1.05417900	1.00379500	-1.72348100
C	1.57243000	0.47904600	-3.07343200
H	2.60604200	0.11922800	-3.00677500
H	1.50758500	1.21595600	-3.88139900
H	1.85433000	1.37963500	-1.07761900
H	0.36187200	1.83806300	-1.88723800
S	2.70064700	-1.93369700	-0.40337600
C	4.02492100	-0.74792300	-0.55169300
C	4.18516300	0.30741300	0.36426000
C	4.97575100	-0.90258800	-1.57662700
C	5.25861100	1.19043700	0.23989300
H	3.47545100	0.42771900	1.17639800
C	6.05935800	-0.02876300	-1.68128700
H	4.85301200	-1.71260900	-2.28997900
C	6.20273700	1.02658100	-0.77760700
H	5.36072800	2.00544400	0.95299500
H	6.78592100	-0.16701300	-2.47929000
H	7.04148200	1.71339600	-0.86469100

H	1.48773200	-1.03258800	-0.52339300
S	-2.54626700	0.48994800	2.24257500
O	0.72454600	-0.62502000	-3.41150300
C	0.05783800	-1.08728500	-2.28514300
O	-0.56482300	-2.12394300	-2.35157300
H	-2.04627900	-5.02989700	0.87374300
H	0.04904500	-4.59344700	2.53877400
H	2.61680500	-0.30498200	4.18309100
H	2.48833600	2.35958700	3.59461000
H	-0.30682500	5.30436600	0.26931500
H	-2.23691000	4.82875600	-1.57058900
H	-4.89463700	0.55023200	-3.12783800
H	-4.91905100	-2.06783200	-2.35237400

int3(*doublet*)

Fe	-0.13497500	0.03637500	-0.21123300
N	1.49870900	-1.07742200	-0.63536900
N	0.98688100	1.71248600	-0.46352300
N	-1.25495000	-1.62640900	0.00490400
N	-1.76378000	1.16421100	0.20544200
C	1.52676800	-2.43865000	-0.76397700
C	0.52364900	3.00089800	-0.43693900
C	2.76330300	-0.63847300	-0.91407800
C	2.31404500	1.78653000	-0.78923000
C	-0.83451100	-2.91071100	-0.19885500
C	-1.83216700	2.53061500	0.17224100
C	-2.56492300	-1.70378800	0.39450200
C	-3.00739500	0.72176700	0.57087400
C	2.85787300	-2.87750100	-1.12620400
C	1.59789600	3.92149200	-0.74127300
C	3.62829700	-1.76033100	-1.21235800
C	2.71168500	3.16726500	-0.95491600
C	-1.91817400	-3.83446700	0.05777100
C	-3.16388200	2.96885800	0.52917600
C	-2.99107300	-3.08613100	0.43510700
C	-3.89204900	1.84560100	0.78422900
C	0.44845400	-3.29348700	-0.57454800
C	-0.77980900	3.38835500	-0.13933400
C	-3.38220200	-0.61452900	0.68402700
C	3.15748700	0.69429000	-0.97020700
H	0.63190900	-4.35718600	-0.69755600
H	-0.99267300	4.45419000	-0.13928300
H	-4.40577300	-0.82306600	0.98388900
H	4.19524700	0.89891500	-1.21910400
C	-2.35935000	-0.20003400	-2.81237300
H	-2.65416500	-1.18176200	-2.42604700
H	-2.97608700	0.56141900	-2.32233000
H	-2.56878400	-0.17475900	-3.88849400
C	0.17227400	-0.04556300	1.92726700
C	0.61682400	1.24535200	2.61628200
C	2.13538200	1.04329900	2.73015100

H	2.57349300	1.48343400	3.63448100
H	2.66412700	1.43799300	1.85621200
H	0.17676500	1.32193600	3.62488100
H	0.36753400	2.16407800	2.08188700
S	-0.57194100	0.11415100	-2.55421800
H	-0.82466600	-0.38125900	2.20707000
O	2.33575800	-0.37691200	2.79147700
C	1.18809000	-1.03347300	2.35629100
O	1.15396700	-2.24734500	2.40154300
H	4.68004300	-1.68019500	-1.45988200
H	3.14472000	-3.91050600	-1.28194800
H	-1.84395000	-4.91165700	-0.03149800
H	-3.98404200	-3.41913000	0.71323500
H	-4.93181200	1.76702800	1.07933000
H	-3.48171200	4.00390700	0.57546900
H	1.49381800	4.99931500	-0.78473000
H	3.71165800	3.49603700	-1.21213800

int3(*quartet*)

Fe	0.05182800	0.14193000	-0.21621700
N	-0.94864800	1.90674200	-0.15741000
N	-1.68471800	-0.79547300	-0.63052500
N	1.80810500	1.08114100	0.17608800
N	1.05254700	-1.62395700	-0.30067900
C	-0.39788000	3.14689300	0.09692500
C	-1.85280200	-2.14683900	-0.86176000
C	-2.27945400	2.13049000	-0.37703300
C	-2.92731300	-0.22583200	-0.80342600
C	1.97186500	2.43475000	0.39140000
C	0.51183000	-2.86166800	-0.58436100
C	3.05788400	0.52148000	0.30283300
C	2.40557500	-1.84040300	-0.13907100
C	-1.39984000	4.15601500	0.04007600
C	-3.24237900	-2.42897000	-1.16840100
C	-2.58555200	3.51634500	-0.26232700
C	-3.90299200	-1.24620000	-1.13630200
C	3.36378900	2.72835500	0.65817300
C	1.52251500	-3.85828200	-0.59043800
C	4.03644800	1.54826900	0.60312900
C	2.71732500	-3.21501900	-0.31062100
C	0.96365900	3.37829800	0.36108800
C	-0.85790500	-3.09638700	-0.83260000
C	3.34412200	-0.82416300	0.16075600
C	-3.21290600	1.11605300	-0.69191900
H	1.25096400	4.40972100	0.55224700
H	-1.14667200	-4.12463900	-1.03531000
H	4.38009700	-1.13145900	0.27894400
H	-4.24279800	1.42467600	-0.84779000
C	2.10434200	0.28889300	-2.98409200
H	2.66304800	1.13863900	-2.57948200
H	2.54951000	-0.63614000	-2.60419100

H	2.19699100	0.29325300	-4.07693100
C	-0.19243900	0.09985300	1.93011500
C	0.74850200	-0.79910600	2.72091400
C	-0.08990700	-2.07518900	2.88392700
H	0.07562300	-2.59404400	3.83518700
H	0.07732700	-2.77745800	2.06190400
H	0.95103300	-0.35619700	3.71046000
H	1.71201900	-0.99484400	2.24776000
S	0.32453500	0.38843300	-2.57674800
H	-0.06989100	1.16651600	2.09705700
O	-1.46254200	-1.64313400	2.85680600
C	-1.54637000	-0.36108700	2.33790400
O	-2.61487700	0.21250400	2.32131300
H	-3.57146800	3.94739500	-0.38732700
H	-1.22705400	5.21337200	0.20289700
H	3.75532300	3.71932300	0.85674800
H	5.09498000	1.36607200	0.74685000
H	3.71041800	-3.64215300	-0.23624100
H	1.35565500	-4.91104700	-0.78547500
H	-3.63344400	-3.41696200	-1.38089600
H	-4.95411400	-1.05256900	-1.31339500

int3(*sextet*)

Fe	0.09400000	0.11602800	-0.27011800
N	-1.15925000	1.78849900	-0.28619700
N	-1.52759500	-1.09969900	-0.73216900
N	1.72271300	1.30836900	0.31232000
N	1.33646600	-1.55158700	-0.21221000
C	-0.77194300	3.06564100	-0.00888000
C	-1.48970600	-2.44683300	-0.93471800
C	-2.48372700	1.79603700	-0.58658500
C	-2.80231000	-0.66745300	-0.97952000
C	1.67020800	2.66229900	0.49397300
C	0.95662000	-2.83651500	-0.49616000
C	3.00661200	0.90008300	0.50186900
C	2.68346100	-1.55333200	0.04927700
C	-1.92015500	3.94334000	-0.14754400
C	-2.81214400	-2.90591100	-1.31860500
C	-2.97745200	3.15808400	-0.50837800
C	-3.62047800	-1.80721100	-1.34708900
C	2.99846100	3.14016000	0.83135600
C	2.11649800	-3.69857800	-0.40737700
C	3.82506900	2.05237600	0.83353800
C	3.18031400	-2.90739300	-0.07180500
C	0.52499500	3.46034700	0.35843900
C	-0.34474800	-3.24920000	-0.81888800
C	3.45085000	-0.42864100	0.38117700
C	-3.23915600	0.65882700	-0.91640000
H	0.66244000	4.52291200	0.54571600
H	-0.47761100	-4.31056900	-1.01356900
H	4.50899100	-0.60368300	0.56046700

H	-4.29101100	0.82736200	-1.13209100
C	2.19670500	0.08143100	-3.13346300
H	2.97737500	0.56604000	-2.53563600
H	2.24856600	-0.99715500	-2.94933600
H	2.41339800	0.26394100	-4.19268600
C	-0.41707300	0.16028100	2.14344000
C	0.49541200	-0.76224600	2.93121100
C	-0.35807200	-2.04085000	2.98664600
H	-0.22777600	-2.62244100	3.90771200
H	-0.15003200	-2.69137400	2.12812600
H	0.67866000	-0.38345500	3.95352500
H	1.47312800	-0.94872200	2.47709600
S	0.54013200	0.75720300	-2.71794400
H	-0.27726000	1.23267600	2.23992900
O	-1.72246300	-1.60782200	2.92292800
C	-1.76958400	-0.30110000	2.41490000
O	-2.85640200	0.23877200	2.28822400
H	-4.00077200	3.46206000	-0.69371400
H	-1.90969300	5.01491200	0.01362000
H	3.25704200	4.17363600	1.03056300
H	4.88951000	2.02518400	1.03639300
H	4.21079400	-3.20787800	0.07905400
H	2.11163400	-4.76824800	-0.58183200
H	-3.07549100	-3.93415800	-1.53691800
H	-4.67537000	-1.76157100	-1.59016800

TS4(*OSS*)

Fe	-1.22490300	0.11686200	0.59108300
N	0.24170600	-0.70630100	1.68607100
N	-1.99342700	-1.71728700	0.29953200
N	-0.33218900	1.91925300	0.70262800
N	-2.57871500	0.90782500	-0.67366900
C	1.28506000	-0.04124600	2.27777400
C	-3.12702500	-2.02019200	-0.41316100
C	0.37356400	-2.01818300	2.06260700
C	-1.57669500	-2.89900800	0.85876900
C	0.79384300	2.22216500	1.42812500
C	-3.63387700	0.24356900	-1.25239400
C	-0.72954400	3.09799100	0.11722600
C	-2.69665700	2.21990200	-1.07225300
C	2.09846500	-0.95897900	3.04223200
C	-3.42171200	-3.43054600	-0.31234500
C	1.52816000	-2.18590100	2.91266900
C	-2.45896100	-3.97561200	0.47871700
C	1.11009600	3.62418300	1.30103500
C	-4.43130000	1.15609100	-2.03392900
C	0.16351900	4.16860100	0.48790600
C	-3.84843700	2.38321600	-1.92357700
C	1.54804000	1.31608300	2.16226600
C	-3.89382400	-1.11553700	-1.13295300
C	-1.83311800	3.24595600	-0.71184200

C	-0.47750900	-3.04614600	1.69048100
H	2.42963000	1.69665700	2.66861100
H	-4.76447300	-1.50364500	-1.65395000
H	-2.03699500	4.23725600	-1.10631200
H	-0.25424600	-4.04290700	2.05804200
C	-3.23262600	2.09549400	2.39545900
H	-2.45418600	2.86321800	2.38395000
H	-3.88242100	2.23171700	1.52667600
H	-3.83190700	2.21681900	3.30539300
C	0.58223700	-0.23681800	-1.61783500
C	-0.04491800	0.34091300	-2.85193600
C	0.00482900	-0.86790300	-3.81321800
H	0.86165900	-0.79345600	-4.49416500
H	-0.91030800	-0.99980700	-4.40002400
H	0.50807200	1.19907000	-3.24702300
H	-1.08137100	0.66015700	-2.68345800
S	-2.51879000	0.41192000	2.44976000
H	1.10683200	0.31631800	-0.85648100
O	0.17836500	-2.03797800	-3.00040900
C	0.70077200	-1.67300100	-1.76277600
O	1.13181000	-2.53173500	-1.01035600
H	1.85421200	-3.13183800	3.32662500
H	2.99562600	-0.68060500	3.58000200
H	1.95974200	4.10683300	1.76757200
H	0.07137500	5.19321600	0.14914300
H	-4.15416100	3.31973200	-2.37397000
H	-5.31498300	0.87644100	-2.59462500
H	-4.25680700	-3.92078200	-0.79759500
H	-2.33352400	-5.00828800	0.77936100
S	3.34693400	0.36050500	-2.71060500
C	4.37163100	0.15953900	-1.29427600
C	4.24551300	-0.95989300	-0.43831500
C	5.36470200	1.11445300	-0.97349000
C	5.07532400	-1.10939900	0.67207400
H	3.47535900	-1.69686000	-0.64678600
C	6.20434800	0.94687700	0.12641400
H	5.46736200	1.99002700	-1.60941600
C	6.06737900	-0.16614900	0.96230100
H	4.94597000	-1.97796900	1.31540900
H	6.96635900	1.69620100	0.33820000
H	6.71967200	-0.29455400	1.82385000

TS4(*triplet*)

Fe	1.16509100	0.09532400	-0.55468700
N	-0.35463900	-0.71331600	-1.59322000
N	1.91111600	-1.75273900	-0.26636600
N	0.32995400	1.92817800	-0.69111300
N	2.61932300	0.88751400	0.60184600
C	-1.40290400	-0.03191600	-2.15315000
C	3.07306900	-2.06497100	0.39227900
C	-0.52780100	-2.02591000	-1.94201300

C	1.44619400	-2.93224100	-0.79067300
C	-0.82139000	2.23935100	-1.36937200
C	3.68865500	0.21023000	1.13391300
C	0.78958600	3.10826400	-0.16204400
C	2.79923600	2.20812600	0.94321800
C	-2.26479900	-0.94236800	-2.87429100
C	3.33455600	-3.48336400	0.30132900
C	-1.71676200	-2.17982400	-2.74810700
C	2.32478900	-4.02088500	-0.43456800
C	-1.09463100	3.65335700	-1.26633600
C	4.56145500	1.12386400	1.83133100
C	-0.09352600	4.19358800	-0.51794200
C	4.00847300	2.36411200	1.71436000
C	-1.62920800	1.33422000	-2.04780300
C	3.90233300	-1.16077700	1.04295500
C	1.94367200	3.24786600	0.59995900
C	0.31438300	-3.06709200	-1.58059100
H	-2.52247500	1.72650200	-2.52433800
H	4.79300500	-1.55803800	1.52181800
H	2.19862000	4.24470000	0.94836600
H	0.05773900	-4.06424200	-1.92488400
C	3.21320000	1.93289000	-2.49514500
H	2.50122800	2.75518500	-2.38064500
H	3.95724600	1.99517600	-1.69543500
H	3.72366700	2.04396900	-3.45884500
C	-0.50321400	-0.13278300	1.53711900
C	0.18261100	0.43750400	2.74595400
C	0.79175400	-0.83030600	3.38305700
H	0.67859700	-0.86412100	4.47194600
H	1.85416200	-0.93469500	3.13467500
H	-0.53701700	0.91144000	3.42680800
H	0.94846700	1.18091200	2.51269000
S	2.36736600	0.30949000	-2.50646300
H	-1.11806900	0.42159900	0.84845300
O	0.08778000	-1.95376600	2.83324200
C	-0.64697800	-1.57210500	1.72023200
O	-1.26212300	-2.41135600	1.08685400
H	-2.07756700	-3.12346300	-3.13804000
H	-3.17366700	-0.65179100	-3.38553400
H	-1.95147200	4.14788400	-1.70684300
H	0.04466600	5.22509600	-0.21752400
H	4.37172100	3.30567600	2.10825100
H	5.47241100	0.83658400	2.34258500
H	4.18452800	-3.98279600	0.75023700
H	2.16811700	-5.05475600	-0.71624000
S	-3.16482400	0.41255300	2.64982700
C	-4.34195600	0.19272100	1.36050000
C	-4.32248300	-0.95642600	0.53754400
C	-5.34372200	1.15976100	1.11855300
C	-5.26754100	-1.12229800	-0.47391400
H	-3.54221100	-1.69632700	0.69125600

C	-6.30111700	0.97231100	0.12292700
H	-5.35960900	2.05833100	1.72980900
C	-6.27015500	-0.16922000	-0.68431800
H	-5.22281000	-2.01124700	-1.10031900
H	-7.06961100	1.72835500	-0.03218200
H	-7.01291700	-0.31160900	-1.46661300

TS4(*quintet*)

Fe	1.19838700	0.09245900	-0.53327800
N	-0.47210000	-0.18478900	-1.72837200
N	1.38997100	-1.97158500	-0.32099200
N	0.91956900	2.16782800	-0.59322200
N	2.80596300	0.37865300	0.76807800
C	-1.23874800	0.80479300	-2.27092800
C	2.34642200	-2.61892200	0.40713300
C	-0.95082200	-1.38271200	-2.16921400
C	0.64433800	-2.91063600	-0.97041200
C	-0.04386900	2.80963100	-1.31657300
C	3.56161100	-0.61431900	1.32959100
C	1.74253700	3.11155800	-0.05154300
C	3.35982900	1.57836100	1.11693100
C	-2.26827500	0.20460400	-3.10237100
C	2.19546600	-4.05070000	0.22106400
C	-2.08739700	-1.14526500	-3.04234900
C	1.14562300	-4.22944800	-0.63251500
C	0.16171400	4.24274800	-1.21139800
C	4.64441000	-0.01496400	2.08658600
C	1.26743600	4.42936100	-0.43274600
C	4.52112700	1.33914900	1.95302200
C	-1.04606200	2.18007600	-2.07065400
C	3.33681000	-1.99086100	1.17703400
C	2.86842800	2.83832300	0.73853300
C	-0.42952300	-2.63658800	-1.82763400
H	-1.74500600	2.83892900	-2.58023000
H	4.02965100	-2.64911600	1.69620700
H	3.42458100	3.69977700	1.10098200
H	-0.92976000	-3.49883300	-2.26140800
C	4.18068500	-0.61151300	-2.10213400
H	4.73078000	-0.02062100	-1.36292700
H	4.06103700	-1.62942300	-1.71838500
H	4.77385000	-0.65643000	-3.02347600
C	-0.44229400	0.24090700	1.31067400
C	0.15546000	0.90330400	2.52337000
C	0.55839000	-0.30790000	3.38718200
H	0.33357400	-0.17446600	4.45080100
H	1.61959700	-0.55159400	3.27625600
H	-0.60031900	1.51033300	3.04176400
H	1.00353800	1.55560000	2.30800800
S	2.55910600	0.14213100	-2.50350800
H	-1.07568400	0.77206800	0.61441200
O	-0.21511200	-1.42312500	2.91409000

C	-0.81143700	-1.12643700	1.70324900
O	-1.52128800	-1.94933100	1.15684300
H	-2.66942500	-1.91835800	-3.52969500
H	-3.02663200	0.75362200	-3.64758700
H	-0.45884600	4.99732200	-1.68028000
H	1.72716500	5.36674100	-0.14175400
H	5.15391700	2.11073500	2.37626700
H	5.39724700	-0.56485000	2.63938500
H	2.81474300	-4.80888500	0.68582600
H	0.73755300	-5.16334500	-1.00061200
S	-3.34563000	1.15163400	2.25863200
C	-4.57347800	0.43404400	1.24715800
C	-4.64260700	-0.96958100	1.07167000
C	-5.53102800	1.23957700	0.58454500
C	-5.63510000	-1.53254400	0.27386200
H	-3.88517000	-1.59113400	1.53702400
C	-6.53541000	0.66528100	-0.18822700
H	-5.46867500	2.31811800	0.69685500
C	-6.59228500	-0.72420000	-0.34910500
H	-5.66411400	-2.61126200	0.13827700
H	-7.27006900	1.30047600	-0.67903600
H	-7.37154500	-1.17143800	-0.96215200

int5(*CSS*)

C	1.33963200	-0.19275600	0.62866700
C	2.56644700	-1.04231900	0.98321600
C	3.58106100	-0.61663400	-0.08855500
H	3.49887500	-1.21592600	-1.00220000
H	4.61797200	-0.62871000	0.25364300
H	2.37167600	-2.11717800	0.98628100
H	2.92874900	-0.75496400	1.97683700
H	0.73333400	0.10201600	1.48615600
S	0.23023600	-1.08712400	-0.56024600
C	-1.38763400	-0.39827500	-0.20500200
C	-2.46417000	-1.29512100	-0.15392600
C	-1.61044300	0.97529700	-0.03417200
C	-3.75811100	-0.81899700	0.06045500
H	-2.28626700	-2.36006400	-0.27275800
C	-2.90645400	1.43490700	0.20915800
H	-0.78286100	1.67522100	-0.09359600
C	-3.98250300	0.54593600	0.25026700
H	-4.58773400	-1.52011700	0.09607400
H	-3.07368200	2.49946100	0.35045400
H	-4.98901600	0.91405600	0.42893200
O	3.24450300	0.74912400	-0.40860500
C	1.97214000	1.04133100	-0.03003400
O	1.47867100	2.12587400	-0.21218500

TS6(*doublet*)

Fe	0.61040300	0.10528700	-0.41305900
N	0.55250500	2.12042400	-0.22098200

N	-0.92539600	0.22179300	-1.73600900
N	1.83534000	-0.01273700	1.20331200
N	0.37039100	-1.91276900	-0.32504000
C	1.34177200	2.88102700	0.60257900
C	-1.54089800	-0.83009200	-2.36449500
C	-0.18914400	3.00688100	-0.95833000
C	-1.47645100	1.35757800	-2.27191200
C	2.44398700	1.04016100	1.83760800
C	-0.41897800	-2.67497300	-1.15141400
C	2.31392600	-1.14795800	1.80914800
C	1.04840100	-2.80078500	0.47628500
C	1.09779900	4.28861000	0.37190500
C	-2.50591500	-0.34424300	-3.32701000
C	0.14551000	4.36712400	-0.59696300
C	-2.46672600	1.01516200	-3.26869400
C	3.33309600	0.55712900	2.87021500
C	-0.23136200	-4.07909000	-0.86643800
C	3.25240300	-0.80262700	2.85353500
C	0.67920200	-4.15788500	0.14463000
C	2.22694700	2.38486600	1.55323700
C	-1.30198800	-2.17606500	-2.10446400
C	1.95278200	-2.44892800	1.47264800
C	-1.13460100	2.65753500	-1.91623900
H	2.78253500	3.11154200	2.14035200
H	-1.86686000	-2.90122000	-2.68464800
H	2.41718200	-3.25641500	2.03274400
H	-1.65110600	3.46647900	-2.42580500
C	3.59294000	-1.17932700	-1.70344300
H	4.02630500	-1.00468500	-0.71155000
H	3.12683900	-2.17183500	-1.69950800
H	4.41117100	-1.19076400	-2.43446800
C	-2.39023000	0.08251500	2.57028100
C	-2.31587000	-1.31462700	2.06731800
C	-3.69063100	-1.45493600	1.37550000
H	-4.17830400	-2.41767500	1.55603100
H	-3.59966800	-1.30081400	0.29352500
H	-2.20825600	-2.03862200	2.89522100
H	-1.48251100	-1.49293400	1.38000500
S	2.38440900	0.13133200	-2.14838800
H	-1.57731600	0.65919600	2.98957700
O	-4.53407900	-0.42344800	1.91855800
C	-3.75101100	0.55223300	2.52984800
O	-4.25222800	1.58091300	2.95334000
H	-0.30417000	5.25112400	-1.03291100
H	1.59424600	5.09587600	0.89726100
H	3.93143000	1.18914200	3.51591200
H	3.76903800	-1.51772100	3.48278000
H	1.07145200	-5.04263900	0.63208100
H	-0.73900100	-4.88707500	-1.38022200
H	-3.12571400	-0.97502700	-3.95328300
H	-3.04752300	1.73288100	-3.83552100

TS6(*quartet*)

Fe	0.17498100	0.15620000	-0.30961300
N	-1.00197100	1.79155000	-0.12096000
N	-1.48041000	-0.98810100	-0.59637400
N	1.79120200	1.24833100	0.24285900
N	1.31173500	-1.49275700	-0.31797500
C	-0.59050800	3.07064700	0.14352000
C	-1.51988400	-2.33189200	-0.83902800
C	-2.35681900	1.85672700	-0.29800000
C	-2.77470900	-0.54210600	-0.70906400
C	1.81632700	2.60608300	0.47308900
C	0.89391900	-2.78093400	-0.58693500
C	3.08238500	0.81386200	0.37576600
C	2.67314900	-1.56937600	-0.10852600
C	-1.72023100	3.97452600	0.12147000
C	-2.87397000	-2.75495700	-1.10309400
C	-2.81728200	3.22015500	-0.15347400
C	-3.65488500	-1.64114900	-1.02105600
C	3.16006300	3.03156300	0.76717800
C	2.02021700	-3.68160000	-0.55366800
C	3.94811000	1.91817500	0.70523500
C	3.11965000	-2.93355500	-0.25779300
C	0.71582700	3.45274100	0.42614600
C	-0.41122600	-3.17716500	-0.83506400
C	3.50418700	-0.50644500	0.21147400
C	-3.18545400	0.77617100	-0.57296700
H	0.89244600	4.50581700	0.62831600
H	-0.58351600	-4.23099900	-1.03545700
H	4.56134600	-0.71729100	0.34578500
H	-4.24684000	0.97920500	-0.67957400
C	1.97806800	0.16287700	-3.30810900
H	2.78274600	0.65291000	-2.74725200
H	2.06587700	-0.91874500	-3.15487800
H	2.13117300	0.37050800	-4.37427300
C	-0.41384700	0.20293500	2.48859700
C	0.45017900	-0.89623400	3.03301800
C	-0.55132500	-2.06977800	3.04528500
H	-0.43093600	-2.74229700	3.90296100
H	-0.47232000	-2.65814300	2.12268600
H	0.80548700	-0.67385600	4.05740700
H	1.33655000	-1.12395300	2.43114100
S	0.32762100	0.78939600	-2.79317900
H	-0.11046400	1.23964400	2.44599200
O	-1.85829500	-1.48738100	3.11537900
C	-1.78777900	-0.13882100	2.72412300
O	-2.81696500	0.51926600	2.66127800
H	-3.85039900	3.53319700	-0.23984800
H	-1.66044100	5.04075100	0.30400800
H	3.45089100	4.05212200	0.98589100
H	5.01701500	1.83919600	0.86479100

H	4.14651800	-3.26020200	-0.14356100
H	1.95906500	-4.74859600	-0.73228000
H	-3.17167400	-3.77409400	-1.31910500
H	-4.72640200	-1.55484600	-1.15277200

TS6(*sextet*)

Fe	0.12130900	0.14758900	-0.28145400
N	-1.08699700	1.85312000	-0.13259300
N	-1.57012500	-1.01122300	-0.63412100
N	1.80485700	1.25810000	0.29199200
N	1.29788700	-1.56430700	-0.29917200
C	-0.64505400	3.10711600	0.16356800
C	-1.59281700	-2.35258000	-0.86904100
C	-2.42492200	1.91092400	-0.35414200
C	-2.84281500	-0.53057900	-0.79456100
C	1.80509700	2.60733200	0.52303200
C	0.85801500	-2.83283600	-0.57868900
C	3.08259600	0.80538900	0.40513800
C	2.65557700	-1.62038000	-0.09969400
C	-1.77092400	4.02452600	0.12009500
C	-2.95000500	-2.75776900	-1.18368900
C	-2.87107300	3.28443700	-0.20373100
C	-3.72016600	-1.63211800	-1.13879900
C	3.16181000	3.03111600	0.81163600
C	1.98915200	-3.73664700	-0.55824300
C	3.95217900	1.91876400	0.73586400
C	3.09577000	-2.98963300	-0.26440900
C	0.68258700	3.44596200	0.47255900
C	-0.47069600	-3.19582000	-0.83655900
C	3.47678900	-0.53290900	0.22213900
C	-3.23210800	0.80625300	-0.67111200
H	0.86664500	4.49615900	0.68803500
H	-0.65096100	-4.24817000	-1.04191700
H	4.53530100	-0.74802700	0.34734400
H	-4.28897700	1.01152100	-0.82052400
C	1.97506200	0.14419000	-3.25859100
H	2.82702500	0.54493500	-2.69723600
H	1.96448200	-0.94358700	-3.13110100
H	2.12902800	0.36728700	-4.32096000
C	-0.31194300	0.17977200	2.23799700
C	0.59908700	-0.81828900	2.91921700
C	-0.31428500	-2.05572300	2.97615700
H	-0.16156500	-2.67885700	3.86581900
H	-0.18774000	-2.67980200	2.08315900
H	0.86757000	-0.49452800	3.94206900
H	1.53507500	-1.02727900	2.39266500
S	0.40118000	0.90752900	-2.69272600
H	-0.10512400	1.24055800	2.32160900
O	-1.65699500	-1.55582500	3.00800000
C	-1.66783200	-0.22858000	2.55379600
O	-2.73154400	0.36788600	2.50395600

H	-3.89341800	3.62447900	-0.31805300
H	-1.71689800	5.08901200	0.31588500
H	3.46289200	4.04816200	1.03433600
H	5.02351800	1.85156000	0.88650900
H	4.12031900	-3.32961600	-0.16578800
H	1.93644200	-4.80301500	-0.74484500
H	-3.26142200	-3.77105200	-1.40876900
H	-4.78541900	-1.54510000	-1.31663500

int7(*doublet*)

C	-0.00760200	1.18285800	-0.03180600
C	-1.41907300	0.73393200	0.03839500
C	-1.27264200	-0.81009500	-0.04325700
H	-1.65215400	-1.20674800	-0.99083900
H	-1.77560600	-1.32883400	0.77727500
H	-2.03940000	1.13848000	-0.77331800
H	-1.90041300	1.05139500	0.97678200
H	0.34652700	2.20473800	-0.06028400
O	0.13043500	-1.10879900	0.03716600
C	0.89096000	0.04177300	-0.00194500
O	2.10346500	0.01506900	0.00059200

int8(*CSS*)

Fe	-0.06649900	0.03847700	-0.30579300
N	-1.53368700	1.45042200	-0.30506500
N	-1.50371400	-1.39708800	-0.44240700
N	1.35914300	1.47339100	-0.30590300
N	1.38711500	-1.36312100	-0.43344800
C	-1.34236900	2.79967500	-0.21996100
C	-1.28597400	-2.74472500	-0.48271200
C	-2.87916200	1.25507000	-0.43255900
C	-2.85370900	-1.21709200	-0.54966100
C	1.14025300	2.81860800	-0.20736500
C	1.19611200	-2.71607100	-0.46227100
C	2.71142300	1.30521300	-0.39744400
C	2.73612300	-1.16042800	-0.50863000
C	-2.61670100	3.48871400	-0.27477300
C	-2.54664200	-3.45026800	-0.60163000
C	-3.57182600	2.52795200	-0.41377600
C	-3.52092400	-2.50005100	-0.64921100
C	2.40301000	3.53096700	-0.22745600
C	2.47272500	-3.39799500	-0.54633100
C	3.37805300	2.59060400	-0.35450400
C	3.42856300	-2.43027900	-0.58405700
C	-0.10598700	3.43734100	-0.14179300
C	-0.03773100	-3.36281600	-0.46084600
C	3.36182600	0.08143700	-0.51033800
C	-3.50381100	0.01545800	-0.54759800
H	-0.11381500	4.52262900	-0.07479800
H	-0.02429800	-4.44954000	-0.49544300
H	4.44670700	0.09510200	-0.57250200

H	-4.58703900	0.00854100	-0.64083200
C	0.84031500	0.13708700	-3.12085500
H	1.55379400	0.97769600	-2.98580500
H	1.45158700	-0.78997900	-3.08292600
H	0.45869300	0.21748300	-4.15981700
C	-0.12404800	-0.02764000	1.51523500
C	-1.35770400	0.05260000	2.37792600
C	-0.94275700	-0.62192800	3.69369400
H	-1.19732500	-1.69129700	3.69328000
H	-1.37230800	-0.16471500	4.59241400
H	-2.23924100	-0.40174900	1.92027300
H	-1.59929300	1.11428600	2.55216500
O	-0.20234400	0.14993900	-2.22267000
C	0.98977400	-0.18431900	2.49532700
O	2.19057200	-0.08104000	2.36380100
O	0.48018000	-0.48395200	3.76184700
H	2.50625600	4.60798000	-0.16284200
H	4.45100900	2.73237000	-0.41008400
H	-2.74208400	4.56446300	-0.22971900
H	-4.64524600	2.65066900	-0.50256500
H	-4.59197500	-2.63522900	-0.74780500
H	-2.65073000	-4.52782800	-0.65644100
H	2.59786400	-4.47402800	-0.58188600
H	4.50415200	-2.54473500	-0.65059600

int8(*OSS*)

Fe	-0.06474400	0.03144200	-0.37657800
N	-1.55855500	1.41507900	-0.34418000
N	-1.47702300	-1.43442600	-0.44421100
N	1.33080400	1.48995500	-0.33856400
N	1.41023100	-1.34698100	-0.44580800
C	-1.39307200	2.76801300	-0.26499200
C	-1.23571800	-2.77835500	-0.46495300
C	-2.90153000	1.19201100	-0.45368300
C	-2.83148000	-1.27972200	-0.53931600
C	1.08765500	2.83150100	-0.24304500
C	1.24407900	-2.70344000	-0.45190300
C	2.68780400	1.34404700	-0.40743900
C	2.75685600	-1.12062000	-0.50297500
C	-2.68093000	3.43083000	-0.31096800
C	-2.48435400	-3.50707300	-0.55980500
C	-3.61841200	2.45061000	-0.43528100
C	-3.47605700	-2.57495700	-0.61240300
C	2.33790600	3.56361300	-0.24496900
C	2.53348200	-3.36206000	-0.50973400
C	3.33109300	2.63962600	-0.35614300
C	3.47245000	-2.37787600	-0.55059400
C	-0.16922600	3.42934300	-0.18963700
C	0.02328400	-3.37382400	-0.44218600
C	3.36100800	0.13134400	-0.50407000
C	-3.50400800	-0.05996400	-0.54861700

H	-0.19663300	4.51418400	-0.12330500
H	0.05692700	-4.46037800	-0.45713600
H	4.44623400	0.16350100	-0.54730700
H	-4.58778100	-0.08802800	-0.62917900
C	0.85981900	0.12638000	-3.14408200
H	1.54001700	0.99066800	-3.00201600
H	1.49455200	-0.78142700	-3.08800200
H	0.48608800	0.18693300	-4.18555400
C	-0.11579100	-0.02864100	1.58162300
C	-1.36493500	0.05878800	2.41948200
C	-0.93909700	-0.49930800	3.78821100
H	-1.18272500	-1.56875200	3.87763800
H	-1.37949100	0.02448300	4.64519400
H	-2.21598900	-0.47652900	1.98885800
H	-1.67248200	1.11411100	2.51061100
O	-0.20306700	0.11193100	-2.26156300
C	0.98458200	-0.14542500	2.54867200
O	2.19226700	-0.08459300	2.40969900
O	0.47926700	-0.33985300	3.84684300
H	2.42245000	4.64200700	-0.17748000
H	4.40223900	2.79937100	-0.39183600
H	-2.82731500	4.50390300	-0.26724000
H	-4.69507400	2.55134300	-0.51004300
H	-4.54558700	-2.73053300	-0.69499600
H	-2.56993000	-4.58701000	-0.59462400
H	2.67866700	-4.43600200	-0.52333000
H	4.55078600	-2.47365300	-0.59689200

int8(*triplet*)

Fe	-0.05027300	0.03328700	-0.40229800
N	-1.52824600	1.43354800	-0.37609000
N	-1.43727400	-1.44635400	-0.30811200
N	1.32033600	1.51607200	-0.48993300
N	1.40404300	-1.35755400	-0.42989800
C	-1.37748700	2.79072400	-0.36725700
C	-1.20562900	-2.79135800	-0.20711700
C	-2.87240800	1.19067900	-0.41718100
C	-2.79585900	-1.28689800	-0.34338900
C	1.09168300	2.86093000	-0.46003100
C	1.26242200	-2.71290700	-0.31265600
C	2.66568000	1.35351000	-0.64418300
C	2.73955500	-1.11796800	-0.58538800
C	-2.67342500	3.43625900	-0.39234300
C	-2.45982500	-3.51068300	-0.17053000
C	-3.60276500	2.44122800	-0.43159600
C	-3.44782300	-2.57647400	-0.26294700
C	2.34248200	3.58317700	-0.58633700
C	2.55637600	-3.35670600	-0.39189200
C	3.31945100	2.64527700	-0.71132800
C	3.47204800	-2.36575700	-0.57231800
C	-0.15921300	3.46467300	-0.37578800

C	0.05196300	-3.38814700	-0.18420100
C	3.33009000	0.13459600	-0.71352900
C	-3.46828100	-0.06813500	-0.41266200
H	-0.18970500	4.55117400	-0.36666800
H	0.09026800	-4.47126600	-0.10248200
H	4.41034800	0.16343500	-0.82733900
H	-4.55453700	-0.10292800	-0.43767400
C	-0.18182200	-1.00532500	-3.10308500
H	0.67651100	-1.69296500	-2.97196300
H	-1.09664700	-1.61214300	-2.95480200
H	-0.17777300	-0.68541800	-4.16264800
C	-0.00231100	0.09208600	1.59888900
C	-1.21769700	0.25425700	2.47354800
C	-0.71728200	-0.14123200	3.87551900
H	-0.95276700	-1.19375200	4.09965200
H	-1.12322500	0.47758000	4.68567900
H	-2.07511000	-0.34527400	2.14974000
H	-1.55308900	1.30546300	2.46155800
O	-0.12254700	0.10485500	-2.27689400
C	1.13550700	0.05481400	2.49962000
O	2.34053400	0.06267200	2.29843500
O	0.69779800	0.02484900	3.84622400
H	2.43604100	4.66284100	-0.58670700
H	4.38663300	2.79186500	-0.82889000
H	-2.83115800	4.50851400	-0.39163300
H	-4.68273200	2.52686000	-0.46612100
H	-4.52096400	-2.72840400	-0.27363900
H	-2.55380800	-4.58759400	-0.09325800
H	2.72053200	-4.42563600	-0.32308700
H	4.54741100	-2.45054200	-0.67477100

int8(*quintet*)

Fe	-0.04281700	0.03586500	-0.39013300
N	-1.65650700	1.38987900	-0.34452000
N	-1.41531400	-1.54089000	-0.31316000
N	1.30344000	1.61540800	-0.45416100
N	1.53365900	-1.32145500	-0.42902200
C	-1.53608000	2.74573400	-0.37519900
C	-1.08946100	-2.86544600	-0.25393700
C	-2.98028800	1.07492100	-0.38030000
C	-2.77537500	-1.43444000	-0.32458800
C	0.97761600	2.93583600	-0.46415500
C	1.42247200	-2.67701400	-0.35650800
C	2.65103300	1.50317200	-0.59684100
C	2.85013500	-1.00350000	-0.55856000
C	-2.86431200	3.33598800	-0.41548300
C	-2.31120700	-3.64953600	-0.22045700
C	-3.75734000	2.30273500	-0.42175500
C	-3.35214900	-2.76634600	-0.26817500
C	2.19538500	3.72149900	-0.60179700
C	2.74978600	-3.26347500	-0.43982200

C	3.22821500	2.83545800	-0.68875600
C	3.63034700	-2.22868100	-0.57140800
C	-0.32487300	3.45513000	-0.40456200
C	0.21427800	-3.38544700	-0.25913900
C	3.36313800	0.29766800	-0.65499900
C	-3.49741200	-0.23000400	-0.36742400
H	-0.40761100	4.53968200	-0.42915900
H	0.29656100	-4.46917800	-0.21247100
H	4.44254600	0.38177200	-0.75733700
H	-4.58143400	-0.32031900	-0.38289500
C	-0.18417400	-0.96849500	-3.10115400
H	0.62076700	-1.70946700	-2.93816700
H	-1.14385800	-1.51068800	-3.00506800
H	-0.10630200	-0.63310000	-4.15250100
C	-0.00877500	0.07825100	1.60033500
C	-1.23541900	0.21672000	2.46048200
C	-0.73432300	-0.19527600	3.85674400
H	-0.94069000	-1.25855700	4.05485300
H	-1.16280100	0.39490700	4.67598100
H	-2.08178600	-0.38893200	2.12204500
H	-1.58121600	1.26390300	2.46332800
O	-0.09184200	0.13085600	-2.25967900
C	1.12776300	0.06836700	2.50424800
O	2.33149400	0.11574900	2.31135900
O	0.67697200	0.01159300	3.84277700
H	2.23886300	4.80418400	-0.63442700
H	4.28448500	3.05034200	-0.80300700
H	-3.07465000	4.39913500	-0.44577700
H	-4.83961600	2.35715000	-0.45800800
H	-4.41376100	-2.98657200	-0.26559000
H	-2.35646000	-4.73167200	-0.17314800
H	2.96690400	-4.32497100	-0.40575100
H	4.70948400	-2.27920000	-0.65979100

TS9(*CSS*)

Fe	-1.02217700	0.04993200	0.52941100
O	-2.43073200	0.23148700	1.78381800
C	-2.72717600	1.36733000	2.51154800
H	-3.04764700	2.22172000	1.88109500
H	-1.89252200	1.73336300	3.14126300
H	-3.57482900	1.14838300	3.18930600
N	-0.24929500	1.88346500	1.02410900
C	0.73352200	2.13858400	1.93919800
C	-0.64187200	3.10152000	0.53661400
C	1.37703200	1.16759200	2.70337400
C	0.98836800	3.55957900	2.02293500
C	-1.64173500	3.30775700	-0.41406800
C	0.13108500	4.15917500	1.14889900
C	1.10986300	-0.19664300	2.66598900
H	2.13808500	1.50507700	3.40255900
H	1.72006100	4.02154500	2.67535800

C	-2.44827500	2.32361600	-0.98617200
H	-1.83919500	4.33648200	-0.70561800
H	0.01583600	5.21518200	0.93396800
C	1.77666700	-1.17578200	3.49744500
N	0.18432000	-0.81044000	1.85902600
C	-3.55522500	2.58253900	-1.88388600
N	-2.35758900	0.98343100	-0.72867000
C	1.23764400	-2.38451100	3.18621900
H	2.55292800	-0.94671300	4.21791100
C	0.23859000	-2.14584700	2.16822500
C	-4.14420400	1.37951200	-2.13077000
H	-3.84049700	3.56217700	-2.24905200
C	-3.39322800	0.38721600	-1.39114000
H	1.47904700	-3.35794500	3.59576900
C	-0.56306700	-3.13700600	1.61702700
H	-5.01034100	1.16624100	-2.74596800
C	-3.71109400	-0.96577000	-1.32820100
C	-1.58645300	-2.92695400	0.69767800
H	-0.40369500	-4.15412800	1.96478000
C	-3.02764300	-1.93182000	-0.60004900
H	-4.57474400	-1.29642900	-1.89923000
C	-2.50499700	-3.95367300	0.24302400
N	-1.91234900	-1.72125200	0.15707400
C	-3.40805100	-3.33003600	-0.55787700
H	-2.45480300	-4.99872200	0.52461900
H	-4.25424000	-3.75582900	-1.08387100
C	0.05033500	0.03059500	-1.09251700
C	0.82349600	1.23723100	-1.59300700
C	-0.28817600	-0.70013800	-2.38233700
H	1.15500700	-0.92230500	-0.57331700
C	1.31755500	0.85009200	-2.99261500
H	1.63086900	1.54628700	-0.92433200
H	0.13633200	2.08990200	-1.67848000
O	0.40596900	-0.15414200	-3.44802100
O	-1.00759400	-1.65004400	-2.58967700
S	2.33658900	-1.91445600	-0.66357800
H	1.29841200	1.67622900	-3.71219700
H	2.32785100	0.42531900	-2.97063100
C	3.74705000	-0.83957600	-0.80372600
C	3.98236000	0.21999100	0.09270400
C	4.69910300	-1.08222900	-1.81252600
C	5.12159300	1.01591500	-0.03138700
H	3.26944800	0.40954800	0.88856300
C	5.84840500	-0.29789200	-1.91642900
H	4.52318900	-1.89095600	-2.51623400
C	6.06463000	0.76080400	-1.03078100
H	5.27686400	1.83561700	0.66707500
H	6.57121100	-0.50762100	-2.70245600
H	6.95519400	1.37878700	-1.11838600

TS9(*OSS*)

Fe	-1.13771200	0.13786300	0.50738800
O	-2.43499200	0.32460800	1.83562800
C	-2.51937000	1.39270600	2.71585000
H	-2.71348400	2.35960800	2.21379700
H	-1.60968700	1.53012300	3.33110700
H	-3.35824400	1.21949800	3.41523200
N	0.35670700	0.64949200	1.77400400
C	0.98475400	-0.19411000	2.65101500
C	0.87638200	1.89811500	1.99682500
C	0.73736900	-1.55734900	2.78587900
C	1.94910300	0.53907000	3.43943700
C	0.46487900	3.06763500	1.36233400
C	1.88609600	1.83861500	3.02958100
C	-0.19149300	-2.29257400	2.05776600
H	1.32338000	-2.09411800	3.52670000
H	2.58229500	0.10224000	4.20252700
C	-0.57104900	3.15491900	0.43719900
H	0.97207700	3.98936600	1.63503400
H	2.45062300	2.68937200	3.39288100
C	-0.45559000	-3.70218000	2.26319200
N	-1.00831700	-1.79780100	1.08040800
C	-1.01073800	4.37894900	-0.19364000
N	-1.31905400	2.09875200	-0.01123000
C	-1.46141800	-4.03641700	1.41096200
H	0.06844200	-4.33148500	2.97253200
C	-1.81004700	-2.83095500	0.68781800
C	-2.03412400	4.04156900	-1.02858600
H	-0.58456900	5.35813000	-0.00914300
C	-2.21809500	2.61205200	-0.90588700
H	-1.94044700	-4.99847500	1.27358300
C	-2.85745200	-2.73975900	-0.22071300
H	-2.62192800	4.68735000	-1.67039200
C	-3.17365500	1.88057500	-1.60788600
C	-3.25870700	-1.57747100	-0.86680700
H	-3.41146200	-3.64895100	-0.43698600
C	-3.39324100	0.51068000	-1.50056400
H	-3.82061400	2.43402500	-2.28363300
C	-4.37305900	-1.49678000	-1.78853500
N	-2.67992100	-0.35194000	-0.71882200
C	-4.45454800	-0.19960100	-2.18766400
H	-4.99405800	-2.33500800	-2.08102500
H	-5.16000900	0.25552000	-2.87282100
C	0.14570800	-0.09440400	-1.12600900
C	0.94061900	1.05574800	-1.71676300
C	-0.10416000	-0.99713300	-2.29349500
H	1.28243600	-0.98618300	-0.47408000
C	1.41793700	0.55517100	-3.09062000
H	1.76482800	1.38775800	-1.07689000
H	0.27900900	1.92127100	-1.84433700
O	0.54676000	-0.52807800	-3.43035600
O	-0.73410200	-2.03042000	-2.36930100

S	2.45020900	-1.94160700	-0.35209800
H	1.34706300	1.30955200	-3.88267100
H	2.44851100	0.17956500	-3.05873800
C	3.83869000	-0.86064800	-0.63103000
C	4.09103800	0.26129900	0.17980200
C	4.75611800	-1.17033100	-1.65181100
C	5.21801600	1.05405200	-0.04017200
H	3.40615200	0.50203400	0.98614000
C	5.89335800	-0.38636500	-1.85239000
H	4.56326300	-2.02977900	-2.28743300
C	6.12773700	0.73403100	-1.05191900
H	5.39031000	1.92168400	0.59308800
H	6.59101700	-0.64562600	-2.64610200
H	7.00867200	1.35075200	-1.21421600

TS9(*triplet*)

Fe	-1.12504200	0.10709100	0.54514300
O	-2.23350200	0.24704100	2.03298600
C	-3.43243500	0.94466700	2.07278500
H	-4.18182700	0.56150400	1.35526000
H	-3.31381100	2.02477800	1.86603600
H	-3.87280600	0.85339900	3.08246900
N	-1.29544400	2.09669800	0.16996600
C	-0.54323700	3.09311500	0.73291400
C	-2.16605500	2.70772800	-0.69287300
C	0.48101500	2.91394700	1.65816400
C	-0.95301200	4.37732700	0.21058600
C	-3.12360800	2.05399000	-1.46394300
C	-1.95803800	4.13798600	-0.67871100
C	0.91260800	1.69215000	2.16839900
H	0.97890300	3.80804000	2.02441400
H	-0.51806000	5.32771400	0.49697400
C	-3.37641100	0.68631000	-1.43491100
H	-3.74739100	2.66470300	-2.11102300
H	-2.51978700	4.85061200	-1.27101800
C	1.93431100	1.54843800	3.18440800
N	0.42495900	0.46489800	1.81541000
C	-4.44240300	0.03428700	-2.16411700
N	-2.69314000	-0.22954300	-0.68082000
C	2.03625200	0.21528800	3.44816200
H	2.48080200	2.36969100	3.63317900
C	1.07784500	-0.45001300	2.59256400
C	-4.39725500	-1.28232400	-1.82254300
H	-5.12727200	0.53607500	-2.83725800
C	-3.29594900	-1.43676100	-0.89789100
H	2.68824300	-0.28643200	4.15310500
C	0.83924700	-1.82045400	2.59596300
H	-5.03345400	-2.09051300	-2.16282300
C	-2.91646500	-2.64775100	-0.33174600
C	-0.13544200	-2.46821700	1.84626000
H	1.44737000	-2.43090900	3.25727900

C	-1.84094100	-2.83913700	0.52762600
H	-3.49768600	-3.52477400	-0.60254000
C	-0.42586200	-3.88428700	1.93542700
N	-0.99229900	-1.86565000	0.96918400
C	-1.48854500	-4.11391500	1.11840500
H	0.12026800	-4.58861000	2.55127800
H	-2.00101600	-5.04787400	0.92108800
C	0.15516600	-0.04712500	-1.10710700
C	0.90163200	1.15341000	-1.66193100
C	-0.12922600	-0.87813300	-2.31132900
H	1.37800400	-0.98151800	-0.58769100
C	1.38822900	0.70475600	-3.05011600
H	1.71731300	1.49675200	-1.01718100
H	0.20909600	1.99812900	-1.76818300
O	0.51578100	-0.36211600	-3.43409600
O	-0.77519000	-1.89905400	-2.43299700
S	2.55777400	-1.91542300	-0.57336500
H	1.32543000	1.48807000	-3.81443300
H	2.41767100	0.32558500	-3.02201900
C	3.91508800	-0.76937000	-0.70676200
C	4.06783400	0.32240500	0.16742900
C	4.90740700	-0.99267200	-1.67886600
C	5.17101900	1.16932400	0.05615000
H	3.32556100	0.49793800	0.93845400
C	6.02020700	-0.15518800	-1.76990400
H	4.79269700	-1.82697300	-2.36506100
C	6.15605300	0.93495900	-0.90728400
H	5.26468700	2.01180900	0.73806500
H	6.77642500	-0.34869800	-2.52807600
H	7.01793000	1.59368000	-0.98475600

TS9(*quintet*)

Fe	-1.08313300	0.10296600	0.52162700
O	-2.15535300	0.23852900	2.04363400
C	-3.37789400	0.89517900	2.10975100
H	-4.15135000	0.43794900	1.46635400
H	-3.31270000	1.96268600	1.83195400
H	-3.75049300	0.85070800	3.14936200
N	-1.19513500	2.18641600	0.23282700
C	-0.40105200	3.12471400	0.82473500
C	-2.07857900	2.82877400	-0.58555300
C	0.62939900	2.85453900	1.73742600
C	-0.79558000	4.43973200	0.35488900
C	-3.07660100	2.20186200	-1.34891600
C	-1.83021500	4.25718200	-0.51931300
C	1.03654900	1.60105900	2.22031700
H	1.15272900	3.71849700	2.14110200
H	-0.33892600	5.37428600	0.66037800
C	-3.39207200	0.83582400	-1.38815900
H	-3.70256200	2.85599700	-1.95156200
H	-2.38487200	5.01326700	-1.06315600

C	2.02132800	1.37839200	3.26574900
N	0.53452000	0.39907600	1.81933200
C	-4.50622900	0.24709600	-2.11020000
N	-2.73529100	-0.14896600	-0.70826800
C	2.06100800	0.03168100	3.49028200
H	2.58494200	2.15594400	3.76865300
C	1.10438600	-0.57661600	2.58208100
C	-4.49988400	-1.08759400	-1.82715800
H	-5.19973000	0.79411400	-2.73831800
C	-3.37621100	-1.32954700	-0.94066000
H	2.67032600	-0.50813200	4.20574300
C	0.78357500	-1.94186900	2.54121100
H	-5.18335200	-1.84870800	-2.18499400
C	-3.01947000	-2.57325400	-0.40299500
C	-0.21091600	-2.57174800	1.78062700
H	1.34628600	-2.58267500	3.21568500
C	-1.94296900	-2.86000000	0.44659300
H	-3.65265800	-3.41307900	-0.67878300
C	-0.59163300	-3.97179800	1.88209100
N	-1.02828100	-1.95415000	0.88425100
C	-1.66377400	-4.14939000	1.05830500
H	-0.10191000	-4.70658400	2.51037300
H	-2.22741400	-5.05813900	0.88189500
C	0.14630100	-0.04319900	-1.12543600
C	0.88417700	1.16369600	-1.67303200
C	-0.17817100	-0.85496500	-2.33569000
H	1.35338600	-0.99052000	-0.63606400
C	1.35663300	0.71651200	-3.06624700
H	1.70484600	1.50069200	-1.03196700
H	0.19011500	2.00719900	-1.77026900
O	0.46408700	-0.33378900	-3.45407000
O	-0.84371900	-1.86065000	-2.45905500
S	2.52581900	-1.93919200	-0.65545900
H	1.30138000	1.50623100	-3.82383800
H	2.37908100	0.31970900	-3.04523000
C	3.89143100	-0.79992500	-0.75900300
C	4.05401000	0.26300700	0.14826300
C	4.87805700	-0.99956600	-1.74193600
C	5.16207800	1.10607200	0.05836700
H	3.31534700	0.41917400	0.92665300
C	5.99580300	-0.16660200	-1.81157900
H	4.75555900	-1.81185900	-2.45278900
C	6.14160500	0.89541000	-0.91611900
H	5.26370200	1.92633200	0.76563000
H	6.74799700	-0.34127800	-2.57824400
H	7.00730300	1.55085600	-0.97674400

int10(*doublet*)

Fe	-0.13497500	0.03637500	-0.21123300
N	1.49870900	-1.07742200	-0.63536900
N	0.98688100	1.71248600	-0.46352300

N	-1.25495000	-1.62640900	0.00490400
N	-1.76378000	1.16421100	0.20544200
C	1.52676800	-2.43865000	-0.76397700
C	0.52364900	3.00089800	-0.43693900
C	2.76330300	-0.63847300	-0.91407800
C	2.31404500	1.78653000	-0.78923000
C	-0.83451100	-2.91071100	-0.19885500
C	-1.83216700	2.53061500	0.17224100
C	-2.56492300	-1.70378800	0.39450200
C	-3.00739500	0.72176700	0.57087400
C	2.85787300	-2.87750100	-1.12620400
C	1.59789600	3.92149200	-0.74127300
C	3.62829700	-1.76033100	-1.21235800
C	2.71168500	3.16726500	-0.95491600
C	-1.91817400	-3.83446700	0.05777100
C	-3.16388200	2.96885800	0.52917600
C	-2.99107300	-3.08613100	0.43510700
C	-3.89204900	1.84560100	0.78422900
C	0.44845400	-3.29348700	-0.57454800
C	-0.77980900	3.38835500	-0.13933400
C	-3.38220200	-0.61452900	0.68402700
C	3.15748700	0.69429000	-0.97020700
H	0.63190900	-4.35718600	-0.69755600
H	-0.99267300	4.45419000	-0.13928300
H	-4.40577300	-0.82306600	0.98388900
H	4.19524700	0.89891500	-1.21910400
C	-2.35935000	-0.20003400	-2.81237300
H	-2.65416500	-1.18176200	-2.42604700
H	-2.97608700	0.56141900	-2.32233000
H	-2.56878400	-0.17475900	-3.88849400
C	0.17227400	-0.04556300	1.92726700
C	0.61682400	1.24535200	2.61628200
C	2.13538200	1.04329900	2.73015100
H	2.57349300	1.48343400	3.63448100
H	2.66412700	1.43799300	1.85621200
H	0.17676500	1.32193600	3.62488100
H	0.36753400	2.16407800	2.08188700
S	-0.57194100	0.11415100	-2.55421800
H	-0.82466600	-0.38125900	2.20707000
O	2.33575800	-0.37691200	2.79147700
C	1.18809000	-1.03347300	2.35629100
O	1.15396700	-2.24734500	2.40154300
H	4.68004300	-1.68019500	-1.45988200
H	3.14472000	-3.91050600	-1.28194800
H	-1.84395000	-4.91165700	-0.03149800
H	-3.98404200	-3.41913000	0.71323500
H	-4.93181200	1.76702800	1.07933000
H	-3.48171200	4.00390700	0.57546900
H	1.49381800	4.99931500	-0.78473000
H	3.71165800	3.49603700	-1.21213800

int10(*quartet*)

Fe	-0.00811000	0.18054500	-0.34115300
N	-1.92242200	1.11486800	-0.25203200
N	-0.90707000	-1.64475100	-0.60061300
N	0.90526100	1.98090500	0.03470800
N	1.90892400	-0.76564900	-0.35363400
C	-2.14455600	2.44085400	-0.08172600
C	-0.26606000	-2.82908300	-0.82169900
C	-3.10895400	0.50435800	-0.47790200
C	-2.24518000	-1.84362300	-0.79006000
C	0.25904800	3.17817400	0.17995600
C	2.13505600	-2.07987100	-0.62078700
C	2.25154200	2.21083500	0.09402600
C	3.11111300	-0.13263800	-0.27503100
C	-3.57486200	2.70244600	-0.19075300
C	-1.25157800	-3.84961600	-1.13547700
C	-4.17221100	1.50054000	-0.44204300
C	-2.47153900	-3.24012200	-1.11847200
C	1.24824900	4.22433500	0.35994400
C	3.56926800	-2.31093900	-0.69341600
C	2.47670900	3.62870400	0.30491400
C	4.17447600	-1.10352500	-0.47849600
C	-1.13104100	3.38873000	0.13836700
C	1.12378000	-3.03591100	-0.81200500
C	3.26538000	1.24511600	-0.04755200
C	-3.25279900	-0.86885300	-0.72713800
H	-1.45424900	4.41966000	0.26859800
H	1.45300000	-4.05296900	-1.01457100
H	4.28649500	1.61667700	0.00836600
H	-4.26604000	-1.22619900	-0.89698600
C	1.07024000	0.78383400	-2.98025300
H	1.56011400	1.73107000	-2.68618500
H	1.85395500	0.00365700	-2.99166800
H	0.72435600	0.90984500	-4.02343500
C	-0.19548000	0.04853000	1.84493700
C	1.09518600	-0.17148400	2.62849100
C	1.06866700	-1.68845200	2.86061600
H	1.51928800	-1.99990400	3.81050400
H	1.55338500	-2.23095800	2.04264000
H	1.05018100	0.35275100	3.59813000
H	2.00470800	0.15183600	2.12140200
H	-0.66044500	1.02279400	1.97225900
O	-0.01004400	0.45937300	-2.17469900
C	-1.08521100	-1.03857000	2.32565600
O	-2.29452900	-1.13609200	2.32887500
O	-0.32203100	-2.04819900	2.89734700
H	1.02338800	5.27584900	0.49887500
H	3.44986100	4.09878600	0.39191000
H	5.23670300	-0.88512700	-0.46957100
H	4.04351000	-3.26608500	-0.89025500
H	-1.02601000	-4.88827700	-1.34862900

H	-3.44166600	-3.68248900	-1.31360900
H	-5.22788800	1.29999500	-0.58652600
H	-4.04725300	3.67401500	-0.09703400

int10(*sextet*)

Fe	-0.01709900	0.18567000	-0.40017400
N	-2.08013900	0.78631700	-0.31964800
N	-0.60303500	-1.75890800	-0.61102600
N	0.57936700	2.08247900	-0.00062500
N	2.04416100	-0.46030300	-0.32585600
C	-2.52641900	2.06810200	-0.14068000
C	0.22976400	-2.84939600	-0.78975800
C	-3.15667900	-0.01180500	-0.51849600
C	-1.88091100	-2.19556300	-0.79122700
C	-0.25482800	3.17325300	0.14464900
C	2.49218900	-1.73696100	-0.55690600
C	1.86870800	2.53650500	0.11699900
C	3.13180300	0.34668700	-0.20598600
C	-3.98156800	2.08099000	-0.22931100
C	-0.55769000	-4.00514500	-1.07031000
C	-4.37208700	0.79761200	-0.46674400
C	-1.87830300	-3.59811400	-1.07410200
C	0.52790900	4.33919100	0.36484400
C	3.94248900	-1.73924500	-0.56569300
C	1.85887100	3.94342700	0.34783400
C	4.34264400	-0.45025700	-0.34757700
C	-1.68187000	3.14737300	0.07669800
C	1.64433400	-2.82306300	-0.75771300
C	3.04880000	1.72831200	0.01448600
C	-3.06438000	-1.38625700	-0.73824400
H	-2.16103000	4.11595600	0.21069600
H	2.12681500	-3.78368800	-0.93168600
H	3.99000600	2.26543300	0.11059100
H	-3.99879900	-1.92333300	-0.88291700
C	1.04801600	0.89033200	-3.00175400
H	1.45898300	1.85326000	-2.65023900
H	1.88569600	0.17103900	-3.04420400
H	0.69579700	1.04432100	-4.03791000
C	-0.24962700	0.07816800	1.83032000
C	1.03938700	0.01885500	2.63865100
C	1.19122700	-1.49070100	2.87248400
H	1.65587500	-1.74673600	3.83173100
H	1.75457400	-1.96829200	2.06490900
H	0.90630200	0.53483300	3.60474600
H	1.91396400	0.45520800	2.15354600
H	-0.82880600	0.99148000	1.92538000
O	-0.01305700	0.43818200	-2.22734400
C	-1.01241200	-1.10599800	2.29250000
O	-2.20398800	-1.33715700	2.27446000
O	-0.14700200	-2.01642200	2.88062300
H	0.13406600	5.33848200	0.51174400

H	2.73892900	4.56272100	0.47738300
H	5.35610400	-0.06853000	-0.29498600
H	4.56832700	-2.61088700	-0.72261400
H	-0.16620700	-5.00027700	-1.24768800
H	-2.76156300	-4.20076700	-1.24971100
H	-5.38138400	0.42154900	-0.58937000
H	-4.60938800	2.95908300	-0.12648500

TS11(*CSS*)

Fe	-1.12535200	0.18088100	0.62838900
N	0.21600300	-0.76374700	1.79149100
N	-2.09811300	-1.59423600	0.32704700
N	-0.16288300	1.91465400	0.90295600
N	-2.49496200	1.13350900	-0.53801500
C	1.30090300	-0.20896300	2.41166400
C	-3.28017600	-1.76653300	-0.33974900
C	0.23574900	-2.09463600	2.11821600
C	-1.77193000	-2.81133100	0.85568200
C	0.97428700	2.11699600	1.64485200
C	-3.63840900	0.58687900	-1.05558600
C	-0.49940600	3.14345800	0.38240600
C	-2.54411900	2.46541000	-0.83106600
C	2.02499800	-1.21369500	3.16134800
C	-3.69815200	-3.15064100	-0.26219700
C	1.35963200	-2.38460100	2.98204000
C	-2.75881100	-3.80089500	0.47955500
C	1.36658000	3.50715000	1.59225000
C	-4.42292100	1.60347900	-1.72353500
C	0.45295500	4.14316900	0.80926200
C	-3.73874200	2.77335900	-1.58829000
C	1.66020500	1.13274500	2.34612700
C	-3.99681000	-0.75708700	-0.98073400
C	-1.59907100	3.40463200	-0.42312600
C	-0.67935200	-3.04726800	1.68815000
H	2.55796600	1.43489000	2.87750500
H	-4.93052200	-1.04477000	-1.45801200
H	-1.74501600	4.43226300	-0.74536600
H	-0.53168400	-4.06649800	2.03501300
C	-0.06785900	-0.47640800	-1.23958100
C	-0.84550200	-0.46411200	-2.52702000
C	-0.12674900	-1.52406900	-3.37976600
H	0.61390900	-1.06754600	-4.04505300
H	-0.80820000	-2.15647100	-3.95758900
H	-0.87322600	0.52140300	-2.99842500
H	-1.88038900	-0.77730400	-2.35498800
H	0.35609300	0.43378900	-0.80038300
O	0.56604200	-2.36926800	-2.44996700
C	0.79584500	-1.69031300	-1.27061500
O	1.58376800	-2.12847600	-0.46290500
H	1.60052000	-3.36615200	3.37195700
H	2.92690200	-1.02709600	3.73139600

H	2.23380600	3.92172900	2.09176500
H	0.41417000	5.18949600	0.53098300
H	-4.00813400	3.75946300	-1.94766500
H	-5.36956300	1.42829500	-2.22114600
H	-4.59683800	-3.55227200	-0.71537600
H	-2.72686900	-4.84606000	0.76318700
S	2.18184100	0.95138000	-2.55114400
C	3.58815700	0.69691000	-1.53178600
C	4.26363000	-0.54482600	-1.49950900
C	4.10074400	1.74181500	-0.72755100
C	5.40319900	-0.72236300	-0.71809400
H	3.87117200	-1.36656900	-2.08893600
C	5.24893500	1.56247800	0.04070800
H	3.57988200	2.69474300	-0.72355800
C	5.91014600	0.32969100	0.05086400
H	5.89903100	-1.69106200	-0.70780300
H	5.62808900	2.38773700	0.64144700
H	6.80389100	0.18927700	0.65511400
O	-2.38033800	0.44146400	1.96817700
C	-2.32984900	-0.18907700	3.20243400
H	-1.40614500	0.02306800	3.77223000
H	-3.18434500	0.16701600	3.80628300
H	-2.42461700	-1.28926100	3.13752900

TS11(*OSS*)

Fe	-1.27526100	0.11750900	0.70881700
N	0.30356700	-0.65453700	1.66614700
N	-1.99437500	-1.73187200	0.35983400
N	-0.45714000	1.94968500	0.86875800
N	-2.78376200	0.88075800	-0.40926400
C	1.41617400	0.00764500	2.12038300
C	-3.11219900	-2.07628500	-0.35323300
C	0.46859700	-1.96523800	2.02767200
C	-1.52574700	-2.89215200	0.91492900
C	0.75138100	2.27832500	1.43180200
C	-3.80562300	0.19478500	-1.01116300
C	-1.02920300	3.13304300	0.47575300
C	-3.05166900	2.21126400	-0.60300500
C	2.30899600	-0.91131100	2.78691600
C	-3.34176600	-3.50084900	-0.26819900
C	1.71207200	-2.13293000	2.74374200
C	-2.36228300	-4.00568200	0.52921600
C	0.95071100	3.70625500	1.38740600
C	-4.73747600	1.11603600	-1.61935600
C	-0.16013700	4.23789700	0.80487200
C	-4.27355000	2.36977700	-1.35797300
C	1.64263500	1.37229500	1.99613200
C	-3.94997900	-1.18750900	-1.01404900
C	-2.24663500	3.26362200	-0.18304600
C	-0.39828100	-3.00384800	1.71662500
H	2.57734000	1.76300800	2.38604200

H	-4.80775400	-1.60129700	-1.53674400
H	-2.57489100	4.27051600	-0.42567100
H	-0.13541100	-3.99557100	2.07258300
C	0.27363000	-0.03257000	-1.48046900
C	-0.40396400	0.61530400	-2.65856800
C	-0.49757300	-0.55763900	-3.66426600
H	0.23565200	-0.44948200	-4.47321000
H	-1.49472500	-0.67299000	-4.10231000
H	0.17912500	1.44788400	-3.06521900
H	-1.40024700	0.99808000	-2.41393800
H	0.93732900	0.48478100	-0.80557000
O	-0.19233300	-1.76083000	-2.94584200
C	0.43552400	-1.45468500	-1.74519400
O	0.97286000	-2.34057300	-1.10268700
H	2.07907700	-3.07778100	3.12528800
H	3.26829300	-0.63878500	3.20760200
H	1.83184600	4.21692800	1.75547100
H	-0.37855900	5.27770800	0.59353200
H	-4.70054300	3.32217700	-1.64849600
H	-5.62690100	0.82453900	-2.16489600
H	-4.15310300	-4.02509000	-0.75828100
H	-2.19495800	-5.03345300	0.82709200
S	2.97927700	0.61657900	-2.76162600
C	4.15930900	0.30787800	-1.49445800
C	4.13789200	-0.88737300	-0.73847300
C	5.17316400	1.24903500	-1.20037500
C	5.08960500	-1.12206100	0.25294400
H	3.35093600	-1.61230700	-0.92512700
C	6.13440100	0.99633100	-0.22318500
H	5.19461900	2.18126300	-1.75891300
C	6.10131400	-0.19138000	0.51471600
H	5.04137100	-2.04736800	0.82418200
H	6.90982100	1.73645300	-0.02918400
H	6.84865500	-0.38669100	1.28118500
O	-2.31478100	0.27391300	2.18360600
C	-1.79156200	0.66685900	3.41940100
H	-1.21056700	1.60104000	3.36552500
H	-2.64030700	0.83878400	4.10194400
H	-1.14709000	-0.10458800	3.87213600

TS11(*triplet*)

Fe	-1.29626200	0.12639200	0.72197900
N	0.29780600	-0.60646100	1.68491100
N	-1.94377200	-1.74269900	0.33381400
N	-0.52623600	1.97937600	0.88769300
N	-2.78510500	0.84948000	-0.45094700
C	1.37784400	0.08743400	2.17161700
C	-3.03689800	-2.11620100	-0.40279800
C	0.50065700	-1.91594700	2.03415300
C	-1.44494700	-2.89422800	0.88072200
C	0.65795000	2.34103100	1.48238000

C	-3.77758800	0.13682800	-1.07214500
C	-1.12242400	3.14862100	0.48591600
C	-3.08988800	2.17299200	-0.64447000
C	2.28762900	-0.80928800	2.84466400
C	-3.22160900	-3.54850900	-0.33675100
C	1.73489800	-2.05033500	2.77219500
C	-2.23800900	-4.03036100	0.46903800
C	0.81696100	3.77428900	1.44815900
C	-4.72357500	1.03277300	-1.69532400
C	-0.29364200	4.27640600	0.83963600
C	-4.30067700	2.29854200	-1.42222000
C	1.56134100	1.46009000	2.06575700
C	-3.88717500	-1.24901800	-1.07584600
C	-2.32771900	3.24725400	-0.20005900
C	-0.32548100	-2.97893300	1.69644900
H	2.47160500	1.87779300	2.48465400
H	-4.72358400	-1.68474400	-1.61498100
H	-2.68039800	4.24511300	-0.44550100
H	-0.03424200	-3.96582000	2.04350300
C	0.48840300	0.05214600	-1.53665700
C	-0.24398500	0.75613300	-2.63879100
C	-0.81831700	-0.43157900	-3.45225900
H	-0.55756300	-0.37934300	-4.51529500
H	-1.90868400	-0.49785100	-3.36220900
H	0.43234700	1.36911700	-3.24790700
H	-1.04031000	1.41408700	-2.27839700
H	1.05278900	0.51907300	-0.74903700
O	-0.25423800	-1.63795900	-2.91979700
C	0.50226200	-1.37728900	-1.78536500
O	1.03188200	-2.29849400	-1.18677400
H	2.12701200	-2.98701400	3.14867800
H	3.22841600	-0.51095600	3.28903900
H	1.67358800	4.30859500	1.83985300
H	-0.53639700	5.31035400	0.62623000
H	-4.74983700	3.23917900	-1.71751100
H	-5.59438900	0.71767700	-2.25744800
H	-4.00677200	-4.09306900	-0.84681500
H	-2.04001200	-5.05569700	0.75609400
S	3.01957900	0.50969000	-2.72763800
C	4.23576900	0.17445700	-1.49680200
C	4.15891800	-0.97235200	-0.67389900
C	5.33096600	1.04645100	-1.30321700
C	5.13482700	-1.22506600	0.28967600
H	3.31570200	-1.64715600	-0.79208300
C	6.31416900	0.77375700	-0.35300200
H	5.39893000	1.94195900	-1.91579700
C	6.22479600	-0.36357600	0.45556900
H	5.04374800	-2.11210100	0.91435300
H	7.15159300	1.46076000	-0.23611000
H	6.98892300	-0.57327300	1.20146900
O	-2.37928800	0.23636900	2.17909300

C	-1.92077700	0.73228700	3.40254100
H	-1.55714100	1.77105600	3.33683500
H	-2.76689100	0.71948900	4.10982700
H	-1.11266400	0.12149400	3.83762100

TS12(*doublet*)

Fe	0.13618600	0.06955000	-0.80237600
N	-1.05510600	1.71439800	-0.45526100
N	-1.50701100	-1.05250100	-1.06738800
N	1.73194100	1.14340700	-0.17537500
N	1.23745900	-1.65689600	-0.53015700
C	-0.63773000	2.99009900	-0.18138600
C	-1.56690700	-2.41384300	-1.22568100
C	-2.40176400	1.79341800	-0.68970400
C	-2.79473700	-0.59878700	-1.20733000
C	1.77333700	2.49212100	0.09344700
C	0.81195500	-2.93566100	-0.77320000
C	3.01300500	0.68228900	0.02249400
C	2.58889100	-1.73701300	-0.31360600
C	-1.75759500	3.90046800	-0.21543100
C	-2.92898300	-2.82962600	-1.50509500
C	-2.85637200	3.15406700	-0.53260900
C	-3.68944800	-1.70419500	-1.49437700
C	3.12147500	2.89613200	0.43770100
C	1.91861800	-3.85734300	-0.67659100
C	3.88953600	1.77482200	0.39266900
C	3.02601900	-3.11009700	-0.39077300
C	0.68397600	3.35454000	0.07818600
C	-0.49745500	-3.29142900	-1.09747000
C	3.41934300	-0.64462600	-0.06063200
C	-3.21296300	0.71607200	-1.04649500
H	0.87706500	4.40172700	0.29745800
H	-0.69989000	-4.34738900	-1.25856800
H	4.47317500	-0.85116000	0.10991900
H	-4.27098000	0.91981500	-1.19105200
C	1.20304900	1.19845500	-3.31174900
H	0.96242900	2.25011500	-3.04059000
H	2.27765000	1.05613000	-3.06359800
H	1.13770900	1.14889400	-4.42036100
C	-0.58919900	0.03272200	2.93713200
C	0.75032100	-0.60594500	3.01829800
C	0.46520500	-1.80107800	3.95598900
H	1.23328400	-1.95358000	4.72040000
H	0.34854200	-2.73096400	3.38553900
H	1.49579400	0.08157600	3.45387700
H	1.14273400	-0.91570200	2.04470400
H	-0.87851500	0.82628500	2.26163300
O	0.36666700	0.27165600	-2.72604800
C	-1.45580200	-0.50357000	3.96015500
O	-2.58248800	-0.18409500	4.29612800
O	-0.77562300	-1.51916200	4.62583800

H	3.41668000	3.90755600	0.69167500
H	4.94824600	1.67282000	0.60148900
H	4.04754200	-3.44599800	-0.25414000
H	1.84895400	-4.92935300	-0.82049900
H	-3.24044500	-3.85468400	-1.66843800
H	-4.75818100	-1.60925200	-1.64671100
H	-3.88108300	3.48450200	-0.65630800
H	-1.69888300	4.96594700	-0.02611400

TS12(*quartet*)

Fe	0.09197300	0.18844500	-0.52688600
N	-1.16646200	1.85890300	-0.21951400
N	-1.59870000	-1.04017300	-0.60829600
N	1.73886300	1.35021100	0.06286600
N	1.30370600	-1.53906000	-0.35316700
C	-0.75231700	3.13605500	-0.00439100
C	-1.59054900	-2.38838000	-0.80148100
C	-2.51284200	1.87159800	-0.39993600
C	-2.88084400	-0.59999100	-0.74569200
C	1.72594000	2.70308400	0.24579200
C	0.88952000	-2.81537000	-0.59642500
C	3.03200400	0.92183200	0.14212700
C	2.66348900	-1.54691700	-0.24472600
C	-1.90523200	4.02463600	-0.04576400
C	-2.94853500	-2.84152900	-1.06037600
C	-2.99505300	3.24083900	-0.29498100
C	-3.74570000	-1.73472500	-1.02732200
C	3.08635500	3.16345100	0.46460900
C	2.04778600	-3.69296000	-0.62876900
C	3.89420200	2.06289000	0.39790000
C	3.14588500	-2.90785100	-0.41098300
C	0.58166500	3.52049600	0.21925000
C	-0.44736500	-3.20579300	-0.78706500
C	3.45787800	-0.41111600	-0.00551000
C	-3.29975600	0.73645600	-0.65180900
H	0.75301400	4.58257000	0.38367700
H	-0.61615400	-4.26602700	-0.96480700
H	4.52998400	-0.58164000	0.07007900
H	-4.36630800	0.91050400	-0.77623700
C	1.40162000	0.31830600	-3.13383500
H	2.19424500	1.02480100	-2.81646400
H	1.84913500	-0.69532600	-3.10573100
H	1.18832100	0.53991600	-4.19828900
C	-0.17887800	0.13601200	2.08565700
C	0.88242200	-0.69900700	2.74472800
C	0.14348100	-2.03408300	2.93928300
H	0.41174200	-2.55734200	3.86368600
H	0.30096900	-2.70365500	2.08828400
H	1.15452400	-0.26630100	3.72438700
H	1.80260500	-0.80836800	2.16891000
H	-0.10182200	1.21139600	2.01634300

O	0.24379500	0.42513700	-2.38323900
C	-1.46763700	-0.43454100	2.48850700
O	-2.58565800	0.03965400	2.48017100
O	-1.25391700	-1.70216800	3.01304600
H	3.37824500	4.19314300	0.63910100
H	4.97217300	2.02145100	0.50855800
H	4.18538100	-3.21475300	-0.37378400
H	2.01978400	-4.76326100	-0.80095600
H	-3.24129500	-3.86914700	-1.24421200
H	-4.81801700	-1.68101600	-1.17711900
H	-4.02938600	3.55091500	-0.39216900
H	-1.87594200	5.09944900	0.09478800

TS12(*sextet*)

Fe	0.00414900	0.21899300	-0.59784200
N	-1.20964800	1.88762700	-0.31658600
N	-1.68641100	-0.97405500	-0.75609700
N	1.67146400	1.36442000	0.04336400
N	1.19074600	-1.52332000	-0.41104600
C	-0.77926700	3.16120200	-0.05488600
C	-1.69727000	-2.33578400	-0.88975800
C	-2.56598000	1.91822800	-0.45982800
C	-2.97317700	-0.53200500	-0.82628700
C	1.68330800	2.71143600	0.23302700
C	0.76383200	-2.79760200	-0.62569400
C	2.95437600	0.90901800	0.14961900
C	2.54392400	-1.55245400	-0.23308200
C	-1.92545800	4.05100800	-0.04770600
C	-3.06628100	-2.77945600	-1.07481700
C	-3.02720800	3.28454600	-0.29796000
C	-3.85354600	-1.66637300	-1.03498900
C	3.04544600	3.14519700	0.48586400
C	1.90283100	-3.69673400	-0.57382200
C	3.83335000	2.03004300	0.43111600
C	3.00542400	-2.92615200	-0.33289100
C	0.54639100	3.53961000	0.18949400
C	-0.57381700	-3.16916000	-0.84548000
C	3.35211600	-0.43158000	0.01855300
C	-3.37873800	0.80482300	-0.71084700
H	0.71554900	4.59767100	0.37697200
H	-0.76144300	-4.23212400	-0.97870900
H	4.41613100	-0.62692000	0.13476000
H	-4.44657400	0.99330400	-0.78624900
C	1.63225800	0.30094200	-3.16695900
H	2.42750700	0.99953300	-2.83883600
H	2.06218500	-0.71836500	-3.10583800
H	1.45027900	0.50684700	-4.24016800
C	-0.19078800	0.02485700	2.16204800
C	0.98665900	-0.56162900	2.89182600
C	0.51724900	-2.01676700	3.08728800
H	0.83626800	-2.45807500	4.04001800

H	0.87203100	-2.65734600	2.27028800
H	1.15068100	-0.07579100	3.87281400
H	1.93714500	-0.51132400	2.35133200
H	-0.32296800	1.09435200	2.06063100
O	0.47099000	0.43571000	-2.43303600
C	-1.34370400	-0.77503500	2.48834000
O	-2.54348100	-0.57438700	2.37008500
O	-0.91403000	-1.98390100	3.06828900
H	3.35103000	4.16779500	0.67619400
H	4.90624700	1.96400100	0.57121300
H	4.03465100	-3.24958800	-0.22716800
H	1.85721600	-4.77192800	-0.70393900
H	-3.37455600	-3.81079500	-1.20037100
H	-4.93226500	-1.60900300	-1.12017500
H	-4.06132000	3.60345500	-0.35748900
H	-1.88388000	5.11867200	0.13504100

TS[PhS$^{\bullet}$+ **int7**](*OSS*)

C	-2.88551300	-0.00555600	1.13420500
C	-3.49358400	0.85814300	0.09388600
C	-2.89270800	0.27154800	-1.21027100
H	-2.16633400	0.95421200	-1.65847100
H	-3.65198600	0.00877000	-1.95162400
H	-3.24050200	1.91880100	0.22296400
H	-4.59331800	0.79680500	0.10638000
H	-2.98775500	0.10081500	2.20589900
S	0.37315100	1.95540800	0.01353200
C	1.60064000	0.74341200	-0.05179000
C	2.91918600	1.03357200	0.39670600
C	1.32180400	-0.56112000	-0.54504900
C	3.90935900	0.06352300	0.35096100
H	3.13104500	2.02858200	0.77491200
C	2.32051900	-1.52515200	-0.58067800
H	0.31852600	-0.79461000	-0.88454700
C	3.61337500	-1.21842100	-0.13615400
H	4.91350200	0.29508400	0.69520500
H	2.09398900	-2.52121400	-0.94955000
H	4.39038800	-1.97748700	-0.16626500
O	-2.19643900	-0.93700700	-0.84815200
C	-2.13631900	-1.08685000	0.52312900
O	-1.53337600	-2.00485300	1.04051600

TS-S1(*CSS*)

Fe	-1.02594700	0.09108200	0.25667800
N	-1.17652000	-1.80630800	0.94932600
N	-2.03774000	-0.42272900	-1.43131000
N	-0.17628400	0.65003700	2.01849300
N	-1.00222300	2.02434400	-0.37103900
C	-0.74217500	-2.28689900	2.15033600
C	-2.41806500	0.40092100	-2.45568300
C	-1.76814700	-2.85903700	0.30668400

C	-2.51447400	-1.66828700	-1.73935100
C	0.10733700	-0.15741900	3.08901900
C	-1.50631700	2.52079200	-1.54524900
C	0.12677600	1.92844600	2.41072100
C	-0.53961900	3.10478100	0.33103400
C	-1.05189500	-3.69848600	2.27048300
C	-3.14175900	-0.35175200	-3.46035700
C	-1.69088400	-4.05425900	1.12485100
C	-3.20163600	-1.63825700	-3.01441900
C	0.64049000	0.63004300	4.18106500
C	-1.31891500	3.95609200	-1.60636200
C	0.64712400	1.92605900	3.76162900
C	-0.71966700	4.31974800	-0.43906400
C	-0.12242200	-1.52999600	3.14148100
C	-2.15467000	1.76946700	-2.52378000
C	-0.01673600	3.06650500	1.62259400
C	-2.37324800	-2.80420400	-0.94523200
H	0.16070000	-2.04555000	4.05586400
H	-2.51553300	2.30163500	-3.40082500
H	0.28728900	4.01380800	2.06137600
H	-2.80039800	-3.72834700	-1.32694400
C	-4.11830000	1.74984500	0.57112000
H	-3.57824900	2.70127400	0.64303900
H	-4.32668000	1.55634700	-0.48791400
H	-5.07893200	1.86499800	1.08937800
C	0.69831500	-0.31114900	-0.68191200
C	0.95101400	0.11196100	-2.13090800
C	0.79252200	-1.22544500	-2.87678400
H	1.44591600	-1.32483900	-3.75014000
H	-0.24146800	-1.40876400	-3.17469000
H	1.97266100	0.48756200	-2.28567500
H	0.25289900	0.86807800	-2.48504000
S	2.32735400	0.64730900	0.50749300
C	3.94368400	0.28284000	-0.16041900
C	4.59211500	1.31123300	-0.86569700
C	4.55741300	-0.97666000	-0.04964300
C	5.84221000	1.08671200	-1.44015000
H	4.11959600	2.28670100	-0.94910000
C	5.81190300	-1.18509100	-0.62184100
H	4.04012000	-1.78478200	0.45606000
C	6.46022700	-0.16056500	-1.31714200
H	6.33666500	1.89094100	-1.97961300
H	6.28154700	-2.16130500	-0.52893400
H	7.43686300	-0.33356300	-1.76190000
S	-3.18989200	0.36746000	1.34572800
O	1.18916300	-2.24535400	-1.93178100
C	1.25442200	-1.71576500	-0.67100000
O	1.72586700	-2.37007200	0.24143700
H	-2.08604300	-5.02328400	0.84333800
H	-0.81203100	-4.31357200	3.12993900
H	0.94324300	0.23052800	5.14213600

H	0.96370300	2.80924600	4.30436900
H	-0.43568600	5.31147300	-0.10598700
H	-1.62994600	4.58715800	-2.43112300
H	-3.55531900	0.06693800	-4.37077300
H	-3.67290400	-2.49395500	-3.48398800
H	2.23661600	-0.41020200	1.34028900

TS-S1(*OSS*)

Fe	-1.03479900	0.09746900	0.27060800
N	-1.21263600	-1.81870300	0.89839400
N	-2.05231600	-0.33867100	-1.42958700
N	-0.15560200	0.57656700	2.03990100
N	-0.96483700	2.04683600	-0.29680200
C	-0.77271000	-2.35115800	2.07607600
C	-2.41099400	0.52396100	-2.43108000
C	-1.83367600	-2.83564400	0.22679100
C	-2.56307200	-1.56212800	-1.77313000
C	0.13205900	-0.27484300	3.07574900
C	-1.45160500	2.59170900	-1.45801400
C	0.17571000	1.83482900	2.47325200
C	-0.48247400	3.09416600	0.44155500
C	-1.11062700	-3.75853200	2.14992700
C	-3.15291700	-0.18053400	-3.45575000
C	-1.77226700	-4.05997600	1.00143300
C	-3.24874100	-1.47694900	-3.04616700
C	0.69690800	0.46303600	4.18528200
C	-1.23323600	4.02261300	-1.47157400
C	0.71838600	1.77353000	3.81366100
C	-0.63379300	4.33614800	-0.28948600
C	-0.12494400	-1.64309300	3.08441100
C	-2.11477600	1.88663700	-2.45984000
C	0.04314400	3.00295500	1.72925900
C	-2.44921700	-2.72536400	-1.01607600
H	0.16251100	-2.19650000	3.97488100
H	-2.46036400	2.45262700	-3.32164300
H	0.36797500	3.92855300	2.19808100
H	-2.90144200	-3.62576500	-1.42437200
C	-4.09493300	1.76853000	0.60081100
H	-3.55189800	2.71897300	0.65772000
H	-4.31497900	1.56316900	-0.45325400
H	-5.04882300	1.88919700	1.12975300
C	0.73244100	-0.31421500	-0.70064600
C	0.94539100	0.11517000	-2.15530300
C	0.74684700	-1.21283200	-2.90780500
H	1.38486300	-1.31804700	-3.79198200
H	-0.29476000	-1.37175900	-3.19353500
H	1.96715200	0.48096000	-2.33658800
H	0.24839600	0.88274100	-2.48662100
S	2.29255000	0.59383600	0.44326800
C	3.93188300	0.25852700	-0.18435300
C	4.60322200	1.31436500	-0.82721700

C	4.53539300	-1.01075200	-0.11904100
C	5.86587300	1.10847300	-1.37871700
H	4.13690600	2.29512300	-0.87824900
C	5.80245600	-1.19997700	-0.66885800
H	4.00099900	-1.83721300	0.33739400
C	6.47432400	-0.14829900	-1.29916700
H	6.37909700	1.93381700	-1.86650900
H	6.26486200	-2.18241800	-0.60968500
H	7.46048500	-0.30702800	-1.72794400
S	-3.16250200	0.39363100	1.38215400
O	1.13380700	-2.24995700	-1.97906400
C	1.22742300	-1.73236600	-0.71356600
O	1.68668200	-2.41078000	0.18993500
H	-2.19007600	-5.01018600	0.69026300
H	-0.87129700	-4.40893400	2.98306500
H	1.00955500	0.02325200	5.12534000
H	1.05939300	2.63069700	4.38257000
H	-0.32948800	5.31016600	0.07612700
H	-1.52558100	4.68621800	-2.27737900
H	-3.55332400	0.27472600	-4.35440100
H	-3.74145300	-2.30628600	-3.54023500
H	2.21023200	-0.46399300	1.27984300

TS-S1(*triplet*)

Fe	-1.09139900	0.28063300	0.28910600
N	-0.11109400	0.64313000	2.03484100
N	-1.46817200	-1.62250600	0.83641100
N	-0.71935400	2.20402100	-0.25989500
N	-2.09145100	-0.05487200	-1.44064300
C	0.43932700	1.82185600	2.46506200
C	-2.14138700	-2.58560900	0.13185400
C	0.06697300	-0.26532700	3.05046400
C	-1.09121000	-2.20251500	2.02188100
C	-0.08290100	3.17456700	0.46495400
C	-2.69315700	-1.21974500	-1.84831300
C	-1.17863700	2.81414000	-1.40492900
C	-2.35529400	0.87836500	-2.41540400
C	1.00416400	1.64991400	3.78212500
C	-2.19575900	-3.81324100	0.89568800
C	0.77336100	0.35312700	4.14383100
C	-1.54404000	-3.57328100	2.06615400
C	-0.10520900	4.42861600	-0.25616100
C	-3.33614200	-1.02465800	-3.12496300
C	-0.78516200	4.20338300	-1.41545200
C	-3.12679400	0.28071500	-3.47388900
C	0.46525000	3.00910400	1.73475100
C	-2.70734300	-2.41258000	-1.12666600
C	-1.93097900	2.20739000	-2.40176200
C	-0.37931200	-1.58435200	3.04100100
H	0.93655500	3.87254500	2.19548700
H	-3.21657700	-3.26293300	-1.57104100

H	-2.22062400	2.82520500	-3.24810200
H	-0.15379300	-2.18564100	3.91789100
C	-4.43182500	-0.01567600	0.88326000
H	-4.62878000	0.03659500	-0.19219100
H	-4.25722800	-1.06170500	1.15394800
H	-5.31931300	0.34086800	1.41939600
C	0.77820200	-0.37881100	-0.69639900
C	0.96487500	0.02572000	-2.15927500
C	0.63789500	-1.27690700	-2.91207800
H	1.26845500	-1.44504900	-3.79215700
H	-0.41236900	-1.32526500	-3.21000500
H	2.00741100	0.31624700	-2.36359900
H	0.32520500	0.84875700	-2.47511800
S	2.35665000	0.34173100	0.40157600
C	3.99583000	-0.07272300	-0.15066200
C	4.80106700	0.96967500	-0.66219600
C	4.46499700	-1.40528000	-0.22115600
C	6.05508000	0.69136100	-1.19076000
H	4.43675400	1.99377500	-0.62233500
C	5.72502200	-1.66496800	-0.75406900
H	3.83345200	-2.21442900	0.13320400
C	6.53103000	-0.62905600	-1.24083200
H	6.67239200	1.50664800	-1.56237300
H	6.08125800	-2.69242800	-0.79412300
H	7.50964800	-0.84433500	-1.66203100
S	-3.01760500	1.04381000	1.36222500
O	0.90332200	-2.34943600	-1.98620400
C	1.03161300	-1.84386000	-0.71231900
O	1.37757900	-2.57888700	0.20184100
H	1.04326100	-0.14711400	5.06645100
H	1.50693100	2.42770900	4.34446200
H	0.33667900	5.35192700	0.09959700
H	-1.01885300	4.90430100	-2.20844300
H	-3.46378400	0.80247500	-4.36215400
H	-3.87857200	-1.79019600	-3.66695900
H	-2.66874700	-4.72799900	0.55923800
H	-1.37070500	-4.25143000	2.89330800
H	2.18904900	-0.74153900	1.20753600

TS-S1(*quintet*)

Fe	-1.07865100	0.25492600	0.22152600
N	-0.15317900	0.91906700	1.98342700
N	-1.36201400	-1.63449300	1.07394700
N	-0.91265800	2.18708700	-0.58633500
N	-2.15293900	-0.34645800	-1.48446400
C	0.26022200	2.19350900	2.24229700
C	-2.00034300	-2.68683900	0.48625000
C	0.04514700	0.16425900	3.10532700
C	-0.95304500	-2.01628100	2.31522800
C	-0.37258800	3.26867500	0.04776200
C	-2.68186400	-1.59088700	-1.68665800

C	-1.43491000	2.60476900	-1.77765200
C	-2.47932800	0.43980100	-2.54967000
C	0.77852100	2.25203300	3.59735300
C	-1.99036400	-3.81341000	1.40482800
C	0.64718000	1.00009800	4.12930900
C	-1.34302800	-3.39910600	2.53273300
C	-0.52475300	4.43636200	-0.80303300
C	-3.36627300	-1.60459900	-2.96789300
C	-1.18008100	4.02693800	-1.92910300
C	-3.24103500	-0.35110800	-3.50040600
C	0.18006400	3.26655200	1.33911100
C	-2.59208700	-2.66725300	-0.78811600
C	-2.13303100	1.79655500	-2.68909400
C	-0.29386300	-1.19150200	3.24159600
H	0.55570100	4.22210500	1.69837100
H	-3.06513100	-3.59347800	-1.10698600
H	-2.47782700	2.28726200	-3.59679100
H	-0.04856100	-1.64989200	4.19709100
C	-4.63575100	-0.14119500	0.88580500
H	-4.77620300	-0.18380400	-0.20085300
H	-4.41992100	-1.15829300	1.23535900
H	-5.57984500	0.18298800	1.34085400
C	0.79176100	-0.42650800	-0.76346100
C	1.00638700	-0.16650700	-2.24529600
C	0.76372800	-1.56842300	-2.84333400
H	1.37457100	-1.79173800	-3.72468800
H	-0.29097000	-1.72210200	-3.08591700
H	2.03645800	0.15334600	-2.46352500
H	0.32603800	0.58048200	-2.65781600
S	2.58153900	0.57266000	0.42425400
C	4.20348400	0.06876300	-0.12004200
C	4.99446100	1.02367000	-0.78274100
C	4.68737200	-1.24268300	0.03373700
C	6.25443700	0.67734900	-1.26697700
H	4.62268300	2.03801700	-0.90463800
C	5.95273600	-1.57372400	-0.44985800
H	4.06199400	-1.99434400	0.50463300
C	6.74305200	-0.62151700	-1.09959800
H	6.85879500	1.42733000	-1.77199000
H	6.31933500	-2.58960800	-0.32283200
H	7.72735300	-0.88933300	-1.47513100
S	-3.28803700	1.01703600	1.34273700
O	1.14165000	-2.50143200	-1.80898100
C	1.24962000	-1.83445600	-0.60797300
O	1.67091100	-2.42281100	0.37695200
H	0.91671900	0.66970700	5.12597600
H	1.17935800	3.13868000	4.07511900
H	-0.18916200	5.43690700	-0.55478500
H	-1.48300600	4.62827300	-2.77882500
H	-3.63616700	0.01319800	-4.44203100
H	-3.88267500	-2.45856200	-3.39135000

H	-2.42606700	-4.78565800	1.20554900
H	-1.14785900	-3.96784700	3.43455100
H	2.34336200	-0.47933500	1.23676000

TS-S2(*CSS*)

Fe	-1.11003500	0.14874200	0.34615600
O	-2.75913300	0.38676200	1.33427800
C	-3.60083900	1.46420300	1.18576600
H	-3.97217000	1.61773500	0.14809100
H	-3.15897100	2.43853400	1.49612500
H	-4.50713000	1.32876300	1.81406000
N	-0.88051400	2.14718300	0.04220100
C	-0.30183400	3.04208700	0.90282500
C	-1.33986100	2.88173800	-1.01951300
C	0.22333100	2.73521400	2.15639000
C	-0.35880400	4.38072400	0.34856200
C	-2.08295000	2.37841400	-2.08624200
C	-1.00031500	4.28026200	-0.84800600
C	0.26495500	1.46915900	2.73721600
H	0.62687300	3.56018200	2.73879100
H	0.03051400	5.26871400	0.83353500
C	-2.50926800	1.05698800	-2.22791300
H	-2.39296100	3.08544900	-2.85224300
H	-1.24875700	5.06885500	-1.54929400
C	0.80358700	1.18451000	4.05087700
N	-0.16743800	0.31335400	2.14274100
C	-3.34846400	0.57067800	-3.30406700
N	-2.21129800	0.03928700	-1.36362200
C	0.67426700	-0.15872300	4.24237400
H	1.21533400	1.92571600	4.72629700
C	0.04683700	-0.68949500	3.04956400
C	-3.56662300	-0.75254200	-3.05910900
H	-3.72781000	1.17741800	-4.11853100
C	-2.85464400	-1.07111200	-1.83761000
H	0.94997400	-0.74542300	5.11130700
C	-0.32903300	-2.02047600	2.87890800
H	-4.15665800	-1.45676500	-3.63448000
C	-2.83075100	-2.33203000	-1.24440200
C	-1.04711300	-2.53045500	1.80130400
H	-0.08687800	-2.71003000	3.68412500
C	-2.18529800	-2.66804500	-0.05727500
H	-3.38655300	-3.12188100	-1.74432500
C	-1.52728100	-3.89747900	1.71207500
N	-1.44369900	-1.81617200	0.70974800
C	-2.23793000	-3.98305300	0.55686200
H	-1.34418100	-4.66808100	2.45199500
H	-2.76116300	-4.83859700	0.14566900
C	0.57184800	-0.26876600	-0.70750700
C	0.79291300	0.27893200	-2.12019800
C	1.00763800	-1.70181200	-0.86358700
C	0.47043800	-0.95853300	-2.97644000

H	1.83668100	0.57478900	-2.30116500
H	0.15162100	1.12481400	-2.36116100
O	0.83803000	-2.09699100	-2.16431600
O	1.46947700	-2.47975800	-0.04601200
S	2.26488200	0.44132600	0.49072400
H	-0.59326800	-1.02721300	-3.21119900
H	1.05338500	-1.02109600	-3.90155100
C	3.84420900	0.09113600	-0.26934600
C	4.53578300	1.17090100	-0.84534600
C	4.38261200	-1.20459500	-0.35871000
C	5.75573500	0.96005100	-1.48555400
H	4.12008300	2.17305700	-0.77713200
C	5.60799900	-1.40004100	-0.99489100
H	3.82889500	-2.04556700	0.04537600
C	6.30044800	-0.32508900	-1.55955200
H	6.28475800	1.80364800	-1.92255500
H	6.01979200	-2.40457800	-1.05579800
H	7.25356400	-0.48761800	-2.05633300
H	2.15191400	-0.71147400	1.18495000

TS-S2(*OSS*)

Fe	-1.14252600	0.17668900	0.39192300
O	-2.69689300	0.47224700	1.41548800
C	-3.63901500	1.44530600	1.13541300
H	-3.23694500	2.47807800	1.16654800
H	-4.12588800	1.32588400	0.14671400
H	-4.44643200	1.39766100	1.89201400
N	-1.50897600	-1.79363000	0.67230700
C	-1.09268500	-2.57139100	1.71734000
C	-2.29117500	-2.59219300	-0.11285000
C	-0.32524700	-2.13425800	2.78978000
C	-1.60804600	-3.91742500	1.57611500
C	-2.94817300	-2.19234900	-1.27277300
C	-2.35766800	-3.93118000	0.44198500
C	0.09782200	-0.82470000	3.00430300
H	-0.06826700	-2.86880700	3.54892100
H	-1.41678400	-4.72805800	2.26953900
C	-2.91674100	-0.91428000	-1.82760000
H	-3.53732400	-2.94306600	-1.79328500
H	-2.90939800	-4.75484800	0.00434500
C	0.78731700	-0.36624600	4.18800100
N	-0.13284200	0.22845700	2.15667500
C	-3.60652700	-0.53252100	-3.04079500
N	-2.22533400	0.15565700	-1.32304700
C	0.93840000	0.98336600	4.05676300
H	1.08973800	-1.00109500	5.01293900
C	0.35018600	1.34506200	2.78557200
C	-3.32431800	0.78593200	-3.25364400
H	-4.22148800	-1.19601400	-3.63759600
C	-2.47338000	1.20937500	-2.16729700
H	1.39888200	1.68103000	4.74658100

C	0.31639000	2.63877000	2.26855000
H	-3.66860600	1.42760600	-4.05675700
C	-1.99646800	2.50780400	-1.98838400
C	-0.21478900	3.00594000	1.03396900
H	0.75484800	3.42757300	2.87445700
C	-1.24014100	2.94782600	-0.90651000
H	-2.26963600	3.24627700	-2.73831100
C	-0.21918500	4.36063000	0.52150700
N	-0.82136800	2.16192800	0.14144200
C	-0.84879200	4.32131900	-0.68640900
H	0.20307800	5.21643300	1.03543200
H	-1.05690200	5.14022600	-1.36559600
C	0.62111200	-0.29080100	-0.72833700
C	0.77765900	0.26080600	-2.14898800
C	0.94242100	-1.73718500	-0.90726600
C	0.39256500	-0.95892300	-3.00324700
H	0.14545400	1.12151400	-2.36000800
H	1.81884600	0.54251000	-2.37005500
O	0.73460600	-2.11603200	-2.21046300
O	1.37657900	-2.54603200	-0.10002400
H	-0.67777300	-0.98715300	-3.21783700
H	0.95198400	-1.03367400	-3.94214500
S	2.22143300	0.35444000	0.39760000
C	3.83139900	0.04515200	-0.30972000
H	2.12323700	-0.81305600	1.08218600
C	4.33702300	-1.25386500	-0.52470700
C	4.56978100	1.15856400	-0.75808700
C	5.57324700	-1.41734900	-1.14683000
H	3.75215400	-2.11470000	-0.21601600
C	5.80108400	0.97809900	-1.38014800
H	4.17652000	2.16004700	-0.60057600
C	6.31366400	-0.31121200	-1.57711000
H	5.95992500	-2.42230400	-1.30145000
H	6.36799800	1.84629900	-1.70883000
H	7.27452500	-0.45012700	-2.06602500

TS-S2(*triplet*)

Fe	-1.05502600	0.04870400	0.74477600
O	-2.45322800	0.37079800	1.90086600
C	-3.77732500	0.52275500	1.50537000
H	-4.18308200	-0.36653000	0.99053500
H	-3.93165700	1.38581200	0.83277700
H	-4.39773900	0.69296600	2.40360400
N	-1.66647600	1.49949700	-0.53684400
C	-1.41286800	2.83905200	-0.41799400
C	-2.49316100	1.35592200	-1.62916600
C	-0.65251300	3.44230600	0.58490900
C	-2.07256800	3.56325100	-1.48173600
C	-3.05161500	0.15688400	-2.05988300
C	-2.73919100	2.64038800	-2.23471800
C	-0.00497600	2.77600700	1.62390100

H	-0.54977500	4.52338500	0.54667200
H	-2.02619600	4.63753900	-1.61716100
C	-2.87720300	-1.08155000	-1.44594600
H	-3.69487100	0.19240100	-2.93562200
H	-3.35559800	2.80282200	-3.11136100
C	0.79803100	3.42121400	2.63873000
N	-0.00381400	1.42159700	1.82036200
C	-3.49918500	-2.30713700	-1.87700000
N	-2.10259200	-1.31237900	-0.33128700
C	1.26872400	2.43358700	3.45543300
H	0.96848900	4.48934200	2.70506200
C	0.74890800	1.18920600	2.94426100
C	-3.10686500	-3.27840400	-0.99986700
H	-4.15609800	-2.39866200	-2.73434600
C	-2.24058000	-2.64330500	-0.03340200
H	1.89873300	2.52709900	4.33234500
C	0.94555800	-0.05710500	3.53219400
H	-3.37301200	-4.32885600	-0.99353400
C	-1.64257500	-3.30244100	1.03979300
C	0.37943500	-1.25096000	3.10489700
H	1.57216900	-0.09418700	4.41959800
C	-0.80405700	-2.71549200	1.98397400
H	-1.84324400	-4.36516500	1.14382700
C	0.53901900	-2.51695000	3.78258600
N	-0.43384200	-1.40071800	2.01241800
C	-0.19874000	-3.42756900	3.09105300
H	1.13988800	-2.66894700	4.67146400
H	-0.32963900	-4.48457500	3.29010600
C	0.70315800	-0.36902500	-0.54987100
C	0.46595500	-0.61678900	-2.04008100
C	1.56136300	-1.51453700	-0.15228100
C	0.59058700	-2.14738300	-2.14340000
H	1.24628200	-0.14434600	-2.65779600
H	-0.49907400	-0.26281000	-2.39947100
O	1.44951500	-2.54784700	-1.05752600
O	2.34588300	-1.61155800	0.78211400
S	2.00057900	1.23728100	-0.34703000
H	-0.37586700	-2.64575200	-2.02926100
H	1.06129700	-2.48895500	-3.07213000
C	3.52666000	1.16934000	-1.25765000
C	3.70905000	2.09453500	-2.30940900
C	4.49408800	0.15827000	-1.05313800
C	4.84478200	2.03467200	-3.10717100
H	2.96011700	2.86499500	-2.47792500
C	5.62661500	0.11379600	-1.86252300
H	4.33993700	-0.57896900	-0.27086700
C	5.81634100	1.04411000	-2.89098500
H	4.98095800	2.76642400	-3.90084100
H	6.37016400	-0.66185800	-1.69015100
H	6.70060300	0.99537200	-3.52127900
H	2.46183200	0.61190300	0.76971800

TS-S2(*quintet*)

Fe	-1.38201100	0.12081000	0.54609400
O	-2.86217200	0.28113600	1.73654100
C	-4.20150500	0.39601600	1.42760400
H	-4.60284400	-0.47503200	0.86667100
H	-4.44094300	1.29441400	0.82081200
H	-4.81142600	0.47449700	2.35167400
N	-2.14699400	1.43787300	-0.92999600
C	-2.01976000	2.79207100	-0.93091900
C	-3.00211400	1.08398500	-1.92807100
C	-1.24121200	3.53069600	-0.01957900
C	-2.83217900	3.34199100	-2.00656200
C	-3.37647100	-0.24060800	-2.23127600
C	-3.44263400	2.28446700	-2.62253700
C	-0.48054000	3.05456400	1.06428200
H	-1.25455800	4.61137800	-0.15021600
H	-2.92718600	4.39512900	-2.24809200
C	-2.98535700	-1.42773300	-1.57960300
H	-4.07582200	-0.36212200	-3.05649800
H	-4.12935100	2.31114400	-3.46166500
C	0.23753300	3.88443800	2.02078900
N	-0.32026700	1.74506100	1.40439200
C	-3.47606300	-2.76353900	-1.87720800
N	-2.11614300	-1.50365600	-0.52989500
C	0.80537100	3.03843600	2.93060300
H	0.28681300	4.96762200	1.99940400
C	0.43629100	1.68715500	2.53495800
C	-2.90339700	-3.60957900	-0.96871600
H	-4.18118300	-3.01151200	-2.66292900
C	-2.05524000	-2.80074300	-0.10940600
H	1.40892100	3.29782200	3.79349800
C	0.79826900	0.50489900	3.21012400
H	-3.04826200	-4.68013000	-0.87587700
C	-1.33081900	-3.26470500	1.00332700
C	0.41699500	-0.81807500	2.90990000
H	1.41889800	0.63396200	4.09504800
C	-0.55707500	-2.52311300	1.91332600
H	-1.38810600	-4.33528800	1.18963200
C	0.76056200	-2.00710700	3.68254900
N	-0.36247800	-1.18139100	1.86055800
C	0.15203100	-3.06208500	3.06710600
H	1.37457700	-2.02161100	4.57640600
H	0.17657300	-4.10621800	3.35851900
C	0.45826200	-0.23870400	-1.02215600
C	0.21530100	0.16294900	-2.45640800
C	1.15112200	-1.58631800	-1.17010100
C	1.14798500	-0.70983100	-3.31104500
H	0.32502300	1.23744900	-2.63318100
H	-0.82856800	-0.08623100	-2.67883300
O	1.44434200	-1.85190400	-2.50001900

O	1.51677400	-2.36851400	-0.32092500
S	2.31957600	0.92945600	-0.31063500
H	0.70102100	-1.06487800	-4.24593700
H	2.09148700	-0.19740600	-3.54768100
C	4.03855000	0.45333700	-0.52903100
C	4.87376600	1.28653100	-1.29051000
C	4.53563800	-0.76593500	-0.03938600
C	6.19442100	0.91539500	-1.53888100
H	4.49022600	2.23045900	-1.67015400
C	5.86114800	-1.12203200	-0.28547100
H	3.87680600	-1.43650600	0.50441100
C	6.69651900	-0.28733200	-1.03353600
H	6.83639200	1.57290100	-2.12086200
H	6.23910900	-2.06530300	0.10154200
H	7.72744900	-0.57372900	-1.22562300
H	2.13125100	0.26893800	0.84647300

TS-S3(*CSS*)

Fe	-1.18555000	0.07146300	0.16991700
N	-1.16696000	-1.92385700	0.49450500
C	-1.64904100	-2.89404500	-0.33561700
C	-0.64550500	-2.57198700	1.57587300
C	-2.26899400	-2.67528600	-1.56339200
C	-1.42998400	-4.20661100	0.24140900
C	-0.06941500	-1.95133600	2.67921400
C	-0.80390300	-4.00554400	1.43193700
C	-2.53207900	-1.43333800	-2.13418100
H	-2.59941000	-3.55346700	-2.11454500
H	-1.72101000	-5.14308000	-0.22227400
C	0.04309300	-0.57720900	2.86595200
H	0.30942200	-2.59337300	3.47150100
H	-0.47167600	-4.74122800	2.15636700
C	-3.24912300	-1.23759700	-3.37771000
N	-2.19012400	-0.22558100	-1.59052800
C	0.59570500	0.04489000	4.05334800
N	-0.37258500	0.37575200	1.98010100
C	-3.34573100	0.10894000	-3.56373400
H	-3.63061100	-2.03648500	-4.00467500
C	-2.68595000	0.73107700	-2.43335600
C	0.50555500	1.38796900	3.86381200
H	1.00122300	-0.49466600	4.90212000
C	-0.10205200	1.58237100	2.56139200
H	-3.82439800	0.64754300	-4.37487400
C	-2.59613200	2.10816500	-2.23117400
H	0.82281700	2.18857700	4.52275700
C	-0.37349600	2.82812500	2.00555100
C	-2.00940500	2.73065100	-1.13055200
H	-3.04516400	2.75113000	-2.98571300
C	-0.99338600	3.05629400	0.78000900
H	-0.09649500	3.70184400	2.59146700
C	-1.96718900	4.16423000	-0.92469300

N	-1.39871600	2.08457300	-0.09111400
C	-1.33285500	4.36701000	0.26454300
H	-2.38321300	4.90096100	-1.60395100
H	-1.11841200	5.30469900	0.76592000
C	0.45865700	0.04302200	-0.82351400
C	0.73530600	1.05394800	-1.91274400
C	1.30588900	-1.14833300	-1.22480800
C	1.95877700	0.53795300	-2.67506900
H	-0.14261500	1.07123000	-2.57324900
H	0.86375900	2.06481600	-1.52161700
O	2.03243100	-0.85928200	-2.37664800
O	1.39509300	-2.26623700	-0.76350000
H	1.87802800	0.64273400	-3.76504200
H	2.88332100	1.01581700	-2.33294800
S	2.69216400	0.84136400	0.59205100
C	4.27170900	0.32680100	0.00324100
C	5.32803300	1.26109700	-0.14766600
C	4.57195800	-1.02383000	-0.30677900
C	6.60339800	0.87101200	-0.55374700
H	5.12281800	2.30663400	0.07115700
C	5.84445500	-1.40430500	-0.72914200
H	3.78552900	-1.76642600	-0.21610700
C	6.87837700	-0.46808400	-0.85185400
H	7.38932400	1.62197100	-0.64647000
H	6.03328900	-2.45240900	-0.96176600
H	7.87260300	-0.77417800	-1.17463300
C	-3.64993000	-1.05996300	2.53318300
H	-2.90658800	-0.91794800	3.32842900
H	-3.51661500	-2.07247900	2.13162100
H	-4.64769400	-1.01023400	2.99354800
S	-3.50065700	0.22309800	1.22527200

TS-S3(*OSS*)

Fe	-1.17671400	0.08269500	0.18255300
N	-1.14292700	-1.91046200	0.51474100
C	-1.61949400	-2.88749800	-0.31047800
C	-0.61562500	-2.55047500	1.59807800
C	-2.23828900	-2.67803300	-1.54038700
C	-1.39160100	-4.19580500	0.27198200
C	-0.04633100	-1.92084000	2.70019800
C	-0.76418000	-3.98554600	1.46035100
C	-2.50122800	-1.44059200	-2.12038200
H	-2.56347300	-3.56053200	-2.08771500
H	-1.67649800	-5.13617300	-0.18758000
C	0.05290200	-0.54533100	2.88289400
H	0.33723200	-2.55685900	3.49508900
H	-0.42588000	-4.71590500	2.18738700
C	-3.21366400	-1.25452000	-3.36808400
N	-2.16602400	-0.22839400	-1.58194700
C	0.59718000	0.08520300	4.06943000
N	-0.36885300	0.40139100	1.99272700

C	-3.31557600	0.09042600	-3.56156700
H	-3.58853400	-2.05847200	-3.99255500
C	-2.66419400	0.72163300	-2.43124300
C	0.49526100	1.42698400	3.87584000
H	1.00558900	-0.44817800	4.92074200
C	-0.11103400	1.61230500	2.57154300
H	-3.79319300	0.62266000	-4.37752100
C	-2.58784100	2.10000900	-2.23340900
H	0.80318000	2.23226700	4.53362000
C	-0.39267600	2.85396900	2.01192100
C	-2.01407200	2.73181400	-1.13106100
H	-3.03831300	2.73618800	-2.99284600
C	-1.00990200	3.07280700	0.78308100
H	-0.12647200	3.73189000	2.59667700
C	-1.98514700	4.16610600	-0.93025400
N	-1.40293300	2.09458300	-0.08641000
C	-1.35804000	4.37859900	0.26139800
H	-2.40405500	4.89690300	-1.61415800
H	-1.15426100	5.31994300	0.76045100
C	0.48356200	0.06403500	-0.81501600
C	0.75868900	1.10173100	-1.88146300
C	1.29104500	-1.13197900	-1.27310800
C	1.96746900	0.59053000	-2.66987200
H	-0.12423800	1.14424100	-2.53382900
H	0.90331500	2.10147000	-1.46811400
O	2.01637300	-0.81735700	-2.42060800
O	1.36044800	-2.26852700	-0.85530700
H	1.88212100	0.73516300	-3.75501800
H	2.90359300	1.03919600	-2.31908500
S	2.66301600	0.76063800	0.61638200
C	4.23929100	0.26211900	0.00246100
C	5.29585700	1.19971200	-0.12151900
C	4.53614700	-1.07817300	-0.35131000
C	6.56971200	0.82110800	-0.54311500
H	5.09238600	2.23792200	0.13104000
C	5.80691600	-1.44659000	-0.78938100
H	3.74866300	-1.82192300	-0.28235900
C	6.84163900	-0.50815800	-0.88463000
H	7.35650500	1.57346200	-0.61395400
H	5.99373400	-2.48686000	-1.05610300
H	7.83452900	-0.80509300	-1.21981500
C	-3.66652600	-1.10062400	2.48642100
H	-2.92357400	-1.00412900	3.28873300
H	-3.55008100	-2.09809400	2.04426600
H	-4.66487800	-1.05135700	2.94557000
S	-3.48996400	0.23214000	1.23243700

TS-S3(*triplet*)

Fe	-1.16632800	0.27679300	0.16024300
N	-1.70548200	-1.61676200	0.63340900
C	-2.20543000	-2.58852400	-0.19245200

C	-1.63527700	-2.16882800	1.88863600
C	-2.46977600	-2.43810800	-1.55139300
C	-2.45780700	-3.79701600	0.56282400
C	-1.17547700	-1.53053900	3.03312100
C	-2.10695500	-3.53076700	1.85361800
C	-2.29308300	-1.25296600	-2.27002100
H	-2.86670100	-3.29747500	-2.08623000
H	-2.84889400	-4.71682900	0.14201100
C	-0.68595400	-0.23189800	3.10956800
H	-1.17291400	-2.11238600	3.95215600
H	-2.14645400	-4.19009500	2.71384800
C	-2.63607200	-1.07370900	-3.65928100
N	-1.80981700	-0.07944400	-1.74942200
C	-0.19975900	0.38835700	4.31639900
N	-0.60118400	0.65023100	2.06276100
C	-2.36431400	0.23453300	-3.96438500
H	-3.03850800	-1.84878200	-4.30246300
C	-1.85032900	0.84382000	-2.76774800
C	0.18162400	1.65567100	3.98051700
H	-0.15296000	-0.09817100	5.28451500
C	-0.07787400	1.80339900	2.56661300
H	-2.49505700	0.74700500	-4.91175600
C	-1.42052200	2.17111400	-2.67582200
H	0.61309300	2.42395400	4.61208000
C	0.14977500	2.97212600	1.83575700
C	-0.87097100	2.77662900	-1.55490500
H	-1.50805400	2.77945200	-3.57381200
C	-0.13920700	3.13513000	0.48612300
H	0.58621700	3.81626300	2.36271300
C	-0.41832500	4.14925500	-1.51010300
N	-0.67824100	2.18272400	-0.33114300
C	0.03876100	4.37210000	-0.24596400
H	-0.45452500	4.83800300	-2.34757900
H	0.46082900	5.27940300	0.17170000
C	0.74648200	-0.37905000	-0.35466300
C	1.25630500	-0.17527200	-1.77345200
C	1.19114600	-1.74576700	0.01345600
C	1.46593600	-1.61034500	-2.28868600
H	0.57322600	0.38774000	-2.40892700
H	2.21274100	0.35932900	-1.76499000
O	1.66080500	-2.42112400	-1.12691300
O	1.23329600	-2.33787900	1.07458700
H	0.58456300	-1.97551900	-2.83411400
H	2.34984600	-1.72230700	-2.92974200
S	2.75633300	0.77469400	0.91571600
C	4.17874600	0.09786900	0.14493900
C	5.03583600	0.89267900	-0.66115500
C	4.54722200	-1.26527600	0.30351300
C	6.19570000	0.37523800	-1.23579200
H	4.76891200	1.93567300	-0.81420300
C	5.70026500	-1.78015800	-0.28371800

H	3.89773900	-1.90599600	0.89226200
C	6.54459100	-0.96823200	-1.05310600
H	6.83157900	1.02472800	-1.83914100
H	5.94556400	-2.83270300	-0.14032300
H	7.44764300	-1.37535300	-1.50610700
C	-4.63184800	0.02709300	0.00600900
H	-4.51710200	-1.02123800	0.30373200
H	-4.57557900	0.07544800	-1.08738900
H	-5.62931300	0.36719600	0.31645000
S	-3.36205600	1.08964800	0.79601300

TS-S3(*quintet*)

Fe	-1.21779800	0.08178100	0.22825100
N	-1.77399300	-1.93266600	0.01423200
C	-2.46885600	-2.46860100	-1.02914800
C	-1.45919000	-2.93276700	0.88272600
C	-3.00409600	-1.74395400	-2.10686300
C	-2.59718600	-3.90154800	-0.82112600
C	-0.76859800	-2.77264400	2.09389500
C	-1.97479500	-4.18651200	0.36098900
C	-2.97991500	-0.35291400	-2.30799100
H	-3.53925000	-2.32562800	-2.85543900
H	-3.10306500	-4.58784900	-1.49191600
C	-0.28874200	-1.58205600	2.65832000
H	-0.59041000	-3.68072700	2.66628700
H	-1.86906700	-5.15260700	0.84257700
C	-3.62590100	0.35930800	-3.39630800
N	-2.36641900	0.55233800	-1.49148300
C	0.39757000	-1.45787300	3.93506400
N	-0.40316000	-0.34712300	2.09965600
C	-3.38823100	1.69165400	-3.19625800
H	-4.19368700	-0.10352200	-4.19669700
C	-2.59488700	1.80352300	-1.98500000
C	0.67968600	-0.13394400	4.10623900
H	0.63331300	-2.28174300	4.59976400
C	0.16428800	0.56180500	2.93809000
H	-3.72412300	2.52631700	-3.80272000
C	-2.13937200	3.00147000	-1.40769600
H	1.19319700	0.33777600	4.93651500
C	0.20572700	1.94821100	2.72504600
C	-1.41253900	3.15862200	-0.21633300
H	-2.40539100	3.91743200	-1.93236100
C	-0.33514300	2.67682700	1.65334300
H	0.70384000	2.53350300	3.49470300
C	-1.00211000	4.42297800	0.37306800
N	-0.98515800	2.14187700	0.58251300
C	-0.33486300	4.12423500	1.52687400
H	-1.20385300	5.40309800	-0.04589400
H	0.11778000	4.81161100	2.23294900
C	0.53156300	-0.09401300	-0.91642300
C	0.81441200	0.76027500	-2.11723300

C	1.35316500	-1.32217400	-1.13771200
C	2.01429100	0.11105300	-2.82746100
H	-0.08043800	0.74741600	-2.76030000
H	0.99120400	1.80633600	-1.84621300
O	2.07648700	-1.22721800	-2.32461000
O	1.41689200	-2.35038500	-0.49217000
H	1.90940200	0.05400500	-3.91904000
H	2.94714200	0.62260300	-2.56818600
S	3.25335300	1.12965400	0.23723500
C	4.78429600	0.36684400	-0.16230000
C	5.96994500	1.12883000	-0.33473800
C	4.91498700	-1.03839000	-0.31957000
C	7.19509000	0.53301300	-0.62956800
H	5.90419400	2.20950400	-0.22710000
C	6.14068800	-1.62661100	-0.62389700
H	4.03176300	-1.65877200	-0.19983800
C	7.29923300	-0.85448800	-0.78032600
H	8.08008500	1.16070900	-0.74817800
H	6.19272400	-2.70964100	-0.73901900
H	8.25524400	-1.32115300	-1.01432100
C	-4.93065800	-0.42522300	0.73049300
H	-4.72821100	-1.49627600	0.59687700
H	-5.06675300	0.00799300	-0.26952900
H	-5.88416800	-0.32876800	1.27026300
S	-3.57296500	0.40611400	1.64607300

TS-S5(*CSS*)

Fe	-1.27578400	0.10318200	0.29004300
N	-0.39436400	0.76465700	1.97300200
N	-1.16413000	-1.79850200	0.97631400
N	-1.54754300	2.02437800	-0.34065000
N	-2.32306600	-0.55672700	-1.34345600
C	-0.15464700	2.06608600	2.31074700
C	-1.63849500	-2.92252900	0.36376200
C	0.08294000	0.00722300	3.00360000
C	-0.57540700	-2.21508500	2.13383300
C	-1.15805500	3.15265300	0.31993200
C	-2.64813800	-1.85212300	-1.63389400
C	-2.23963300	2.44247300	-1.44182600
C	-2.89832600	0.21311200	-2.31551700
C	0.50222700	2.13758200	3.60273400
C	-1.34365100	-4.09626300	1.16358300
C	0.65073800	0.85614700	4.03328700
C	-0.67943800	-3.65552100	2.26540000
C	-1.58324800	4.33427800	-0.40570100
C	-3.43197000	-1.91207900	-2.85148900
C	-2.25911800	3.89144700	-1.50351500
C	-3.58856900	-0.62581300	-3.27590900
C	-0.49333500	3.17731100	1.54431400
C	-2.31813300	-2.95698200	-0.85096400
C	-2.85234500	1.60674500	-2.37413500

C	0.01637300	-1.38102100	3.07774000
H	-0.23503800	4.15401600	1.94888000
H	-2.63780800	-3.93276600	-1.21189600
H	-3.36335700	2.08411700	-3.20858300
H	0.44828700	-1.85279300	3.95797000
C	-3.57613600	-0.38812600	2.11525300
H	-3.80506200	-1.43972300	1.80935600
H	-2.93656000	-0.48253400	3.02734400
H	-4.54850700	0.02397700	2.48292400
C	0.36051500	-0.07894100	-0.77272900
C	0.56102300	0.75488700	-2.02150500
C	1.73652300	0.12715900	-2.77508100
H	2.68154500	0.63842900	-2.55859000
H	1.59354200	0.08142500	-3.86319600
H	0.70229200	1.81461800	-1.80192100
H	-0.35675600	0.66664700	-2.61917300
S	2.55859400	0.86980500	0.40887400
C	4.12194900	0.31962300	-0.19349900
C	5.14319100	1.25132500	-0.51058000
C	4.44586900	-1.05214300	-0.34847700
C	6.40928100	0.84254600	-0.92726300
H	4.91808900	2.31102700	-0.41310300
C	5.70793800	-1.45349500	-0.78261900
H	3.68573400	-1.79483100	-0.12767800
C	6.70820400	-0.51682700	-1.07063900
H	7.16847600	1.59357300	-1.15067300
H	5.91582600	-2.51794300	-0.89280700
H	7.69488700	-0.83841700	-1.40160400
O	1.82305600	-1.21539000	-2.28984300
C	1.16211500	-1.33045900	-1.06588400
O	1.27340100	-2.37845400	-0.46481200
H	1.10403400	0.49761900	4.95112000
H	0.80954400	3.05637500	4.09052000
H	-1.39458400	5.35625400	-0.09374500
H	-2.74124400	4.47405200	-2.28195600
H	-4.12566700	-0.26125500	-4.14561600
H	-3.81314600	-2.82362700	-3.30000400
H	-1.61195200	-5.11253800	0.89482400
H	-0.28705600	-4.23193400	3.09643900
O	-3.05275200	0.39895000	1.12888700

TS-S5(*OSS*)

Fe	-1.27343600	0.10848700	0.30153300
N	-0.39880800	0.77789800	1.98272500
N	-1.14944000	-1.79224200	0.99171100
N	-1.54737300	2.03097400	-0.33595100
N	-2.28403400	-0.55935500	-1.34223400
C	-0.16952100	2.08254800	2.32075400
C	-1.61995900	-2.91923000	0.38224900
C	0.08641900	0.02376800	3.01476000
C	-0.55968500	-2.20372200	2.15079400

C	-1.17370500	3.16257500	0.32732700
C	-2.60358100	-1.85772700	-1.63153900
C	-2.22989700	2.44275700	-1.44579900
C	-2.85076700	0.20532700	-2.32543300
C	0.48907400	2.15832600	3.61164600
C	-1.32574200	-4.08850500	1.18641500
C	0.64926700	0.87814600	4.04176300
C	-0.66111600	-3.64250300	2.28721000
C	-1.60115900	4.33943200	-0.40269800
C	-3.36824400	-1.92410400	-2.86129000
C	-2.26153000	3.88971000	-1.50860600
C	-3.52227500	-0.64063200	-3.29300900
C	-0.51659200	3.19188500	1.55696200
C	-2.28849300	-2.95851800	-0.83926700
C	-2.82031100	1.59825900	-2.38549200
C	0.02922700	-1.36333100	3.09242300
H	-0.26846400	4.17015000	1.96417300
H	-2.60404400	-3.93551400	-1.20033300
H	-3.32467700	2.06822500	-3.22816800
H	0.46463800	-1.83027800	3.97351400
C	-3.55803500	-0.38394200	2.12535100
H	-3.77091500	-1.44364700	1.84023300
H	-2.91460600	-0.44834900	3.03602600
H	-4.53473400	0.02336700	2.48448000
C	0.40548100	-0.06415000	-0.76656700
C	0.59585600	0.79776400	-2.00123700
C	1.74690600	0.16405600	-2.78709500
H	2.70923600	0.63980000	-2.56362200
H	1.59436800	0.16177700	-3.87500900
H	0.76124000	1.85018500	-1.76357100
H	-0.32971200	0.73736400	-2.58949000
S	2.49570800	0.77055800	0.45388000
C	4.05886700	0.25266900	-0.18257900
C	5.06742700	1.20439500	-0.47811500
C	4.39422500	-1.11034500	-0.38052200
C	6.33508600	0.82119100	-0.91414200
H	4.83183500	2.25817600	-0.34761600
C	5.65736100	-1.48567700	-0.83447200
H	3.64225800	-1.86639700	-0.17791900
C	6.64608900	-0.53031000	-1.09975800
H	7.08549000	1.58595100	-1.11947500
H	5.87539600	-2.54401600	-0.97809700
H	7.63378200	-0.83180800	-1.44619800
O	1.79746200	-1.19672300	-2.34987700
C	1.14272600	-1.33346000	-1.12172300
O	1.22866200	-2.40693900	-0.56182600
H	1.10714200	0.52363300	4.95893900
H	0.78940600	3.07965000	4.09914100
H	-1.42431700	5.36324600	-0.08973900
H	-2.73938200	4.46783800	-2.29304700
H	-4.04698600	-0.28108200	-4.17232100

H	-3.73881400	-2.83887300	-3.31205700
H	-1.59110800	-5.10629200	0.92056700
H	-0.26809500	-4.21547100	3.12039500
O	-3.04790100	0.39191400	1.12107200

TS-S5(*triplet*)

Fe	-1.28646500	0.27632800	0.26613300
O	-2.94670600	0.84188700	0.95138800
C	-4.17292200	0.46401100	0.43813900
H	-4.35686300	0.83658400	-0.58993700
H	-4.98702700	0.87212000	1.07373800
H	-4.31852900	-0.63399300	0.40339300
N	-1.86364300	-1.66666300	0.28130300
C	-1.79593400	-2.50306900	1.36832300
C	-2.41857500	-2.39372600	-0.73880500
C	-1.31065900	-2.16711900	2.62457700
C	-2.31685100	-3.80312200	1.01990600
C	-2.70828900	-1.91295200	-2.01188100
C	-2.70005600	-3.74116200	-0.28688000
C	-0.78151200	-0.93512600	3.00162300
H	-1.32082900	-2.95002900	3.38000400
H	-2.36611800	-4.64808500	1.69837800
C	-2.49572700	-0.59625700	-2.43912000
H	-3.14802500	-2.60703600	-2.72429700
H	-3.13188800	-4.52131600	-0.90442800
C	-0.28967800	-0.62433000	4.32007400
N	-0.67067100	0.16169300	2.18908300
C	-2.84756000	-0.08547800	-3.73902100
N	-1.95797500	0.40357000	-1.67012500
C	0.11764600	0.68023700	4.28799500
H	-0.25725000	-1.32314900	5.14907900
C	-0.13229100	1.15604700	2.94672700
C	-2.52251600	1.24837200	-3.73733600
H	-3.28787700	-0.67278000	-4.53775000
C	-1.97100400	1.54012800	-2.44362300
H	0.55987400	1.27209100	5.08168800
C	0.11847500	2.46077100	2.50681900
H	-2.64263200	1.97215100	-4.53691200
C	-1.48959100	2.79497800	-2.04745400
C	-0.16667500	2.94406200	1.23660000
H	0.57138900	3.14890600	3.21590500
C	-0.90840600	3.09911300	-0.82549300
H	-1.56288700	3.60086500	-2.77529400
C	0.03856200	4.31855100	0.81930500
N	-0.72316300	2.22696900	0.21758800
C	-0.42321100	4.41386400	-0.45776600
H	0.48099900	5.09091400	1.43892800
H	-0.44512600	5.28357800	-1.10630600
C	0.59630400	-0.30533800	-0.43843800
C	1.10304500	0.17395700	-1.79040300
C	1.05184000	-1.71375000	-0.34617700

C	1.31017100	-1.13168000	-2.57927800
H	0.41372400	0.84900700	-2.29752600
H	2.05852800	0.69877400	-1.68291400
O	1.51173600	-2.15427300	-1.60157500
O	1.09825800	-2.50510100	0.57624500
H	0.42419800	-1.38217100	-3.18014100
H	2.18886500	-1.11450000	-3.23699100
C	4.08606600	0.02088300	0.08732800
C	4.95426100	0.94433200	-0.55307100
C	4.42192100	-1.35370800	-0.04395300
S	2.69149300	0.55735300	1.00502700
C	6.09361100	0.53001800	-1.24134100
H	4.71240800	2.00235400	-0.48468900
C	5.55410400	-1.76286500	-0.74417300
H	3.76394400	-2.08702800	0.41227800
C	6.41011000	-0.82973200	-1.34470800
H	6.73857100	1.27530300	-1.70936300
H	5.77370400	-2.82782100	-0.82410800
H	7.29693900	-1.15545300	-1.88700300

TS-S5(*quintet*)

Fe	-1.36519100	0.09764300	0.38032400
N	-0.41942100	-0.52134100	2.13460200
N	-1.88655600	-1.90021700	-0.05685000
N	-0.96142400	2.10948800	0.83502400
N	-2.44693000	0.72960300	-1.33965300
C	0.17856600	0.30075300	3.03453000
C	-2.62582200	-2.32431700	-1.11874800
C	-0.33051000	-1.80180800	2.58148700
C	-1.57994600	-2.97420500	0.72036800
C	-0.28074100	2.53338100	1.93305300
C	-3.10932800	-0.08780600	-2.20548900
C	-1.36151600	3.19596200	0.12045100
C	-2.63305700	2.02270500	-1.72873300
C	0.69671200	-0.50502100	4.13190800
C	-2.78731400	-3.76871800	-1.02813500
C	0.38054200	-1.80376600	3.85188500
C	-2.14190000	-4.16744500	0.10886700
C	-0.22645700	3.98866600	1.91611000
C	-3.74778000	0.73073300	-3.22386200
C	-0.89424400	4.39785500	0.79673900
C	-3.45119900	2.03462500	-2.92891100
C	0.24891500	1.70174400	2.93543000
C	-3.17216200	-1.49248500	-2.11363700
C	-2.12066600	3.15318300	-1.06310700
C	-0.86420300	-2.92597100	1.92943800
H	0.77496500	2.20839100	3.74222700
H	-3.74324100	-1.99462000	-2.89324400
H	-2.35735200	4.11687100	-1.51232500
H	-0.69868500	-3.88351700	2.42058000
C	-4.33629300	-0.13625500	1.16626200

H	-4.76746800	0.31329400	0.24020400
H	-4.42715200	-1.23953200	1.02669500
H	-5.05439600	0.12021200	1.98269500
C	0.43726700	-0.08211700	-0.85733400
C	0.61327700	0.70210600	-2.13272800
C	1.78245600	0.04497600	-2.88267900
H	2.72340100	0.57370200	-2.69249900
H	1.62631500	-0.04531800	-3.96675500
H	0.76132500	1.77130400	-1.95172300
H	-0.31793100	0.60256200	-2.71200900
S	2.89348900	1.07601400	0.18701800
C	4.43685500	0.38197600	-0.29115500
C	5.55454000	1.20713600	-0.58278100
C	4.64756500	-1.01855400	-0.38668500
C	6.79639400	0.67420300	-0.92480300
H	5.42295100	2.28575400	-0.52823000
C	5.88800300	-1.54395800	-0.74224200
H	3.81543900	-1.68478700	-0.18035500
C	6.98134700	-0.71028900	-1.01104800
H	7.62901700	1.34837300	-1.13321100
H	6.00422200	-2.62612900	-0.80746000
H	7.94981100	-1.12849500	-1.28278900
O	1.88141000	-1.27491900	-2.34322100
C	1.22105600	-1.33069100	-1.10924100
O	1.32102400	-2.34999800	-0.45268800
H	0.60892500	-2.68614000	4.44061500
H	1.23745800	-0.12041500	4.98997500
H	0.26486400	4.60506300	2.66137400
H	-1.05972700	5.41462700	0.45508300
H	-3.76446100	2.92458800	-3.46576200
H	-4.34641400	0.35452000	-4.04730900
H	-3.32696300	-4.38540100	-1.73955400
H	-2.05058100	-5.17438100	0.50293100
O	-3.06581200	0.28394400	1.44428500

TS-S6(*CSS*)

Fe	-0.97806000	0.11047400	0.36715800
N	-1.98833500	-1.57508500	-0.13658000
N	-1.95337700	1.13816600	-1.11882800
N	-0.18528300	-0.83810700	1.94292400
N	-0.11129900	1.85033200	0.95483900
C	-1.92852900	-2.78590000	0.48582100
C	-1.88415100	2.47847600	-1.38349100
C	-2.87830800	-1.71807400	-1.16604600
C	-2.85586200	0.61527800	-2.00603600
C	-0.37888400	-2.14750600	2.30370400
C	-0.26864600	3.09337400	0.39579700
C	0.62448000	-0.29425200	2.90643700
C	0.71826500	2.02124800	2.03016600
C	-2.79695600	-3.73882500	-0.17581100
C	-2.75485700	2.81549800	-2.49092100

C	-3.38716900	-3.07487100	-1.20400900
C	-3.35611000	1.65620600	-2.87956800
C	0.34375000	-2.44335600	3.52300600
C	0.51526100	4.07194400	1.11850700
C	0.96546800	-1.29297300	3.89819000
C	1.13181300	3.40528100	2.13375400
C	-1.17039500	-3.06256500	1.61986300
C	-1.08992000	3.39145200	-0.68953700
C	1.06888300	1.02361600	2.93830100
C	-3.26751400	-0.71367200	-2.04629000
H	-1.22236200	-4.07163300	2.02041300
H	-1.12626700	4.42852400	-1.01399400
H	1.72109500	1.30755800	3.76046400
H	-3.98697200	-0.98397700	-2.81488300
C	-3.11121400	2.29576200	2.08170700
H	-2.25358200	2.63932800	2.67010300
H	-3.18483700	2.92058800	1.18454200
H	-4.02178100	2.44374200	2.67551900
C	0.40614200	-0.25908300	-1.01415200
C	0.94065000	0.84827300	-1.91650100
C	0.43074600	0.46349800	-3.31748400
H	1.14675000	0.67075400	-4.12098200
H	-0.52063000	0.94938000	-3.55495800
H	2.03594800	0.86034400	-1.91842900
H	0.60970800	1.84127400	-1.62313500
S	-2.98238800	0.51893400	1.65111600
O	0.22592900	-0.95955800	-3.28178500
C	0.26958000	-1.42218800	-1.98446700
O	0.23897300	-2.61537700	-1.77723500
H	-4.10404600	-3.44578300	-1.92682100
H	-2.92648800	-4.77132000	0.12615900
H	0.35351800	-3.40847700	4.01570400
H	1.59445700	-1.11543100	4.76265600
H	1.78971300	3.79952200	2.89955800
H	0.56427700	5.12714700	0.87583500
H	-2.88433600	3.81239600	-2.89606800
H	-4.08177800	1.50419400	-3.66989600
C	2.08907300	-1.06773000	0.05028900
H	1.46061700	-1.88256300	0.37990800
H	2.18527400	-0.24136100	0.74288000
C	3.07453500	-1.33483900	-0.87575600
H	2.98387500	-2.25778500	-1.44622700
C	4.19149800	-0.48657500	-1.23854400
C	5.09298400	-0.91648400	-2.24202100
C	4.45307900	0.76503900	-0.62713100
C	6.19423500	-0.15021000	-2.60891700
H	4.91049200	-1.87130200	-2.73022600
C	5.55270000	1.53050700	-1.00069700
H	3.78317800	1.13419800	0.14366100
C	6.43422000	1.08147800	-1.99098100
H	6.86773200	-0.51146100	-3.38323000

H	5.72514900	2.48839700	-0.51504200
H	7.29299500	1.68349600	-2.27743200

TS-S6(*OSS*)

Fe	0.06510900	0.04128100	-0.48171800
N	-1.66540500	-0.99450000	-0.63382800
N	1.08523500	-1.66249800	-0.87036200
N	-0.96010900	1.76710300	-0.19826700
N	1.79354800	1.10801300	-0.47026400
C	-2.92718300	-0.46547300	-0.59859800
C	2.44159200	-1.77915700	-0.98366400
C	-1.81502100	-2.33308600	-0.87781000
C	0.57427500	-2.91041200	-1.07457900
C	-2.32296900	1.90286400	-0.19053700
C	3.05132300	0.59786800	-0.64481600
C	-0.44663200	3.02828900	-0.03286600
C	1.94323700	2.45896500	-0.29741700
C	-3.90991400	-1.50760300	-0.80626500
C	2.80330000	-3.15377800	-1.26796600
C	-3.21914200	-2.66811100	-0.97429200
C	1.64157600	-3.85570500	-1.32612600
C	-2.68431500	3.28796100	0.01829600
C	4.03118900	1.65957600	-0.57654400
C	-1.51889200	3.98626500	0.11963100
C	3.34315100	2.81610100	-0.36274100
C	-3.24115900	0.87224600	-0.38000900
C	3.35918900	-0.74159400	-0.86466100
C	0.90435900	3.35836000	-0.06966900
C	-0.77648800	-3.23600700	-1.06908800
H	-4.29475100	1.13800200	-0.36295800
H	4.40994400	-0.99480800	-0.97754500
H	1.16784500	4.40455700	0.06139700
H	-1.04261000	-4.27314600	-1.25292800
C	0.14471800	2.05000000	-3.30581300
H	-0.65923900	2.65276600	-2.86972500
H	1.10370900	2.46402800	-2.97574800
H	0.08888600	2.13681500	-4.39751100
C	0.29824500	-0.24654500	1.56811200
C	0.80520400	0.88482800	2.44496100
C	1.45427100	0.19859800	3.66202800
H	0.82492500	0.24905100	4.55915300
H	2.44410200	0.60001600	3.90958000
H	0.01433200	1.58502800	2.73588100
H	1.55338900	1.47007100	1.90482200
S	-0.01378600	0.28070000	-2.85800400
O	1.61235400	-1.17872500	3.30695000
C	0.86642600	-1.48003700	2.17455100
O	0.73943900	-2.65011400	1.86298800
H	-3.60439800	-3.66364900	-1.15952800
H	-4.98198000	-1.35097600	-0.81854000
H	-3.70085600	3.66011800	0.06740100

H	-1.37997300	5.05096800	0.26648300
H	3.72988700	3.82310000	-0.25916900
H	5.10017800	1.52039000	-0.68606900
H	3.81773400	-3.50955100	-1.40245900
H	1.49722600	-4.91232800	-1.51667400
C	-1.69291700	-0.64869500	2.45094000
H	-1.74021500	-1.61845900	1.97001400
H	-2.06463100	0.18038000	1.86562300
C	-1.76813500	-0.53925900	3.83008500
H	-1.95012900	0.45366000	4.24409300
C	-1.64368200	-1.59441300	4.81966400
C	-1.94699600	-1.30883500	6.17194700
C	-1.25368900	-2.91878200	4.50542300
C	-1.88785600	-2.29115000	7.15594300
H	-2.24191500	-0.29544600	6.43896000
C	-1.19251300	-3.89537000	5.49420900
H	-0.95910800	-3.16529300	3.49079500
C	-1.51313100	-3.59645800	6.82363700
H	-2.13266000	-2.03848200	8.18581200
H	-0.87926800	-4.90172800	5.22547000
H	-1.46179100	-4.36675200	7.58960300

TS-S6(*triplet*)

Fe	-0.96849300	0.39467200	0.55910100
N	-2.05915100	-1.24462100	0.15726200
N	-1.99573100	1.45957400	-0.82773200
N	0.01428500	-0.64312100	2.00242100
N	0.10220200	2.06490000	0.99636000
C	-1.96475400	-2.47348800	0.74937900
C	-1.85679900	2.78932800	-1.13599400
C	-3.05622900	-1.34168400	-0.77350800
C	-3.00258900	0.98286100	-1.62252900
C	-0.17665000	-1.94559800	2.36422600
C	-0.04076100	3.31573500	0.45571300
C	0.97554500	-0.14687000	2.83902200
C	1.07479300	2.16685400	1.95417300
C	-2.93766100	-3.37878500	0.17833400
C	-2.79747300	3.16076300	-2.16895500
C	-3.61574600	-2.67704900	-0.76700400
C	-3.50745200	2.03791200	-2.47328800
C	0.69784000	-2.29375300	3.46421400
C	0.88777500	4.23450100	1.07432600
C	1.41351700	-1.17511800	3.76041400
C	1.58405700	3.51963900	2.00194900
C	-1.09086900	-2.81242400	1.77338200
C	-0.95004400	3.66150700	-0.54175400
C	1.49031300	1.14523400	2.80485000
C	-3.49237600	-0.32038700	-1.60870700
H	-1.13412300	-3.82988400	2.15164000
H	-0.95337200	4.69436100	-0.87949500
H	2.26613000	1.38854900	3.52594800

H	-4.29430000	-0.55618700	-2.30277800
C	-3.22900200	2.58283600	1.99386600
H	-2.46942300	3.37114100	2.03823900
H	-3.72558900	2.63689100	1.01973700
H	-3.97347500	2.77552400	2.77532400
C	0.40531000	-0.10670600	-0.98453700
C	0.96422000	0.97032400	-1.89691800
C	0.38278400	0.60730300	-3.27586700
H	1.06801300	0.79671800	-4.11033700
H	-0.56174200	1.13085400	-3.46997900
H	2.06016100	0.91564600	-1.93947900
H	0.70153800	1.98463000	-1.60045800
S	-2.49463100	0.93075100	2.29086600
O	0.13057700	-0.80425500	-3.22977500
C	0.11761000	-1.23634600	-1.90686800
O	-0.06482200	-2.41893500	-1.68537400
H	-4.41782100	-3.01187300	-1.41358200
H	-3.06426000	-4.41300800	0.47451700
H	0.74093200	-3.26870300	3.93470400
H	2.17023500	-1.03890000	4.52378000
H	2.36211800	3.86281900	2.67344700
H	0.97858900	5.28450800	0.82279400
H	-2.89038100	4.15405300	-2.59194200
H	-4.30432700	1.91850600	-3.19762800
C	2.29088700	-1.17159400	-0.10364500
H	1.59826000	-1.97404900	0.11093900
H	2.39730000	-0.41386700	0.66221500
C	3.24579100	-1.34158400	-1.07328400
H	3.14011700	-2.19489400	-1.74292500
C	4.37428700	-0.46901600	-1.35366400
C	4.64635000	0.71631200	-0.62657000
C	5.27715400	-0.80731100	-2.38927900
C	5.75414800	1.50388000	-0.92142900
H	3.97212500	1.02153700	0.16829700
C	6.38607600	-0.01809100	-2.68039200
H	5.09081000	-1.71006800	-2.96749700
C	6.63668000	1.14626700	-1.94809500
H	5.93094000	2.41051400	-0.34633000
H	7.05800600	-0.31076800	-3.48494100
H	7.50066400	1.76652500	-2.17420400

TS-S6(*quintet*)

Fe	-0.07965500	0.15273800	-0.45612500
N	-1.97881200	-0.67371200	-0.68489600
N	0.78034800	-1.72374000	-0.76618600
N	-0.96090900	2.07583400	-0.30359800
N	1.79527400	1.01943900	-0.37142700
C	-3.16299600	0.00569100	-0.67388500
C	2.11183300	-1.98238200	-0.84643600
C	-2.24696400	-1.99208100	-0.90831500
C	0.10579100	-2.88654700	-0.97155200

C	-2.29486500	2.34855600	-0.35474100
C	2.98120000	0.35172900	-0.49112000
C	-0.28636900	3.25733500	-0.22531900
C	2.06705200	2.35345900	-0.24257000
C	-4.24944300	-0.93622500	-0.88356900
C	2.30529200	-3.39834900	-1.11055000
C	-3.68359200	-2.16927600	-1.02790100
C	1.06496700	-3.95912300	-1.18370300
C	-2.48607700	3.78563400	-0.27923400
C	4.06922200	1.30837400	-0.40318300
C	-1.24309400	4.34859000	-0.20282300
C	3.50602800	2.54231600	-0.24972500
C	-3.30931500	1.39007500	-0.49929700
C	3.12601000	-1.02683800	-0.70913100
C	1.11236900	3.38052900	-0.17279000
C	-1.28929600	-3.01270900	-1.01971300
H	-4.32876600	1.76868900	-0.51990900
H	4.14699000	-1.39244700	-0.78713900
H	1.50425700	4.39202700	-0.09323500
H	-1.67619400	-4.01312500	-1.19911000
C	0.99548700	1.63337400	-3.44370300
H	0.74866800	2.63717200	-3.08158500
H	2.01152500	1.38480400	-3.12284100
H	0.97295700	1.64659500	-4.54032100
C	0.00934500	-0.01897700	1.65502200
C	-0.14981600	1.24413700	2.47336100
C	0.54263900	0.93934400	3.81389100
H	-0.17298900	0.66518900	4.59836400
H	1.16523600	1.76363300	4.18129300
H	-1.19454700	1.55065700	2.59590900
H	0.36361000	2.07254800	1.97378700
S	-0.22564200	0.39203100	-2.86825500
O	1.39414400	-0.18327100	3.56764500
C	1.05915900	-0.79373100	2.36344200
O	1.59265000	-1.85250900	2.08752000
H	-4.18101200	-3.11538900	-1.20671200
H	-5.30082400	-0.67565800	-0.92118700
H	-3.44545200	4.28992400	-0.29834100
H	-0.99048100	5.40114200	-0.14456700
H	4.00779200	3.49874700	-0.15906400
H	5.12199200	1.05774300	-0.46026500
H	3.26648800	-3.88671000	-1.21999200
H	0.81015200	-4.99579400	-1.37070800
C	-1.65930600	-1.38608400	2.39992900
H	-1.14347500	-2.23097300	1.95749200
H	-2.30233800	-0.83253200	1.73015800
C	-1.91333400	-1.33279600	3.75372600
H	-2.61231800	-0.57183000	4.10403000
C	-1.36845500	-2.18584500	4.79844500
C	-1.91829700	-2.11808100	6.09937200
C	-0.31742000	-3.10847900	4.58291800

C	-1.46377300	-2.93972600	7.12714400
H	-2.72283300	-1.41015600	6.29126300
C	0.13494600	-3.92529300	5.61440700
H	0.16934400	-3.15289900	3.61413600
C	-0.43402900	-3.85504300	6.89136800
H	-1.91255700	-2.86496100	8.11582600
H	0.95157800	-4.61749400	5.42196300
H	-0.07266300	-4.49622500	7.69200400

S7

C	-1.17216600	1.11783300	0.90534100
C	-2.63062300	1.60607800	0.79254500
H	-3.19874700	1.42047900	1.71129900
H	-2.72129700	2.66223500	0.52952500
H	-0.82245200	1.11706000	1.94146800
H	-0.49877300	1.76032700	0.32615000
O	-3.23996100	0.84139900	-0.26989000
C	-2.52130700	-0.28897300	-0.52447700
O	-2.89561600	-1.14028700	-1.29418400
C	-1.25948200	-0.26411300	0.28291300
C	-0.82554100	-1.55302700	0.95503000
C	-0.06942400	-1.06711400	-0.24227900
H	-0.37701600	-1.45382200	1.93994000
H	-1.46862600	-2.41911900	0.82740400
H	-0.30564000	-1.58794700	-1.16939500
C	1.31188800	-0.49435300	-0.17749300
C	1.76997000	0.29745500	-1.24373700
C	2.17615800	-0.72230000	0.90113000
C	3.04959400	0.85070700	-1.22785500
H	1.11418200	0.47469100	-2.09326100
C	3.45795800	-0.16766000	0.92072800
H	1.85352900	-1.35213500	1.72530700
C	3.89858600	0.62201500	-0.14181000
H	3.38472900	1.45935400	-2.06360600
H	4.11440000	-0.36070600	1.76523400
H	4.89666300	1.05140500	-0.12768400

TS-S8(*CSS*)

Fe	-1.17615100	0.05258500	0.61195700
O	-2.56815100	0.20716400	1.91491600
C	-3.23488500	1.37130100	2.23042400
H	-3.82366500	1.79034100	1.38691800
H	-2.57536000	2.19045400	2.58612200
H	-3.96279800	1.17130300	3.04238800
N	-1.15242700	2.07005300	0.24966300
C	-0.32521500	2.99710900	0.82160700
C	-1.98542400	2.76617900	-0.58464200
C	0.63381600	2.71827900	1.79293200
C	-0.62535100	4.32038600	0.31700000
C	-2.99150500	2.20422400	-1.37118000
C	-1.66353400	4.17681000	-0.55416500

C	0.86679300	1.47078900	2.36528600
H	1.21980600	3.55348200	2.16882400
H	-0.11389200	5.22878600	0.61384800
C	-3.33453600	0.85224700	-1.42373200
H	-3.57598200	2.88505400	-1.98549900
H	-2.17679700	4.94259400	-1.12439300
C	1.81366000	1.22974800	3.43341900
N	0.23329000	0.30327400	2.01929600
C	-4.43259700	0.31077600	-2.20032200
N	-2.71753200	-0.14577300	-0.72165400
C	1.73315600	-0.09555300	3.73469800
H	2.44083800	1.98866700	3.88666300
C	0.74074200	-0.66432500	2.84841200
C	-4.48010200	-1.02217100	-1.92743000
H	-5.07946200	0.89142300	-2.84776500
C	-3.41275700	-1.29256300	-0.98553000
H	2.28175600	-0.65153900	4.48606900
C	0.36519900	-2.00434000	2.84938200
H	-5.17279900	-1.76436500	-2.30656600
C	-3.17736100	-2.52853100	-0.39028400
C	-0.60955400	-2.57329700	2.03373800
H	0.85545100	-2.65540800	3.56902700
C	-2.21977300	-2.79943900	0.58166200
H	-3.81910100	-3.35175700	-0.69396800
C	-1.05101000	-3.95381900	2.12285100
N	-1.31859600	-1.90691300	1.08111500
C	-2.05737400	-4.09194600	1.22056800
H	-0.64322800	-4.69303700	2.80248400
H	-2.64788500	-4.97208500	0.99478300
C	-0.02035700	-0.27658300	-1.01105000
C	0.09252000	0.79096000	-2.09169500
C	-0.06284400	-1.55988300	-1.82627800
C	0.46136600	0.06147800	-3.38988300
H	0.78458000	1.59936600	-1.83572600
H	-0.89022300	1.25195700	-2.21988500
O	0.09352200	-1.30329400	-3.17663400
O	-0.17057600	-2.71165700	-1.46822900
H	-0.08298700	0.42407600	-4.26934200
H	1.53725400	0.09891900	-3.60535600
C	1.90961300	-0.53674000	-0.28743100
H	1.66041400	-1.37272600	0.35484400
H	1.88435900	0.42810600	0.20143200
C	2.82311600	-0.70570600	-1.32000200
H	3.21390200	0.19686000	-1.79146100
C	3.33526000	-1.94273400	-1.86970900
C	4.33549500	-1.88854500	-2.87078300
C	2.92144500	-3.22497200	-1.43214300
C	4.90314200	-3.04375300	-3.39699800
H	4.66600700	-0.91439200	-3.22682900
C	3.48874200	-4.37640400	-1.96651200
H	2.12938100	-3.31002600	-0.69741000

C	4.48492800	-4.30001900	-2.94678800
H	5.67173300	-2.96640300	-4.16341700
H	3.14352400	-5.34742600	-1.61917700
H	4.92312000	-5.20610000	-3.35838600

TS-S8(*OSS*)

Fe	-1.20008200	0.18905000	0.61230900
O	-2.50431500	0.46093700	1.93259200
C	-2.51614200	1.51219800	2.83454400
H	-2.61467100	2.50407900	2.35189400
H	-1.61119900	1.55858900	3.47128500
H	-3.38125600	1.40094700	3.51517700
N	-1.29248800	2.14495600	0.07239400
C	-0.51336100	3.17542300	0.52853000
C	-2.16577700	2.68851300	-0.82907900
C	0.51957000	3.05184400	1.45414400
C	-0.90552200	4.41381400	-0.10704200
C	-3.14558900	1.99059400	-1.53122000
C	-1.93139600	4.11076800	-0.95159000
C	0.88897300	1.87140100	2.09356900
H	1.06176500	3.95517700	1.72129900
H	-0.44779100	5.37800700	0.08082300
C	-3.41963400	0.63169700	-1.41337000
H	-3.76391500	2.56311000	-2.21771600
H	-2.49110600	4.77548600	-1.59908600
C	1.89844200	1.78026600	3.12502200
N	0.30989700	0.64604700	1.89051500
C	-4.49517500	-0.04504300	-2.11373900
N	-2.75130800	-0.24805200	-0.61316400
C	1.89722600	0.48879500	3.55955300
H	2.50558900	2.60845700	3.47134600
C	0.89216200	-0.20929800	2.78816900
C	-4.46321200	-1.34149100	-1.70869700
H	-5.17259600	0.43027700	-2.81323500
C	-3.36732100	-1.45371600	-0.76693900
H	2.50639100	0.03669000	4.33349100
C	0.56171400	-1.55208100	2.96081700
H	-5.10673300	-2.16024100	-2.00759400
C	-3.02288200	-2.62527000	-0.10446700
C	-0.40686400	-2.25141100	2.24552600
H	1.10614700	-2.10053600	3.72512300
C	-2.00984200	-2.74566200	0.83999700
H	-3.60650400	-3.51460000	-0.32626700
C	-0.73955400	-3.64334600	2.47042400
N	-1.17701000	-1.73963400	1.23943000
C	-1.73346500	-3.95164100	1.59341500
H	-0.26649800	-4.28082000	3.20809400
H	-2.25118600	-4.89442400	1.46214000
C	0.13828900	-0.13017900	-0.97727200
C	1.12862400	0.94919000	-1.38351800
C	-0.22523200	-0.79794600	-2.25359800

C	1.48411300	0.64851900	-2.85095300
H	2.01361400	0.98487000	-0.73809800
H	0.65333800	1.93180300	-1.31134900
O	0.48109200	-0.25603200	-3.32292100
O	-0.97832400	-1.72932200	-2.47718700
H	1.46941400	1.53660800	-3.49422800
H	2.46096600	0.16035700	-2.95424100
C	1.47953700	-1.80593400	-0.43030900
H	0.67197200	-2.52053200	-0.53703600
H	1.56695200	-1.34517900	0.54300000
C	2.63803000	-1.93271000	-1.18167800
C	2.86016200	-2.76799700	-2.34765200
C	4.17320900	-2.90422700	-2.85818000
C	1.82940300	-3.48279400	-3.00538800
C	4.45129700	-3.72307200	-3.94846500
H	4.98131300	-2.35811200	-2.37437500
C	2.11342100	-4.29701400	-4.09691300
H	0.80099600	-3.36255100	-2.68104600
C	3.42196000	-4.43128600	-4.57608400
H	5.47359200	-3.80811400	-4.31221000
H	1.29959700	-4.82528800	-4.58876600
H	3.63351900	-5.06933900	-5.43103800
H	3.50234300	-1.34306900	-0.87234900

TS-S8(*triplet*)

Fe	-1.27760400	0.17701100	0.63886800
O	-2.27484000	0.32093000	2.20930400
C	-3.42344000	1.08638500	2.35064900
H	-4.23048100	0.79069800	1.65398200
H	-3.25087000	2.16855500	2.19769300
H	-3.81998400	0.96367500	3.37549300
N	-1.47047300	2.16082200	0.24836400
C	-0.69688200	3.16549200	0.76606300
C	-2.40567400	2.76383900	-0.54883100
C	0.39892900	2.99377300	1.60867500
C	-1.15603200	4.44692700	0.27584200
C	-3.41858700	2.10073200	-1.23522200
C	-2.21341500	4.19683800	-0.54646700
C	0.88712700	1.77553400	2.07447900
H	0.91773900	3.89184800	1.93396700
H	-0.71358200	5.40181200	0.53449100
C	-3.66418600	0.73302400	-1.17150300
H	-4.08918000	2.70203800	-1.84292800
H	-2.82148900	4.90330600	-1.09894000
C	2.00302400	1.64184200	2.98759000
N	0.36918900	0.54472300	1.78118200
C	-4.76590500	0.06866300	-1.83408100
N	-2.92893700	-0.17093400	-0.45595800
C	2.12909300	0.31314600	3.25730800
H	2.58984800	2.46783800	3.37215700
C	1.08798800	-0.36083600	2.51069900

C	-4.67982000	-1.24704200	-1.50277600
H	-5.49503600	0.56229900	-2.46527400
C	-3.52227000	-1.38607000	-0.64547700
H	2.84058800	-0.17973600	3.90934200
C	0.82539700	-1.72640800	2.58598400
H	-5.32228800	-2.06425200	-1.80790600
C	-3.09846400	-2.59411200	-0.10361000
C	-0.22254500	-2.38019600	1.94448200
H	1.47428900	-2.32498600	3.21978300
C	-1.99000600	-2.77352600	0.71770000
H	-3.68667100	-3.47609000	-0.34226500
C	-0.51151200	-3.79337700	2.07869300
N	-1.12367900	-1.79224900	1.10387300
C	-1.61017700	-4.03862400	1.31438000
H	0.06051300	-4.48707800	2.68338900
H	-2.13226500	-4.97571200	1.16155000
C	-0.06274700	0.01797100	-1.09558000
C	0.98975100	1.08093100	-1.35830000
C	-0.56854000	-0.35388600	-2.43496400
C	1.19678400	1.08239100	-2.88645800
H	1.92414700	0.89435100	-0.81618300
H	0.63080800	2.05903700	-1.02553200
O	0.11410400	0.32977700	-3.43869800
O	-1.41501100	-1.16585600	-2.77131700
H	1.17152400	2.08742000	-3.32582100
H	2.13605900	0.59933500	-3.18268800
C	1.20400600	-1.84413600	-1.01036800
H	0.32893100	-2.46245200	-1.17378800
H	1.39379700	-1.56689000	0.01652800
C	2.28262700	-1.89823200	-1.87441200
H	3.21460800	-1.43686500	-1.54406000
C	2.34108300	-2.51191400	-3.18923100
C	3.59472300	-2.65545900	-3.82998400
C	1.20275900	-3.00525300	-3.87255500
C	3.71495800	-3.27645700	-5.06975600
H	4.48402700	-2.27671100	-3.32877700
C	1.32921000	-3.62323000	-5.11242100
H	0.21595800	-2.86298800	-3.44389000
C	2.58129000	-3.77155600	-5.72125300
H	4.69618900	-3.37387000	-5.53087100
H	0.43546100	-3.98332400	-5.61749500
H	2.66956000	-4.25456400	-6.69173300

TS-S8(*quintet*)

Fe	-1.10222400	0.37622900	0.58984800
O	-2.19430100	0.32955100	2.11183100
C	-3.34367200	1.09080300	2.28176900
H	-4.07146000	0.96631200	1.45906700
H	-3.14480800	2.17441700	2.37772300
H	-3.85023300	0.77161200	3.21164700
N	-1.61911100	2.33859000	0.12677200

C	-1.05776600	3.46795400	0.65173400
C	-2.63169300	2.71547900	-0.70984000
C	0.00270000	3.50153100	1.57260900
C	-1.73698300	4.62919100	0.10553000
C	-3.49794200	1.84362900	-1.38654100
C	-2.70463100	4.16471700	-0.73839500
C	0.68855900	2.41060900	2.12933000
H	0.31800000	4.48877500	1.90291900
H	-1.49882200	5.65924500	0.34499400
C	-3.53439300	0.44312000	-1.31151000
H	-4.24669700	2.31125500	-2.02162300
H	-3.41460200	4.74042200	-1.32085100
C	1.72841900	2.48432800	3.14172800
N	0.45205800	1.10374200	1.82801200
C	-4.48770500	-0.42257200	-1.98520900
N	-2.68945000	-0.32003600	-0.56822500
C	2.07384600	1.19895500	3.44658700
H	2.12208000	3.39977400	3.56853100
C	1.24247400	0.33315300	2.62606400
C	-4.18209600	-1.70068500	-1.62214400
H	-5.27867000	-0.08632500	-2.64539100
C	-3.03981100	-1.62373600	-0.72662800
H	2.80396700	0.85885500	4.17214300
C	1.20033900	-1.06862100	2.70558200
H	-4.67337900	-2.61688800	-1.92860300
C	-2.40867500	-2.71356300	-0.11028800
C	0.31573000	-1.94212500	2.05256000
H	1.89699000	-1.52858600	3.40310000
C	-1.31620400	-2.68915000	0.77027200
H	-2.82693600	-3.69409300	-0.32648200
C	0.25177400	-3.38253300	2.24932900
N	-0.62992400	-1.57569800	1.14524400
C	-0.75640200	-3.84443400	1.45548500
H	0.89339500	-3.95091500	2.91280300
H	-1.10567400	-4.86462200	1.34548600
C	0.18993600	0.41103500	-1.07074800
C	1.21315300	1.52635800	-1.14859100
C	-0.25036600	0.18883900	-2.47364500
C	1.47543900	1.73593500	-2.65368800
H	2.13344900	1.29292100	-0.60320900
H	0.81487700	2.44188800	-0.70262200
O	0.46031500	1.00519500	-3.34864900
O	-1.04647200	-0.60031600	-2.94422200
H	1.40866800	2.78670300	-2.96118900
H	2.45254700	1.34542200	-2.96148200
C	1.48682400	-1.47623700	-1.13453100
H	0.58424100	-2.00885400	-1.40597500
H	1.67237500	-1.38395800	-0.07289700
C	2.51798200	-1.38235700	-2.04303100
H	2.29937000	-1.61034100	-3.08608200
C	3.88103400	-0.95710900	-1.77548500

C	4.81369900	-0.89600900	-2.83860300
C	4.35466300	-0.61178500	-0.48522400
C	6.13666800	-0.51618800	-2.63060300
H	4.47785300	-1.15501700	-3.84076400
C	5.67661200	-0.23035200	-0.28196800
H	3.67464100	-0.64201300	0.36101800
C	6.58191500	-0.17869400	-1.34906100
H	6.82426100	-0.48038300	-3.47342300
H	6.00597600	0.03219200	0.72118400
H	7.61386900	0.12106200	-1.18350300

TS-S9(*doublet*)

Fe	0.16223500	0.14063000	-0.14957500
N	-1.04700900	1.75380800	-0.08032700
N	-1.45397400	-1.02365600	-0.49907400
N	1.79178000	1.30305500	0.18660800
N	1.38407900	-1.47021400	-0.27697500
C	-0.64926200	3.04709900	0.10440400
C	-1.43634800	-2.36143700	-0.78887700
C	-2.40439800	1.78633500	-0.22248000
C	-2.76179500	-0.62856800	-0.57891700
C	1.78557200	2.66116900	0.34953000
C	1.00235500	-2.74803700	-0.58895800
C	3.09290200	0.90120000	0.32659200
C	2.74065900	-1.50875200	-0.08458200
C	-1.79595000	3.93267600	0.06706700
C	-2.78150500	-2.83299700	-1.03914900
C	-2.88652000	3.14866800	-0.13442900
C	-3.60510600	-1.75729000	-0.90231300
C	3.12939400	3.13782200	0.59362500
C	2.15368600	-3.62362200	-0.59358200
C	3.94161800	2.04388900	0.58357700
C	3.23256900	-2.85515000	-0.27330500
C	0.65714200	3.47541500	0.30754900
C	-0.30325700	-3.16791100	-0.82999000
C	3.54120900	-0.41240500	0.22113400
C	-3.21522900	0.67860600	-0.43816200
H	0.81123600	4.54129300	0.45321700
H	-0.45035700	-4.21825900	-1.06763700
H	4.60543100	-0.59046400	0.35125500
H	-4.28429100	0.84959700	-0.52706600
C	2.05648300	0.27772100	-3.02557500
H	2.73727400	0.96053600	-2.50572400
H	2.39136200	-0.74888600	-2.84179800
H	2.12450500	0.47608400	-4.10196100
C	0.00723400	-0.07551800	2.02232900
C	0.22383000	-1.47063300	2.61578700
C	-1.21827100	-1.96256200	2.80994100
H	-1.34952800	-2.61816900	3.67980200
H	-1.59156700	-2.48090200	1.92027000
H	0.72573400	-1.40628200	3.59610000
H	0.80694000	-2.15573400	1.99767100
S	0.32047900	0.52983500	-2.49568200
H	0.77972500	0.64638700	2.28054900
O	-2.00316500	-0.78175400	3.02683900

C	-1.28886300	0.33828300	2.60765600
O	-1.76999100	1.43937800	2.79024200
H	-3.92669300	3.44103200	-0.21212300
H	-1.74839200	5.00810900	0.18958900
H	3.39694900	4.17591000	0.75187600
H	5.01450100	1.99742700	0.72912200
H	4.27035300	-3.15307500	-0.18019400
H	2.12198600	-4.68438900	-0.81324800
H	-3.04101000	-3.85544100	-1.28739400
H	-4.68131100	-1.71042700	-1.01781300

S10(*doublet*)

Fe	0.05636500	0.14840100	-0.20748900
N	-1.08419900	1.82109800	-0.16832500
N	-1.59706000	-0.92736900	-0.64755400
N	1.72251400	1.22371300	0.22120300
N	1.20384900	-1.52087600	-0.28928800
C	-0.63863100	3.08568700	0.09822700
C	-1.64329200	-2.27504100	-0.87591900
C	-2.42152700	1.92695600	-0.42291100
C	-2.86785500	-0.46020900	-0.84578700
C	1.76474100	2.57312400	0.44440100
C	0.76342200	-2.78425800	-0.58111300
C	3.00849900	0.76970300	0.34265400
C	2.56237200	-1.61439800	-0.12485700
C	-1.73633200	4.02744900	0.01262000
C	-2.99271300	-2.67809900	-1.21304100
C	-2.84266200	3.30704400	-0.31615600
C	-3.75144400	-1.54957000	-1.19819200
C	3.12280000	2.98739600	0.72280400
C	1.87547500	-3.70882800	-0.59182600
C	3.89616800	1.86758200	0.65683400
C	2.99309700	-2.98196500	-0.30951800
C	0.67370000	3.43796300	0.40043100
C	-0.55776000	-3.14364900	-0.83353600
C	3.41047200	-0.55360900	0.18104500
C	-3.26047300	0.86839300	-0.74935600
H	0.86947100	4.48867400	0.59818100
H	-0.75422200	-4.19193500	-1.04227900
H	4.46869700	-0.77398300	0.29342300
H	-4.30756400	1.09509100	-0.92839700
C	2.07478100	0.28171400	-3.02291600
H	2.73706900	0.97090300	-2.48752900
H	2.40599400	-0.74187700	-2.81627100
H	2.17926800	0.46805500	-4.09853600
C	-0.24250800	0.03981400	1.92255800
C	0.72938800	-0.81332100	2.73751200
C	-0.05887600	-2.12075100	2.90073600
H	0.13049200	-2.63875300	3.84887900
H	0.13396100	-2.81535100	2.07582700
H	0.91058800	-0.36533100	3.72921600
H	1.70189400	-0.97839400	2.27121700
S	0.32091000	0.53235200	-2.55381800
H	-0.17091700	1.10940700	2.11335400
O	-1.44400900	-1.74291400	2.87595300
C	-1.57241000	-0.46798500	2.33179700

O	-2.67414200	0.04198800	2.28698100
H	-3.85660100	3.65637200	-0.46975100
H	-1.64917700	5.09431500	0.18121700
H	3.42696400	4.00629000	0.93198400
H	4.96614800	1.77580400	0.80214700
H	4.01910900	-3.32250000	-0.23372700
H	1.79404100	-4.77010600	-0.79522800
H	-3.29582700	-3.69478900	-1.43306800
H	-4.81056300	-1.44336900	-1.39952000

TS-S11(*doublet*)

Fe	0.16223500	0.14063000	-0.14957500
N	-1.04700900	1.75380800	-0.08032700
N	-1.45397400	-1.02365600	-0.49907400
N	1.79178000	1.30305500	0.18660800
N	1.38407900	-1.47021400	-0.27697500
C	-0.64926200	3.04709900	0.10440400
C	-1.43634800	-2.36143700	-0.78887700
C	-2.40439800	1.78633500	-0.22248000
C	-2.76179500	-0.62856800	-0.57891700
C	1.78557200	2.66116900	0.34953000
C	1.00235500	-2.74803700	-0.58895800
C	3.09290200	0.90120000	0.32659200
C	2.74065900	-1.50875200	-0.08458200
C	-1.79595000	3.93267600	0.06706700
C	-2.78150500	-2.83299700	-1.03914900
C	-2.88652000	3.14866800	-0.13442900
C	-3.60510600	-1.75729000	-0.90231300
C	3.12939400	3.13782200	0.59362500
C	2.15368600	-3.62362200	-0.59358200
C	3.94161800	2.04388900	0.58357700
C	3.23256900	-2.85515000	-0.27330500
C	0.65714200	3.47541500	0.30754900
C	-0.30325700	-3.16791100	-0.82999000
C	3.54120900	-0.41240500	0.22113400
C	-3.21522900	0.67860600	-0.43816200
H	0.81123600	4.54129300	0.45321700
H	-0.45035700	-4.21825900	-1.06763700
H	4.60543100	-0.59046400	0.35125500
H	-4.28429100	0.84959700	-0.52706600
C	2.05648300	0.27772100	-3.02557500
H	2.73727400	0.96053600	-2.50572400
H	2.39136200	-0.74888600	-2.84179800
H	2.12450500	0.47608400	-4.10196100
C	0.00723400	-0.07551800	2.02232900
C	0.22383000	-1.47063300	2.61578700
C	-1.21827100	-1.96256200	2.80994100
H	-1.34952800	-2.61816900	3.67980200
H	-1.59156700	-2.48090200	1.92027000
H	0.72573400	-1.40628200	3.59610000
H	0.80694000	-2.15573400	1.99767100
S	0.32047900	0.52983500	-2.49568200
H	0.77972500	0.64638700	2.28054900
O	-2.00316500	-0.78175400	3.02683900
C	-1.28886300	0.33828300	2.60765600
O	-1.76999100	1.43937800	2.79024200

H	-3.92669300	3.44103200	-0.21212300
H	-1.74839200	5.00810900	0.18958900
H	3.39694900	4.17591000	0.75187600
H	5.01450100	1.99742700	0.72912200
H	4.27035300	-3.15307500	-0.18019400
H	2.12198600	-4.68438900	-0.81324800
H	-3.04101000	-3.85544100	-1.28739400
H	-4.68131100	-1.71042700	-1.01781300

S12(*doublet*)

Fe	0.07461700	0.16205700	-0.32292600
N	-1.12721300	1.79386800	-0.25462900
N	-1.55519500	-0.99362600	-0.64782900
N	1.71400400	1.31227200	0.00906100
N	1.28061200	-1.46784900	-0.41484400
C	-0.72263800	3.07951100	-0.03851600
C	-1.56071800	-2.34528400	-0.84253300
C	-2.47264600	1.84046700	-0.46839500
C	-2.84450100	-0.57461800	-0.81478200
C	1.71380500	2.66638300	0.20324800
C	0.87745900	-2.75392800	-0.65301700
C	3.02128400	0.91126600	0.06582200
C	2.64814300	-1.50141000	-0.32680100
C	-1.85905300	3.97780000	-0.10763300
C	-2.90700300	-2.80547900	-1.11919400
C	-2.94600600	3.20695600	-0.38134400
C	-3.70333800	-1.70328600	-1.10717400
C	3.06721300	3.13883500	0.40036600
C	2.02467900	-3.63367300	-0.70310200
C	3.88035900	2.04893300	0.31110600
C	3.12514400	-2.85507600	-0.50268000
C	0.58838900	3.48835600	0.19383900
C	-0.43982600	-3.17036600	-0.83213000
C	3.46667800	-0.39886600	-0.09474600
C	-3.28086000	0.74221300	-0.73843600
H	0.75273700	4.55011600	0.35956300
H	-0.60380100	-4.23069700	-1.00612500
H	4.53778100	-0.57414000	-0.03704600
H	-4.34148600	0.92584900	-0.88595800
C	1.30410800	0.33347700	-2.94916800
H	2.10303600	1.03345100	-2.63543000
H	1.75169900	-0.67999700	-2.94172700
H	1.06896500	0.57027400	-4.00472500
C	-0.12505100	0.08784200	1.82542600
C	0.90823400	-0.71384900	2.62123600
C	0.16947700	-2.04035700	2.84790200
H	0.41963200	-2.53346600	3.79564700
H	0.34570900	-2.74590800	2.02808400
H	1.11821200	-0.23900200	3.59496700
H	1.86530100	-0.86208400	2.11762300
H	-0.07998400	1.16236100	2.00068900
O	0.15409000	0.43182800	-2.18423300
C	-1.41665800	-0.44664800	2.31017700
O	-2.53722100	0.02457200	2.30315900
O	-1.22539300	-1.70472000	2.88146400
H	3.34176500	4.17279100	0.57434500

H	4.95956500	2.00237300	0.39900400
H	4.16703800	-3.15235100	-0.47669700
H	1.97683300	-4.70253600	-0.87585900
H	-3.18206400	-3.83749600	-1.30245600
H	-4.77213000	-1.63880400	-1.27274700
H	-3.97767500	3.51296100	-0.50809400
H	-1.80847600	5.05152800	0.03075500

IX. NMR Spectra

7.3166
7.3133
7.2981
7.2952
7.2922
7.2833
7.2778
7.2757
7.2736
7.2658
7.2641
7.2601
7.2539
7.2479
7.2445
7.2429
7.2403
7.2378
7.2355
7.2317
7.2248
7.2226
7.2193
4.4696
4.4624
4.4471
4.4407
4.4229
4.4185
4.4166
4.4006
4.3985
4.3943
2.6675
2.6643
2.6468
2.6421
2.6398
2.6322
2.6260
2.6169
2.6101
2.6082
2.5854
2.3005
2.2933
2.2826
2.2753
2.2687
2.2615
2.2509
1.9467
1.9334
1.9273
1.9141
1.5549
1.5417
1.5327
1.5196
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.19 (m, 5H), 4.51 – 4.36 (m, 2H), 2.74 – 2.54 (m, 2H), 2.27 (ddd, *J* = 12.7, 7.2, 2.9 Hz, 1H), 1.93 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.54 (dd, *J* = 8.9, 5.3 Hz, 1H).
O
O
F (m)
7.27
E (m)
4.42
C (m)
2.63
A (ddd)
2.27
B (dd)
1.93
D (dd)
1.54
5.18
2.00
1.99
1.00
1.01
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

175.9660
135.3836
129.0249
128.2449
127.1882
65.6560
34.7631
32.0954
27.8264
17.3309
^{13}C NMR (101 MHz, $CDCl_3$) δ 175.97, 135.38, 129.02, 128.24, 127.19, 65.66, 34.76, 32.10, 27.83, 17.33.
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.05 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 4.40 (td, *J* = 9.0, 5.5 Hz, 1H), 4.26 (td, *J* = 8.9, 6.9 Hz, 1H), 3.80 (s, 3H), 2.71 (dd, *J* = 9.4, 7.1 Hz, 1H), 2.12 (ddd, *J* = 13.0, 8.9, 6.9 Hz, 1H), 1.88 (ddd, *J* = 13.0, 8.7, 5.5 Hz, 1H), 1.77 (dd, *J* = 9.4, 5.1 Hz, 1H), 1.40 (dd, *J* = 7.1, 5.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.66, 158.84, 129.31, 127.99, 114.18, 66.02, 55.44, 30.64, 27.29, 25.56, 18.52.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.17 (d, *J* = 8.3 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.46 (td, *J* = 9.0, 2.9 Hz, 1H), 4.40 (ddd, *J* = 9.8, 9.0, 7.3 Hz, 1H), 3.77 (s, 3H), 2.61 (dt, *J* = 12.1, 9.1 Hz, 2H), 2.25 (ddd, *J* = 12.7, 7.1, 2.8 Hz, 1H), 1.87 (dd, *J* = 7.6, 5.2 Hz, 1H), 1.51 (dd, *J* = 8.9, 5.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 176.15, 158.69, 130.04, 127.42, 113.70, 65.67, 55.34, 34.27, 32.05, 27.66, 17.47.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.22 – 7.15 (m, 1H), 6.74 (ddd, *J* = 8.3, 2.6, 0.9 Hz, 1H), 6.64 (dp, *J* = 7.7, 0.8 Hz, 1H), 6.62 – 6.57 (m, 1H), 4.34 (td, *J* = 8.9, 5.7 Hz, 1H), 4.21 (td, *J* = 8.9, 6.7 Hz, 1H), 3.74 (s, 3H), 2.66 (dd, *J* = 9.3, 7.1 Hz, 1H), 2.09 (ddd, *J* = 13.1, 8.9, 6.8 Hz, 1H), 1.86 (ddd, *J* = 13.0, 8.8, 5.7 Hz, 1H), 1.71 (dd, *J* = 9.3, 5.1 Hz, 1H), 1.38 (dd, *J* = 7.1, 5.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.38, 159.80, 137.67, 129.64, 120.28, 114.14, 112.24, 65.96, 55.25, 31.01, 27.44, 25.46, 18.47.

7.1535
7.1339
7.1142
6.7837
6.7820
6.7801
6.7782
6.7765
6.7650
6.7631
6.7611
6.7592
6.7575
6.7393
6.7334
6.7290
6.7075
6.7064
6.7012
6.7000
6.6871
6.6860
6.6808
6.6795
4.4178
4.4026
4.3954
4.3800
4.3725
4.3541
4.3497
4.3475
4.3319
4.3295
4.3252
4.3073
3.7214
2.5691
2.5615
2.5464
2.5377
2.5264
2.5147
2.2204
2.2133
2.2025
2.1957
2.1885
2.1813
2.1709
2.1635
1.8566
1.8433
1.8373
1.8241
1.4732
1.4599
1.4510
1.4379
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.13 (t, *J* = 7.9 Hz, 1H), 6.77 (ddd, *J* = 6.9, 1.5, 0.8 Hz, 1H), 6.73 (t, *J* = 2.1 Hz, 1H), 6.69 (dd, *J* = 8.2, 2.5 Hz, 1H), 4.43 – 4.30 (m, 2H), 3.72 (s, 3H), 2.63 – 2.48 (m, 2H), 2.19 (ddd, *J* = 12.9, 7.1, 2.9 Hz, 1H), 1.84 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.46 (dd, *J* = 8.8, 5.3 Hz, 1H).
H (ddd) 6.77
G (t) 7.13
I (t) 6.73
J (dd) 6.69
F (m) 4.35
E (s) 3.72
D (m) 2.54
B (dd) 1.84
A (ddd) 2.19
C (dd) 1.46
0.99
1.00
0.99
0.97
2.03
3.04
2.01
1.01
1.01
0.99
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

175.7899
159.3344
136.8911
129.0819
121.3065
114.8869
112.3428
65.5307
55.1701
34.6331
32.0231
27.7735
17.3251
^{13}C NMR (101 MHz, $CDCl_3$) δ 175.79, 159.33, 136.89, 129.08, 121.31, 114.89, 112.34, 65.53, 55.17, 34.63, 32.02, 27.77, 17.33.
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.14 (d, *J* = 7.9 Hz, 2H), 7.01 (d, *J* = 8.1 Hz, 2H), 4.40 (td, *J* = 8.9, 5.6 Hz, 1H), 4.26 (td, *J* = 8.9, 6.8 Hz, 1H), 2.72 (dd, *J* = 9.4, 7.1 Hz, 1H), 2.34 (s, 3H), 2.14 (ddd, *J* = 13.0, 8.9, 6.8 Hz, 1H), 1.89 (ddd, *J* = 12.9, 8.7, 5.5 Hz, 1H), 1.78 (dd, *J* = 9.3, 5.1 Hz, 1H), 1.43 (dd, *J* = 7.1, 5.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.63, 136.96, 132.99, 129.44, 128.09, 66.03, 30.94, 27.40, 25.54, 21.19, 18.47.

7.1478
7.1275
7.1031
7.0829
4.4880
4.4808
4.4657
4.4584
4.4431
4.4359
4.4179
4.4138
4.4115
4.3957
4.3934
4.3891
4.3711
2.6569
2.6553
2.6327
2.6243
2.6132
2.6097
2.6025
2.6007
2.5917
2.5783
2.5766
2.3017
2.2520
2.2448
2.2342
2.2270
1.9156
1.9024
1.8963
1.8832
1.5286
1.5153
1.5064
1.4933
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 (q, *J* = 8.1 Hz, 4H), 4.49 – 4.37 (m, 2H), 2.69 – 2.54 (m, 2H), 2.30 (s, 3H), 2.24 (dd, *J* = 7.1, 2.9 Hz, 1H), 1.90 (dd, *J* = 7.7, 5.2 Hz, 1H), 1.51 (dd, *J* = 8.9, 5.3 Hz, 1H).
O
O
G (q)
7.12
F (m)
4.42
E (m)
2.61
C (dd)
2.24
D (s)
2.30
A (dd)
1.90
B (dd)
1.51
3.99
2.03
2.02
3.00
1.01
1.01
1.01
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

176.0942
136.7884
132.3263
129.0057
128.8828
65.6558
34.5674
32.1154
27.7306
21.2679
17.3444
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.09, 136.79, 132.33, 129.01, 128.88, 65.66, 34.57, 32.12, 27.73, 21.27, 17.34.
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 (d, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 8.1 Hz, 2H), 4.41 (td, *J* = 9.0, 5.8 Hz, 1H), 4.28 (td, *J* = 8.9, 6.5 Hz, 1H), 2.72 (dd, *J* = 9.3, 7.1 Hz, 1H), 2.14 (ddd, *J* = 13.1, 8.9, 6.5 Hz, 1H), 1.88 (ddd, *J* = 13.0, 8.8, 5.8 Hz, 1H), 1.80 (dd, *J* = 9.3, 5.2 Hz, 1H), 1.42 (dd, *J* = 7.1, 5.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.19, 134.71, 133.12, 129.50, 128.96, 65.98, 30.34, 27.61, 25.49, 18.70.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 (d, *J* = 8.5 Hz, 2H), 7.18 (d, *J* = 8.3 Hz, 2H), 4.47 (td, *J* = 9.0, 3.0 Hz, 1H), 4.40 (ddd, *J* = 9.6, 9.0, 7.4 Hz, 1H), 2.68 – 2.54 (m, 2H), 2.28 (ddd, *J* = 12.7, 7.3, 2.9 Hz, 1H), 1.89 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.55 (dd, *J* = 8.9, 5.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.85, 133.89, 133.00, 130.37, 128.41, 65.69, 33.93, 31.91, 27.92, 17.61.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.4 Hz, 2H), 7.00 (d, *J* = 8.5 Hz, 2H), 4.41 (td, *J* = 9.0, 5.8 Hz, 1H), 4.28 (td, *J* = 8.9, 6.6 Hz, 1H), 2.77 – 2.63 (m, 1H), 2.14 (ddd, *J* = 13.1, 8.9, 6.5 Hz, 1H), 1.88 (ddd, *J* = 13.2, 8.8, 5.8 Hz, 1H), 1.80 (dd, *J* = 9.3, 5.2 Hz, 1H), 1.42 (dd, *J* = 7.1, 5.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.15, 135.25, 131.90, 129.85, 121.17, 65.98, 30.40, 27.61, 25.48, 18.66.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 4.47 (td, *J* = 9.0, 3.0 Hz, 1H), 4.40 (ddd, *J* = 9.6, 9.0, 7.4 Hz, 1H), 2.66 – 2.54 (m, 2H), 2.28 (ddd, *J* = 13.0, 7.5, 3.2 Hz, 1H), 1.88 (dd, *J* = 7.7, 5.4 Hz, 1H), 1.55 (dd, *J* = 8.8, 5.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.84, 134.43, 131.33, 130.73, 121.14, 65.69, 33.97, 31.89, 27.91, 17.56.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 7.9 Hz, 2H), 7.24 (d, *J* = 8.7 Hz, 2H), 4.43 (td, *J* = 9.0, 5.9 Hz, 1H), 4.29 (td, *J* = 9.0, 6.4 Hz, 1H), 2.80 (dd, *J* = 9.3, 7.1 Hz, 1H), 2.17 (ddd, *J* = 13.1, 8.9, 6.4 Hz, 1H), 1.94 – 1.82 (m, 2H), 1.51 (dd, *J* = 7.1, 5.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 178.94, 140.47, 129.54 (130.02, 129.70, 129.37, 129.05, q, *J* = 32.5 Hz), 128.45, 125.73 (125.79, 125.75, 125.71, 125.67, q, *J* =3.8 Hz), 124.16 (128.21, 125.51, 122.81, 120.11, q, *J* = 271.8 Hz), 65.98, 30.48, 28.00, 25.46, 18.91.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.1 Hz, 2H), 7.37 (d, *J* = 8.6 Hz, 2H), 4.49 (td, *J* = 9.0, 3.1 Hz, 1H), 4.42 (td, *J* = 9.3, 7.4 Hz, 1H), 2.74 – 2.57 (m, 2H), 2.32 (ddd, *J* = 12.8, 7.3, 3.1 Hz, 1H), 1.96 (dd, *J* = 7.7, 5.4 Hz, 1H), 1.61 (dd, *J* = 8.8, 5.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.69, 139.45, 129.39, 129.33 (129.81, 129.49, 129.16, 128.84, q, *J* = 32.5 Hz), 125.19 (125.24, 125.21, 125.17, 125.13, q, *J* = 3.8 Hz), 124.29 (128.34, 125.64, 122.94, 120.22, q, *J* = 271.9 Hz), 65.73, 34.06, 31.89, 28.23, 17.69.

7.2845 7.2833 7.2668 7.2642 7.2628 7.2603 7.2578 7.1434 7.1409 7.1250 7.1220 7.1061 7.1031 7.1007 7.0982 7.0900 7.0884 7.0844 7.0828 7.0807 7.0779 7.0760 7.0721 7.0696 7.0656 7.0553 7.0521 4.4176 4.4168 4.4053 4.4043 4.3953 4.3945 4.3829 4.3820 4.3671 4.3483 4.3457 4.3270 4.3240 4.3053 2.7840 2.7654 2.7623 2.7429 2.1664 2.1626 2.1525 2.1339 2.1299 2.1114 1.8314 1.8188 1.7955 1.7862 1.4679 1.4552 1.4498 1.4373

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.23 (m, 1H), 7.12 (td, *J* = 7.5, 1.1 Hz, 1H), 7.10 – 7.02 (m, 2H), 4.41 (dtd, *J* = 8.9, 4.9, 0.3 Hz, 1H), 4.34 (td, *J* = 8.6, 7.5 Hz, 1H), 2.84 – 2.70 (m, 1H), 2.15 (ddd, *J* = 13.0, 9.0, 7.4 Hz, 1H), 1.84 – 1.74 (m, 2H), 1.45 (dd, *J* = 7.2, 5.0 Hz, 1H).

179.3232 163.7235 161.2661 129.4130 129.3765 129.2243 129.1434 124.4045 124.3681 123.8005 123.6554 115.7259 115.5131 66.1518 26.4883 25.8949 25.5154 25.4792 17.4338 17.4189

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.32, 162.49 (163.72, 161.27, d, *J* = 248.2 Hz), 129.39 (129.41, 129.38, d, *J* = 3.7 Hz), 129.18 (129.22, 129.14, d, *J* = 8.2 Hz), 124.39 (124.40, 124.37, d, *J* = 3.7 Hz), 123.73 (123.80, 123.66, d, *J* = 14.7 Hz), 115.62 (115.73, 115.51, d, *J* = 21.5 Hz), 66.15, 26.49, 25.89, 25.50 (25.52, 25.48, d, *J* = 3.7 Hz), 17.43 (17.43, 17.42, d, *J* = 1.5 Hz).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 – 7.17 (m, 2H), 7.09 (td, *J* = 7.5, 1.1 Hz, 1H), 6.99 (ddd, *J* = 9.6, 8.3, 1.2 Hz, 1H), 4.52 – 4.44 (m, 2H), 2.68 – 2.54 (m, 2H), 2.33 (ddd, *J* = 12.7, 6.3, 4.0 Hz, 1H), 1.86 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.54 (dd, *J* = 8.7, 5.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 176.26, 162.33 (163.54, 161.11, d, J = 245.9 Hz), 130.43 (130.45, 130.41, d, J = 3.7 Hz), 128.97 (129.01, 128.93, d, J = 8.3 Hz), 123.90 (123.92, 123.88, d, J = 3.5 Hz), 123.15 (123.22, 123.07, d, J = 14.8 Hz), 114.94 (115.04, 114.83, d, J = 21.4 Hz), 65.92, 31.56, 28.11 (28.13, 28.09, d, J = 3.8 Hz), 26.95, 16.51.

7.8421
7.8303
7.8266
7.8199
7.8090
7.8032
7.7859
7.5710
7.5696
7.5143
7.5015
7.4970
7.4921
7.4849
7.4777
7.4727
7.4684
7.2746
7.2701
7.2535
7.2490
4.4331
4.4193
4.4107
4.3969
4.3884
4.3745
4.2927
4.2757
4.2706
4.2536
4.2484
4.2313
2.9446
2.9266
2.9216
2.9036
2.2113
2.1944
2.1889
2.1785
2.1720
2.1615
2.1563
2.1393
1.9226
1.9087
1.9028
1.9006
1.8899
1.8867
1.8797
1.8760
1.8669
1.8542
1.6417
1.6288
1.6238
1.6109
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.76 (m, 3H), 7.60 – 7.55 (m, 1H), 7.53 – 7.44 (m, 2H), 7.26 (dd, *J* = 8.4, 1.8 Hz, 1H), 4.40 (td, *J* = 9.0, 5.5 Hz, 1H), 4.26 (td, *J* = 8.9, 6.8 Hz, 1H), 2.92 (dd, *J* = 9.2, 7.2 Hz, 1H), 2.18 (ddd, *J* = 13.1, 8.9, 6.8 Hz, 1H), 1.95 – 1.82 (m, 2H), 1.63 (dd, *J* = 7.2, 5.2 Hz, 1H).
H (m) 7.49
J (m) 7.82
G (dd) 7.26
I (m) 7.57
F (td) 4.26
E (td) 4.40
A (dd) 2.92
C (m) 1.89
B (ddd) 2.18
D (dd) 1.63
3.05
1.00
2.02
1.59
1.00
1.00
0.96
1.00
2.00
1.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
179.4823
133.6982
133.4690
132.6450
128.4745
127.8154
127.7028
126.6991
126.5802
126.5022
126.1060
66.0708
31.3611
27.7993
25.6080
18.5290
^{13}C NMR (101 MHz, $CDCl_3$) δ 179.48, 133.70, 133.47, 132.64, 128.47, 127.82, 127.70, 126.70, 126.58, 126.50, 126.11, 66.07, 31.36, 27.80, 25.61, 18.53.
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

7.8034
7.8009
7.7957
7.7939
7.7912
7.7865
7.7844
7.7795
7.7770
7.7750
7.7719
7.7701
7.7506
7.7156
7.7132
7.7109
7.7086
7.4590
7.4460
7.4414
7.4358
7.4290
7.4221
7.4166
7.4123
7.3801
7.3757
7.3588
7.3544
4.4995
4.4908
4.4768
4.4731
4.4683
4.4665
4.4503
4.4491
2.8201
2.7994
2.7787
2.6827
2.6747
2.6510
2.6279
2.3657
2.3576
2.3485
2.3403
2.3340
2.3257
2.3168
2.0863
2.0731
2.0669
2.0538
1.6389
1.6257
1.6169
1.6035
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 – 7.74 (m, 3H), 7.71 (dd, *J* = 1.9, 1.0 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.37 (dd, *J* = 8.5, 1.8 Hz, 1H), 4.52 – 4.42 (m, 2H), 2.80 (t, *J* = 8.3 Hz, 1H), 2.67 (dt, *J* = 12.5, 9.3 Hz, 1H), 2.34 (ddd, *J* = 12.7, 6.9, 3.3 Hz, 1H), 2.07 (dd, *J* = 7.7, 5.3 Hz, 1H), 1.62 (dd, *J* = 8.8, 5.3 Hz, 1H).
H (m) 7.43
J (m) 7.78
G (dd) 7.37
I (dd) 7.71
F (m) 4.47
E (dt) 2.67
B (dd) 2.07
D (t) 2.80
A (ddd) 2.34
C (dd) 1.62
3.04
0.98
2.05
0.99
2.02
0.99
1.03
1.01
0.99
1.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
175.9662
133.3053
132.8852
132.7170
127.9090
127.8671
127.8513
127.7508
127.1389
126.1290
125.8071
65.7079
34.9676
32.1510
17.6013
^{13}C NMR (101 MHz, CDCl$_3$) δ 175.97, 133.31, 132.89, 132.72, 127.91, 127.87, 127.85, 127.75, 127.14, 126.13, 125.81, 65.71, 34.97, 32.15, 17.60.
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

7.2963
7.2915
7.2798
7.2767
7.2741
7.2600
7.2088
7.2054
7.2028
7.1934
7.1902
7.1857
7.1715
4.3904
4.3817
4.3681
4.3594
4.3457
4.3370
4.2126
4.1913
4.1702
4.1486
2.6989
2.6808
2.6714
2.6631
2.6530
2.6349
2.6190
2.4266
2.4042
2.3955
2.3815
2.3729
2.3504
2.0294
2.0218
2.0101
2.0005
1.9927
1.9900
1.9848
1.9789
1.9730
1.9653
1.9575
1.9466
1.9286
1.3227
1.3038
1.2852
1.1841
1.1726
1.1664
1.1557
1.1450
1.1346
1.1232
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.26 (m, 2H), 7.23 – 7.13 (m, 3H), 4.36 (td, *J* = 9.0, 3.5 Hz, 1H), 4.18 (q, *J* = 8.6 Hz, 1H), 2.79 – 2.54 (m, 2H), 2.39 (dt, *J* = 12.5, 9.0 Hz, 1H), 2.09 – 1.83 (m, 3H), 1.30 (p, *J* = 7.4 Hz, 1H), 1.23 – 1.10 (m, 2H).
I (m) 7.27
H (m) 7.19
B (q) 4.18
A (td) 4.36
G (m) 2.67
F (dt) 2.39
E (m) 1.98
D (m) 1.16
C (p) 1.30
2.03
2.99
1.01
1.01
2.00
1.00
2.99
1.06
2.02
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

178.5149
141.5955
128.7133
128.4811
126.0238
65.7884
35.8216
31.8728
30.3595
28.5593
24.1842
20.2240
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.51, 141.60, 128.71, 128.48, 126.02, 65.79, 35.82, 31.87, 30.36, 28.56, 24.18, 20.22.
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

f2 (ppm)
f1 (ppm)

f2 (ppm)
f1 (ppm)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.26 (m, 2H), 7.24 – 7.15 (m, 3H), 4.37 (td, *J* = 8.6, 6.7 Hz, 1H), 4.20 (td, *J* = 8.7, 6.4 Hz, 1H), 2.83 – 2.68 (m, 2H), 2.17 – 2.05 (m, 2H), 1.74 – 1.59 (m, 2H), 1.51 (dq, *J* = 9.1, 6.8 Hz, 1H), 1.40 (dd, *J* = 9.1, 4.2 Hz, 1H), 0.60 (dd, *J* = 6.7, 4.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 180.22, 141.31, 128.51, 128.48, 126.13, 65.92, 35.64, 31.89, 25.59, 25.52, 24.17, 21.13.

f2 (ppm)
f1 (ppm)

f2 (ppm)
f1 (ppm)

7.5719 7.5684 7.5651 7.5629 7.5602 7.5587 7.5553 7.5512 7.5479 7.5445 7.5422 7.3560 7.3541 7.3503 7.3472 7.3448 7.3417 7.3392 7.3378 7.3341 7.3304 4.2708 4.2666 4.2631 4.2516 4.2482 4.2443 4.2286 4.2260 4.2219 4.2096 4.2054 4.2033 3.8798 3.8643 3.8582 3.8427 2.6993 2.6965 2.6941 2.6819 2.6800 2.6776 2.6748 2.6654 2.6628 2.6602 2.6583 2.6464 2.6437 2.6412 2.3128 2.2976 2.2942 2.2825 2.2791 2.2638 2.2604 2.2452

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.50 (m, 2H), 7.39 – 7.29 (m, 3H), 4.31 – 4.17 (m, 2H), 3.86 (dd, *J* = 8.6, 6.2 Hz, 1H), 2.67 (dddd, *J* = 13.4, 8.7, 7.7, 6.6 Hz, 1H), 2.27 (ddt, *J* = 13.5, 7.4, 6.1 Hz, 1H).

175.1007 133.7312 131.8099 129.4032 128.8644 66.6226 44.5381 30.1008

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.10, 133.73, 131.81, 129.40, 128.86, 66.62, 44.54, 30.10.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 – 7.21 (m, 1H), 7.12 (dt, *J* = 7.4, 1.6 Hz, 2H), 6.87 (ddd, *J* = 8.4, 2.3, 1.3 Hz, 1H), 4.31 – 4.20 (m, 2H), 3.88 (dd, *J* = 8.7, 6.4 Hz, 1H), 3.80 (s, 3H), 2.68 (dddd, *J* = 13.5, 8.7, 7.5, 6.6 Hz, 1H), 2.28 (ddt, *J* = 13.6, 7.4, 6.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.12, 160.00, 133.04, 130.17, 125.53, 118.46, 114.82, 66.65, 55.51, 44.53, 30.17.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (dd, *J* = 8.9, 5.3 Hz, 2H), 7.05 (dd, *J* = 8.9, 8.5 Hz, 2H), 4.31 – 4.17 (m, 2H), 3.77 (dd, *J* = 8.7, 6.2 Hz, 1H), 2.66 (dddd, *J* = 13.5, 8.7, 7.7, 6.6 Hz, 1H), 2.25 (ddt, *J* = 13.5, 7.4, 6.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.80, 163.41 (164.66, 162.17, d, *J* = 150.8 Hz), 136.72 (136.76, 136.67, d, *J* = 8.5 Hz), 126.49 (126.51, 126.48, d, *J* = 3.6 Hz), 116.49 (116.60, 116.39, d, *J* = 22.1 Hz), 66.43, 44.82 (44.83, 44.81, d, *J* = 1.4 Hz), 29.73.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 8.6 Hz, 2H), 7.31 (d, *J* = 8.5 Hz, 2H), 4.27 (t, *J* = 6.9 Hz, 2H), 3.82 (dd, *J* = 8.7, 6.3 Hz, 1H), 2.74 – 2.62 (m, 1H), 2.25 (td, *J* = 13.4, 6.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.83, 135.31, 135.12, 130.26, 129.59, 66.59, 44.55, 29.93.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.36 (m, 4H), 4.28 (td, *J* = 7.0, 1.0 Hz, 2H), 3.83 (dd, *J* = 8.7, 6.4 Hz, 1H), 2.68 (ddtd, *J* = 14.1, 8.7, 7.0, 0.6 Hz, 1H), 2.25 (dqd, *J* = 13.4, 6.7, 1.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.81, 135.20, 132.54, 130.98, 123.40, 66.60, 44.43, 29.95.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 4.27 – 4.15 (m, 2H), 3.78 (dd, *J* = 8.7, 6.0 Hz, 1H), 2.64 (dddd, *J* = 13.5, 8.7, 7.8, 6.7 Hz, 1H), 2.35 (s, 3H), 2.31 – 2.21 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.19, 139.44, 134.52, 130.22, 127.85, 66.62, 44.82, 29.99, 21.38.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 4.28 – 4.14 (m, 2H), 3.80 (dd, *J* = 8.7, 6.1 Hz, 1H), 2.90 (hept, *J* = 7.0 Hz, 1H), 2.65 (dddd, *J* = 13.5, 8.7, 7.7, 6.6 Hz, 1H), 2.27 (ddt, *J* = 13.5, 7.4, 6.0 Hz, 1H), 1.24 (d, *J* = 7.0 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.25, 150.17, 134.42, 128.26, 127.60, 66.61, 44.80, 33.97, 30.10, 23.95.

7.6445
7.6237
7.5915
7.5708
4.4070
4.3911
4.3884
4.3841
4.3722
4.3681
4.3655
4.3625
4.3493
4.3472
4.3437
4.3396
4.3284
4.3243
4.3208
4.3056
4.0003
3.9841
3.9786
3.9624
2.7987
2.7826
2.7800
2.7771
2.7643
2.7610
2.7583
2.7487
2.7460
2.7427
2.7300
2.7271
2.7244
2.7084
2.3347
2.3191
2.3161
2.3032
2.3005
2.2846
2.2821
2.2693
2.2662
2.2505
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 8.3 Hz, 2H), 4.36 (qdd, *J* = 9.1, 7.5, 6.2 Hz, 2H), 3.98 (dd, *J* = 8.7, 6.5 Hz, 1H), 2.75 (dddd, *J* = 13.7, 8.7, 7.5, 6.4 Hz, 1H), 2.29 (ddt, *J* = 13.7, 7.5, 6.3 Hz, 1H).
F (d) 7.58
E (d) 7.63
D (qdd) 4.36
A (dd) 3.98
B (dddd) 2.75
C (ddt) 2.29
2.00
1.98
2.07
0.99
1.05
1.03
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

174.4848
137.5082
131.6777
130.5066
130.1812
129.8553
129.5300
127.9037
126.0927
126.0558
126.0184
125.9809
125.1991
122.4948
119.7912
66.5313
43.4813
29.9833
^{13}C NMR (101 MHz, $CDCl_3$) δ 174.48, 137.51, 131.68, 130.02 (130.51, 130.18, 129.86, 129.53, q, *J* = 32.3 Hz), 126.04 (126.09, 126.06, 126.02, 125.98, q, *J* = 3.8 Hz), 123.85 (127.90, 125.20, 122.49, 119.79, q, *J* = 273.1 Hz), 66.53, 43.48, 29.98.
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.15 (d, *J* = 2.1 Hz, 1H), 6.85 (d, *J* = 8.3 Hz, 1H), 4.24 (ddd, *J* = 8.9, 7.8, 5.8 Hz, 1H), 4.15 (ddd, *J* = 8.9, 7.6, 6.5 Hz, 1H), 3.90 (s, 6H), 3.75 (dd, *J* = 8.8, 6.2 Hz, 1H), 2.66 (dddd, *J* = 13.4, 8.7, 7.8, 6.5 Hz, 1H), 2.28 (ddt, *J* = 13.5, 7.6, 6.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.41, 150.38, 149.20, 128.46, 121.81, 117.98, 111.50, 66.57, 56.16, 56.03, 45.26, 29.73.

8.0648
8.0604
7.8386
7.8328
7.8301
7.8284
7.8238
7.8212
7.8132
7.8062
7.8015
7.7988
7.7954
7.6089
7.6042
7.5875
7.5827
7.5297
7.5213
7.5144
7.5124
7.5067
7.5048
7.4976
4.2764
4.2749
4.2720
4.2607
4.2583
4.2557
4.2540
4.2421
4.2405
4.2373
3.9827
3.9669
3.9611
3.9453
2.7160
2.7131
2.7009
2.6991
2.6966
2.6944
2.6842
2.6823
2.6795
2.6776
2.6628
2.6605
2.3387
2.3368
2.3230
2.3208
2.3189
2.3051
2.3031
2.2871
2.2853
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 1.7 Hz, 1H), 7.85 – 7.78 (m, 3H), 7.60 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.55 – 7.47 (m, 2H), 4.30 – 4.21 (m, 2H), 3.96 (dd, *J* = 8.7, 6.3 Hz, 1H), 2.74 – 2.64 (m, 1H), 2.36 – 2.27 (m, 1H).
S
O
O
F (m) 7.51
H (d) 8.06
E (dd) 7.60
G (m) 7.81
D (m) 4.26
C (dd) 3.96
A (m) 2.69
B (m) 2.31
1.00
3.03
1.00
2.00
2.04
0.98
1.02
1.03
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

175.0958
133.6674
133.1641
133.0652
130.2440
129.1318
129.0819
127.8553
127.0170
126.8860
66.6677
44.5848
30.1120
^{13}C NMR (101 MHz, $CDCl_3$) δ 175.10, 133.67, 133.16, 133.07, 130.24, 129.13, 129.08, 127.86, 127.02, 126.89, 66.67, 44.58, 30.11.
S
O
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

XIII. References

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