

Supporting Information

Iron Porphyrin Catalyzed Bromination of Unactivated C-H Bonds: Inhibition of Oxygen Rebound by Redox-Inactive Metal Ions

Yiran Xu,^{a,‡} Peng Wu,^{b,‡} Duanfeng Xie,^a Yue Cui,^a Yuheng Zhang,^a Binju Wang,^{c,*}
Mian Guo^{a,*}

^a College of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, PR China

^b State Key Laboratory of High-Efficiency Utilization of Coal and Green Chemical Engineering, School of Chemistry and Chemical Engineering, Ningxia University, Yinchuan 750021, P. R. China

^c Key Laboratory of Physical Chemistry of Solid Surfaces and Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China

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General Information

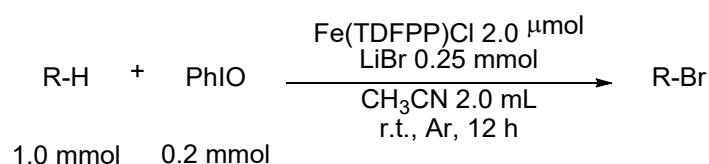
Materials

Commercially available chemicals were used without further purification unless otherwise noted. Dichloromethane (analytical pure grade) was distilled from calcium hydride and chloroform (analytical pure grade) was distilled from anhydrous potassium carbonate before use.^{S1} Iodosylbenzene (PhIO) was synthesized according to a literature method from iodobenzene diacetate purchased from Bide Pharmatech Ltd.^{S2} Metal bromides, *n*-Bu₄N⁺OTf⁻, *cis*- and *trans*- decalin, *n*-dodecane were purchased from Shanghai Titan Co. Ltd. *Meso*-tetramesistylporphyrinatoiron(III) chloride [Fe(TMP)Cl], *meso*-tetrakis(2,6-difluorophenyl)porphyrinatoiron(III) chloride [Fe(TDFPP)Cl], *meso*-tetrakis(2-fluorophenyl)porphyrinatoiron(III) chloride [Fe(TMFP)Cl], *meso*-tetrakis(pentafluorophenyl)porphyrinatoiron(III) chloride [Fe(TPFPP)Cl], and *meso*-tetrakis(2,6-dichlorophenyl)porphyrinatoiron(III) chloride [Fe(TDCPP)Cl] were synthesized according to previously reported procedures.^{S3}

Instrumentation

Gas chromatography/mass spectrometry (GC/MS) was recorded on an Agilent 8890 GC system with 5977 EI MSD Bundle equipped with a capillary column (J&W, HP-5ms, 30 m × 0.25 mm × 0.25 μm). The products of the iron-porphyrin catalyzed bromination reaction were confirmed by comparing the retention time and the mass spectrometry of standard compounds. UV-vis spectrums were recorded on an Agilent Cary 60 UV-vis spectrophotometer equipped with a UNISOKU USP-203 cryostat system. Electrospray ionization mass spectrometry (ESI-MS) was collected on a Thermo Fisher Scientific LTQ Orbitrap Elite Mass Spectrometer by infusing samples directly into the source using a sample syringe. The spray voltage was set at 2.5 kV and the capillary temperature at 120 °C. Cyclic voltammetry was recorded on a CHI760E electrochemical workstation at room temperature. *N*-Bu₄N⁺OTf⁻ (195.0 mg, 0.5 mmol) was used as the supporting electrolyte and CH₃CN was used as solvent. The working electrode was a glassy carbon, the counter electrode was a platinum wire. Ag wire was used as pseudo-reference electrode and ferrocene was used as internal standard. Atomic absorption spectroscopy was recorded on an AnalytikJena contrAA700 at 670 nm.

Procedure A: Standard procedure of iron porphyrin catalyzed bromination of hydrocarbons



In a glove box filled with argon, [Fe(TDFPP)Cl] (1.7 mg, 2.0 μ mol), PhIO (44.0 mg, 0.2 mmol), and LiBr (21.7 mg, 0.25 mmol) were added to a 10 ml sealed vial equipped with a magnetic stirrer. Then substrate (1.0 mmol) and CH₃CN (2.0 mL, HPLC grade) were added to the vial via syringe. The solution turned red and the insoluble PhIO disappeared gradually. The reactions were run at room temperature and completion of the reaction was indicated by the disappearance of the red color of high-valent iron-oxo porphyrin intermediate after 12 h. Once the reaction was completed, the reaction was added with 10 mL of *n*-dodecane and 5 mL of water were added to the reaction residue and the reaction solution was retracted with 2 mL of *n*-hexane. And the organic layer was then analyzed by GC/MS. The assignment of the product was based on the comparison with the GC retention time and the MS spectra of the corresponding authentic samples. The TON of brominated products and side products was based on the added iron porphyrin and determined with *n*-dodecane as internal standard.

Procedure B: Competitive kinetic isotope experiments.

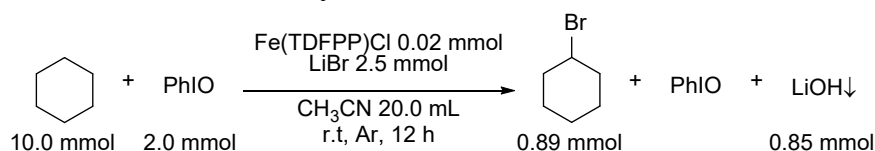
Following the procedure A, the substrate was replaced by the mixture of 0.5 mmol of cyclohexane and 0.5 mmol of cyclohexane-*d*₁₂ in the reaction of cyclohexane, or the mixture of 0.5 mmol of toluene and 0.5 mmol of toluene-*d*₈ in the reaction of toluene. Then the mixture was extracted and analyzed by GC-MS following procedure A.

Procedure C: Generation and characterization of Li⁺-bound iron(IV)-oxo porphyrin species

Following procedure A and using cyclohexane as substrate, the reaction mixture was immediately filtrated after the reaction started for 1 min to remove unreacted PhIO and 1.0 mM solution of Li⁺-bound iron(IV)-oxo porphyrin species in CH₃CN was obtained as mother liquor. The ESI-MS sample was prepared by diluting 50 μ L of mother liquor to 1 mL solution with CH₃CN at 263 K and stored at 195 K. UV-vis spectrum of 0.025 mM and 0.005 mM Li⁺-bound iron(IV)-oxo porphyrin species was recorded in a 10 mm cuvette at 263 K.

Non-Li⁺-bound compound II was prepared according to previously reported procedure and the UV-vis spectra was recorded in a 10 mm cuvette at 263 K.^{S4}

Procedure D: Quantitative analysis of LiOH



In a glove box filled with argon, [Fe(TDFPP)Cl] (17 mg, 0.02 mmol), PhIO (440 mg, 2.0 mmol), LiBr (215 mg, 2.5 mmol) was added to a 50 ml flask and sealed with septum. Then cyclohexane (1.06 mL, 10.0 mmol) and CH₃CN (20.0 mL, HPLC grade) were added to the flask via syringe and stirred under argon for 12 h. Once the reaction was completed, 0.1 mL dodecane was added as internal standard and the supernatant was analyzed by GC-MS. Then

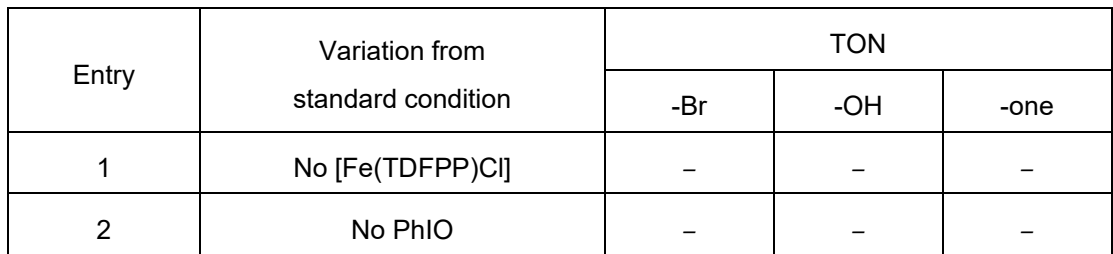
the mixture was filtered through Celite and washed with 20 mL CH₃CN and 10 mL CH₂Cl₂ successively. The residue was washed with 20 mL deionized water twice and the filtrate was diluted to 100 mL. 1 mL of the dilute filtrate was taken out and further diluted to 100 mL for AAS analysis and the rest filtrate was titrated by 0.1 M of HCl with methyl orange as indicator to determine the amount of OH⁻, which was formed during the bromination of cyclohexane. GC-MS result showed 0.89 mmol of C₆H₁₁Br was generated. The AAS analysis showed the amount of Li in the residue was 1.10 mmol and the titration experiment showed the amount of OH⁻ was 0.85 mmol.

Procedure E: Cyclic voltammetry

In an oven dried two neck round-bottom bottle equipped with working electrode, counter electrode and reference electrode. LiBr (8.7 mg, 0.1 mmol) and supporting electrolyte was added to the bottle. Then the bottle was purged and charged with argon three times and added anhydrous CH₃CN (5.0 mL). CV was recorded under room temperature. The scan range was between -0.5 V to 1.5 V (positive) and scan rate was 0.1 V/s. *N*-Bu₄N⁺Br⁻ was tested with the same procedure.

DFT Calculations

All calculations were performed with the Gaussian 16 software package.^{S5} The geometries of investigated species were optimized in conjunction with the SMD^{S6} continuum solvation model at the B3LYP^{S7}/def2-SVP^{S8} level of theory, in which the solvent of CH₃CN was used. Gibbs energy corrections were obtained at 312K. The electronic energies were further refined with the larger basis set def2-TZVP^{S8} for all atoms.



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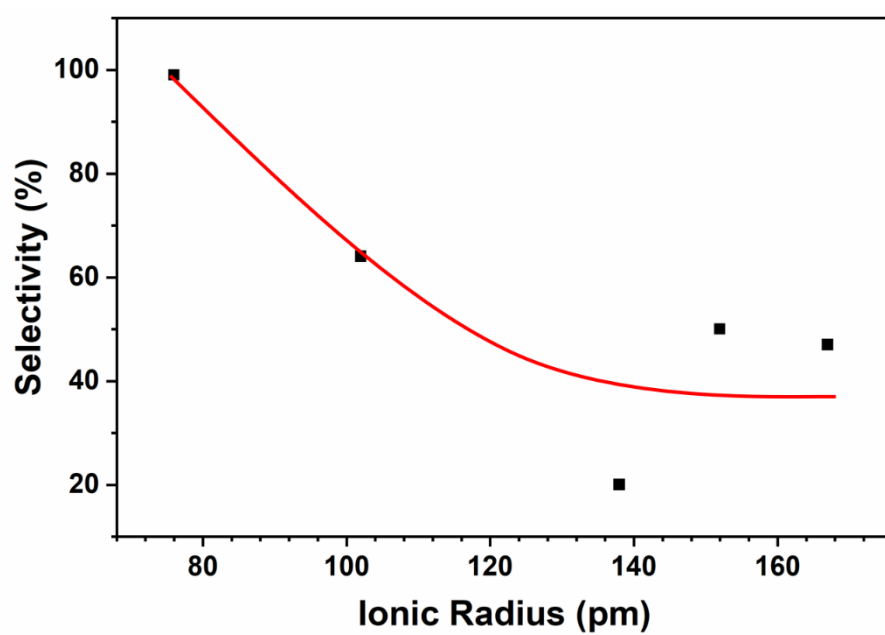


Figure S1. Correlation of the selectivity of iron porphyrin catalyzed bromination and the ionic radii of metal ions.

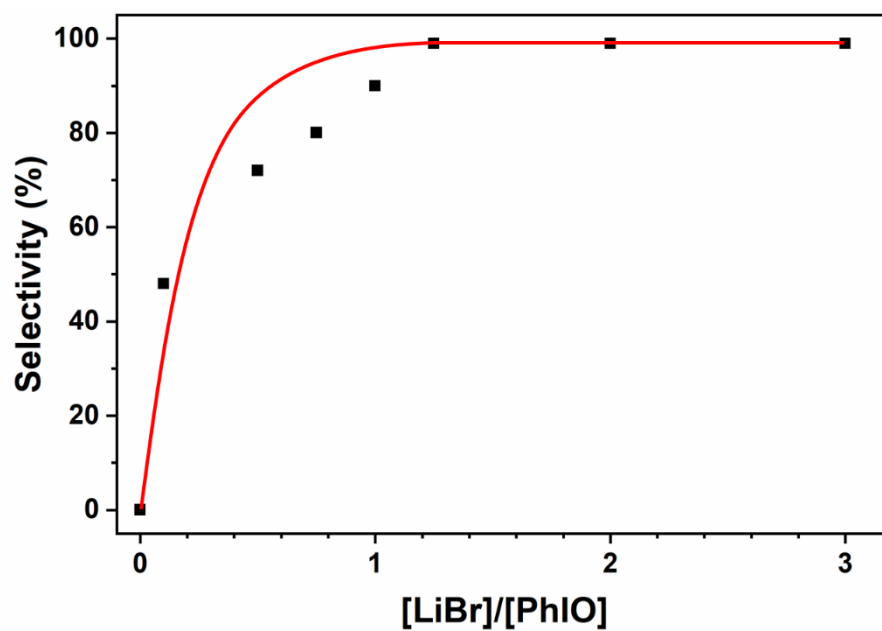


Figure S2. Correlation of the selectivity of iron porphyrin catalyzed bromination and the loading of LiBr.

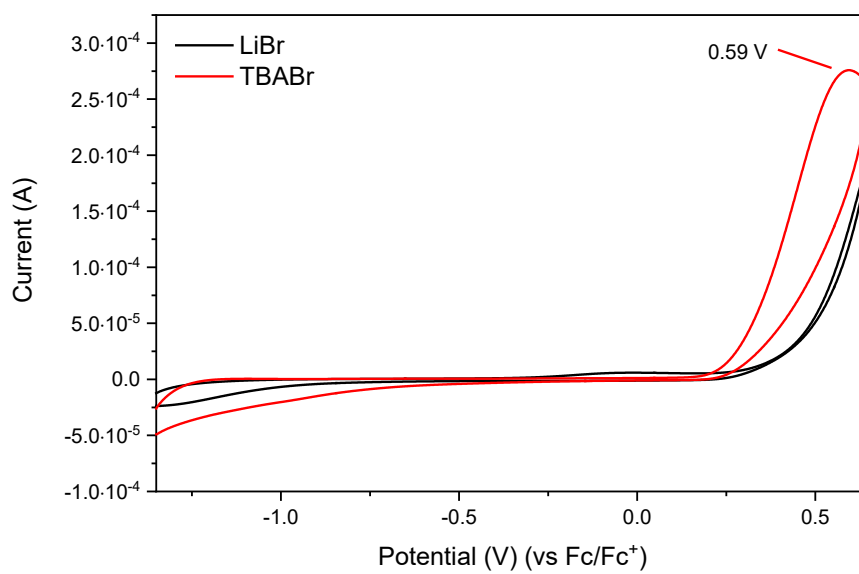


Figure S3. Cyclic voltammetry of LiBr (black line) and TBABr (red line).

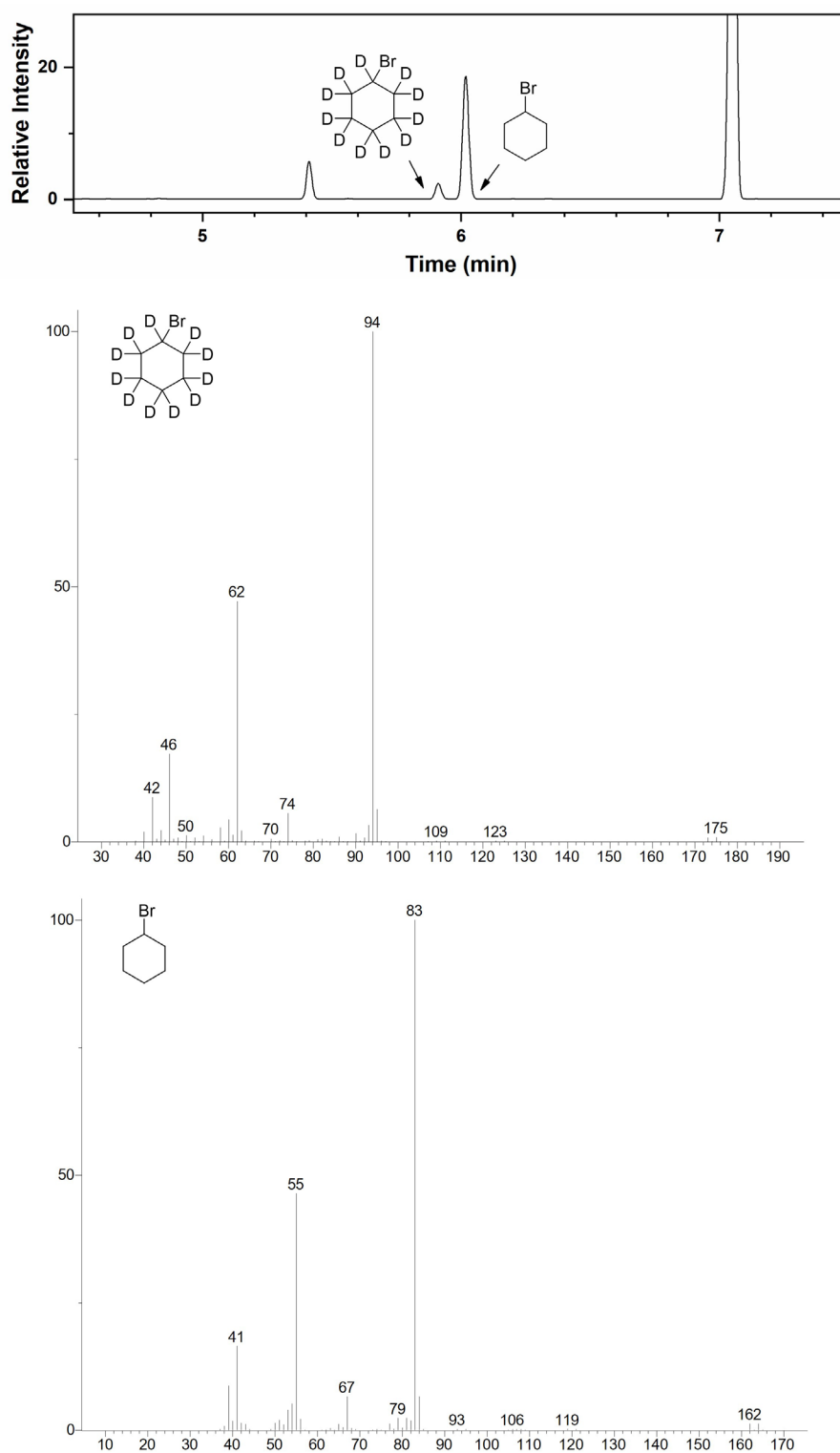


Figure S4. Competitive kinetic isotope experiments of cyclohexane and cyclohexane- d_{12} : (a) GC-MS TIC analysis of [Fe(TDFPP)Cl] catalyzed bromination of 1:1 molar ratio mixture of cyclohexane and cyclohexane- d_{12} ; (b) MS spectroscopy of bromocyclohexane- d_{11} generated in the reaction; (c) MS spectroscopy of bromocyclohexane generated in the reaction.

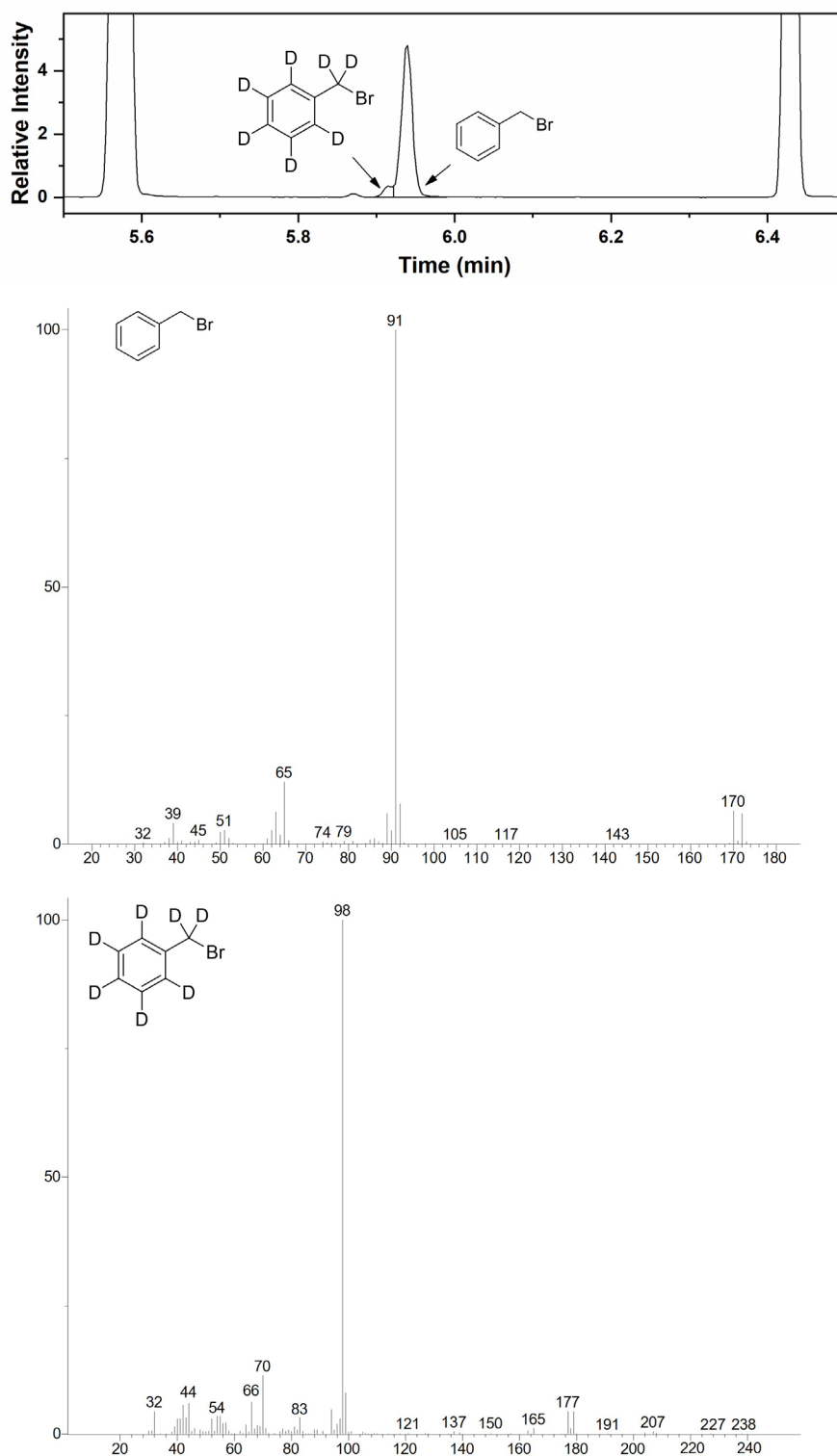


Figure S5. Competitive kinetic isotope experiments of toluene and toluene- d_8 : (a) GC-MS TIC analysis of [Fe(TDFPP)Cl] catalyzed bromination of 1:1 molar ratio mixture of toluene and toluene- d_8 ; (b) MS spectroscopy of benzylbromide- d_7 generated in the reaction; (c) MS spectroscopy of benzylbromide generated in the reaction.

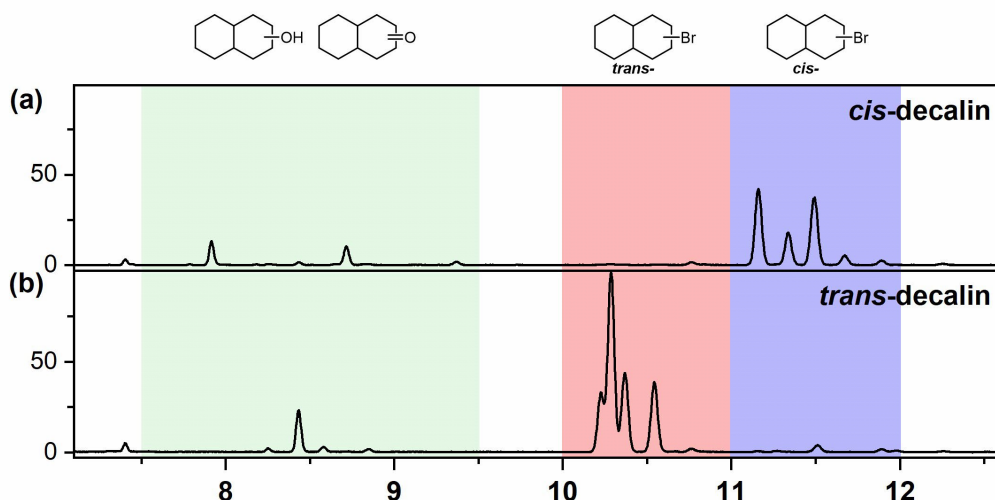


Figure S6. GC-MS TIC of iron porphyrin-catalyzed bromination of decalin as diagnostic substrates. (a) *cis*-decalin as the substrate; (b) *trans*-decalin as the substrate.

To probe the lifetime of the incipient radical which was generated from H atom abstraction by high-valent iron-oxo intermediate, decalin was selected as the diagnostic substrate. When *cis*-decalin was used, if a long-lived radical was involved in the reaction, *trans*-brominated decalin through radical rearrangement would be obtained. To the opposite, only configuration retained product *trans*-brominated decalin would be obtained when *trans*-decalin was used, since no radical rearrangement can occur in this case. The brominated products obtained in the reaction of *cis*-decalin exhibited the retention time in the range of 11-12 min (Figure S5a, blue region), while the brominated products obtained in the reaction of *trans*-decalin exhibited the retention time in the range of 10-11 min (Figure S5b, red region). As discussed above, only *trans*-brominated decalin would be obtained in the bromination of *trans*-decalin. Therefore, the brominated products with the retention time from 10-11 min can be assigned as *trans*-brominated decalin. Consequently, the brominated products with the retention time from 11-12 min can be assigned as *cis*-brominated decalin in the reaction of *cis*-decalin. This result unambiguously demonstrated that no radical rearrangement occurred in the bromination of *cis*-decalin, suggesting a carbon cation process as discussed in the text. Small amounts of byproducts with the retention time in the range of 7.5-9.5 min were the oxygenated compounds, such as ketone and alcohol products (Figure S5, green region).

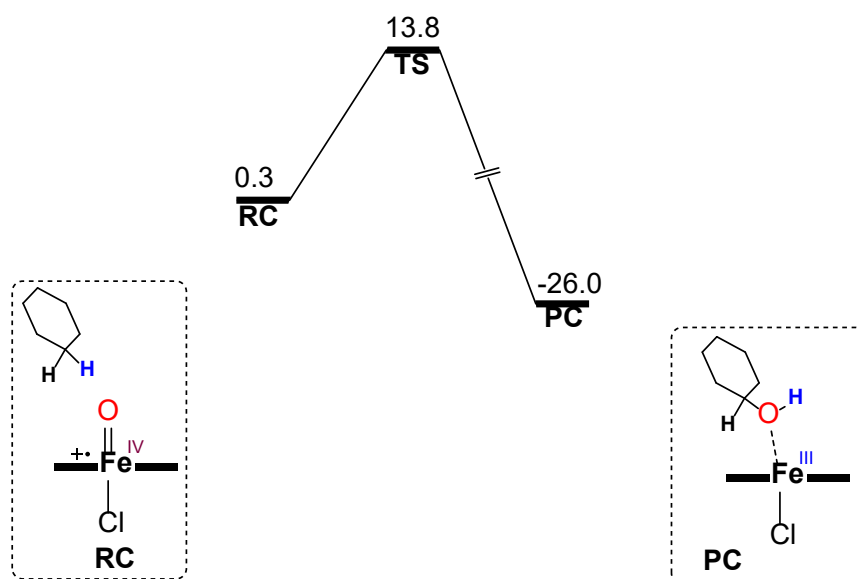


Figure S7. Gibbs free energy profile (kcal/mol) for the bromination of CHA by **Cpd I** without LiBr in doublet.

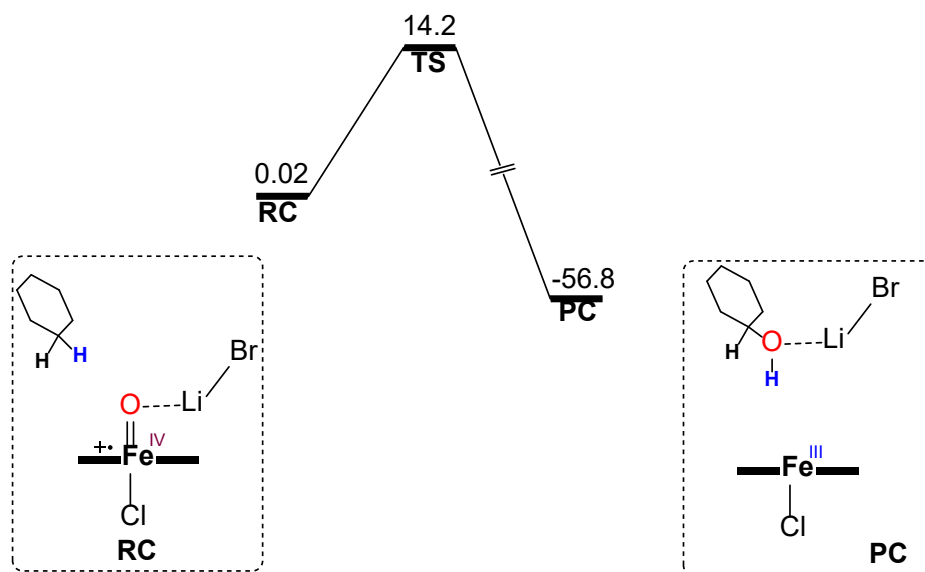


Figure S8. Gibbs free energy profile (kcal/mol) for the bromination of CHA by Cpd I with 1 LiBr in doublet.

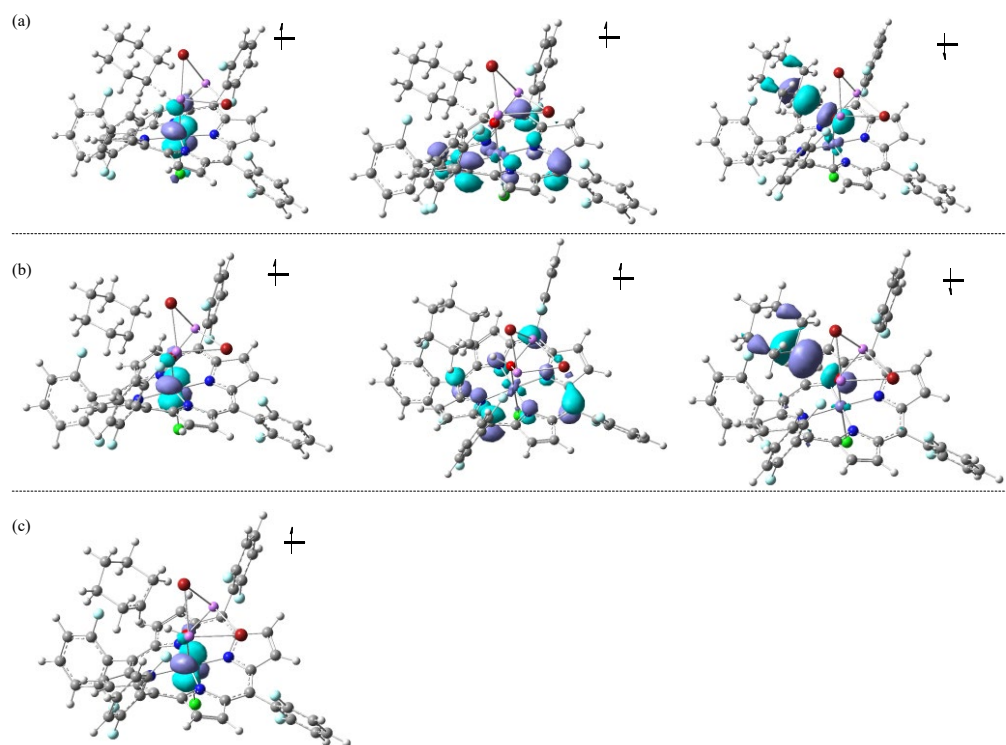


Figure S9. Singly occupied molecular orbitals (SOMOs) of key structures during the bromination of cyclohexane on the doublet. (a) TSA1; (b) A1; and (c) A2

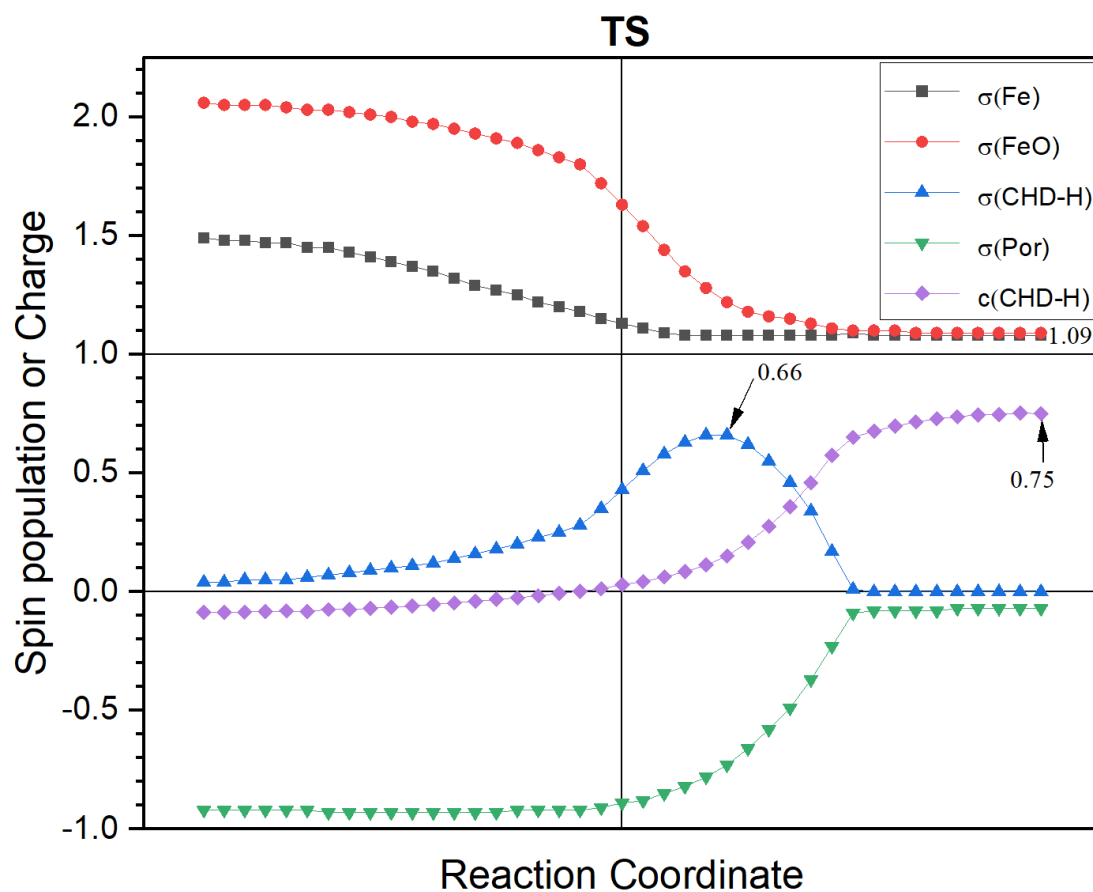


Figure S10. Evolution of charge and spin population along the reaction path for the HAT of CHA in doublet.

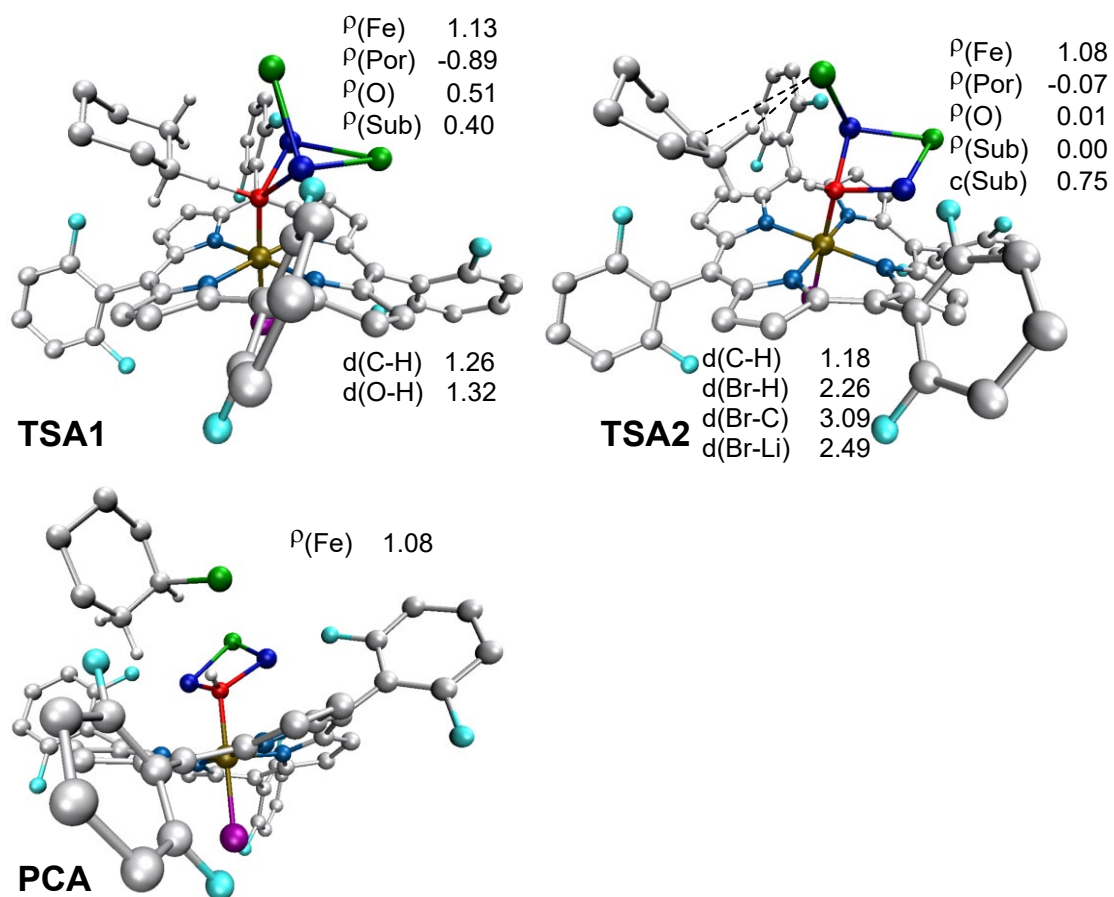


Figure S11. Some key structures involved in the reaction of the bromination of CHA by **Cpd I** with 2 LiBr. Key distances, spin and charge population are given. Some atoms are omitted for clarity.

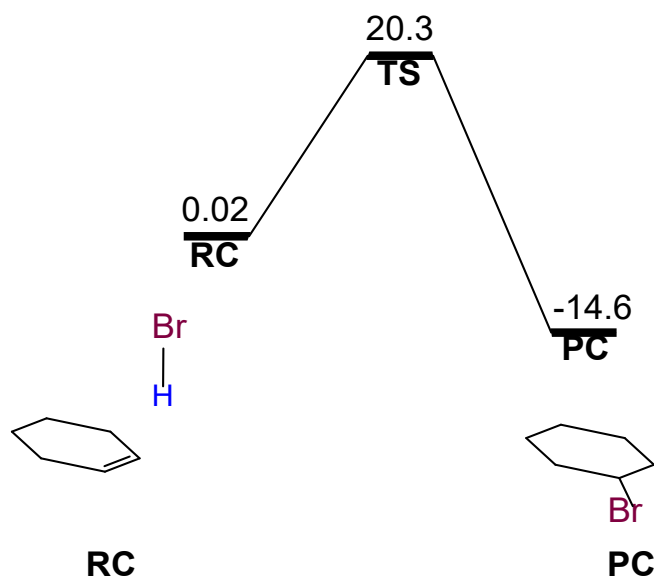


Figure S12. Gibbs free energy profile (kcal/mol) for the addition of HBr to cyclohexene without Li^+ .

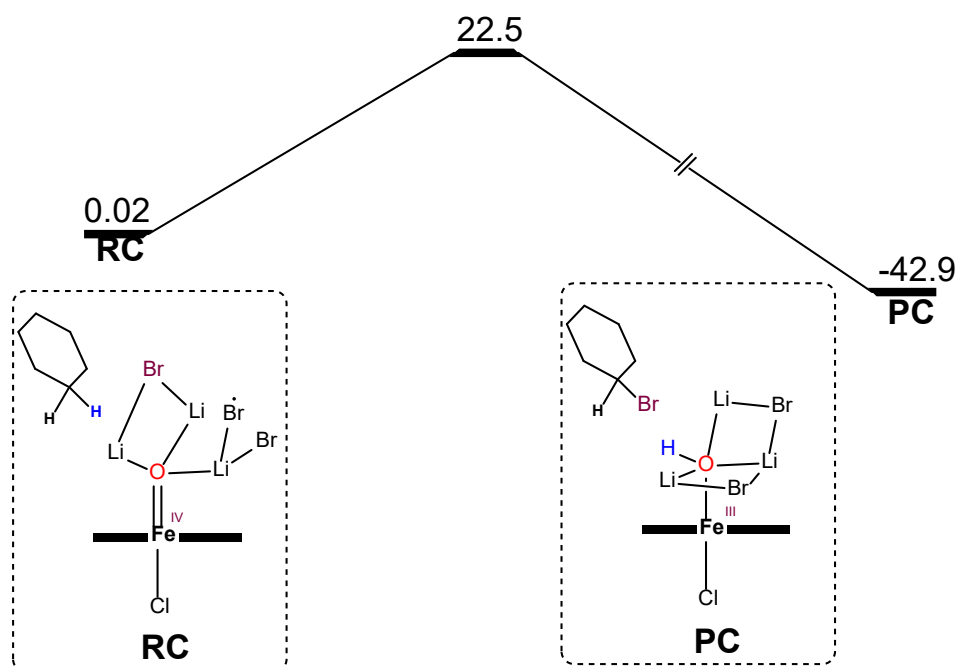


Figure S13. Gibbs free energy profile (kcal/mol) for the bromination of CHA by **Cpd I** with 3 LiBr in doublet.

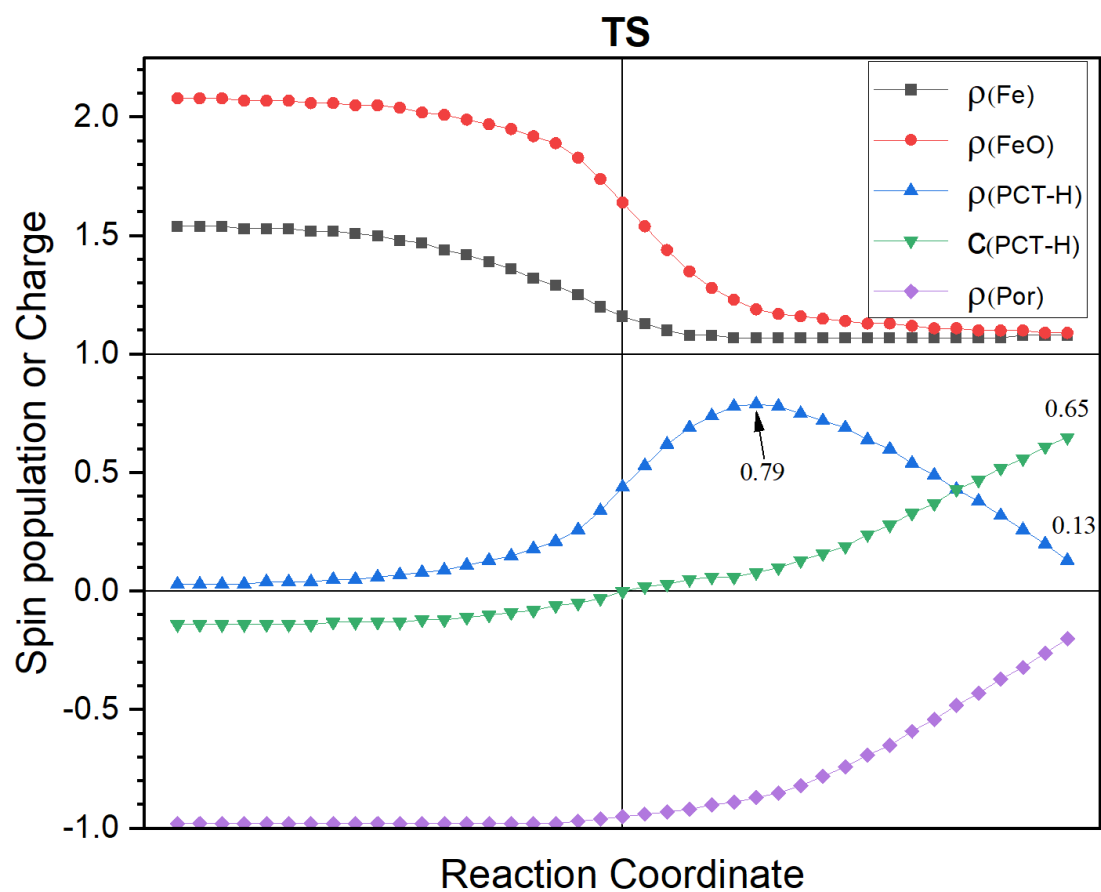


Figure S14. Evolution of charge and spin population along the reaction path for the HAT of PCT in doublet.

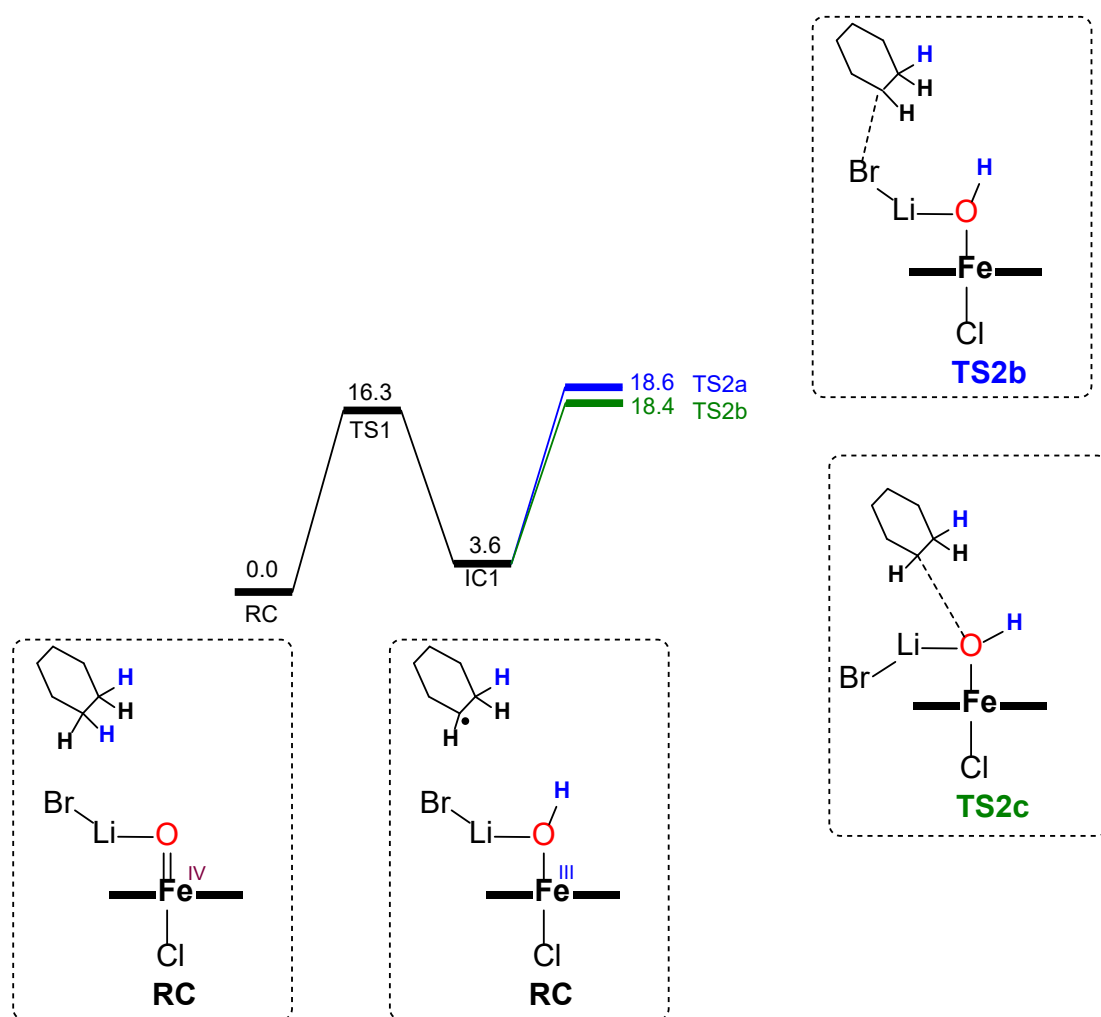


Figure S15. Gibbs free energy profile (kcal/mol) for the bromination and hydroxylation of CHA by **Cpd II** with 1 LiBr in triplet. Bromination in blue and hydroxylation in green.

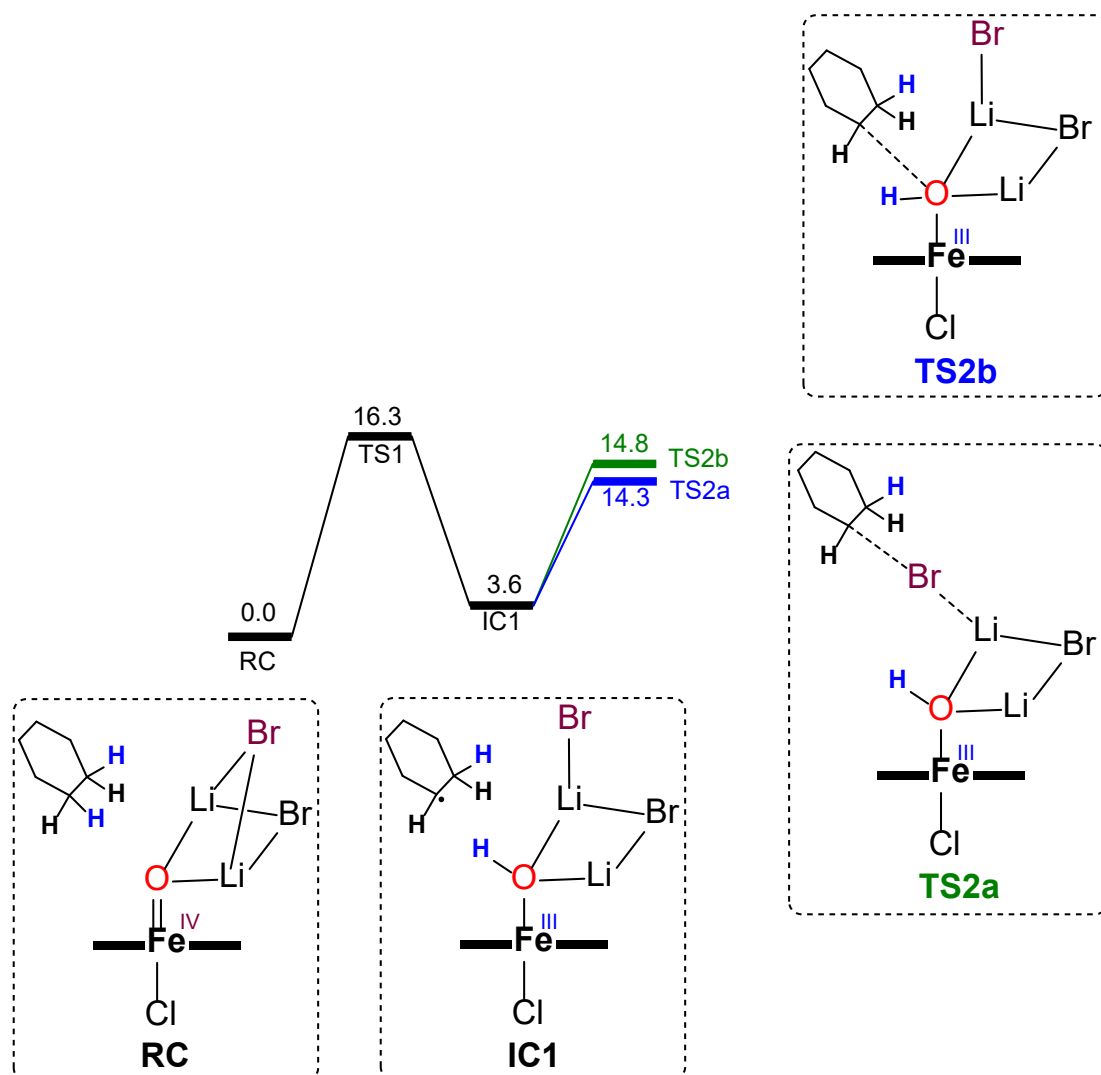


Figure S16. Gibbs free energy profile (kcal/mol) for the bromination and hydroxylation of CHA by **Cpd II** with 2 LiBr in triplet. Bromination in blue and hydroxylation in green.

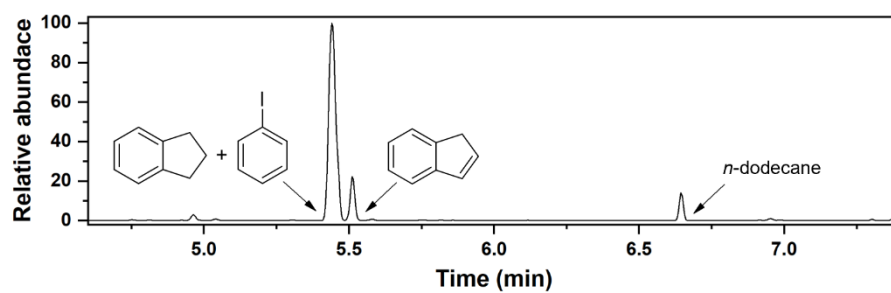


Figure S17. Indane as substrate under standard condition with *n*-dodecane as internal standard. Indene was afforded as the only product and no oxygenated product could be detected.

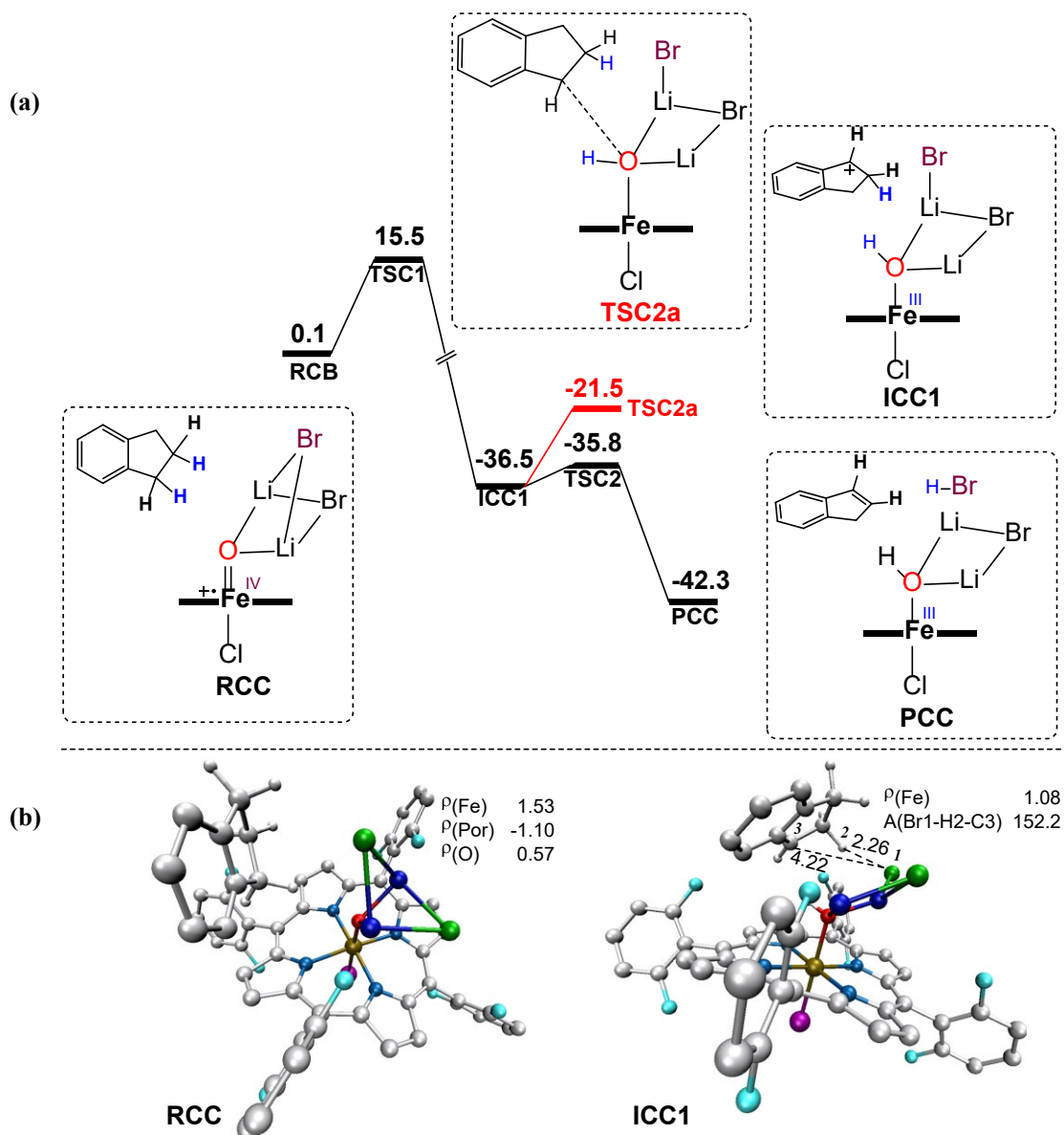


Figure S18. (a) Gibbs free energy profile (kcal/mol) for the oxidation of Indane by **Cpd I** with 2 molecules of LiBr. (b) Key structures on doublet involved in reactions. Key distances (in angstroms) and spin population are given. Some atoms are omitted for clarity.

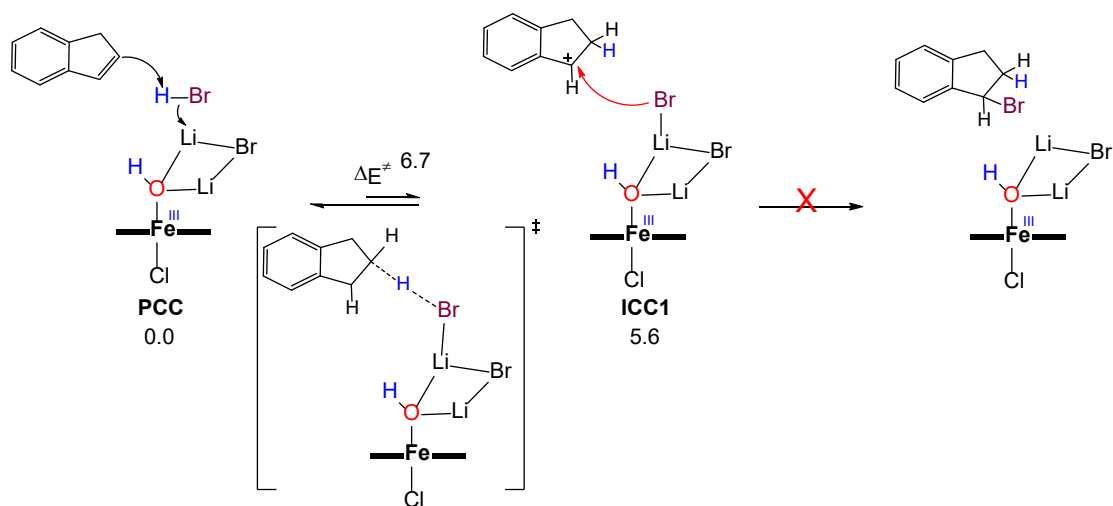


Figure S19. Gibbs free energy profile (kcal/mol) for the addition of HBr to indene from **PCC**.

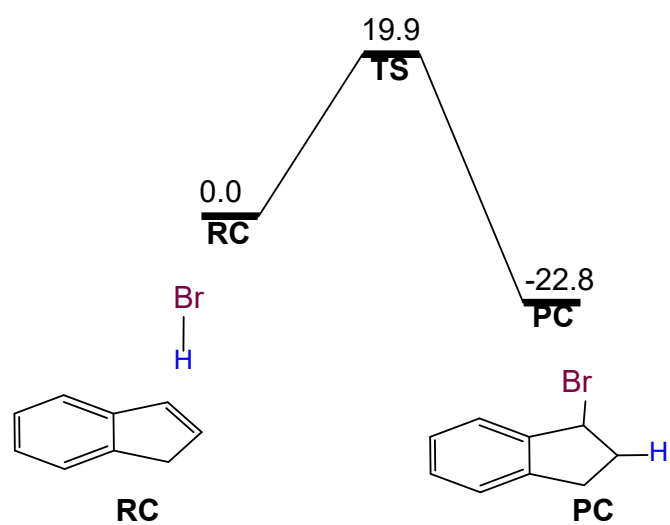


Figure S20. Gibbs free energy profile (kcal/mol) for the addition of HBr to indene without Li^+ .

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Appendix

Coordinates

RCA-Quartet							
Fe	-0.254304000	0.174548000	-0.885746000	C	6.721827000	1.390913000	-2.349569000
N	1.391191000	-0.880015000	-1.241481000	C	6.717788000	2.214881000	-3.478041000
N	-1.350598000	-1.460221000	-1.021364000	H	5.479742000	3.262091000	-4.940865000
N	0.842307000	1.830604000	-0.906013000	H	7.664823000	2.552165000	-3.904816000
N	-1.907994000	1.244589000	-0.744360000	H	7.647111000	1.074258000	-1.865502000
C	2.589298000	-0.417340000	-1.758545000	C	0.807968000	-4.337655000	0.064165000
C	-2.689759000	-1.555297000	-1.135982000	C	1.324046000	-5.475519000	-0.566084000
C	1.515872000	-2.210069000	-1.073211000	C	0.624693000	-4.438097000	1.449937000
C	-0.878098000	-2.717050000	-0.705844000	C	1.638766000	-6.640519000	0.125592000
C	2.138307000	1.958946000	-1.263625000	C	0.926581000	-5.569479000	2.189841000
C	-3.194976000	0.862577000	-1.063549000	C	1.438256000	-6.679395000	1.508189000
C	0.470326000	3.006117000	-0.290114000	H	2.032096000	-7.496190000	-0.425732000
C	-1.961027000	2.528059000	-0.332604000	H	1.683615000	-7.586665000	2.064216000
C	3.465762000	-1.546066000	-1.991614000	H	0.766420000	-5.569541000	3.268954000
C	-3.109367000	-2.928929000	-0.930177000	C	-5.000224000	-0.778424000	-1.609667000
C	2.827944000	-2.649365000	-1.503459000	C	-6.078549000	-0.505463000	-0.752043000
C	-1.990768000	-3.639596000	-0.613562000	C	-5.320502000	-1.445057000	-2.804605000
C	2.631083000	3.265587000	-0.876080000	C	-7.390770000	-0.850922000	-1.059883000
C	-4.073170000	2.004090000	-0.920515000	C	-6.616307000	-1.800700000	-3.155826000
C	1.610377000	3.894567000	-0.221840000	C	-7.654499000	-1.497089000	-2.270079000
C	-3.319177000	3.021730000	-0.411264000	H	-8.180962000	-0.613640000	-0.345665000
H	4.461628000	-1.493804000	-2.423971000	H	-8.680732000	-1.770422000	-2.525110000
H	-4.135201000	-3.285502000	-0.982865000	H	-6.792154000	-2.305887000	-4.106970000
H	3.192341000	-3.672689000	-1.479748000	C	-1.127492000	4.453232000	0.972563000
H	-1.905345000	-4.699571000	-0.383776000	C	-1.601147000	4.183605000	2.263518000
H	3.639635000	3.633317000	-1.051536000	C	-0.972121000	5.805300000	0.646830000
H	-5.136514000	2.015389000	-1.144408000	C	-1.902256000	5.161983000	3.196319000
H	1.613619000	4.887906000	0.219805000	C	-1.266351000	6.829365000	1.541891000
H	-3.634401000	4.029216000	-0.148107000	C	-1.730520000	6.498873000	2.817984000
C	2.950794000	0.925274000	-1.817221000	H	-2.257034000	4.876994000	4.187886000
C	-3.586773000	-0.455905000	-1.292334000	H	-1.130278000	7.865409000	1.227314000
C	-0.840351000	3.309551000	0.072763000	H	-1.961862000	7.293504000	3.530368000
C	0.465812000	-3.060191000	-0.610752000	F	1.512318000	-5.428955000	-1.894333000
C	4.267510000	1.331679000	-2.375758000	F	0.138135000	-3.344516000	2.110185000
C	4.322161000	2.176691000	-3.496736000	F	3.159290000	2.568368000	-4.042776000
C	5.505443000	0.970022000	-1.823864000	F	-0.529961000	6.113264000	-0.581613000
C	5.512815000	2.616245000	-4.061909000	F	5.518397000	0.197922000	-0.722550000
				F	-1.756124000	2.871905000	2.616690000

F	-4.314992000	-1.743234000	-3.644453000	C	-1.987400000	-3.640281000	-0.619346000
F	-5.834127000	0.096783000	0.418425000	C	2.633936000	3.268178000	-0.867065000
Cl	-0.459387000	0.394583000	-3.216522000	C	-4.072698000	2.005087000	-0.930289000
O	-0.149028000	0.022376000	0.780294000	C	1.610186000	3.897688000	-0.218747000
C	3.235724000	-1.913486000	2.212277000	C	-3.319010000	3.025015000	-0.425594000
C	3.226227000	-0.506075000	1.606692000	H	4.469017000	-1.488164000	-2.419621000
C	3.996987000	0.492172000	2.477224000	H	-4.133487000	-3.284939000	-0.976925000
C	5.427002000	0.008541000	2.756279000	H	3.195356000	-3.670688000	-1.489977000
C	5.434394000	-1.402297000	3.362180000	H	-1.900961000	-4.700689000	-0.391954000
C	4.666730000	-2.396722000	2.479751000	H	3.643438000	3.635538000	-1.037753000
H	2.719315000	-2.615445000	1.537235000	H	-5.136057000	2.015042000	-1.154201000
H	2.663565000	-1.900387000	3.157002000	H	1.610854000	4.891660000	0.221478000
H	2.192143000	-0.162156000	1.456364000	H	-3.634164000	4.033633000	-0.166749000
H	3.701157000	-0.549230000	0.615929000	C	2.957759000	0.928349000	-1.808537000
H	4.018196000	1.482182000	1.987163000	C	-3.586107000	-0.455814000	-1.290925000
H	3.450196000	0.622024000	3.428292000	C	-0.841121000	3.313625000	0.064737000
H	5.951100000	0.713864000	3.425005000	C	0.468705000	-3.060640000	-0.621272000
H	5.992530000	-0.005061000	1.806408000	C	4.276291000	1.335897000	-2.361951000
H	6.471253000	-1.747520000	3.519556000	C	4.334735000	2.184286000	-3.480186000
H	4.959146000	-1.368107000	4.360754000	C	5.512436000	0.972030000	-1.807537000
H	4.657162000	-3.397364000	2.946453000	C	5.527207000	2.625356000	-4.040303000
H	5.196523000	-2.504122000	1.514023000	C	6.730564000	1.394191000	-2.328212000
Li	-0.380274000	-1.385579000	2.132348000	C	6.730273000	2.221792000	-3.454013000
Br	0.442308000	0.088087000	4.028651000	H	5.496986000	3.273988000	-4.917307000
Li	-1.109686000	0.935678000	2.275954000	H	7.678724000	2.560152000	-3.876776000
Br	-2.872416000	-0.880338000	2.257346000	H	7.654250000	1.075588000	-1.842373000
RCA-Doublet				C	0.811171000	-4.338034000	0.053680000
Fe	-0.250668000	0.176229000	-0.887627000	C	1.330171000	-5.474922000	-0.575939000
N	1.395208000	-0.877929000	-1.242560000	C	0.625131000	-4.439436000	1.439079000
N	-1.348565000	-1.460354000	-1.027556000	C	1.645279000	-6.639758000	0.115826000
N	0.845157000	1.832989000	-0.906233000	C	0.927266000	-5.570715000	2.179059000
N	-1.906895000	1.246884000	-0.750100000	C	1.442025000	-6.679562000	1.497995000
C	2.595580000	-0.413595000	-1.754319000	H	2.041051000	-7.494570000	-0.435084000
C	-2.687951000	-1.555133000	-1.135100000	H	1.687689000	-7.586686000	2.054133000
C	1.518877000	-2.208688000	-1.080531000	H	0.764950000	-5.571476000	3.257851000
C	-0.874917000	-2.717597000	-0.715413000	C	-5.000032000	-0.779557000	-1.605092000
C	2.142743000	1.961289000	-1.256483000	C	-6.077033000	-0.503806000	-0.746683000
C	-3.194240000	0.862791000	-1.067679000	C	-5.322229000	-1.449898000	-2.797426000
C	0.469874000	3.009702000	-0.292987000	C	-7.389666000	-0.850760000	-1.051202000
C	-1.960911000	2.531146000	-0.343716000	C	-6.618466000	-1.807202000	-3.145292000
C	3.471882000	-1.541949000	-1.990423000	C	-7.655244000	-1.501096000	-2.258738000
C	-3.107277000	-2.928866000	-0.928896000	H	-8.178760000	-0.611148000	-0.336547000
C	2.831916000	-2.646954000	-1.509686000	H	-8.681822000	-1.775603000	-2.511109000
				H	-6.795759000	-2.315466000	-4.094525000

C	-1.131373000	4.455701000	0.965619000	N	1.324217000	-1.343090000	-1.100264000
C	-1.607938000	4.183337000	2.254942000	N	-1.481506000	-1.357928000	-0.908380000
C	-0.976176000	5.808406000	0.642665000	N	1.298719000	1.431079000	-1.047836000
C	-1.912271000	5.159832000	3.188676000	N	-1.519203000	1.384266000	-0.869278000
C	-1.273465000	6.830661000	1.538804000	C	2.605956000	-1.175850000	-1.573126000
C	-1.740696000	6.497530000	2.813094000	C	-2.804747000	-1.226195000	-1.146346000
H	-2.269309000	4.872830000	4.178848000	C	1.200996000	-2.637658000	-0.725515000
H	-1.137261000	7.867371000	1.226480000	C	-1.268649000	-2.650391000	-0.491318000
H	-1.974496000	7.290724000	3.526270000	C	2.588551000	1.294415000	-1.456504000
F	1.521190000	-5.427491000	-1.903795000	C	-2.841119000	1.243644000	-1.215289000
F	0.135553000	-3.347054000	2.099044000	C	1.153186000	2.712302000	-0.588000000
F	3.173602000	2.578054000	-4.028479000	C	-1.328844000	2.684533000	-0.534391000
F	-0.530613000	6.118768000	-0.583959000	C	3.298884000	-2.445195000	-1.532718000
F	5.521913000	0.196188000	-0.708805000	C	-3.478276000	-2.486274000	-0.904011000
F	-1.762539000	2.870826000	2.605364000	C	2.446010000	-3.341038000	-0.950567000
F	-4.318017000	-1.750308000	-3.638105000	C	-2.532380000	-3.356312000	-0.445580000
F	-5.831086000	0.103111000	0.420990000	C	3.297808000	2.541047000	-1.264634000
Cl	-0.455149000	0.397204000	-3.221538000	C	-3.492442000	2.533613000	-1.149924000
O	-0.151226000	0.021262000	0.778540000	C	2.419542000	3.406993000	-0.673916000
C	3.230074000	-1.918330000	2.214342000	C	-2.571249000	3.416834000	-0.664440000
C	3.222390000	-0.509709000	1.611545000	H	4.318697000	-2.620271000	-1.867401000
C	3.990888000	0.486782000	2.486071000	H	-4.544474000	-2.662817000	-1.025947000
C	5.419982000	0.002420000	2.768510000	H	2.630946000	-4.390141000	-0.735880000
C	5.425347000	-1.409532000	3.371827000	H	-2.658916000	-4.394904000	-0.146781000
C	4.660236000	-2.402175000	2.485203000	H	4.342828000	2.713830000	-1.511996000
H	2.715855000	-2.618834000	1.536201000	H	-4.529459000	2.734118000	-1.403580000
H	2.654961000	-1.907232000	3.157294000	H	2.603247000	4.433537000	-0.367831000
H	2.188702000	-0.165256000	1.459244000	H	-2.697491000	4.478314000	-0.461511000
H	3.699988000	-0.550982000	0.622030000	C	3.201361000	0.068390000	-1.813592000
H	4.013727000	1.477659000	1.997785000	C	-3.464788000	0.005276000	-1.421575000
H	3.441328000	0.615122000	3.435732000	C	-0.080066000	3.274435000	-0.218043000
H	5.942182000	0.706425000	3.440092000	C	-0.013096000	-3.221642000	-0.268985000
H	5.988388000	-0.009556000	1.820334000	C	4.612045000	0.123329000	-2.286346000
H	6.461690000	-1.755170000	3.531660000	C	4.927723000	0.566224000	-3.577406000
H	4.947091000	-1.377113000	4.369048000	C	5.696633000	-0.210279000	-1.465237000
H	4.649292000	-3.403696000	2.949859000	C	6.233648000	0.655536000	-4.047486000
H	5.192887000	-2.507683000	1.520848000	C	7.018833000	-0.133054000	-1.887025000
Li	-0.385741000	-1.387942000	2.125950000	C	7.279374000	0.300257000	-3.190653000
Br	0.432202000	0.084237000	4.027001000	H	6.410914000	0.999545000	-5.067869000
Li	-1.115493000	0.932406000	2.269663000	H	8.311541000	0.365789000	-3.541661000
Br	-2.879416000	-0.885127000	2.253208000	H	7.817587000	-0.405112000	-1.195156000
				C	0.029205000	-4.476308000	0.523743000
TSA1-Quartet				C	0.356426000	-5.741606000	0.022536000
Fe	-0.097738000	0.028165000	-0.932677000	C	-0.281960000	-4.423653000	1.889079000

C	0.375172000	-6.883398000	0.816877000	H	2.713954000	1.993458000	1.800682000
C	-0.273031000	-5.526160000	2.728021000	H	2.240321000	1.213956000	3.331202000
C	0.059515000	-6.767231000	2.173421000	H	4.655653000	1.860149000	3.413389000
H	0.632187000	-7.842050000	0.363170000	H	4.969465000	0.950269000	1.921551000
H	0.072019000	-7.655063000	2.809097000	H	5.663579000	-0.400689000	3.893977000
H	-0.518392000	-5.405816000	3.784280000	H	4.045906000	-0.243960000	4.599733000
C	-4.880626000	-0.070299000	-1.859894000	H	4.263846000	-2.463403000	3.497191000
C	-5.966842000	0.452154000	-1.138340000	H	4.741415000	-1.687070000	1.974991000
C	-5.206566000	-0.743861000	-3.050766000	Li	-0.884197000	-1.209973000	2.207816000
C	-7.285043000	0.331396000	-1.567769000	Br	-0.207851000	0.106982000	4.311211000
C	-6.506312000	-0.879732000	-3.520957000	Li	-0.954829000	1.214532000	2.165349000
C	-7.549384000	-0.334764000	-2.766600000	Br	-3.155172000	-0.113726000	2.022881000
H	-8.080516000	0.756465000	-0.953381000				
H	-8.579495000	-0.432872000	-3.116113000	TSA1-Doublet			
H	-6.680996000	-1.405309000	-4.461196000	Fe	-0.070580000	0.028063000	-0.949660000
C	-0.127165000	4.530721000	0.569925000	N	1.345250000	-1.345978000	-1.094302000
C	-0.600032000	4.476096000	1.888180000	N	-1.468827000	-1.359690000	-0.934633000
C	0.249549000	5.797796000	0.109472000	N	1.327397000	1.425869000	-1.045680000
C	-0.695158000	5.577559000	2.722791000	N	-1.497932000	1.394268000	-0.898561000
C	0.168170000	6.938938000	0.901261000	C	2.635548000	-1.183009000	-1.547499000
C	-0.304723000	6.820422000	2.210989000	C	-2.794256000	-1.218356000	-1.152860000
H	-1.062955000	5.455894000	3.742713000	C	1.210331000	-2.645309000	-0.733832000
H	0.471618000	7.899399000	0.481341000	C	-1.261154000	-2.652783000	-0.520513000
H	-0.370549000	7.707987000	2.843752000	C	2.623875000	1.285845000	-1.429768000
F	0.655085000	-5.845063000	-1.281935000	C	-2.821878000	1.253777000	-1.238028000
F	-0.597908000	-3.205870000	2.425710000	C	1.177457000	2.712784000	-0.594155000
F	3.915070000	0.915451000	-4.387124000	C	-1.305047000	2.694804000	-0.575099000
F	0.694737000	5.905814000	-1.151777000	C	3.320996000	-2.456084000	-1.508978000
F	5.437839000	-0.603536000	-0.202962000	C	-3.473961000	-2.474150000	-0.906313000
F	-0.972216000	3.254983000	2.378617000	C	2.455645000	-3.352205000	-0.947545000
F	-4.201117000	-1.272527000	-3.768711000	C	-2.528019000	-3.352567000	-0.464876000
F	-5.731777000	1.078722000	0.020733000	C	3.333876000	2.531209000	-1.229065000
Cl	-0.244825000	0.071073000	-3.247386000	C	-3.468997000	2.546380000	-1.186608000
O	-0.002465000	0.001611000	0.921620000	C	2.448665000	3.401682000	-0.657957000
C	2.640405000	-1.433216000	2.467916000	C	-2.543410000	3.431944000	-0.713344000
C	2.448321000	-0.151024000	1.683815000	H	4.344399000	-2.633448000	-1.831137000
C	2.862574000	1.099907000	2.428617000	H	-4.542979000	-2.642247000	-1.014092000
C	4.347709000	0.972242000	2.834550000	H	2.632184000	-4.404142000	-0.739855000
C	4.592820000	-0.310344000	3.641102000	H	-2.657794000	-4.391162000	-0.167588000
C	4.123503000	-1.558463000	2.881009000	H	4.383624000	2.699632000	-1.458734000
H	2.335080000	-2.306549000	1.868810000	H	-4.506160000	2.747615000	-1.438873000
H	2.011020000	-1.408732000	3.372178000	H	2.630056000	4.428915000	-0.353004000
H	1.234061000	-0.052123000	1.328639000	H	-2.665341000	4.495855000	-0.520971000
H	2.941646000	-0.209598000	0.708332000	C	3.239531000	0.058381000	-1.776922000

C	-3.452277000	0.016183000	-1.425678000	F	-0.994510000	3.256716000	2.334020000
C	-0.055847000	3.281200000	-0.245455000	F	-4.203689000	-1.281229000	-3.756867000
C	-0.007789000	-3.228447000	-0.293438000	F	-5.711836000	1.121728000	0.010247000
C	4.656894000	0.109895000	-2.228927000	Cl	-0.210771000	0.072246000	-3.266185000
C	4.994125000	0.565446000	-3.510231000	O	-0.032786000	-0.000298000	0.902424000
C	5.727762000	-0.238457000	-1.395812000	C	2.594972000	-1.422308000	2.467062000
C	6.307215000	0.652947000	-3.960155000	C	2.414246000	-0.130652000	1.696511000
C	7.056417000	-0.163846000	-1.797437000	C	2.802801000	1.112051000	2.468575000
C	7.338404000	0.282397000	-3.092188000	C	4.276811000	0.985546000	2.914363000
H	6.501226000	1.007353000	-4.973920000	C	4.506070000	-0.305798000	3.710820000
H	8.375933000	0.346166000	-3.427352000	C	4.066287000	-1.545758000	2.920860000
H	7.843455000	-0.447835000	-1.096985000	H	2.311480000	-2.288525000	1.847317000
C	0.024871000	-4.483938000	0.499110000	H	1.941296000	-1.414026000	3.354567000
C	0.354253000	-5.749828000	0.001147000	H	1.217783000	-0.039491000	1.328473000
C	-0.299699000	-4.430998000	1.861343000	H	2.930096000	-0.171307000	0.731606000
C	0.363624000	-6.891715000	0.795631000	H	2.667124000	2.012838000	1.848367000
C	-0.301051000	-5.533515000	2.700333000	H	2.156584000	1.211766000	3.356039000
C	0.034981000	-6.775150000	2.149030000	H	4.563288000	1.867598000	3.512737000
H	0.623551000	-7.850747000	0.344378000	H	4.924028000	0.979075000	2.018819000
H	0.039923000	-7.663019000	2.784760000	H	5.569641000	-0.393675000	3.993200000
H	-0.556771000	-5.412851000	3.754094000	H	3.931404000	-0.255102000	4.654005000
C	-4.870581000	-0.056578000	-1.857360000	H	4.193149000	-2.458425000	3.528369000
C	-5.952255000	0.480414000	-1.139336000	H	4.710270000	-1.658929000	2.031306000
C	-5.203980000	-0.740965000	-3.040257000	Li	-0.924183000	-1.216929000	2.176061000
C	-7.272352000	0.360779000	-1.563411000	Br	-0.282064000	0.097880000	4.292145000
C	-6.505737000	-0.875819000	-3.504982000	Li	-0.997157000	1.213545000	2.133844000
C	-7.543927000	-0.317791000	-2.753538000	Br	-3.201325000	-0.116950000	1.994004000
H	-8.063647000	0.797353000	-0.951709000	IC1A-Quartet			
H	-8.575592000	-0.414805000	-3.098733000	Fe	-0.319100000	-0.108360000	-1.219970000
H	-6.685564000	-1.410515000	-4.439087000	N	1.125470000	-1.487760000	-1.243030000
C	-0.110464000	4.535526000	0.545423000	N	-1.691550000	-1.496290000	-0.829140000
C	-0.607186000	4.478115000	1.854888000	N	1.078540000	1.308340000	-1.412720000
C	0.279556000	5.802707000	0.096687000	N	-1.746480000	1.267080000	-1.035830000
C	-0.712366000	5.576662000	2.692018000	C	2.397350000	-1.340750000	-1.737830000
C	0.189115000	6.941156000	0.891453000	C	-3.053170000	-1.360460000	-0.898540000
C	-0.307359000	6.819736000	2.192112000	C	1.004890000	-2.778650000	-0.809870000
H	-1.098947000	5.452757000	3.704703000	C	-1.433020000	-2.763540000	-0.376470000
H	0.504255000	7.901858000	0.480832000	C	2.386780000	1.126210000	-1.772930000
H	-0.380545000	7.705128000	2.827102000	C	-3.100860000	1.082790000	-1.183920000
F	0.665481000	-5.853986000	-1.300439000	C	0.936740000	2.618620000	-1.032760000
F	-0.619619000	-3.212629000	2.395032000	C	-1.534800000	2.605380000	-0.861290000
F	3.995415000	0.929281000	-4.330811000	C	3.078020000	-2.617580000	-1.687340000
F	0.747815000	5.913772000	-1.155931000	C	-3.679300000	-2.599180000	-0.496280000
F	5.448949000	-0.643874000	-0.141832000				

C	2.239140000	-3.491080000	-1.055180000	H	-7.549100000	-1.559520000	-3.469800000
C	-2.678110000	-3.453490000	-0.126470000	C	-0.291960000	4.534560000	0.015570000
C	3.098050000	2.379830000	-1.642490000	C	-0.719360000	4.579000000	1.350190000
C	-3.758900000	2.369400000	-1.164730000	C	0.086200000	5.763500000	-0.537330000
C	2.213970000	3.289520000	-1.134020000	C	-0.771510000	5.734440000	2.113290000
C	-2.797170000	3.306520000	-0.907980000	C	0.051350000	6.956450000	0.179060000
H	4.084900000	-2.811690000	-2.049010000	C	-0.379020000	6.934180000	1.508500000
H	-4.751940000	-2.777040000	-0.460980000	H	-1.108440000	5.686340000	3.149850000
H	2.422760000	-4.536050000	-0.816200000	H	0.356410000	7.881160000	-0.313830000
H	-2.765760000	-4.471360000	0.248210000	H	-0.410100000	7.862660000	2.082550000
H	4.152260000	2.529900000	-1.864790000	F	0.222710000	-6.054410000	-1.190100000
H	-4.825060000	2.535890000	-1.298380000	F	-0.266300000	-3.135470000	2.484210000
H	2.405040000	4.330370000	-0.884960000	F	3.777470000	0.823810000	-4.561140000
H	-2.920400000	4.382290000	-0.800110000	F	0.494810000	5.782380000	-1.816490000
C	3.007210000	-0.110550000	-2.032990000	F	5.231750000	-0.945180000	-0.444020000
C	-3.743730000	-0.164690000	-1.165250000	F	-1.099080000	3.400760000	1.936240000
C	-0.281350000	3.223910000	-0.684410000	F	-4.975890000	-1.461180000	-3.317210000
C	-0.157610000	-3.340680000	-0.256060000	F	-5.633200000	0.937480000	0.682970000
C	4.425340000	-0.085960000	-2.489520000	Cl	-0.644020000	-0.270350000	-3.585680000
C	4.769650000	0.402950000	-3.758230000	O	0.017640000	0.067360000	0.945390000
C	5.498710000	-0.491570000	-1.683250000	C	3.176930000	-1.220120000	1.950880000
C	6.080220000	0.474240000	-4.218960000	C	3.382640000	0.239290000	1.639410000
C	6.825550000	-0.438150000	-2.096730000	C	4.163040000	1.053620000	2.376350000
C	7.110210000	0.047420000	-3.376200000	C	4.903900000	0.596920000	3.605550000
H	6.272710000	0.860190000	-5.221480000	C	4.431720000	-0.779260000	4.096440000
H	8.146160000	0.096490000	-3.718760000	C	4.237330000	-1.748130000	2.924310000
H	7.609790000	-0.770000000	-1.414240000	H	3.186210000	-1.791600000	1.010590000
C	-0.037400000	-4.553330000	0.597770000	H	2.165180000	-1.371090000	2.374510000
C	0.143120000	-5.860520000	0.135940000	H	0.974280000	0.182030000	0.990730000
C	-0.104040000	-4.404950000	1.988140000	H	2.899100000	0.645880000	0.746240000
C	0.245850000	-6.954130000	0.991580000	H	4.297550000	2.094660000	2.060620000
C	-0.007730000	-5.453340000	2.888980000	H	2.203860000	1.276960000	3.147990000
C	0.168310000	-6.741880000	2.370770000	H	4.797890000	1.353700000	4.402790000
H	0.383190000	-7.950500000	0.567950000	H	5.984980000	0.571810000	3.368460000
H	0.246950000	-7.590610000	3.053500000	H	5.149220000	-1.185040000	4.827630000
H	-0.066380000	-5.258080000	3.960840000	H	3.469740000	-0.664030000	4.627710000
C	-5.223060000	-0.238350000	-1.319710000	H	3.953440000	-2.749280000	3.286960000
C	-6.125540000	0.303040000	-0.392330000	H	5.193700000	-1.860660000	2.382510000
C	-5.799630000	-0.908600000	-2.409450000	Li	-0.794960000	-1.269040000	1.914730000
C	-7.507000000	0.207100000	-0.532100000	Br	1.090280000	1.621530000	4.039750000
C	-7.172820000	-1.028930000	-2.593480000	Li	-1.043150000	1.349270000	1.763160000
C	-8.026850000	-0.462830000	-1.642810000	Br	-2.669810000	-0.087750000	2.913950000
H	-8.149550000	0.651890000	0.229770000				
H	-9.108690000	-0.546930000	-1.767920000				

ICA1-Doublet

Fe	-0.289870000	-0.041200000	-1.171370000	C	0.021140000	-4.484960000	1.899970000
N	1.180760000	-1.404430000	-1.278150000	C	0.414940000	-7.025780000	0.816740000
N	-1.639310000	-1.491950000	-0.875100000	C	0.136480000	-5.571040000	2.780740000
N	1.069830000	1.433050000	-1.341080000	C	0.334580000	-6.854680000	2.216690000
N	-1.759880000	1.311920000	-0.993050000	H	0.571000000	-8.018120000	0.356680000
C	2.457760000	-1.206800000	-1.787590000	H	0.429070000	-7.732720000	2.881560000
C	-3.015240000	-1.385120000	-0.969120000	H	0.075290000	-5.406390000	3.870880000
C	1.102110000	-2.725600000	-0.882150000	C	-5.229600000	-0.287380000	-1.402200000
C	-1.358800000	-2.781440000	-0.448920000	C	-6.166070000	0.231420000	-0.469780000
C	2.391200000	1.291320000	-1.733070000	C	-5.784760000	-0.960830000	-2.520920000
C	-3.119500000	1.095640000	-1.198620000	C	-7.560360000	0.109610000	-0.632610000
C	0.905890000	2.741810000	-0.914500000	C	-7.170180000	-1.108620000	-2.728900000
C	-1.589610000	2.668510000	-0.784200000	C	-8.056500000	-0.565070000	-1.770850000
C	3.181420000	-2.479420000	-1.784330000	H	-8.225960000	0.539570000	0.132650000
C	-3.632220000	-2.664170000	-0.607550000	H	-9.146660000	-0.668280000	-1.915350000
C	2.364400000	-3.405320000	-1.165110000	H	-7.524350000	-1.639850000	-3.626900000
C	-2.608530000	-3.517600000	-0.238700000	C	-0.402800000	4.603670000	0.223110000
C	3.089150000	2.571860000	-1.566190000	C	-0.880020000	4.563180000	1.558330000
C	-3.817990000	2.379530000	-1.177380000	C	-0.037020000	5.885130000	-0.254500000
C	2.182980000	3.454890000	-1.006410000	C	-0.994580000	5.687740000	2.390540000
C	-2.880690000	3.347270000	-0.863940000	C	-0.130010000	7.049350000	0.532830000
H	4.204120000	-2.637460000	-2.166500000	C	-0.611030000	6.942850000	1.857650000
H	-4.711350000	-2.866420000	-0.599280000	H	-1.365660000	5.572150000	3.422010000
H	2.580500000	-4.467460000	-0.959630000	H	0.172650000	8.018200000	0.095830000
H	-2.678620000	-4.559270000	0.106860000	H	-0.686770000	7.850090000	2.486380000
H	4.149820000	2.753480000	-1.801770000	F	0.374810000	-6.051020000	-1.364330000
H	-4.892990000	2.525110000	-1.351920000	F	-0.164240000	-3.218110000	2.440630000
H	2.355860000	4.503440000	-0.725640000	F	3.745110000	1.077470000	-4.604270000
H	-3.033220000	4.431520000	-0.740720000	F	0.415730000	5.988220000	-1.531680000
C	3.040480000	0.063490000	-2.049090000	F	5.345480000	-0.737820000	-0.496580000
C	-3.738180000	-0.183900000	-1.220790000	F	-1.245200000	3.329310000	2.076490000
C	-0.340530000	3.317280000	-0.551130000	F	-4.931130000	-1.491930000	-3.437680000
C	-0.057620000	-3.340150000	-0.335340000	F	-5.698920000	0.868310000	0.633820000
C	4.466310000	0.137010000	-2.535620000	Cl	-0.592730000	-0.136150000	-3.447070000
C	4.774800000	0.664040000	-3.816840000	O	-0.022560000	0.049650000	0.831470000
C	5.577650000	-0.252850000	-1.748720000	C	3.281260000	-1.112410000	1.850300000
C	6.090670000	0.779410000	-4.307850000	C	3.490810000	0.392540000	1.735980000
C	6.910880000	-0.157390000	-2.190850000	C	4.244250000	1.112940000	2.616740000
C	7.158930000	0.362120000	-3.483650000	C	4.953880000	0.493430000	3.814290000
H	6.257430000	1.190140000	-5.318750000	C	4.487300000	-0.962160000	4.096320000
H	8.201850000	0.442770000	-3.847680000	C	4.334610000	-1.768430000	2.781180000
H	7.728340000	-0.484430000	-1.520680000	H	3.315430000	-1.564000000	0.836130000
C	0.089560000	-4.590700000	0.489940000	H	2.252150000	-1.320010000	2.236850000
C	0.293010000	-5.894500000	-0.016340000	H	0.917020000	0.308250000	0.944250000

H	3.032420000	0.919470000	0.875390000	C	3.039860000	0.495320000	-1.812490000
H	4.382280000	2.201050000	2.449070000	C	-3.672730000	-0.117430000	-1.298670000
H	2.183910000	1.119630000	3.300130000	C	-0.478550000	3.357070000	-0.075210000
H	4.802030000	1.137650000	4.713960000	C	0.058010000	-3.133590000	-0.524130000
H	6.057070000	0.517580000	3.617560000	C	4.414410000	0.703350000	-2.346020000
H	5.203990000	-1.463840000	4.791600000	C	4.611210000	1.414070000	-3.542610000
H	3.500490000	-0.937550000	4.620460000	C	5.578160000	0.257400000	-1.704400000
H	4.051260000	-2.827020000	2.995680000	C	5.871850000	1.647860000	-4.084530000
H	5.319420000	-1.797460000	2.249600000	C	6.856780000	0.472560000	-2.206980000
Li	-0.749290000	-1.350370000	1.873810000	C	6.996290000	1.169970000	-3.408970000
Br	0.929870000	1.155920000	4.104830000	H	5.948280000	2.198980000	-5.022770000
Li	-1.273880000	1.283150000	1.601100000	H	7.992330000	1.347200000	-3.819910000
Br	-2.750360000	-0.276720000	2.825140000	H	7.715960000	0.098670000	-1.648620000
TSA2-Doublet				C	0.237980000	-4.421470000	0.191310000
Fe	-0.269420000	0.149940000	-0.993970000	C	0.616590000	-5.635470000	-0.397530000
N	1.274790000	-1.098590000	-1.188530000	C	0.018260000	-4.464020000	1.576370000
N	-1.563770000	-1.339250000	-0.955360000	C	0.768280000	-6.812520000	0.330450000
N	1.033450000	1.663600000	-0.982910000	C	0.158690000	-5.608400000	2.348250000
N	-1.804520000	1.394380000	-0.802320000	C	0.537240000	-6.791980000	1.707810000
C	2.529390000	-0.808190000	-1.699590000	H	1.059330000	-7.723650000	-0.194180000
C	-2.920710000	-1.290650000	-1.102460000	H	0.653360000	-7.708450000	2.289880000
C	1.215260000	-2.440370000	-1.022420000	H	-0.023940000	-5.556340000	3.422180000
C	-1.243120000	-2.626490000	-0.624660000	C	-5.128950000	-0.266940000	-1.552140000
C	2.345660000	1.637020000	-1.357410000	C	-6.111980000	0.182850000	-0.653880000
C	-3.125040000	1.172570000	-1.150050000	C	-5.598140000	-0.924170000	-2.702050000
C	0.793980000	2.902370000	-0.442780000	C	-7.474470000	0.006770000	-0.882530000
C	-1.694790000	2.708550000	-0.489700000	C	-6.950760000	-1.111740000	-2.968790000
C	3.254530000	-2.031300000	-1.894890000	C	-7.888980000	-0.640590000	-2.047850000
C	-3.484620000	-2.600620000	-0.858100000	H	-8.182380000	0.374500000	-0.138540000
C	2.448830000	-3.050160000	-1.441960000	H	-8.954830000	-0.782520000	-2.239220000
C	-2.451830000	-3.419560000	-0.515200000	H	-7.242040000	-1.621740000	-3.887970000
C	2.967250000	2.906960000	-1.047320000	C	-0.652800000	4.502120000	0.848100000
C	-3.840990000	2.407600000	-1.098130000	C	-1.238490000	4.260300000	2.101940000
C	2.021850000	3.671130000	-0.425840000	C	-0.303970000	5.835510000	0.593320000
C	-2.958000000	3.364350000	-0.645520000	C	-1.467930000	5.239870000	3.054190000
H	4.258650000	-2.113010000	-2.302920000	C	-0.516880000	6.858320000	1.514420000
H	-4.543080000	-2.843810000	-0.896490000	C	-1.100300000	6.554120000	2.745860000
H	2.663750000	-4.114280000	-1.437880000	H	-1.916310000	4.966120000	4.009840000
H	-2.488880000	-4.473840000	-0.251710000	H	-0.226770000	7.875550000	1.247550000
H	4.004340000	3.165050000	-1.248390000	H	-1.270070000	7.348210000	3.475680000
H	-4.893500000	2.539740000	-1.333050000	F	0.834540000	-5.659150000	-1.718860000
H	2.128100000	4.685740000	-0.053610000	F	-0.337110000	-3.311520000	2.200480000
H	-3.147510000	4.419740000	-0.464050000	F	3.538110000	1.881070000	-4.184130000
				F	0.246710000	6.135480000	-0.589890000

F	5.458310000	-0.389780000	-0.529970000	C	-3.447170000	-2.860100000	-0.928810000
F	-1.580700000	2.975820000	2.406710000	C	2.533910000	-2.851010000	-1.566840000
F	-4.700980000	-1.385390000	-3.579600000	C	-2.338810000	-3.637430000	-0.741030000
F	-5.730340000	0.791520000	0.469390000	C	2.547690000	3.125100000	-1.437850000
Cl	-0.428950000	0.275580000	-3.239860000	C	-4.167830000	2.078480000	-0.487560000
O	-0.165410000	0.072180000	0.935710000	C	1.591110000	3.833070000	-0.770020000
C	3.607510000	-1.256960000	1.440810000	C	-3.318700000	3.078680000	-0.108910000
C	3.262510000	0.094800000	1.747830000	H	4.244470000	-1.775080000	-2.441520000
C	4.311530000	0.996110000	2.426450000	H	-4.488060000	-3.176490000	-0.941610000
C	5.626680000	0.263880000	2.730940000	H	2.873770000	-3.879310000	-1.472950000
C	5.360180000	-1.156540000	3.241580000	H	-2.287790000	-4.713830000	-0.590090000
C	4.678630000	-1.989100000	2.149660000	H	3.547230000	3.452750000	-1.715520000
H	2.970610000	-1.819310000	0.757540000	H	-5.254900000	2.103990000	-0.507120000
H	2.404360000	-0.095650000	2.535250000	H	1.648020000	4.859010000	-0.413730000
H	0.717180000	0.331760000	1.230730000	H	-3.568710000	4.082430000	0.228920000
H	2.720180000	0.584830000	0.926120000	C	2.773190000	0.702850000	-2.104040000
H	4.502090000	1.865450000	1.776980000	C	-3.828470000	-0.366750000	-1.046080000
H	3.878400000	1.393760000	3.358890000	C	-0.806810000	3.336070000	-0.129130000
H	6.214060000	0.837890000	3.464940000	C	0.144600000	-3.171950000	-0.800910000
H	6.236040000	0.201510000	1.812680000	C	4.138950000	0.984670000	-2.631880000
H	6.293040000	-1.647440000	3.559910000	C	4.320390000	1.627330000	-3.864880000
H	4.701460000	-1.111560000	4.126510000	C	5.311780000	0.676300000	-1.929660000
H	4.269950000	-2.939670000	2.544410000	C	5.572210000	1.933680000	-4.388720000
H	5.412250000	-2.307540000	1.378170000	C	6.585980000	0.961950000	-2.408830000
Li	-0.674200000	-1.268170000	2.267030000	C	6.708720000	1.593810000	-3.649600000
Br	0.875710000	-0.308390000	3.997040000	H	5.637770000	2.430030000	-5.358420000
Li	-1.601880000	1.037970000	1.697720000	H	7.700700000	1.826250000	-4.043320000
Br	-3.071210000	-0.675520000	2.444470000	H	7.455000000	0.691950000	-1.806370000
PCA-Doublet				C	0.429710000	-4.478280000	-0.151050000
Fe	-0.455650000	0.140220000	-1.165480000	C	0.864230000	-5.641190000	-0.795200000
N	1.128680000	-1.026050000	-1.486010000	C	0.267240000	-4.580400000	1.236350000
N	-1.618790000	-1.463470000	-1.009920000	C	1.118760000	-6.829290000	-0.115600000
N	0.722140000	1.741770000	-1.202200000	C	0.506660000	-5.732930000	1.967170000
N	-2.022460000	1.280070000	-0.735550000	C	0.937480000	-6.867670000	1.269670000
C	2.356230000	-0.629750000	-1.950730000	H	1.452290000	-7.702930000	-0.678280000
C	-2.989360000	-1.493840000	-1.059060000	H	1.134410000	-7.793070000	1.815120000
C	1.208120000	-2.369950000	-1.242430000	H	0.361170000	-5.732790000	3.048420000
C	-1.197740000	-2.754360000	-0.830380000	C	-5.297490000	-0.596830000	-1.147380000
C	2.008820000	1.797810000	-1.662830000	C	-6.171200000	-0.441060000	-0.062930000
C	-3.347530000	0.934610000	-0.828010000	C	-5.883520000	-1.028490000	-2.345630000
C	0.438250000	2.965410000	-0.657560000	C	-7.540000000	-0.675190000	-0.148160000
C	-1.976640000	2.575510000	-0.302660000	C	-7.245780000	-1.275250000	-2.482200000
C	3.224550000	-1.785180000	-2.065070000	C	-8.073540000	-1.093200000	-1.370670000
				H	-8.161200000	-0.533040000	0.737850000

H	-9.145880000	-1.282220000	-1.457330000	RCB-Quartet			
H	-7.634560000	-1.603660000	-3.447640000	Fe	0.423043000	0.074242000	0.874654000
C	-0.905590000	4.530780000	0.750520000	N	-0.928068000	-1.355445000	1.158911000
C	-1.076160000	4.340360000	2.126670000	N	1.878080000	-1.259741000	0.912739000
C	-0.848730000	5.862790000	0.327790000	N	-1.025402000	1.425205000	1.030137000
C	-1.189280000	5.367120000	3.049790000	N	1.781339000	1.508230000	0.792552000
C	-0.958630000	6.937230000	1.206510000	C	-2.196199000	-1.221721000	1.695991000
C	-1.130730000	6.680900000	2.569630000	C	3.204366000	-1.044719000	1.033808000
H	-1.315930000	5.137670000	4.108900000	C	-0.734179000	-2.667982000	0.911711000
H	-0.909940000	7.953880000	0.812670000	C	1.711930000	-2.575931000	0.540737000
H	-1.218020000	7.514560000	3.269660000	C	-2.296353000	1.236724000	1.453697000
F	1.041790000	-5.596790000	-2.125600000	C	3.128677000	1.423662000	1.072101000
F	-0.146090000	-3.459430000	1.910550000	C	-0.948321000	2.703288000	0.524190000
F	3.224810000	1.963090000	-4.567780000	C	1.525421000	2.786672000	0.442519000
F	-0.680020000	6.102060000	-0.982370000	C	-2.781694000	-2.536745000	1.844138000
F	5.195730000	0.078800000	-0.728870000	C	3.931285000	-2.271200000	0.771102000
F	-1.119570000	3.046790000	2.586220000	C	-1.903378000	-3.427791000	1.299176000
F	-5.081940000	-1.212520000	-3.409110000	C	3.007849000	-3.208763000	0.415939000
F	-5.654770000	-0.053290000	1.116830000	C	-3.069272000	2.443369000	1.236822000
Cl	-0.869400000	0.298900000	-3.390540000	C	3.716206000	2.741515000	0.966302000
O	-0.081520000	0.002430000	0.780030000	C	-2.247555000	3.333019000	0.606331000
C	2.271070000	-0.868870000	3.307850000	C	2.735171000	3.576922000	0.515730000
C	2.687680000	-1.749350000	2.135130000	H	-3.755746000	-2.751449000	2.274398000
C	4.191270000	-1.700030000	1.851350000	H	5.012177000	-2.381118000	0.814822000
C	5.008390000	-2.004420000	3.113040000	H	-2.017195000	-4.504836000	1.214523000
C	4.626280000	-1.069250000	4.268340000	H	3.171832000	-4.248205000	0.139851000
C	3.119790000	-1.109250000	4.549820000	H	-4.123259000	2.566437000	1.473529000
H	1.200130000	-0.957790000	3.533270000	H	4.753663000	2.989579000	1.172803000
H	2.106220000	-1.509460000	1.233730000	H	-2.486808000	4.338889000	0.270872000
H	0.866900000	0.187780000	0.859150000	H	2.802653000	4.639985000	0.294541000
H	2.396730000	-2.776550000	2.422820000	C	-2.845579000	-0.002952000	1.895196000
H	4.433980000	-2.411870000	1.046060000	C	3.821747000	0.224480000	1.239705000
H	4.451820000	-0.699080000	1.470440000	C	0.242007000	3.313014000	0.127454000
H	6.087020000	-1.922040000	2.898020000	C	0.484995000	-3.221537000	0.420619000
H	4.824830000	-3.051050000	3.419140000	C	-4.204868000	0.044921000	2.493344000
H	5.177960000	-1.339190000	5.183770000	C	-4.440532000	0.808574000	3.650288000
H	4.919640000	-0.035140000	4.015940000	C	-5.332290000	-0.582866000	1.940174000
H	2.838820000	-0.408220000	5.350730000	C	-5.692884000	0.939369000	4.236467000
H	2.840650000	-2.120560000	4.901770000	C	-6.606949000	-0.468804000	2.483913000
Li	-0.803350000	-1.549660000	1.547410000	C	-6.780920000	0.294955000	3.640410000
Br	2.398600000	1.101110000	2.771830000	H	-5.797562000	1.541014000	5.140763000
Li	-0.915830000	1.127900000	2.041700000	H	-7.775354000	0.390955000	4.081655000
Br	-1.906730000	-0.570320000	3.490580000	H	-7.438526000	-0.974273000	1.990448000
				C	0.460105000	-4.512102000	-0.313758000

C	0.229100000	-5.768447000	0.257711000	H	-1.835408000	-3.094248000	-1.575173000
C	0.677196000	-4.502245000	-1.698422000	C	-3.431375000	-1.789627000	-2.208896000
C	0.210425000	-6.941825000	-0.488932000	C	-4.807881000	-1.968144000	-2.417595000
C	0.661782000	-5.637685000	-2.491520000	C	-5.725543000	-0.940919000	-2.168187000
C	0.425691000	-6.868006000	-1.867855000	C	-5.250812000	0.287346000	-1.709687000
H	0.030168000	-7.891263000	0.018004000	C	-3.884785000	0.503580000	-1.514144000
H	0.410571000	-7.781023000	-2.466648000	C	-2.986668000	-0.535791000	-1.752554000
H	0.827965000	-5.549832000	-3.566177000	H	-5.178298000	-2.933286000	-2.775326000
C	5.274487000	0.228034000	1.544475000	H	-6.795949000	-1.099927000	-2.312684000
C	6.253924000	0.779729000	0.702121000	H	-3.529742000	1.472397000	-1.165127000
C	5.750295000	-0.394862000	2.711236000	Cl	-6.388435000	1.572009000	-1.310542000
C	7.612889000	0.734323000	0.997486000				
C	7.095901000	-0.454779000	3.049728000				
C	8.028832000	0.116927000	2.179559000	RCB-Doublet			
H	8.320594000	1.177963000	0.295194000	Fe	0.421926000	0.073923000	0.876066000
H	9.092478000	0.077837000	2.424570000	N	-0.930903000	-1.354443000	1.161616000
H	7.390825000	-0.944732000	3.979110000	N	1.877742000	-1.262693000	0.915970000
C	0.220321000	4.540971000	-0.704201000	N	-1.025505000	1.426783000	1.031278000
C	0.661876000	4.452179000	-2.031198000	N	1.783396000	1.507585000	0.796741000
C	-0.197722000	5.807497000	-0.281305000	C	-2.200781000	-1.218476000	1.695452000
C	0.693645000	5.522990000	-2.908721000	C	3.204460000	-1.048338000	1.029136000
C	-0.180552000	6.919279000	-1.117896000	C	-0.736704000	-2.667936000	0.921364000
C	0.266436000	6.768517000	-2.433356000	C	1.709071000	-2.579613000	0.547507000
H	1.040632000	5.376709000	-3.932702000	C	-2.298587000	1.239037000	1.447184000
H	-0.514024000	7.882448000	-0.728120000	C	3.131724000	1.420062000	1.073693000
H	0.281832000	7.632934000	-3.100505000	C	-0.944817000	2.706345000	0.527667000
F	0.024048000	-5.830139000	1.582783000	C	1.529048000	2.787365000	0.453593000
F	0.899166000	-3.295733000	-2.300990000	C	-2.786125000	-2.533046000	1.849083000
F	-3.394526000	1.438037000	4.210614000	C	3.929753000	-2.275527000	0.764953000
F	-0.621192000	5.943809000	0.984265000	C	-1.906398000	-3.426391000	1.310777000
F	-5.179932000	-1.311747000	0.825199000	C	3.004112000	-3.213562000	0.417461000
F	1.068148000	3.225710000	-2.480651000	C	-3.070086000	2.446250000	1.227049000
F	4.848339000	-0.953037000	3.536025000	C	3.720174000	2.738216000	0.974800000
F	5.868723000	1.359802000	-0.441122000	C	-2.244606000	3.336242000	0.602664000
Cl	0.614672000	0.192964000	3.213169000	C	2.739242000	3.576859000	0.530493000
O	0.320833000	0.001264000	-0.798918000	H	-3.761118000	-2.745829000	2.278128000
Li	0.949209000	-1.258525000	-2.194937000	H	5.010817000	-2.385659000	0.803235000
Br	-0.238922000	-0.032842000	-4.055024000	H	-2.019516000	-4.503896000	1.231375000
Li	1.002539000	1.180354000	-2.249207000	H	3.165999000	-4.253889000	0.143485000
Br	3.198488000	-0.106079000	-2.291253000	H	-4.125307000	2.569294000	1.458213000
H	-1.922450000	-0.365004000	-1.580407000	H	4.758129000	2.984201000	1.181329000
C	-2.437706000	-2.889703000	-2.473393000	H	-2.481134000	4.342890000	0.267626000
H	-1.735406000	-2.587191000	-3.267856000	H	2.806988000	4.641072000	0.315031000
H	-2.929414000	-3.827294000	-2.773355000	C	-2.850433000	0.000264000	1.889101000
				C	3.824146000	0.220471000	1.234476000

C	0.246332000	3.315923000	0.136561000	F	4.857552000	-0.965186000	3.523721000
C	0.481746000	-3.224131000	0.430712000	F	5.866504000	1.360859000	-0.448741000
C	-4.211313000	0.050398000	2.483454000	Cl	0.613924000	0.193587000	3.217736000
C	-4.450212000	0.818133000	3.637026000	O	0.321576000	0.000918000	-0.797620000
C	-5.337273000	-0.579320000	1.929493000	Li	0.950013000	-1.259610000	-2.190227000
C	-5.704196000	0.951378000	4.219112000	Br	-0.235089000	-0.032283000	-4.052873000
C	-6.613484000	-0.463005000	2.469132000	Li	1.006747000	1.178634000	-2.244974000
C	-6.790669000	0.305052000	3.622271000	Br	3.202118000	-0.111867000	-2.291242000
H	-5.811308000	1.556362000	5.120884000	H	-1.925666000	-0.357589000	-1.581635000
H	-7.786356000	0.402870000	4.060282000	C	-2.435443000	-2.886020000	-2.466903000
H	-7.443713000	-0.970210000	1.975180000	H	-1.731417000	-2.584784000	-3.260133000
C	0.453996000	-4.514633000	-0.303672000	H	-2.924988000	-3.825003000	-2.765664000
C	0.221207000	-5.770653000	0.267779000	H	-1.835548000	-3.087451000	-1.566522000
C	0.669944000	-4.504863000	-1.688567000	C	-3.431303000	-1.786592000	-2.208023000
C	0.199508000	-6.943866000	-0.479009000	C	-4.807146000	-1.968181000	-2.418414000
C	0.651497000	-5.640202000	-2.481792000	C	-5.727011000	-0.941813000	-2.173772000
C	0.413525000	-6.870172000	-1.858137000	C	-5.255174000	0.288632000	-1.718138000
H	0.017927000	-7.893048000	0.027937000	C	-3.889827000	0.507894000	-1.521024000
H	0.396012000	-7.783051000	-2.457078000	C	-2.989418000	-0.530556000	-1.754925000
H	0.816878000	-5.552529000	-3.556583000	H	-5.175280000	-2.935125000	-2.773639000
C	5.277893000	0.221977000	1.534594000	H	-6.796896000	-1.103167000	-2.319535000
C	6.254917000	0.776062000	0.690950000	H	-3.537133000	1.478438000	-1.174312000
C	5.757200000	-0.405015000	2.697714000	Cl	-6.395717000	1.572527000	-1.324859000
C	7.614822000	0.728782000	0.981739000	TSB1-Quartet			
C	7.103858000	-0.467050000	3.031546000				
C	8.034289000	0.107017000	2.160257000	Fe	0.406550000	0.323404000	-0.838479000
H	8.320483000	1.174597000	0.278772000	N	-0.067013000	2.235762000	-0.619108000
H	9.098706000	0.066479000	2.401661000	N	2.310307000	0.722917000	-0.627544000
H	7.401518000	-0.960341000	3.958282000	N	-1.500598000	-0.066417000	-1.187070000
C	0.228493000	4.544675000	-0.694069000	N	0.885552000	-1.560007000	-1.133220000
C	0.671910000	4.455881000	-2.020417000	C	-1.209125000	2.874904000	-1.022136000
C	-0.186702000	5.811798000	-0.270335000	C	3.373842000	-0.027396000	-1.016320000
C	0.708495000	5.527718000	-2.896540000	C	0.707217000	3.155113000	0.019264000
C	-0.164806000	6.924527000	-1.105568000	C	2.804293000	1.824325000	0.016169000
C	0.284194000	6.773957000	-2.420360000	C	-2.474147000	0.816559000	-1.564108000
H	1.056897000	5.381773000	-3.920087000	C	2.095596000	-2.085214000	-1.497317000
H	-0.496241000	7.888207000	-0.715305000	C	-2.088365000	-1.289838000	-1.069404000
H	0.303407000	7.639147000	-3.086407000	C	0.015916000	-2.600707000	-1.009790000
F	0.017294000	-5.832147000	1.593064000	C	-1.130781000	4.271270000	-0.657514000
F	0.894069000	-3.298780000	-2.291122000	C	4.603094000	0.631362000	-0.632278000
F	-3.405661000	1.449356000	4.198167000	C	0.030169000	4.431615000	0.047640000
F	-0.612311000	5.947615000	0.994583000	C	4.249057000	1.757022000	0.055669000
F	-5.181784000	-1.312657000	0.817889000	C	-3.721613000	0.108960000	-1.741753000
F	1.075226000	3.228583000	-2.470292000	C	1.969468000	-3.516916000	-1.660327000

C	-3.497166000	-1.188045000	-1.375620000	C	-2.359656000	-5.104916000	1.740470000
C	0.697028000	-3.846545000	-1.289259000	C	-3.712218000	-5.479038000	-0.243804000
H	-1.876900000	5.029582000	-0.878202000	C	-3.355926000	-5.817431000	1.064279000
H	5.604887000	0.253679000	-0.823426000	H	-2.064557000	-5.341306000	2.763747000
H	0.413361000	5.345753000	0.493238000	H	-4.478508000	-6.027601000	-0.793950000
H	4.898965000	2.500390000	0.512654000	H	-3.858424000	-6.648095000	1.563994000
H	-4.666751000	0.560455000	-2.032588000	F	2.864881000	5.640577000	-0.020641000
H	2.757904000	-4.191375000	-1.981745000	F	2.529084000	2.050175000	3.022932000
H	-4.220894000	-1.995966000	-1.333198000	F	-3.173601000	2.171371000	-4.219031000
H	0.235533000	-4.831628000	-1.266577000	F	-3.393408000	-4.102850000	-2.127802000
C	-2.336014000	2.219832000	-1.558852000	F	-3.962563000	3.914913000	0.087522000
C	3.290127000	-1.341414000	-1.538737000	F	-0.789388000	-3.344243000	1.741269000
C	-1.373797000	-2.480503000	-0.800943000	F	4.637041000	-0.281577000	-3.719575000
C	2.031651000	2.911787000	0.456747000	F	4.622601000	-3.651743000	-0.422559000
C	-3.490225000	3.021083000	-2.046686000	Cl	0.657246000	0.691708000	-3.115875000
C	-3.884055000	2.956125000	-3.392990000	O	0.215582000	0.038133000	0.963427000
C	-4.274045000	3.839664000	-1.221308000	Li	1.573616000	0.359979000	2.407768000
C	-4.965744000	3.664305000	-3.903259000	Br	0.191159000	-0.648223000	4.290825000
C	-5.369855000	4.559145000	-1.682795000	Li	0.381942000	-1.688963000	1.929694000
C	-5.709071000	4.469392000	-3.035716000	Br	2.891190000	-1.736369000	1.907515000
H	-5.208880000	3.573911000	-4.963249000	H	-2.160693000	-1.388840000	2.890017000
H	-6.564897000	5.030419000	-3.417318000	C	-1.861087000	1.167236000	2.007902000
H	-5.938507000	5.170464000	-0.980217000	H	-1.398493000	1.183272000	3.004027000
C	2.663096000	3.817092000	1.450057000	H	-1.966489000	2.164049000	1.562283000
C	3.064966000	5.135593000	1.206466000	H	-0.882838000	0.613744000	1.404490000
C	2.908883000	3.333351000	2.741723000	C	-3.062353000	0.320639000	1.911333000
C	3.667034000	5.928920000	2.177905000	C	-4.251010000	0.797556000	1.320963000
C	3.498068000	4.080098000	3.748962000	C	-5.378261000	-0.014475000	1.192847000
C	3.879200000	5.393364000	3.451163000	C	-5.312928000	-1.340233000	1.626561000
H	3.962384000	6.948095000	1.923102000	C	-4.159059000	-1.842079000	2.240734000
H	4.348913000	6.005975000	4.223557000	C	-3.054121000	-1.009071000	2.391204000
H	3.649015000	3.637779000	4.734826000	H	-4.290025000	1.822924000	0.953277000
C	4.542249000	-1.948357000	-2.056847000	H	-6.287025000	0.366806000	0.723762000
C	5.175202000	-3.068358000	-1.493168000	H	-4.125839000	-2.877202000	2.583693000
C	5.196677000	-1.365492000	-3.156538000	Cl	-6.681297000	-2.409520000	1.368320000
C	6.365671000	-3.590590000	-1.989691000				
C	6.380414000	-1.859311000	-3.689940000	TSB1-Doublet			
C	6.963864000	-2.981753000	-3.095367000	Fe	0.385673000	0.335287000	-0.854767000
H	6.805646000	-4.460224000	-1.498714000	N	-0.110115000	2.236096000	-0.630878000
H	7.896490000	-3.384196000	-3.496740000	N	2.297825000	0.760526000	-0.653714000
H	6.824325000	-1.361886000	-4.553785000	N	-1.513870000	-0.084057000	-1.187467000
C	-2.071083000	-3.659060000	-0.231698000	N	0.895451000	-1.553268000	-1.147525000
C	-1.748000000	-4.056360000	1.074235000	C	-1.267303000	2.860495000	-1.024923000
C	-3.065114000	-4.416123000	-0.864833000	C	3.368423000	0.010491000	-1.010519000

C	0.661838000	3.172393000	-0.015469000	C	4.566646000	-1.903232000	-2.034151000
C	2.777432000	1.870643000	-0.012365000	C	5.204297000	-3.022299000	-1.473395000
C	-2.507710000	0.782177000	-1.540116000	C	5.228092000	-1.304683000	-3.121564000
C	2.116639000	-2.063999000	-1.505521000	C	6.406533000	-3.526798000	-1.960038000
C	-2.083187000	-1.321834000	-1.066509000	C	6.423097000	-1.781083000	-3.645160000
C	0.041387000	-2.601342000	-1.036095000	C	7.011620000	-2.902140000	-3.052957000
C	-1.197554000	4.261698000	-0.678283000	H	6.849631000	-4.396207000	-1.471491000
C	4.590293000	0.677029000	-0.615283000	H	7.953317000	-3.291140000	-3.446311000
C	-0.028661000	4.442283000	0.007017000	H	6.871470000	-1.271701000	-4.499676000
C	4.221942000	1.811538000	0.049640000	C	-2.024735000	-3.689928000	-0.238734000
C	-3.748774000	0.057719000	-1.697218000	C	-1.675491000	-4.085837000	1.060907000
C	2.005652000	-3.494911000	-1.682798000	C	-3.017640000	-4.459411000	-0.858277000
C	-3.499643000	-1.236734000	-1.342539000	C	-2.261528000	-5.144463000	1.734072000
C	0.732934000	-3.839213000	-1.325029000	C	-3.639320000	-5.533303000	-0.229953000
H	-1.954911000	5.009236000	-0.896986000	C	-3.257803000	-5.869796000	1.071455000
H	5.595876000	0.298941000	-0.784099000	H	-1.946915000	-5.379103000	2.751940000
H	0.351426000	5.365507000	0.436172000	H	-4.406185000	-6.091569000	-0.769429000
H	4.861750000	2.563464000	0.506800000	H	-3.740355000	-6.708958000	1.576606000
H	-4.704970000	0.497444000	-1.968971000	F	2.792806000	5.686917000	-0.065170000
H	2.803077000	-4.159582000	-2.002391000	F	2.491495000	2.103879000	2.991470000
H	-4.210474000	-2.055487000	-1.291970000	F	-3.285674000	2.098967000	-4.180570000
H	0.280162000	-4.828484000	-1.312785000	F	-3.371075000	-4.147372000	-2.114759000
C	-2.390946000	2.190002000	-1.540744000	F	-4.004032000	3.886805000	0.120729000
C	3.302589000	-1.311196000	-1.528157000	F	-0.716229000	-3.361518000	1.714152000
C	-1.352763000	-2.499552000	-0.813796000	F	4.663149000	-0.222409000	-3.682728000
C	1.991840000	2.950173000	0.418970000	F	4.645517000	-3.623436000	-0.416260000
C	-3.565326000	2.971307000	-2.012265000	Cl	0.632535000	0.689869000	-3.138453000
C	-3.988193000	2.884829000	-3.348705000	O	0.241086000	0.033562000	0.947241000
C	-4.342064000	3.790127000	-1.180044000	Li	1.597520000	0.379306000	2.381575000
C	-5.089915000	3.572304000	-3.843882000	Br	0.243599000	-0.670866000	4.268986000
C	-5.457072000	4.489473000	-1.626351000	Li	0.445349000	-1.693281000	1.901254000
C	-5.824661000	4.378624000	-2.970175000	Br	2.961443000	-1.699133000	1.894925000
H	-5.354679000	3.465554000	-4.897136000	H	-2.109003000	-1.437024000	2.851721000
H	-6.695862000	4.923879000	-3.339663000	C	-1.836304000	1.137362000	2.015310000
H	-6.018100000	5.102220000	-0.918897000	H	-1.365395000	1.146381000	3.007997000
C	2.608753000	3.866715000	1.411497000	H	-1.951408000	2.138062000	1.580945000
C	2.995228000	5.189110000	1.164586000	H	-0.864995000	0.596204000	1.403354000
C	2.855726000	3.390880000	2.705967000	C	-3.035502000	0.287502000	1.923689000
C	3.583625000	5.993698000	2.135103000	C	-4.236470000	0.771553000	1.364720000
C	3.431763000	4.148828000	3.712477000	C	-5.363573000	-0.041740000	1.243763000
C	3.797612000	5.465633000	3.411181000	C	-5.285320000	-1.375102000	1.651168000
H	3.867215000	7.015503000	1.877492000	C	-4.117770000	-1.884990000	2.232522000
H	4.256816000	6.086901000	4.182984000	C	-3.013112000	-1.051043000	2.377796000
H	3.584717000	3.712115000	4.700531000	H	-4.285250000	1.803468000	1.017001000

H	-6.282744000	0.345067000	0.800245000	H	-5.298304000	3.294078000	-4.971497000
H	-4.074526000	-2.926514000	2.554528000	H	-6.668008000	4.761484000	-3.447947000
Cl	-6.655673000	-2.443372000	1.402132000	H	-6.008373000	4.991476000	-1.026941000
ICBI-Quartet				C	2.692757000	3.896449000	1.250147000
Fe	0.466474000	0.285064000	-0.909277000	C	3.071457000	5.209143000	0.945549000
N	-0.044140000	2.193805000	-0.708221000	C	2.956712000	3.473325000	2.559555000
N	2.370377000	0.704036000	-0.682840000	C	3.667443000	6.054051000	1.876220000
N	-1.447772000	-0.141638000	-1.170331000	C	3.540302000	4.273571000	3.528186000
N	0.970472000	-1.612635000	-1.085720000	C	3.897225000	5.578558000	3.170110000
C	-1.208234000	2.804927000	-1.098554000	H	3.944234000	7.065672000	1.574762000
C	3.445856000	-0.059396000	-1.007100000	H	4.361839000	6.232288000	3.911252000
C	0.732054000	3.149310000	-0.125505000	H	3.705488000	3.877771000	4.531361000
C	2.848460000	1.839952000	-0.087338000	C	4.650684000	-2.030795000	-1.903428000
C	-2.452310000	0.711220000	-1.529332000	C	5.264918000	-3.114628000	-1.254225000
C	2.190395000	-2.147270000	-1.410121000	C	5.345302000	-1.506502000	-3.007793000
C	-2.014190000	-1.371866000	-0.991727000	C	6.475168000	-3.657515000	-1.674786000
C	0.112088000	-2.653432000	-0.918357000	C	6.550124000	-2.023235000	-3.466993000
C	-1.142505000	4.213784000	-0.787178000	C	7.113634000	-3.107907000	-2.788934000
C	4.664822000	0.623439000	-0.634319000	H	6.898305000	-4.496111000	-1.119215000
C	0.036584000	4.416445000	-0.125158000	H	8.062378000	-3.527004000	-3.131159000
C	4.292421000	1.784254000	-0.018552000	H	7.025580000	-1.572082000	-4.339376000
C	-3.697623000	-0.015768000	-1.626437000	C	-1.960909000	-3.702455000	-0.080272000
C	2.076343000	-3.585227000	-1.510203000	C	-1.640368000	-4.032291000	1.244472000
C	-3.436634000	-1.298573000	-1.237253000	C	-2.941472000	-4.499820000	-0.683130000
C	0.801844000	-3.905938000	-1.138185000	C	-2.238229000	-5.060549000	1.953739000
H	-1.910608000	4.949548000	-1.009386000	C	-3.574660000	-5.544558000	-0.018386000
H	5.671811000	0.240204000	-0.781895000	C	-3.218289000	-5.819471000	1.304372000
H	0.416268000	5.351190000	0.278487000	H	-1.946211000	-5.245580000	2.988445000
H	4.930625000	2.553662000	0.410776000	H	-4.332711000	-6.126345000	-0.545170000
H	-4.659752000	0.413918000	-1.891875000	H	-3.710129000	-6.635045000	1.838373000
H	2.872780000	-4.268128000	-1.791703000	F	2.853706000	5.656180000	-0.300870000
H	-4.143272000	-2.117098000	-1.147902000	F	2.602718000	2.197597000	2.898306000
H	0.346849000	-4.892078000	-1.072397000	F	-3.215059000	1.967884000	-4.217283000
C	-2.338730000	2.116961000	-1.579239000	F	-3.274788000	-4.239808000	-1.956715000
C	3.380786000	-1.401215000	-1.460713000	F	-3.985896000	3.819771000	0.046185000
C	-1.280154000	-2.539449000	-0.700718000	F	-0.704506000	-3.267149000	1.884234000
C	2.065472000	2.939898000	0.302612000	F	4.805599000	-0.457368000	-3.650201000
C	-3.519380000	2.877827000	-2.068138000	F	4.673694000	-3.639364000	-0.174226000
C	-3.933105000	2.760038000	-3.405070000	Cl	0.688053000	0.562748000	-3.173794000
C	-4.312627000	3.698451000	-1.254278000	O	0.275069000	0.067502000	0.985239000
C	-5.040895000	3.423426000	-3.918959000	Li	1.631828000	0.477550000	2.364716000
C	-5.434116000	4.374556000	-1.720001000	Br	-0.014327000	-0.215157000	4.174852000
C	-5.791665000	4.234963000	-3.063748000	Li	0.436474000	-1.585685000	2.013019000
				Br	2.933009000	-1.641832000	2.097578000

H	-2.429255000	-0.895818000	2.887810000	H	-4.866102000	0.331900000	-1.200907000
C	-2.756151000	1.707464000	2.257041000	H	-2.461478000	-4.375963000	-1.431667000
H	-1.837465000	1.513291000	2.817502000	C	-1.138146000	3.059578000	-1.512154000
H	-2.977857000	2.728389000	1.941754000	C	1.963159000	-3.010474000	-1.338389000
H	-0.550330000	0.511619000	1.241936000	C	-2.679322000	-1.549010000	-1.010576000
C	-3.663788000	0.661514000	1.994028000	C	3.298945000	1.546083000	-0.242539000
C	-4.913332000	0.898821000	1.338329000	C	-1.812403000	4.361250000	-1.792433000
C	-5.789093000	-0.138512000	1.051075000	C	-2.361794000	4.636567000	-3.052819000
C	-5.436062000	-1.452150000	1.395172000	C	-1.970367000	5.367342000	-0.830350000
C	-4.232096000	-1.728635000	2.061828000	C	-3.013996000	5.826574000	-3.358351000
C	-3.364738000	-0.689224000	2.362086000	C	-2.615467000	6.573265000	-1.083849000
H	-5.171435000	1.919223000	1.047744000	C	-3.136696000	6.798046000	-2.360972000
H	-6.730887000	0.055690000	0.534144000	H	-3.412776000	5.973302000	-4.363565000
H	-3.980411000	-2.756684000	2.326379000	H	-3.645910000	7.739095000	-2.580466000
Cl	-6.485673000	-2.781608000	0.938461000	H	-2.701140000	7.309892000	-0.283162000
IC1B-Doublet				C	4.439662000	2.105228000	0.530427000
Fe	0.381745000	0.035879000	-1.109488000	C	5.354137000	3.051491000	0.053383000
N	0.997886000	1.932047000	-1.019159000	C	4.654437000	1.665428000	1.845777000
N	2.261966000	-0.596073000	-0.898707000	C	6.397947000	3.554911000	0.823976000
N	-1.531467000	0.625475000	-1.235583000	C	5.675266000	2.136613000	2.659039000
N	-0.229498000	-1.902363000	-1.071647000	C	6.550758000	3.093401000	2.134183000
C	0.241018000	3.047912000	-1.275602000	H	7.073808000	4.292159000	0.387160000
C	2.734873000	-1.871026000	-1.061483000	H	7.364042000	3.479304000	2.752698000
C	2.220359000	2.373958000	-0.597817000	H	5.774354000	1.753615000	3.675973000
C	3.324172000	0.167481000	-0.494854000	C	2.676070000	-4.298415000	-1.565509000
C	-1.956561000	1.912884000	-1.432836000	C	2.599371000	-5.372842000	-0.668164000
C	0.562520000	-3.002600000	-1.338341000	C	3.493421000	-4.498932000	-2.686969000
C	-2.658728000	-0.150864000	-1.133604000	C	3.274024000	-6.574341000	-0.858603000
C	-1.530926000	-2.348694000	-1.112913000	C	4.185737000	-5.681848000	-2.924202000
C	1.047040000	4.238006000	-1.081319000	C	4.069727000	-6.722579000	-1.998317000
C	4.155339000	-1.908358000	-0.780051000	H	3.170497000	-7.367531000	-0.116149000
C	2.252162000	3.822257000	-0.607157000	H	4.606600000	-7.658916000	-2.166008000
C	4.514294000	-0.651209000	-0.397442000	H	4.799944000	-5.769539000	-3.822022000
C	-3.403543000	1.950187000	-1.479951000	C	-3.964515000	-2.252712000	-0.756152000
C	-0.267048000	-4.167412000	-1.531765000	C	-4.141362000	-2.952965000	0.446302000
C	-3.838586000	0.678322000	-1.259838000	C	-5.042086000	-2.297306000	-1.649675000
C	-1.560746000	-3.770673000	-1.358671000	C	-5.307508000	-3.632774000	0.775212000
H	0.715892000	5.260346000	-1.245671000	C	-6.231231000	-2.963671000	-1.369954000
H	4.784392000	-2.793761000	-0.838612000	C	-6.358814000	-3.628961000	-0.147319000
H	3.096648000	4.439437000	-0.314945000	H	-5.379313000	-4.145619000	1.734921000
H	5.498302000	-0.295885000	-0.099892000	H	-7.031734000	-2.957253000	-2.111843000
H	-4.005847000	2.843893000	-1.623587000	H	-7.286040000	-4.156352000	0.087365000
H	0.094490000	-5.165113000	-1.769608000	F	5.213111000	3.488704000	-1.210664000
				F	3.821027000	0.714641000	2.343463000

F	-2.253432000	3.694266000	-4.005375000	C	3.906205000	2.425712000	0.106887000
F	-4.913766000	-1.670968000	-2.832116000	C	3.743288000	-2.596059000	0.005610000
F	-1.477687000	5.151500000	0.404529000	C	-1.726599000	3.593297000	-1.756270000
F	-3.117088000	-2.953609000	1.327047000	C	-1.931426000	-3.303947000	-1.981558000
F	3.609860000	-3.492534000	-3.570869000	C	-2.732537000	2.676701000	-1.800971000
F	1.839689000	-5.226894000	0.432261000	C	-2.868703000	-2.314553000	-2.042825000
Cl	0.550907000	-0.021787000	-3.374979000	H	3.237646000	4.491467000	-0.260494000
O	0.227371000	0.112600000	0.837974000	H	2.934448000	-4.600985000	-0.411086000
Li	1.584471000	0.332160000	2.212327000	H	4.902514000	2.531504000	0.528252000
Br	1.043275000	2.602481000	2.950086000	H	4.765415000	-2.774963000	0.328972000
Li	-0.201640000	-1.601338000	1.261865000	H	-1.802381000	4.670131000	-1.885682000
Br	1.110592000	-1.961716000	3.255035000	H	-2.054719000	-4.351169000	-2.246395000
H	-1.080041000	1.079821000	3.211292000	H	-3.788735000	2.863205000	-1.973870000
C	-2.554861000	2.621252000	1.599611000	H	-3.903357000	-2.391049000	-2.368693000
H	-1.548742000	3.011693000	1.790581000	C	0.711594000	3.478197000	-1.166712000
H	-3.237878000	3.218016000	0.992478000	C	0.461203000	-3.407587000	-1.222720000
H	-0.148013000	0.985225000	1.026780000	C	-2.831201000	0.165104000	-1.651946000
C	-2.963104000	1.425236000	2.150941000	C	3.780250000	-0.088071000	0.129669000
C	-4.284684000	0.911836000	1.904063000	C	0.780867000	4.967697000	-1.196827000
C	-4.703497000	-0.258159000	2.499091000	C	1.517018000	5.663063000	-2.164059000
C	-3.811978000	-0.943188000	3.353837000	C	0.132803000	5.755526000	-0.236532000
C	-2.497167000	-0.491983000	3.598597000	C	1.605203000	7.051264000	-2.198574000
C	-2.079154000	0.680285000	3.009332000	C	0.190636000	7.144858000	-0.225816000
H	-4.958881000	1.471613000	1.254930000	C	0.934009000	7.789324000	-1.219480000
H	-5.706257000	-0.651524000	2.329671000	H	2.193506000	7.529512000	-2.983554000
H	-1.828066000	-1.062163000	4.244600000	H	0.992043000	8.880002000	-1.229534000
Cl	-4.359581000	-2.368125000	4.151738000	H	-0.338514000	7.696635000	0.552950000
TSB2a-Doublet				C	5.174841000	-0.155129000	0.653913000
Fe	0.547677000	0.049332000	-1.009051000	C	6.274120000	0.316349000	-0.079182000
N	1.961411000	1.415761000	-0.619309000	C	5.475454000	-0.711623000	1.907215000
N	1.819733000	-1.444696000	-0.551021000	C	7.582730000	0.271455000	0.389862000
N	-0.773601000	1.519470000	-1.403929000	C	6.767520000	-0.775620000	2.420476000
N	-0.907599000	-1.351687000	-1.282768000	C	7.823033000	-0.276360000	1.652913000
C	1.848144000	2.778178000	-0.739975000	H	8.386880000	0.659034000	-0.237940000
C	1.625535000	-2.794261000	-0.739565000	H	8.843479000	-0.319894000	2.040019000
C	3.219014000	1.172734000	-0.120689000	H	6.925489000	-1.217036000	3.406059000
C	3.117164000	-1.298921000	-0.119348000	C	0.487282000	-4.877825000	-1.469378000
C	-0.510268000	2.865517000	-1.469139000	C	-0.284357000	-5.784401000	-0.728109000
C	-0.716838000	-2.705876000	-1.493027000	C	1.297763000	-5.441208000	-2.465925000
C	-2.125546000	1.377006000	-1.605063000	C	-0.261056000	-7.158763000	-0.946606000
C	-2.211943000	-1.095752000	-1.641549000	C	1.354085000	-6.806772000	-2.723388000
C	3.064242000	3.418455000	-0.290464000	C	0.566211000	-7.665998000	-1.952129000
C	2.820076000	-3.520309000	-0.377980000	H	-0.886141000	-7.805691000	-0.328651000
				H	0.596572000	-8.741970000	-2.137779000

H	2.006809000	-7.173092000	-3.517613000	N	-1.436093000	0.035828000	-1.362771000
C	-4.319205000	0.162499000	-1.658882000	N	0.800301000	-1.749962000	-1.204568000
C	-5.013457000	-0.405205000	-0.578859000	C	-0.817680000	2.932337000	-1.236475000
C	-5.117834000	0.670833000	-2.691204000	C	3.451757000	-0.548530000	-0.893049000
C	-6.398570000	-0.446046000	-0.490180000	C	1.146540000	3.033139000	-0.245863000
C	-6.508704000	0.648965000	-2.655704000	C	3.057293000	1.461411000	-0.094877000
C	-7.145658000	0.090730000	-1.543718000	C	-2.328037000	1.029203000	-1.665576000
H	-6.866457000	-0.883249000	0.393188000	C	1.971528000	-2.428204000	-1.448303000
H	-7.068487000	1.063518000	-3.495807000	C	-2.145701000	-1.130733000	-1.281961000
H	-8.236698000	0.070009000	-1.498689000	C	-0.205664000	-2.674436000	-1.225724000
F	6.047336000	0.835425000	-1.299328000	C	-0.568659000	4.328701000	-0.937251000
F	4.471808000	-1.219906000	2.636979000	C	4.723276000	-0.022962000	-0.438630000
F	2.169896000	4.946192000	-3.094666000	C	0.613979000	4.381438000	-0.263424000
F	-4.505481000	1.198859000	-3.764944000	C	4.472825000	1.207245000	0.093433000
F	-0.579959000	5.128792000	0.720711000	C	-3.649644000	0.460522000	-1.833095000
F	-4.287483000	-0.932680000	0.434142000	C	1.682599000	-3.828304000	-1.665898000
F	2.056353000	-4.613506000	-3.206021000	C	-3.547946000	-0.868535000	-1.540601000
F	-1.082954000	-5.299521000	0.234764000	C	0.341119000	-3.992065000	-1.474735000
Cl	1.125441000	-0.090833000	-3.187838000	H	-1.232985000	5.156754000	-1.170629000
O	0.030080000	0.174894000	0.896536000	H	5.674770000	-0.547566000	-0.490890000
Li	0.723694000	-1.071134000	2.330104000	H	1.100445000	5.262120000	0.146188000
Br	1.756855000	0.637551000	3.643630000	H	5.180372000	1.899984000	0.544110000
Li	-1.463419000	-0.950052000	0.822675000	H	-4.547318000	1.020202000	-2.085807000
Br	-1.223881000	-2.509715000	2.613987000	H	2.415504000	-4.593406000	-1.910781000
H	-1.450725000	0.609156000	4.123737000	H	-4.341701000	-1.609884000	-1.539008000
C	-1.082313000	2.054026000	1.900567000	H	-0.240297000	-4.909221000	-1.542017000
H	-0.193062000	1.999135000	2.536552000	C	-2.033398000	2.410526000	-1.698107000
H	-1.029133000	2.634334000	0.979606000	C	3.251150000	-1.865429000	-1.339784000
H	0.714482000	0.743218000	1.292783000	C	-1.579910000	-2.403713000	-1.085681000
C	-2.310070000	1.597954000	2.379241000	C	2.422401000	2.672258000	0.228534000
C	-3.513958000	1.887028000	1.667101000	C	-3.103433000	3.331368000	-2.176203000
C	-4.730697000	1.446387000	2.144351000	C	-3.534132000	3.288694000	-3.511885000
C	-4.754551000	0.667465000	3.317107000	C	-3.762720000	4.262444000	-1.361827000
C	-3.590008000	0.362139000	4.046004000	C	-4.532475000	4.111882000	-4.021382000
C	-2.374991000	0.832875000	3.585461000	C	-4.767527000	5.106930000	-1.821641000
H	-3.458516000	2.468153000	0.745410000	C	-5.148578000	5.027324000	-3.163735000
H	-5.656923000	1.660735000	1.611134000	H	-4.809120000	4.024854000	-5.073479000
H	-3.652158000	-0.246273000	4.948668000	H	-5.935030000	5.682876000	-3.544114000
Cl	-6.274412000	0.048009000	3.867184000	H	-5.235331000	5.804847000	-1.125233000
TSB2-Doublet				C	3.131894000	3.555024000	1.193055000
Fe	0.526093000	0.221810000	-1.050448000	C	3.650642000	4.824222000	0.911391000
N	0.259818000	2.180917000	-0.837159000	C	3.332680000	3.101004000	2.504827000
N	2.468830000	0.379953000	-0.686015000	C	4.299763000	5.606810000	1.861894000
				C	3.968451000	3.837487000	3.492866000

C	4.452892000	5.106561000	3.157639000	C	-4.571101000	-2.181295000	2.595556000
H	4.678785000	6.588446000	1.572394000	C	-3.285658000	-1.709956000	2.934589000
H	4.959170000	5.709208000	3.914751000	C	-2.879330000	-0.483585000	2.452040000
H	4.078601000	3.417680000	4.493952000	H	-5.695996000	0.347615000	0.625843000
C	4.450252000	-2.711026000	-1.594195000	H	-6.424243000	-1.870107000	1.505664000
C	4.796064000	-3.807723000	-0.791899000	H	-2.639607000	-2.302230000	3.583083000
C	5.330386000	-2.427838000	-2.649038000	Cl	-5.114851000	-3.677634000	3.256063000
C	5.924486000	-4.590051000	-1.016071000				
C	6.469630000	-3.180093000	-2.915320000	PCB-Doublet			
C	6.761253000	-4.268758000	-2.088555000	Fe	-0.873876000	0.266484000	0.843999000
H	6.132186000	-5.428699000	-0.349350000	N	0.215475000	1.947045000	0.777319000
H	7.651720000	-4.871467000	-2.280599000	N	-2.528775000	1.247723000	0.227815000
H	7.105652000	-2.904813000	-3.758390000	N	0.760594000	-0.731982000	1.382244000
C	-2.404453000	-3.537410000	-0.595685000	N	-1.966638000	-1.403939000	0.811998000
C	-2.128819000	-4.043817000	0.683953000	C	1.486298000	2.138599000	1.258950000
C	-3.419033000	-4.196986000	-1.297915000	C	-3.839509000	0.831142000	0.363755000
C	-2.784480000	-5.123984000	1.250665000	C	-0.192039000	3.146113000	0.247785000
C	-4.118917000	-5.280680000	-0.774259000	C	-2.576829000	2.576446000	-0.128710000
C	-3.793736000	-5.741885000	0.503829000	C	1.958296000	-0.218190000	1.806106000
H	-2.517710000	-5.454785000	2.254870000	C	-3.334171000	-1.532966000	0.813378000
H	-4.898107000	-5.750670000	-1.376818000	C	0.912949000	-2.092284000	1.307259000
H	-4.334631000	-6.590731000	0.927117000	C	-1.452601000	-2.669257000	0.841246000
F	3.516218000	5.301698000	-0.338346000	C	1.892578000	3.510191000	1.035858000
F	2.882738000	1.853273000	2.822358000	C	-4.729350000	1.917578000	0.044147000
F	-2.946459000	2.403243000	-4.334938000	C	0.873538000	4.121131000	0.370719000
F	-3.716766000	-3.767250000	-2.535792000	C	-3.949566000	2.990484000	-0.287359000
F	-3.415266000	4.334255000	-0.061077000	C	2.888793000	-1.299121000	2.057103000
F	-1.154957000	-3.421929000	1.419193000	C	-3.692038000	-2.933308000	0.871987000
F	5.052215000	-1.374408000	-3.436844000	C	2.258371000	-2.454418000	1.700502000
F	3.999710000	-4.110268000	0.248631000	C	-2.526774000	-3.640599000	0.839145000
Cl	0.883088000	0.464059000	-3.302196000	H	2.843940000	3.943981000	1.333489000
O	0.202999000	-0.006574000	0.831830000	H	-5.815671000	1.862752000	0.052258000
Li	1.294810000	0.560908000	2.336710000	H	0.834298000	5.149533000	0.020692000
Br	-0.602332000	2.309015000	3.070738000	H	-4.274343000	3.985218000	-0.584277000
Li	0.270124000	-1.802266000	1.318419000	H	3.911042000	-1.182533000	2.407950000
Br	1.806440000	-1.740059000	3.180992000	H	-4.705651000	-3.324817000	0.911005000
H	-1.913999000	-0.063159000	2.744086000	H	2.662365000	-3.463055000	1.722987000
C	-3.369536000	1.545643000	1.159289000	H	-2.395886000	-4.720431000	0.858115000
H	-2.394886000	1.977666000	1.412855000	C	2.313680000	1.140392000	1.796070000
H	-4.077826000	2.147735000	0.588580000	C	-4.244210000	-0.476701000	0.668134000
H	-0.492382000	0.629096000	1.069832000	C	-0.091007000	-3.005296000	0.947311000
C	-3.749093000	0.297663000	1.617489000	C	-1.473744000	3.440963000	-0.242464000
C	-5.037559000	-0.235125000	1.272856000	C	3.689745000	1.491457000	2.250733000
C	-5.444628000	-1.460062000	1.753749000	C	4.090129000	1.329082000	3.584580000

C	4.687117000	1.927854000	1.366974000	Li	-1.963252000	0.485761000	-1.852585000
C	5.384416000	1.580287000	4.028220000	Br	2.183444000	-2.035661000	-2.665817000
C	5.997292000	2.183013000	1.757827000	Li	-0.495689000	-1.789891000	-1.851063000
C	6.340032000	2.007078000	3.101392000	Br	-2.431095000	-1.369147000	-3.313289000
H	5.624120000	1.434442000	5.082890000	H	4.583217000	-1.599153000	-0.050161000
H	7.363475000	2.202046000	3.429345000	C	2.853896000	-0.361898000	-1.744897000
H	6.725055000	2.501057000	1.009499000	H	2.433203000	-0.445509000	-0.738812000
C	-1.725056000	4.760657000	-0.887082000	H	2.382860000	0.457570000	-2.299521000
C	-1.738824000	5.977097000	-0.193463000	H	0.419882000	0.432816000	-1.164690000
C	-2.005300000	4.834921000	-2.258936000	C	4.338150000	-0.260382000	-1.731773000
C	-1.997471000	7.198353000	-0.808136000	C	5.000196000	0.583729000	-2.635836000
C	-2.268299000	6.029207000	-2.920385000	C	6.378317000	0.786146000	-2.546197000
C	-2.261080000	7.215914000	-2.180782000	C	7.096277000	0.127626000	-1.543831000
H	-1.993106000	8.109168000	-0.206988000	C	6.464495000	-0.746408000	-0.652324000
H	-2.466213000	8.165411000	-2.680252000	C	5.087667000	-0.935839000	-0.755027000
H	-2.473659000	6.014860000	-3.992118000	H	4.429189000	1.114163000	-3.402444000
C	-5.705355000	-0.748382000	0.785148000	H	6.889335000	1.460351000	-3.235677000
C	-6.423618000	-1.485151000	-0.166117000	H	7.041458000	-1.253311000	0.122990000
C	-6.452002000	-0.251146000	1.862724000	Cl	8.818293000	0.421111000	-1.383355000
C	-7.789495000	-1.731690000	-0.063914000				
C	-7.817619000	-0.470811000	2.010136000	PCBa-Doublet			
C	-8.483794000	-1.219052000	1.035326000	Fe	0.367608000	0.760565000	-1.194672000
H	-8.284722000	-2.314073000	-0.842806000	N	-0.408642000	2.367342000	-0.360413000
H	-9.556099000	-1.403033000	1.132517000	N	2.150374000	1.283695000	-0.577217000
H	-8.334011000	-0.056606000	2.877768000	N	-1.459730000	0.058860000	-1.437182000
C	0.278855000	-4.399323000	0.582263000	N	1.095826000	-1.026204000	-1.564367000
C	0.131598000	-4.813455000	-0.747622000	C	-1.662230000	2.879726000	-0.612540000
C	0.759925000	-5.371189000	1.466793000	C	3.338538000	0.769509000	-1.039389000
C	0.441730000	-6.084026000	-1.206811000	C	0.204443000	3.232426000	0.516610000
C	1.085419000	-6.663481000	1.064729000	C	2.470111000	2.293598000	0.301134000
C	0.924572000	-7.013690000	-0.278755000	C	-2.589476000	0.825546000	-1.589482000
H	0.306312000	-6.328966000	-2.261397000	C	2.394986000	-1.305183000	-1.929480000
H	1.454813000	-7.373839000	1.806337000	C	-1.858443000	-1.256693000	-1.511481000
H	1.176662000	-8.023945000	-0.608142000	C	0.403388000	-2.204321000	-1.636915000
F	-1.493961000	5.954878000	1.128129000	C	-1.821644000	4.129149000	0.094582000
F	-2.019039000	3.685336000	-2.963330000	C	4.438091000	1.498781000	-0.459455000
F	3.174850000	0.896340000	4.469153000	C	-0.694211000	4.311341000	0.845719000
F	0.908866000	-5.032913000	2.758143000	C	3.902786000	2.407302000	0.412603000
F	4.358475000	2.094184000	0.073338000	C	-3.726772000	-0.033145000	-1.830801000
F	-0.346448000	-3.897905000	-1.643640000	C	2.502343000	-2.698665000	-2.294416000
F	-5.809155000	0.476663000	2.792724000	C	-3.285839000	-1.319967000	-1.716088000
F	-5.757441000	-1.971949000	-1.225561000	C	1.287064000	-3.270174000	-2.044861000
Cl	-1.431420000	0.655555000	3.013050000	H	-2.699536000	4.769334000	0.057779000
O	-0.396346000	-0.069172000	-1.022652000	H	5.490348000	1.303236000	-0.654391000

H	-0.472862000	5.131656000	1.524452000	H	-3.532935000	-6.277701000	-2.032086000
H	4.425577000	3.114285000	1.053516000	H	-2.772349000	-7.171781000	0.192948000
H	-4.749292000	0.304263000	-1.982205000	F	1.987146000	5.988151000	1.095504000
H	3.403268000	-3.190057000	-2.652022000	F	2.056870000	1.810245000	3.293097000
H	-3.879029000	-2.227522000	-1.775718000	F	-3.588680000	2.739090000	-3.876491000
H	0.994409000	-4.310506000	-2.172413000	F	-2.785464000	-4.016727000	-3.030269000
C	-2.684032000	2.194289000	-1.289616000	F	-4.541868000	3.029266000	0.728231000
C	3.467825000	-0.415374000	-1.782537000	F	-0.191145000	-3.529937000	0.874439000
C	-0.980830000	-2.349466000	-1.455059000	F	4.694858000	1.086618000	-3.775642000
C	1.539337000	3.133901000	0.932891000	F	5.111745000	-2.603112000	-0.875929000
C	-3.983583000	2.871670000	-1.560178000	Cl	0.571930000	1.565021000	-3.261998000
C	-4.405932000	3.109969000	-2.876542000	O	-0.078183000	-0.593733000	2.089145000
C	-4.881194000	3.257880000	-0.556234000	Li	1.700304000	0.270159000	2.094053000
C	-5.623350000	3.704758000	-3.190748000	Br	0.006817000	-3.471787000	4.361941000
C	-6.110325000	3.852998000	-0.817634000	Li	0.789302000	-2.477488000	2.356789000
C	-6.476124000	4.076792000	-2.147837000	Br	3.072579000	-1.637136000	1.837543000
H	-5.883982000	3.864469000	-4.238371000	H	-2.171632000	-2.722138000	2.805025000
H	-7.437246000	4.543825000	-2.373905000	C	-1.163405000	-0.191989000	2.988627000
H	-6.758467000	4.124803000	0.017166000	H	-0.938509000	-0.699340000	3.937324000
C	2.007177000	3.878778000	2.131187000	H	-1.118077000	0.898648000	3.128642000
C	2.229464000	5.258356000	2.195570000	H	-0.399240000	-0.490059000	1.170256000
C	2.273897000	3.167985000	3.307248000	C	-2.494381000	-0.613279000	2.431884000
C	2.689140000	5.893703000	3.345849000	C	-3.375508000	0.340440000	1.903311000
C	2.730513000	3.743215000	4.481296000	C	-4.584333000	-0.046902000	1.320864000
C	2.939130000	5.127504000	4.487475000	C	-4.893868000	-1.405514000	1.247331000
H	2.847019000	6.973430000	3.330000000	C	-4.037472000	-2.377356000	1.773757000
H	3.300541000	5.613472000	5.396170000	C	-2.843111000	-1.974476000	2.372609000
H	2.912538000	3.121400000	5.359090000	H	-3.116370000	1.400834000	1.932991000
C	4.817378000	-0.755180000	-2.311825000	H	-5.260738000	0.697881000	0.903080000
C	5.602763000	-1.820015000	-1.846847000	H	-4.298036000	-3.435189000	1.706174000
C	5.400836000	0.041000000	-3.310291000	Cl	-6.362582000	-1.904997000	0.425252000
C	6.873700000	-2.097121000	-2.343220000				
C	6.664719000	-0.197846000	-3.838146000	RC-Quartet with 1 LiBr			
C	7.400823000	-1.279057000	-3.345573000	Fe	-0.261267000	0.340763000	-0.575163000
H	7.428742000	-2.942795000	-1.933533000	N	0.872153000	-1.244241000	-1.035666000
H	8.396488000	-1.484037000	-3.745234000	N	-1.897945000	-0.814832000	-0.675812000
H	7.049717000	0.460604000	-4.618704000	N	1.364874000	1.501275000	-0.640620000
C	-1.482518000	-3.700519000	-1.095080000	N	-1.407270000	1.961396000	-0.287914000
C	-1.070531000	-4.253893000	0.126983000	C	2.172491000	-1.239670000	-1.486064000
C	-2.371934000	-4.483204000	-1.840031000	C	-3.193268000	-0.395536000	-0.664095000
C	-1.509015000	-5.473113000	0.618525000	C	0.487406000	-2.545258000	-0.975177000
C	-2.840447000	-5.718210000	-1.400809000	C	-1.927271000	-2.182385000	-0.545475000
C	-2.407905000	-6.206409000	-0.164543000	C	2.610271000	1.162424000	-1.077140000
H	-1.155466000	-5.821435000	1.589910000	C	-2.771905000	2.036040000	-0.390364000

C	1.454334000	2.776697000	-0.152034000	C	-7.151688000	1.125478000	-2.057391000
C	-0.976552000	3.190885000	0.118594000	C	-7.878724000	1.580232000	-0.953354000
C	2.597507000	-2.591835000	-1.762447000	H	-7.788089000	2.177471000	1.144980000
C	-4.083192000	-1.530891000	-0.544729000	H	-8.956128000	1.735649000	-1.042622000
C	1.562768000	-3.407407000	-1.408587000	H	-7.624988000	0.917051000	-3.018345000
C	-3.294948000	-2.633182000	-0.417508000	C	0.701034000	4.871353000	0.909218000
C	3.525735000	2.259680000	-0.870240000	C	1.371570000	4.919990000	2.141588000
C	-3.213201000	3.378047000	-0.082962000	C	0.412195000	6.107015000	0.314265000
C	2.812133000	3.255787000	-0.269391000	C	1.717049000	6.111236000	2.768165000
C	-2.104340000	4.080742000	0.282855000	C	0.744724000	7.323300000	0.899892000
H	3.566897000	-2.880112000	-2.161165000	C	1.397169000	7.316582000	2.136091000
H	-5.168397000	-1.477416000	-0.505378000	H	2.228736000	6.078731000	3.731389000
H	1.512218000	-4.491946000	-1.468671000	H	0.495024000	8.249933000	0.380400000
H	-3.610193000	-3.660229000	-0.262594000	H	1.663309000	8.263070000	2.611712000
H	4.581753000	2.256363000	-1.128948000	F	-2.374515000	-4.925414000	-2.064013000
H	-4.240880000	3.729846000	-0.113989000	F	0.599604000	-4.139609000	1.503849000
H	3.161936000	4.238916000	0.036420000	F	3.908154000	1.063185000	-3.920161000
H	-2.054764000	5.116032000	0.608226000	F	-0.200459000	6.106235000	-0.881079000
C	2.997123000	-0.111358000	-1.548429000	F	5.024580000	-1.558335000	-0.174097000
C	-3.627793000	0.946594000	-0.620109000	F	1.686564000	3.755597000	2.735345000
C	0.374833000	3.562572000	0.283633000	F	-5.076078000	0.481672000	-2.967632000
C	-0.799496000	-3.012274000	-0.608742000	F	-5.255211000	1.857912000	1.527668000
C	4.392815000	-0.263844000	-2.040420000	Cl	-0.492181000	0.707651000	-2.882231000
C	4.810958000	0.346513000	-3.231786000	O	-0.126881000	0.080660000	1.051464000
C	5.370744000	-0.985052000	-1.341878000	C	2.261067000	-1.464288000	2.389849000
C	6.106857000	0.238903000	-3.723074000	C	2.933831000	-0.099898000	2.190285000
C	6.680374000	-1.114703000	-1.788601000	C	3.886081000	0.231944000	3.344153000
C	7.041143000	-0.499436000	-2.990973000	C	4.920580000	-0.884062000	3.546777000
H	6.363345000	0.731478000	-4.662482000	C	4.240167000	-2.242357000	3.769739000
H	8.064992000	-0.592836000	-3.359523000	C	3.282059000	-2.585579000	2.621670000
H	7.393345000	-1.686124000	-1.192034000	H	1.651373000	-1.705589000	1.504755000
C	-0.918457000	-4.451962000	-0.272849000	H	1.597758000	-1.410896000	3.279311000
C	-1.704207000	-5.367184000	-0.986705000	H	2.170526000	0.683646000	2.064248000
C	-0.200441000	-4.972667000	0.817369000	H	3.508610000	-0.130203000	1.250672000
C	-1.804909000	-6.709414000	-0.638304000	H	4.388430000	1.196346000	3.154961000
C	-0.279003000	-6.302743000	1.208729000	H	3.302338000	0.358759000	4.275533000
C	-1.090419000	-7.170353000	0.471063000	H	5.586335000	-0.644895000	4.393825000
H	-2.431818000	-7.369372000	-1.240098000	H	5.560432000	-0.947014000	2.646833000
H	-1.162078000	-8.220871000	0.761197000	H	4.997177000	-3.037064000	3.885342000
H	0.291884000	-6.638576000	2.075917000	H	3.671111000	-2.209085000	4.717935000
C	-5.092103000	1.188229000	-0.724197000	H	2.760039000	-3.536474000	2.817163000
C	-5.869295000	1.632708000	0.354685000	H	3.862492000	-2.727290000	1.693360000
C	-5.782345000	0.931900000	-1.918037000	Li	-0.316841000	-1.281185000	2.264723000
C	-7.242051000	1.833667000	0.264948000	Br	-2.020286000	-2.557897000	3.144402000

RC-Doublet with 1 LiBr

Fe	-0.255063000	0.344352000	-0.571011000	C	-0.912539000	-4.453673000	-0.305105000
N	0.880771000	-1.239677000	-1.033642000	C	-1.697573000	-5.362747000	-1.027501000
N	-1.894634000	-0.814601000	-0.680576000	C	-0.197014000	-4.982884000	0.782545000
N	1.369581000	1.506687000	-0.631536000	C	-1.798753000	-6.707779000	-0.690161000
N	-1.406791000	1.965313000	-0.289291000	C	-0.276071000	-6.316153000	1.162869000
C	2.184951000	-1.232792000	-1.475666000	C	-1.086007000	-7.177727000	0.416560000
C	-3.189269000	-0.398547000	-0.656692000	H	-2.424884000	-7.362828000	-1.298108000
C	0.494505000	-2.540154000	-0.989332000	H	-1.158094000	-8.230597000	0.697964000
C	-1.921016000	-2.183846000	-0.558349000	H	0.293116000	-6.659024000	2.028429000
C	2.618457000	1.167929000	-1.055421000	C	-5.092515000	1.181719000	-0.705023000
C	-2.773634000	2.034819000	-0.387478000	C	-5.863844000	1.628711000	0.377040000
C	1.453176000	2.787502000	-0.151687000	C	-5.789638000	0.919974000	-1.893691000
C	-0.979923000	3.198253000	0.104830000	C	-7.237546000	1.826603000	0.295055000
C	2.609675000	-2.582760000	-1.762933000	C	-7.160135000	1.110378000	-2.025302000
C	-4.077428000	-1.535251000	-0.537034000	C	-7.881229000	1.567595000	-0.918359000
C	1.570967000	-3.399803000	-1.425287000	H	-7.778788000	2.172633000	1.177181000
C	-3.287148000	-2.637462000	-0.423542000	H	-8.959456000	1.720678000	-1.001528000
C	3.531375000	2.267199000	-0.847269000	H	-7.638931000	0.897764000	-2.982612000
C	-3.217458000	3.378294000	-0.090087000	C	0.690974000	4.889825000	0.886514000
C	2.811634000	3.266847000	-0.260611000	C	1.353711000	4.952269000	2.122435000
C	-2.109237000	4.087376000	0.264198000	C	0.400854000	6.118832000	0.278516000
H	3.581330000	-2.868548000	-2.157962000	C	1.691108000	6.150674000	2.739811000
H	-5.162330000	-1.483159000	-0.488891000	C	0.725358000	7.341747000	0.854642000
H	1.518731000	-4.483558000	-1.497019000	C	1.370581000	7.348861000	2.094658000
H	-3.599595000	-3.666010000	-0.272811000	H	2.197056000	6.129124000	3.706373000
H	4.589515000	2.263331000	-1.097103000	H	0.475151000	8.262641000	0.325275000
H	-4.246311000	3.726797000	-0.120172000	H	1.630477000	8.300712000	2.562988000
H	3.157219000	4.253026000	0.040111000	F	-2.367005000	-4.911841000	-2.101533000
H	-2.061154000	5.125629000	0.580148000	F	0.600875000	-4.154889000	1.477433000
C	3.009996000	-0.105715000	-1.526023000	F	3.937659000	1.080816000	-3.885454000
C	-3.627052000	0.943973000	-0.609022000	F	-0.205400000	6.104213000	-0.919986000
C	0.371607000	3.574618000	0.270821000	F	5.026980000	-1.562549000	-0.146797000
C	-0.793642000	-3.011286000	-0.629455000	F	1.669040000	3.794802000	2.729083000
C	4.408823000	-0.256405000	-2.009541000	F	-5.088824000	0.467568000	-2.946026000
C	4.835241000	0.359330000	-3.195237000	F	-5.243004000	1.859863000	1.545268000
C	5.381315000	-0.982895000	-1.308892000	Cl	-0.484674000	0.713372000	-2.882145000
C	6.133958000	0.252429000	-3.679049000	O	-0.133685000	0.080294000	1.056064000
C	6.693527000	-1.112048000	-1.748155000	C	2.247408000	-1.479577000	2.394475000
C	7.062662000	-0.491006000	-2.944976000	C	2.923123000	-0.114900000	2.207254000
H	6.396915000	0.749427000	-4.614336000	C	3.867099000	0.209744000	3.369978000
H	8.088638000	-0.583984000	-3.307683000	C	4.898841000	-0.908472000	3.574490000
H	7.401870000	-1.687799000	-1.150240000	C	4.215388000	-2.267216000	3.784893000
				C	3.265591000	-2.603194000	2.627774000
				H	1.643346000	-1.715129000	1.503987000

H	1.577954000	-1.430434000	3.279491000	C	3.036230000	-0.882141000	-1.407786000
H	2.161414000	0.670004000	2.079361000	C	-3.232386000	1.715363000	-0.624664000
H	3.504891000	-0.140817000	1.271774000	C	1.272820000	3.388303000	0.126118000
H	4.372104000	1.174504000	3.189810000	C	-1.381189000	-2.783246000	-0.627375000
H	3.276501000	0.332203000	4.297621000	C	4.381968000	-1.413516000	-1.760040000
H	5.558312000	-0.674501000	4.427904000	C	5.036784000	-1.055909000	-2.947230000
H	5.545580000	-0.967237000	2.679200000	C	5.079080000	-2.277605000	-0.903306000
H	4.970730000	-3.063319000	3.901926000	C	6.300241000	-1.535607000	-3.282174000
H	3.639193000	-2.238521000	4.728933000	C	6.343741000	-2.776293000	-1.196216000
H	2.741270000	-3.554598000	2.814300000	C	6.949321000	-2.400070000	-2.398017000
H	3.852865000	-2.740609000	1.703132000	H	6.750720000	-1.224120000	-4.225533000
Li	-0.335024000	-1.289716000	2.256750000	H	7.941409000	-2.782943000	-2.646353000
Br	-2.026680000	-2.583847000	3.133117000	H	6.831114000	-3.441509000	-0.482272000
TS-Doublet with 1 LiBr				C	-1.886166000	-4.162252000	-0.396165000
Fe	-0.062483000	0.364489000	-0.639905000	C	-2.821327000	-4.792252000	-1.230105000
N	0.685923000	-1.459827000	-0.963330000	C	-1.424490000	-4.917045000	0.696869000
N	-1.943623000	-0.387368000	-0.660847000	C	-3.305344000	-6.074396000	-0.991775000
N	1.788044000	1.103834000	-0.661934000	C	-1.892176000	-6.197087000	0.975297000
N	-0.834308000	2.204399000	-0.345411000	C	-2.838980000	-6.771251000	0.125172000
C	1.959009000	-1.784202000	-1.337950000	H	-4.030678000	-6.502501000	-1.684861000
C	-3.121738000	0.325591000	-0.696284000	H	-3.212833000	-7.776591000	0.330710000
C	-0.011995000	-2.637813000	-0.903638000	H	-1.506493000	-6.716645000	1.853124000
C	-2.293073000	-1.701713000	-0.595317000	C	-4.602179000	2.299516000	-0.684400000
C	2.939971000	0.468805000	-1.052478000	C	-5.225012000	2.860734000	0.439628000
C	-2.138526000	2.583025000	-0.406080000	C	-5.356229000	2.281401000	-1.867014000
C	2.151280000	2.356902000	-0.272644000	C	-6.511452000	3.389729000	0.404989000
C	-0.119991000	3.318988000	0.018838000	C	-6.644436000	2.803570000	-1.945935000
C	2.069544000	-3.208699000	-1.551771000	C	-7.217430000	3.359391000	-0.800077000
C	-4.246556000	-0.582817000	-0.656479000	H	-6.936636000	3.808317000	1.318121000
C	0.853501000	-3.742411000	-1.254322000	H	-8.227904000	3.771060000	-0.845543000
C	-3.734536000	-1.835711000	-0.546859000	H	-7.173026000	2.763943000	-2.899303000
C	4.067986000	1.358137000	-0.910707000	C	1.895604000	4.638317000	0.646127000
C	-2.265723000	3.992215000	-0.099070000	C	2.580090000	4.640692000	1.871476000
C	3.580885000	2.526877000	-0.407269000	C	1.870880000	5.855374000	-0.049703000
C	-1.017468000	4.438904000	0.205102000	C	3.192397000	5.775304000	2.393639000
H	2.963890000	-3.730330000	-1.881046000	C	2.473947000	7.012898000	0.434296000
H	-5.292150000	-0.288026000	-0.645972000	C	3.134088000	6.965144000	1.663986000
H	0.552020000	-4.785192000	-1.300690000	H	3.701027000	5.707393000	3.356177000
H	-4.276690000	-2.767075000	-0.427455000	H	2.418991000	7.925442000	-0.160780000
H	5.099583000	1.111364000	-1.146777000	H	3.610821000	7.865270000	2.057664000
H	-3.192690000	4.558310000	-0.096443000	F	-3.258286000	-4.131927000	-2.311911000
H	4.133174000	3.432150000	-0.169782000	F	-0.487801000	-4.392076000	1.486794000
H	-0.726302000	5.441999000	0.502465000	F	4.417500000	-0.218424000	-3.783898000
				F	1.244002000	5.899879000	-1.230959000

F	4.497065000	-2.624263000	0.255290000	C	-3.242911000	-1.967259000	-0.952801000
F	2.643652000	3.495599000	2.564392000	C	4.579606000	0.930609000	0.141362000
F	-4.810427000	1.736418000	-2.957897000	C	-1.637791000	3.842946000	-0.757253000
F	-4.547933000	2.879765000	1.594929000	C	4.108766000	2.206003000	0.123648000
Cl	-0.234736000	0.692500000	-2.887376000	C	-0.370355000	4.310180000	-0.573786000
O	-0.042790000	0.170033000	1.143480000	H	3.499608000	-4.133348000	-0.702282000
C	1.754894000	-2.316301000	2.371915000	H	-4.757582000	-0.381416000	-0.785735000
C	2.050346000	-0.847149000	2.143290000	H	1.000857000	-5.050521000	-1.126285000
C	2.270178000	-0.052795000	3.415509000	H	-3.810645000	-2.893090000	-0.948698000
C	3.394867000	-0.696071000	4.252838000	H	5.596275000	0.597199000	0.329554000
C	3.104192000	-2.177994000	4.523114000	H	-2.548642000	4.419272000	-0.896035000
C	2.874725000	-2.954410000	3.220639000	H	4.665628000	3.124644000	0.285429000
H	1.654936000	-2.849295000	1.416038000	H	-0.044252000	5.345382000	-0.525250000
H	0.790633000	-2.435800000	2.898082000	C	3.561228000	-1.318328000	-0.260834000
H	1.062000000	-0.329885000	1.578089000	C	-2.674607000	1.568105000	-0.835057000
H	2.854548000	-0.693251000	1.407148000	C	1.863332000	3.244014000	-0.236206000
H	2.502280000	0.998992000	3.185168000	C	-0.956801000	-2.980482000	-0.992286000
H	1.340295000	-0.053801000	4.014419000	C	4.893217000	-1.957092000	-0.057970000
H	3.522673000	-0.143221000	5.199284000	C	5.949363000	-1.795531000	-0.966001000
H	4.349434000	-0.604869000	3.702801000	C	5.160465000	-2.757537000	1.062241000
H	3.931779000	-2.629772000	5.096701000	C	7.196819000	-2.387320000	-0.786981000
H	2.202262000	-2.259170000	5.157729000	C	6.392265000	-3.366588000	1.281783000
H	2.621002000	-4.006738000	3.433712000	C	7.411416000	-3.175629000	0.345760000
H	3.807539000	-2.965543000	2.630144000	H	7.973028000	-2.221863000	-1.535352000
Li	-1.392184000	-0.553155000	2.109621000	H	8.384375000	-3.646526000	0.501309000
Br	-2.716171000	-2.230014000	2.881015000	H	6.531078000	-3.974175000	2.177018000
PC-Doublet with 1LiBr				C	-1.570088000	-4.335463000	-1.091587000
Fe	0.477274000	0.141307000	-0.844914000	C	-2.246438000	-4.768834000	-2.241253000
N	1.154222000	-1.734996000	-0.648835000	C	-1.518103000	-5.248177000	-0.027930000
N	-1.406697000	-0.552392000	-0.892163000	C	-2.834242000	-6.026795000	-2.342988000
N	2.308617000	0.810583000	-0.301536000	C	-2.093476000	-6.513668000	-0.084789000
N	-0.255735000	1.996120000	-0.539633000	C	-2.753231000	-6.898075000	-1.254523000
C	2.470132000	-2.139642000	-0.542791000	H	-3.341967000	-6.299707000	-3.269097000
C	-2.578731000	0.177524000	-0.872203000	H	-3.210356000	-7.887839000	-1.317882000
C	0.433814000	-2.886352000	-0.882121000	H	-2.017356000	-7.170069000	0.783056000
C	-1.803517000	-1.871562000	-0.964573000	C	-4.028089000	2.188987000	-0.802954000
C	3.459420000	0.070203000	-0.145980000	C	-4.507843000	2.812599000	0.352334000
C	-1.562230000	2.409000000	-0.737674000	C	-4.912626000	2.166587000	-1.889790000
C	2.695463000	2.124872000	-0.152221000	C	-5.763689000	3.384802000	0.466997000
C	0.487364000	3.163653000	-0.451701000	C	-6.182990000	2.733765000	-1.834079000
C	2.574299000	-3.564343000	-0.726013000	C	-6.602777000	3.343585000	-0.649640000
C	-3.724649000	-0.699664000	-0.883794000	H	-6.070965000	3.826193000	1.414925000
C	1.313400000	-4.026899000	-0.939286000	H	-7.600582000	3.783111000	-0.591676000
				H	-6.821402000	2.684825000	-2.717283000

C	2.475600000	4.595787000	-0.075727000	N	1.029994000	1.490421000	-0.566049000
C	2.923596000	5.057890000	1.169458000	N	-1.776965000	1.323958000	-0.221884000
C	2.633047000	5.475877000	-1.155158000	C	2.499263000	-1.070425000	-0.883961000
C	3.497909000	6.313054000	1.348684000	C	-2.965538000	-1.417565000	-0.361694000
C	3.202016000	6.739711000	-1.021470000	C	1.148308000	-2.662287000	-0.226254000
C	3.634508000	7.152722000	0.240708000	C	-1.319493000	-2.831551000	-0.059463000
H	3.824522000	6.609145000	2.346492000	C	2.321603000	1.396205000	-1.025096000
H	3.296053000	7.373737000	-1.904169000	C	-3.108546000	1.057088000	-0.250014000
H	4.082951000	8.140992000	0.362615000	C	0.786655000	2.809665000	-0.364141000
F	-2.330525000	-3.931021000	-3.280403000	C	-1.650371000	2.661254000	0.060308000
F	-0.881287000	-4.881106000	1.094510000	C	3.287726000	-2.282105000	-0.813558000
F	5.744118000	-1.035006000	-2.047248000	C	-3.556678000	-2.737433000	-0.302222000
F	2.207638000	5.081675000	-2.360700000	C	2.453565000	-3.266516000	-0.379699000
F	4.180785000	-2.942761000	1.958752000	C	-2.540148000	-3.610515000	-0.069640000
F	2.796384000	4.246329000	2.227569000	C	2.887431000	2.719303000	-1.168973000
F	-4.514963000	1.571128000	-3.018649000	C	-3.865662000	2.261942000	0.020946000
F	-3.677756000	2.838525000	1.439553000	C	1.947612000	3.596188000	-0.722602000
Cl	0.824546000	0.326903000	-3.002158000	C	-2.958532000	3.249270000	0.252285000
O	-1.346102000	0.890099000	2.196616000	H	4.346681000	-2.358990000	-1.044643000
C	-1.382307000	-1.152830000	3.496529000	H	-4.614940000	-2.961700000	-0.400264000
C	-0.643748000	-0.352204000	2.432921000	H	2.686472000	-4.314093000	-0.208648000
C	0.808863000	-0.093426000	2.819963000	H	-2.605784000	-4.687369000	0.053901000
C	1.538614000	-1.419698000	3.067281000	H	3.880997000	2.944202000	-1.545852000
C	0.814768000	-2.266820000	4.120886000	H	-4.949588000	2.329676000	0.060835000
C	-0.658898000	-2.483305000	3.750836000	H	2.014146000	4.679779000	-0.671375000
H	-2.425333000	-1.325354000	3.182183000	H	-3.156242000	4.287413000	0.502240000
H	-1.413970000	-0.555798000	4.426804000	C	3.026091000	0.201130000	-1.199554000
H	-0.887147000	1.369608000	1.483598000	C	-3.690738000	-0.220309000	-0.400125000
H	-0.662319000	-0.934544000	1.494832000	C	-0.442150000	3.367638000	0.054618000
H	1.311834000	0.476703000	2.022004000	C	-0.022804000	-3.375719000	0.055195000
H	0.822510000	0.535690000	3.727439000	C	4.440201000	0.260171000	-1.663436000
H	2.582293000	-1.231313000	3.363073000	C	4.826494000	-0.310201000	-2.887244000
H	1.590027000	-1.981866000	2.120185000	C	5.465327000	0.853103000	-0.910274000
H	1.325122000	-3.236994000	4.240400000	C	6.138183000	-0.286507000	-3.351683000
H	0.872792000	-1.757427000	5.100764000	C	6.789875000	0.893017000	-1.335545000
H	-1.180183000	-3.041835000	4.545262000	C	7.119949000	0.320876000	-2.565893000
H	-0.720473000	-3.107049000	2.841923000	H	6.364811000	-0.742224000	-4.316468000
Li	-3.206874000	1.110030000	2.336862000	H	8.154477000	0.345949000	-2.914775000
Br	-5.119430000	-0.133050000	2.352992000	H	7.535330000	1.365521000	-0.694600000
RC-Quartet without LiBr				C	0.127140000	-4.806626000	0.443805000
Fe	-0.276264000	-0.005986000	-0.291161000	C	-0.237854000	-5.871208000	-0.391665000
N	1.213906000	-1.325874000	-0.520837000	C	0.685264000	-5.154817000	1.683904000
N	-1.602529000	-1.513031000	-0.240775000	C	-0.072859000	-7.205102000	-0.030013000
				C	0.864325000	-6.475265000	2.085543000

C	0.480398000	-7.500290000	1.218017000	H	1.156785000	-1.853556000	4.556203000
H	-0.375505000	-7.984185000	-0.730956000	H	2.673881000	-1.112057000	5.093344000
H	0.615710000	-8.541795000	1.517248000	H	3.013536000	-2.304928000	2.927117000
H	1.298888000	-6.675107000	3.065888000	H	1.700869000	-1.367007000	2.194781000
C	-5.174716000	-0.280343000	-0.518908000	H	3.897150000	-0.397416000	1.543401000
C	-5.996494000	-0.816255000	0.483947000	H	4.346412000	-0.203973000	3.239991000
C	-5.833037000	0.241945000	-1.643572000				
C	-7.384180000	-0.853964000	0.383143000	RC-Doublet without LiBr			
C	-7.217413000	0.219278000	-1.785673000	Fe	-0.266791000	-0.004514000	-0.292094000
C	-7.990352000	-0.334161000	-0.762613000	N	1.211983000	-1.336843000	-0.515640000
H	-7.961665000	-1.283047000	1.203054000	N	-1.611447000	-1.502816000	-0.255093000
H	-9.078004000	-0.357758000	-0.857776000	N	1.051564000	1.481258000	-0.564578000
H	-7.662225000	0.634672000	-2.690910000	N	-1.763124000	1.340916000	-0.235095000
C	-0.424198000	4.799542000	0.459827000	C	2.503003000	-1.092600000	-0.862042000
C	0.307174000	5.204729000	1.589208000	C	-2.974988000	-1.392726000	-0.367771000
C	-1.077481000	5.817516000	-0.250080000	C	1.129573000	-2.676137000	-0.233370000
C	0.373686000	6.528661000	2.010976000	C	-1.341461000	-2.824077000	-0.087176000
C	-1.031414000	7.154497000	0.134731000	C	2.347450000	1.374903000	-1.010973000
C	-0.302992000	7.503447000	1.273965000	C	-3.095447000	1.083400000	-0.247936000
H	0.952326000	6.771074000	2.903285000	C	0.814490000	2.803569000	-0.381212000
H	-1.560331000	7.895166000	-0.466538000	C	-1.624998000	2.679003000	0.039342000
H	-0.259199000	8.548056000	1.589313000	C	3.279638000	-2.311759000	-0.790595000
F	-0.763933000	-5.586635000	-1.589287000	C	-3.578436000	-2.707752000	-0.319352000
F	1.059192000	-4.171661000	2.510019000	C	2.430898000	-3.291522000	-0.375644000
F	3.888811000	-0.900601000	-3.633718000	C	-2.569126000	-3.592565000	-0.101854000
F	-1.764937000	5.488367000	-1.350143000	C	2.922345000	2.692836000	-1.164421000
F	5.158338000	1.393630000	0.275401000	C	-3.842764000	2.294468000	0.024280000
F	0.964436000	4.270580000	2.285882000	C	1.982684000	3.579837000	-0.738717000
F	-5.092656000	0.783030000	-2.614900000	C	-2.927353000	3.277459000	0.239522000
F	-5.418726000	-1.303360000	1.588508000	H	4.340440000	-2.396945000	-1.009852000
Cl	-0.522746000	-0.033364000	-2.641881000	H	-4.639206000	-2.920979000	-0.414867000
O	-0.125382000	0.012232000	1.336503000	H	2.651541000	-4.342801000	-0.211366000
C	2.796417000	1.164686000	2.583815000	H	-2.644065000	-4.669987000	0.010648000
C	2.175462000	1.439448000	3.959912000	H	3.920720000	2.907692000	-1.534395000
C	1.209404000	0.318321000	4.370041000	H	-4.925771000	2.369269000	0.074569000
C	1.885412000	-1.059590000	4.317048000	H	2.054354000	4.663602000	-0.699839000
C	2.510303000	-1.323521000	2.940786000	H	-3.115675000	4.318403000	0.485076000
C	3.483244000	-0.206546000	2.545871000	C	3.044502000	0.175031000	-1.172793000
H	3.507741000	1.961125000	2.309128000	C	-3.689498000	-0.190201000	-0.393938000
H	1.991575000	1.175874000	1.831937000	C	-0.412061000	3.375127000	0.028702000
H	1.650786000	2.409665000	3.947121000	C	-0.049171000	-3.381023000	0.031085000
H	2.981473000	1.525032000	4.715011000	C	4.463781000	0.222131000	-1.621776000
H	0.808272000	0.509253000	5.381505000	C	4.859612000	-0.354188000	-2.839728000
H	0.355045000	0.318666000	3.672808000	C	5.484413000	0.810661000	-0.859085000

C	6.176398000	-0.340795000	-3.289735000	C	2.140470000	1.430545000	3.967859000
C	6.813829000	0.840241000	-1.269854000	C	1.162036000	0.318450000	4.373247000
C	7.153546000	0.262189000	-2.494773000	C	1.826611000	-1.065334000	4.328180000
H	6.410547000	-0.800688000	-4.250731000	C	2.459891000	-1.337789000	2.957338000
H	8.192004000	0.279241000	-2.832274000	C	3.445567000	-0.229914000	2.568318000
H	7.555351000	1.309712000	-0.622154000	H	3.490060000	1.936919000	2.326439000
C	0.084515000	-4.815167000	0.413334000	H	1.971127000	1.162871000	1.839465000
C	-0.287621000	-5.871876000	-0.428950000	H	1.623824000	2.405032000	3.948023000
C	0.632203000	-5.175058000	1.654836000	H	2.941126000	1.511895000	4.729117000
C	-0.138875000	-7.209116000	-0.072804000	H	0.755256000	0.514953000	5.381397000
C	0.794747000	-6.499244000	2.051159000	H	0.312974000	0.324408000	3.669674000
C	0.404462000	-7.516019000	1.176780000	H	1.089255000	-1.852389000	4.563494000
H	-0.446095000	-7.981629000	-0.779006000	H	2.608634000	-1.123036000	5.110625000
H	0.526972000	-8.560297000	1.471826000	H	2.954789000	-2.323525000	2.949712000
H	1.221838000	-6.708361000	3.032850000	H	1.655921000	-1.375459000	2.204966000
C	-5.174921000	-0.237879000	-0.500114000	H	3.866609000	-0.426393000	1.569877000
C	-5.991726000	-0.772362000	0.507606000	H	4.302966000	-0.233123000	3.269570000
C	-5.839311000	0.293963000	-1.616681000	TS-Doublet without LiBr			
C	-7.380510000	-0.799231000	0.418977000	Fe	0.234244000	0.061765000	-0.374925000
C	-7.224985000	0.282213000	-1.746621000	N	-1.609078000	0.803566000	-0.545709000
C	-7.992924000	-0.269883000	-0.719053000	N	0.991140000	1.905780000	-0.237761000
H	-7.953908000	-1.227754000	1.242042000	N	-0.522013000	-1.766641000	-0.511240000
H	-9.081523000	-0.285012000	-0.804632000	N	2.087300000	-0.690760000	-0.279152000
H	-7.674690000	0.704718000	-2.646128000	C	-2.732744000	0.139440000	-0.946306000
C	-0.383123000	4.809165000	0.425302000	C	2.303400000	2.272934000	-0.354621000
C	0.350592000	5.215785000	1.552683000	C	-1.983272000	2.080700000	-0.236619000
C	-1.029767000	5.827338000	-0.290398000	C	0.273533000	3.043792000	0.003964000
C	0.426220000	6.541656000	1.966661000	C	-1.782013000	-2.120383000	-0.931759000
C	-0.974335000	7.166216000	0.086514000	C	3.259504000	0.005455000	-0.370384000
C	-0.243499000	7.516776000	1.223710000	C	0.145436000	-2.927545000	-0.217684000
H	1.006173000	6.785280000	2.857784000	C	2.404731000	-1.985492000	0.018517000
H	-1.498231000	7.906992000	-0.519001000	C	-3.867419000	1.033018000	-0.897692000
H	-0.192491000	8.562891000	1.532920000	C	2.419251000	3.706161000	-0.207261000
F	-0.804517000	-5.575847000	-1.627812000	C	-3.409147000	2.226386000	-0.429889000
F	1.012299000	-4.199923000	2.487571000	C	1.168632000	4.179849000	0.047473000
F	3.925922000	-0.939980000	-3.594905000	C	-1.905441000	-3.558940000	-0.907330000
F	-1.720120000	5.496275000	-1.388002000	C	4.383827000	-0.887842000	-0.155894000
F	5.167959000	1.357181000	0.321268000	C	-0.729319000	-4.055590000	-0.427796000
F	1.000623000	4.281047000	2.255397000	C	3.850534000	-2.108553000	0.127845000
F	-5.103421000	0.833546000	-2.592344000	H	-4.886592000	0.762980000	-1.154632000
F	-5.407853000	-1.269173000	1.604525000	H	3.348696000	4.265166000	-0.249602000
Cl	-0.520910000	-0.032085000	-2.650348000	H	-3.975325000	3.133517000	-0.243192000
O	-0.146161000	0.013319000	1.336583000	H	0.868602000	5.206269000	0.230718000
C	2.770033000	1.147091000	2.597504000				

H	-2.800203000	-4.106101000	-1.185896000	F	-1.272079000	5.414397000	-1.563135000
H	5.428742000	-0.589523000	-0.170611000	F	-2.334307000	3.529443000	2.610902000
H	-0.447578000	-5.096715000	-0.280569000	F	-3.853611000	-0.537777000	-3.735938000
H	4.395503000	-3.012386000	0.387155000	F	3.251472000	-4.752068000	-1.344535000
C	-2.825078000	-1.231664000	-1.220336000	F	-4.599884000	-2.924697000	0.257497000
C	3.387903000	1.395802000	-0.490510000	F	0.717086000	-4.175103000	2.582792000
C	1.498186000	-3.046718000	0.132403000	F	4.855014000	0.904164000	-2.812906000
C	-1.122080000	3.129808000	0.103742000	F	4.851990000	2.962751000	1.419590000
C	-4.135059000	-1.731657000	-1.724218000	Cl	0.443652000	0.177125000	-2.615447000
C	-4.620825000	-1.332823000	-2.982141000	O	0.064515000	-0.011436000	1.396519000
C	-4.997194000	-2.538091000	-0.967703000	C	-1.544438000	-1.736477000	2.835069000
C	-5.869564000	-1.712330000	-3.469722000	C	-0.814894000	-1.381476000	4.094213000
C	-6.253144000	-2.941288000	-1.414653000	C	-0.922001000	0.111900000	4.452387000
C	-6.684958000	-2.522723000	-2.676130000	C	-2.365116000	0.617807000	4.342118000
H	-6.177603000	-1.362985000	-4.456309000	C	-2.928876000	0.363062000	2.940974000
H	-7.669657000	-2.827194000	-3.039847000	C	-2.881642000	-1.129415000	2.580535000
H	-6.871562000	-3.565657000	-0.767534000	H	-1.298650000	-2.693690000	2.358039000
C	-1.751628000	4.417825000	0.507226000	H	-0.469378000	-0.660606000	1.708358000
C	-1.819423000	5.523216000	-0.348175000	H	0.232754000	-1.712588000	4.043219000
C	-2.358670000	4.567131000	1.762277000	H	-1.277011000	-1.983382000	4.914733000
C	-2.434566000	6.719651000	0.010673000	H	-0.526454000	0.279321000	5.467049000
C	-2.983648000	5.742871000	2.161911000	H	-0.285843000	0.680454000	3.755206000
C	-3.017036000	6.822774000	1.273893000	H	-2.409175000	1.694115000	4.572632000
H	-2.455525000	7.544364000	-0.704261000	H	-2.997114000	0.105562000	5.093840000
H	-3.511163000	7.751234000	1.566764000	H	-3.959610000	0.739680000	2.856241000
H	-3.430552000	5.799963000	3.158100000	H	-2.326296000	0.918120000	2.207988000
C	4.764378000	1.928209000	-0.694966000	H	-3.206712000	-1.308538000	1.545151000
C	5.468979000	2.665008000	0.267124000	H	-3.624427000	-1.675173000	3.212176000
C	5.468911000	1.632127000	-1.871955000				
C	6.783638000	3.083681000	0.089554000	PC-Doublet without LiBr			
C	6.787138000	2.025335000	-2.091212000	Fe	0.149504000	0.062267000	-0.554130000
C	7.442220000	2.756297000	-1.097227000	N	1.800257000	1.213319000	-0.269054000
H	7.274450000	3.648481000	0.880269000	N	1.338037000	-1.574165000	-0.402804000
H	8.477411000	3.068146000	-1.243461000	N	-1.036008000	1.688564000	-0.488315000
H	7.277964000	1.749034000	-3.027236000	N	-1.497455000	-1.091304000	-0.601991000
C	1.967493000	-4.384897000	0.593497000	C	1.811035000	2.574537000	-0.089184000
C	1.536214000	-4.916604000	1.818795000	C	0.907930000	-2.871471000	-0.282832000
C	2.812236000	-5.208443000	-0.164770000	C	3.114760000	0.817494000	-0.347951000
C	1.908099000	-6.177987000	2.275421000	C	2.708915000	-1.616131000	-0.431230000
C	3.208439000	-6.477837000	0.250111000	C	-0.628235000	2.978149000	-0.264742000
C	2.751406000	-6.957370000	1.479039000	C	-1.525356000	-2.456840000	-0.489567000
H	1.539930000	-6.520002000	3.242285000	C	-2.384397000	1.741711000	-0.744263000
H	3.860148000	-7.066580000	-0.397250000	C	-2.787232000	-0.690009000	-0.843036000
H	3.051769000	-7.952962000	1.816733000	C	3.175511000	3.048481000	-0.025935000

C	2.046924000	-3.759705000	-0.208004000	H	-1.509404000	-8.494797000	0.784542000
C	3.979844000	1.967437000	-0.219793000	H	-0.507094000	-7.841594000	-1.432428000
C	3.160558000	-2.985419000	-0.325931000	C	-4.683777000	0.890831000	-1.110598000
C	-1.760100000	3.873585000	-0.363051000	C	-5.605676000	0.621495000	-0.088886000
C	-2.879880000	-2.934429000	-0.660011000	C	-5.213421000	1.430264000	-2.290622000
C	-2.843235000	3.109678000	-0.675379000	C	-6.971753000	0.854147000	-0.218077000
C	-3.656746000	-1.842674000	-0.901078000	C	-6.572879000	1.679770000	-2.463941000
H	3.477620000	4.081027000	0.125742000	C	-7.450442000	1.385617000	-1.418203000
H	1.996850000	-4.838852000	-0.090453000	H	-7.631393000	0.621367000	0.618995000
H	5.065598000	1.945843000	-0.256972000	H	-6.917389000	2.097456000	-3.411016000
H	4.199288000	-3.305146000	-0.313358000	H	-8.519263000	1.575276000	-1.538272000
H	-1.720393000	4.951410000	-0.227812000	F	4.892686000	-1.551640000	-2.709769000
H	-3.185804000	-3.976781000	-0.620795000	F	5.331567000	-0.028204000	1.719740000
H	-3.867939000	3.436868000	-0.830854000	F	1.868612000	5.360218000	-1.733423000
H	-4.725982000	-1.814308000	-1.093559000	F	-4.371513000	1.723105000	-3.287837000
C	0.684544000	3.405863000	-0.018433000	F	-0.095752000	4.473535000	2.449443000
C	-0.426190000	-3.298407000	-0.267964000	F	-5.144020000	0.120494000	1.067205000
C	-3.225627000	0.637472000	-0.931230000	F	0.084198000	-5.425207000	-2.101077000
C	3.565634000	-0.505809000	-0.446875000	F	-1.526907000	-4.200591000	2.147183000
C	0.880222000	4.841443000	0.337499000	Cl	0.310532000	0.138910000	-2.750906000
C	1.457167000	5.778134000	-0.530163000	O	0.152377000	-0.145647000	1.730443000
C	0.468498000	5.331555000	1.585234000	C	-0.523162000	0.581577000	2.781720000
C	1.624445000	7.119140000	-0.192884000	C	-2.026424000	0.380076000	2.607360000
C	0.615543000	6.662302000	1.965210000	C	-2.449862000	-1.076920000	2.819447000
C	1.198601000	7.555876000	1.063439000	C	-1.963291000	-1.619949000	4.168082000
H	2.080703000	7.794069000	-0.918417000	C	-0.448864000	-1.430584000	4.327999000
H	1.322243000	8.604291000	1.343180000	C	-0.044756000	0.037623000	4.132454000
H	0.274509000	6.973253000	2.953646000	H	-0.275432000	1.654234000	2.685136000
C	5.034199000	-0.760127000	-0.498601000	H	1.104928000	-0.149157000	1.904212000
C	5.653336000	-1.284718000	-1.642855000	H	-2.329131000	0.730620000	1.614452000
C	5.876083000	-0.516917000	0.596163000	H	-2.530752000	1.034454000	3.339902000
C	7.019943000	-1.543667000	-1.713147000	H	-3.544650000	-1.157294000	2.732085000
C	7.246435000	-0.760303000	0.570276000	H	-2.026447000	-1.693030000	2.013483000
C	7.814854000	-1.276170000	-0.596620000	H	-2.220470000	-2.687780000	4.259892000
H	7.434183000	-1.947901000	-2.637855000	H	-2.484591000	-1.093688000	4.990321000
H	8.888283000	-1.473672000	-0.635266000	H	-0.112664000	-1.783584000	5.317129000
H	7.839131000	-0.547107000	1.460947000	H	0.067350000	-2.050960000	3.575603000
C	-0.709555000	-4.737784000	0.003648000	H	1.050366000	0.162616000	4.218909000
C	-1.266148000	-5.141586000	1.226014000	H	-0.487587000	0.663730000	4.926926000
C	-0.453284000	-5.758280000	-0.921461000				
C	-1.559094000	-6.468594000	1.525929000	RC-Quartet with 3LiBr			
C	-0.729901000	-7.099117000	-0.664844000	Fe	-0.096849000	0.168147000	-1.042142000
C	-1.286243000	-7.447930000	0.567720000	N	1.512233000	-0.921337000	-1.305247000
H	-1.990169000	-6.710714000	2.498323000	N	-1.250819000	-1.428013000	-1.185130000

N	1.028840000	1.778000000	-1.054252000	C	1.345807000	-6.805106000	1.282904000
N	-1.758148000	1.279960000	-0.901451000	H	1.291374000	-7.728079000	-0.692380000
C	2.735521000	-0.515210000	-1.777683000	H	1.562846000	-7.738300000	1.807082000
C	-2.594833000	-1.480453000	-1.461416000	H	1.331450000	-5.583690000	3.097846000
C	1.583371000	-2.262407000	-1.062986000	C	-4.859302000	-0.623108000	-1.995639000
C	-0.835302000	-2.700295000	-0.906011000	C	-5.930122000	-0.434567000	-1.110470000
C	2.329666000	1.882355000	-1.464935000	C	-5.193618000	-1.108813000	-3.268175000
C	-3.033320000	0.939522000	-1.308616000	C	-7.253405000	-0.689706000	-1.456287000
C	0.652604000	2.987055000	-0.539479000	C	-6.500761000	-1.375702000	-3.661034000
C	-1.788038000	2.595292000	-0.501251000	C	-7.532312000	-1.160248000	-2.742609000
C	3.598076000	-1.671394000	-1.893579000	H	-8.038600000	-0.522788000	-0.716965000
C	-3.035766000	-2.854321000	-1.382064000	H	-8.565627000	-1.364732000	-3.031592000
C	2.911894000	-2.736521000	-1.381000000	H	-6.689599000	-1.745299000	-4.670360000
C	-1.961829000	-3.601169000	-0.985674000	C	-0.777454000	4.536028000	0.728975000
C	2.797683000	3.225828000	-1.207242000	C	-0.267883000	4.453664000	2.031315000
C	-3.887568000	2.090661000	-1.168489000	C	-1.359920000	5.761253000	0.386369000
C	1.779623000	3.893787000	-0.584882000	C	-0.321034000	5.481828000	2.957601000
C	-3.136212000	3.090969000	-0.611981000	C	-1.441824000	6.830919000	1.273332000
H	4.617833000	-1.658783000	-2.270313000	C	-0.919890000	6.683844000	2.561132000
H	-4.054885000	-3.192743000	-1.555307000	H	0.093659000	5.337854000	3.956326000
H	3.247059000	-3.766584000	-1.278032000	H	-1.908064000	7.760336000	0.941907000
H	-1.919633000	-4.672092000	-0.798273000	H	-0.978333000	7.515538000	3.266452000
H	3.793703000	3.595144000	-1.442357000	F	0.778321000	-5.607197000	-2.093611000
H	-4.943718000	2.124064000	-1.424753000	F	0.816448000	-3.284865000	2.006815000
H	1.768386000	4.922847000	-0.231815000	F	3.316312000	2.186459000	-4.343869000
H	-3.459070000	4.096073000	-0.354022000	F	-1.856234000	5.901711000	-0.853673000
C	3.127845000	0.822683000	-1.932233000	F	5.716440000	0.234201000	-0.788685000
C	-3.443176000	-0.369300000	-1.616174000	F	0.317120000	3.270656000	2.409421000
C	-0.649906000	3.346792000	-0.151429000	F	-4.195927000	-1.324547000	-4.142504000
C	0.500612000	-3.083634000	-0.711852000	F	-5.657530000	0.001512000	0.129197000
C	4.442214000	1.166783000	-2.543584000	Cl	-0.256636000	0.386981000	-3.337333000
C	4.484150000	1.866795000	-3.760859000	O	-0.029183000	0.053913000	0.703982000
C	5.688158000	0.878581000	-1.970215000	C	3.756747000	-1.918450000	2.329820000
C	5.667661000	2.241280000	-4.387042000	C	3.606461000	-0.617738000	1.535494000
C	6.898952000	1.234175000	-2.555040000	C	4.212801000	0.580851000	2.275872000
C	6.880921000	1.917748000	-3.773507000	C	5.680278000	0.322777000	2.644481000
H	5.621663000	2.777238000	-5.336518000	C	5.833881000	-0.979668000	3.442531000
H	7.821912000	2.204114000	-4.248358000	C	5.225719000	-2.173490000	2.693112000
H	7.830056000	0.976586000	-2.047455000	H	3.353452000	-2.764714000	1.748740000
C	0.785890000	-4.399799000	-0.079575000	H	3.151993000	-1.849216000	3.251177000
C	0.921319000	-5.613339000	-0.759806000	H	2.549185000	-0.422214000	1.293899000
C	0.944899000	-4.456347000	1.308597000	H	4.120773000	-0.729787000	0.572048000
C	1.196699000	-6.812014000	-0.106833000	H	4.128701000	1.491071000	1.655797000
C	1.219640000	-5.617436000	2.013114000	H	3.628576000	0.764613000	3.195338000

H	6.089278000	1.173177000	3.217368000	C	3.612506000	-0.652885000	1.476459000
H	6.275281000	0.250889000	1.715863000	C	1.113370000	3.276531000	0.046072000
H	6.897972000	-1.169003000	3.667247000	C	-0.614520000	-3.002012000	0.906563000
H	5.321384000	-0.868002000	4.416618000	C	-4.076729000	1.683021000	2.662231000
H	5.319668000	-3.093195000	3.296396000	C	-3.991044000	2.480977000	3.815983000
H	5.801813000	-2.345467000	1.764151000	C	-5.374454000	1.443720000	2.189961000
Li	0.108196000	-1.403712000	1.993172000	C	-5.102070000	2.993583000	4.475777000
Br	0.752298000	-0.017867000	3.926788000	C	-6.516578000	1.936914000	2.812264000
Li	0.718473000	1.320715000	1.917423000	C	-6.372299000	2.713930000	3.964329000
Br	-2.488929000	-1.964207000	2.250901000	H	-4.956617000	3.599271000	5.371817000
Li	-1.841519000	0.213187000	1.084233000	H	-7.258242000	3.108791000	4.466416000
Br	-3.384928000	0.852466000	2.816396000	H	-7.494147000	1.710456000	2.383272000
RC-Doublet with 3 LiBr				C	-1.079152000	-4.297333000	0.343325000
				C	-1.167160000	-5.504593000	1.042389000
Fe	0.287639000	0.204880000	1.075598000	C	-1.479639000	-4.335942000	-0.996342000
N	-1.404655000	-0.724247000	1.420905000	C	-1.628891000	-6.679212000	0.454368000
N	1.308440000	-1.507442000	1.216851000	C	-1.946297000	-5.472934000	-1.635779000
N	-0.678556000	1.905253000	1.043116000	C	-2.018570000	-6.654211000	-0.887857000
N	2.044412000	1.147949000	0.858112000	H	-1.677897000	-7.590819000	1.052299000
C	-2.566479000	-0.187910000	1.922151000	H	-2.383297000	-7.568475000	-1.360830000
C	2.657872000	-1.684553000	1.415460000	H	-2.240259000	-5.426623000	-2.685317000
C	-1.595889000	-2.065952000	1.276499000	C	5.036506000	-1.038679000	1.671618000
C	0.760069000	-2.745288000	1.004379000	C	5.952726000	-1.038797000	0.611662000
C	-1.956339000	2.142530000	1.465501000	C	5.525920000	-1.466941000	2.911708000
C	3.305029000	0.686291000	1.175778000	C	7.281090000	-1.422714000	0.757115000
C	-0.208446000	3.051936000	0.465054000	C	6.846426000	-1.858527000	3.108819000
C	2.182849000	2.429006000	0.386730000	C	7.722248000	-1.831551000	2.019669000
C	-3.508956000	-1.258648000	2.162699000	H	7.943409000	-1.401262000	-0.109948000
C	2.965509000	-3.094737000	1.340754000	H	8.762363000	-2.136242000	2.155312000
C	-2.936276000	-2.408440000	1.697587000	H	7.166395000	-2.176729000	4.102471000
C	1.802269000	-3.744287000	1.036220000	C	1.354342000	4.443211000	-0.844366000
C	-2.311479000	3.508709000	1.150711000	C	0.865063000	4.398974000	-2.155378000
C	4.265189000	1.731935000	0.921406000	C	2.030828000	5.615076000	-0.489215000
C	-1.250426000	4.055404000	0.484863000	C	1.023455000	5.417929000	-3.080612000
C	3.580100000	2.785949000	0.383405000	C	2.218480000	6.672945000	-1.374074000
H	-4.502729000	-1.137094000	2.586163000	C	1.711189000	6.566491000	-2.672005000
H	3.957955000	-3.522924000	1.461999000	H	0.619251000	5.307000000	-4.087895000
H	-3.354975000	-3.412619000	1.683873000	H	2.754261000	7.561139000	-1.034882000
H	1.652620000	-4.810904000	0.883241000	H	1.852357000	7.388843000	-3.376522000
H	-3.267551000	3.973731000	1.381920000	F	-0.790710000	-5.514866000	2.330046000
H	5.335866000	1.655655000	1.096191000	F	-1.393598000	-3.172077000	-1.714038000
H	-1.155227000	5.062070000	0.083111000	F	-2.768844000	2.757611000	4.301678000
H	3.985195000	3.739507000	0.054720000	F	2.515019000	5.711052000	0.759335000
C	-2.831645000	1.186086000	2.013627000	F	-5.524417000	0.712303000	1.071656000

F	0.194619000	3.268144000	-2.539814000	C	3.513173000	-2.444845000	-1.426252000
F	4.672485000	-1.500590000	3.948487000	C	-3.258070000	-2.583873000	-1.387633000
F	5.510507000	-0.658707000	-0.601076000	C	2.637601000	-3.333004000	-0.868800000
Cl	0.540161000	0.452297000	3.353533000	C	-2.336305000	-3.441008000	-0.849726000
O	0.172882000	0.016654000	-0.645349000	C	3.426102000	2.558877000	-1.323111000
C	-4.372646000	-2.032785000	-2.230123000	C	-3.337648000	2.455658000	-1.540468000
C	-4.151183000	-0.834523000	-1.300176000	C	2.504138000	3.412092000	-0.784949000
C	-4.704501000	0.461296000	-1.902410000	C	-2.461531000	3.359438000	-1.003937000
C	-6.187356000	0.315365000	-2.267462000	H	4.550273000	-2.617899000	-1.705044000
C	-6.415892000	-0.881043000	-3.201890000	H	-4.293791000	-2.794958000	-1.644048000
C	-5.854709000	-2.178054000	-2.602271000	H	2.810798000	-4.378023000	-0.619480000
H	-4.005960000	-2.958061000	-1.754434000	H	-2.460962000	-4.495738000	-0.612352000
H	-3.771980000	-1.888662000	-3.145899000	H	4.469645000	2.759670000	-1.556689000
H	-3.080225000	-0.712999000	-1.068672000	H	-4.359727000	2.636992000	-1.864004000
H	-4.652836000	-1.029595000	-0.339686000	H	2.633666000	4.457488000	-0.511454000
H	-4.564375000	1.295481000	-1.195291000	H	-2.624919000	4.420268000	-0.827251000
H	-4.119838000	0.706035000	-2.806120000	C	3.410075000	0.066369000	-1.803748000
H	-6.563421000	1.242423000	-2.734635000	C	-3.270456000	-0.076767000	-1.792528000
H	-6.773573000	0.169952000	-1.340792000	C	0.005447000	3.250296000	-0.412086000
H	-7.490792000	-0.995629000	-3.426114000	C	0.150526000	-3.248412000	-0.386294000
H	-5.912369000	-0.683939000	-4.167079000	C	4.820741000	0.127143000	-2.278341000
H	-5.995163000	-3.017477000	-3.305503000	C	5.125229000	0.511742000	-3.591169000
H	-6.431669000	-2.430936000	-1.692391000	C	5.916918000	-0.151423000	-1.453502000
Li	-0.584878000	-1.320825000	-1.808945000	C	6.427260000	0.601850000	-4.073287000
Br	-1.352710000	0.074880000	-3.665744000	C	7.236378000	-0.074991000	-1.885355000
Li	0.068244000	1.278702000	-2.119781000	C	7.483886000	0.302921000	-3.208473000
Br	1.979364000	-2.174354000	-2.584735000	H	6.592983000	0.902099000	-5.109359000
Li	2.012296000	-0.398589000	-0.850608000	H	8.512982000	0.368629000	-3.568501000
Br	2.656448000	0.745921000	-2.949064000	H	8.042443000	-0.304752000	-1.186574000
TS-Doublet with 3 LiBr				C	0.183555000	-4.537412000	0.358394000
Fe	0.100939000	-0.003950000	-1.077068000	C	0.228617000	-5.805766000	-0.228499000
N	1.520318000	-1.342568000	-1.122626000	C	0.169553000	-4.515676000	1.756283000
N	-1.314643000	-1.396584000	-1.072489000	C	0.256168000	-6.979954000	0.519302000
N	1.461312000	1.390565000	-1.106158000	C	0.194066000	-5.648298000	2.554049000
N	-1.380766000	1.335095000	-1.085506000	C	0.238391000	-6.892423000	1.914065000
C	2.815453000	-1.178407000	-1.535544000	H	0.290459000	-7.940156000	0.001790000
C	-2.622147000	-1.293887000	-1.495932000	H	0.258858000	-7.805310000	2.513048000
C	1.369848000	-2.639852000	-0.730455000	H	0.180709000	-5.550282000	3.640560000
C	-1.105478000	-2.697571000	-0.704858000	C	-4.686732000	-0.138803000	-2.242388000
C	2.767683000	1.277589000	-1.487401000	C	-5.755681000	0.274053000	-1.435058000
C	-2.673395000	1.176026000	-1.549259000	C	-5.030748000	-0.659164000	-3.497979000
C	1.254967000	2.677773000	-0.702526000	C	-7.084739000	0.198188000	-1.838834000
C	-1.221177000	2.656679000	-0.772193000	C	-6.343643000	-0.752988000	-3.947439000
				C	-7.371517000	-0.317133000	-3.106263000

H	-7.868926000	0.536240000	-1.159303000	Li	-1.907124000	0.026436000	0.554336000
H	-8.409103000	-0.383469000	-3.440992000	Br	-2.883490000	1.600779000	2.202746000
H	-6.539870000	-1.162530000	-4.939798000				
C	-0.014802000	4.543077000	0.324956000	PC-Doublet with 3 LiBr			
C	0.150904000	4.532764000	1.713732000	Fe	0.077965000	-0.008496000	-1.132538000
C	-0.187177000	5.802859000	-0.256486000	N	1.512909000	-1.333577000	-1.142918000
C	0.153420000	5.668728000	2.506825000	N	-1.327210000	-1.394823000	-1.096214000
C	-0.192103000	6.979881000	0.487088000	N	1.451966000	1.384230000	-1.101374000
C	-0.019851000	6.904249000	1.872015000	N	-1.386854000	1.335057000	-1.099722000
H	0.286363000	5.580080000	3.586108000	C	2.807833000	-1.167873000	-1.566575000
H	-0.329971000	7.933228000	-0.025934000	C	-2.645413000	-1.289039000	-1.480888000
H	-0.022014000	7.819622000	2.467517000	C	1.368088000	-2.630209000	-0.756832000
F	0.244884000	-5.878447000	-1.568072000	C	-1.110691000	-2.694385000	-0.725760000
F	0.131106000	-3.290118000	2.372008000	C	2.763049000	1.280997000	-1.473606000
F	4.104987000	0.805528000	-4.414414000	C	-2.680084000	1.181979000	-1.560818000
F	-0.356837000	5.864017000	-1.586343000	C	1.251561000	2.659070000	-0.656080000
F	5.672887000	-0.495640000	-0.173325000	C	-1.218094000	2.660916000	-0.796919000
F	0.314006000	3.313949000	2.323186000	C	3.509485000	-2.431793000	-1.478052000
F	-4.037986000	-1.087174000	-4.296144000	C	-3.282000000	-2.577658000	-1.352098000
F	-5.475357000	0.750731000	-0.211163000	C	2.636781000	-3.321693000	-0.906229000
Cl	0.053398000	0.003302000	-3.369265000	C	-2.344253000	-3.436508000	-0.843579000
O	0.050290000	-0.003658000	0.862556000	C	3.429293000	2.548678000	-1.262394000
C	2.883419000	-1.365280000	2.421520000	C	-3.328479000	2.468809000	-1.587068000
C	2.607638000	-0.103569000	1.626098000	C	2.509570000	3.382797000	-0.689104000
C	2.999399000	1.174894000	2.340400000	C	-2.445054000	3.376199000	-1.057959000
C	4.505535000	1.111292000	2.683285000	H	4.542116000	-2.606154000	-1.784065000
C	4.831020000	-0.142523000	3.503908000	H	-4.324562000	-2.784368000	-1.573784000
C	4.384742000	-1.422347000	2.786706000	H	2.813356000	-4.367027000	-0.658879000
H	2.600650000	-2.259729000	1.844760000	H	-2.462158000	-4.491713000	-0.604519000
H	2.293427000	-1.357023000	3.351835000	H	4.482646000	2.741422000	-1.465501000
H	1.432985000	-0.057052000	1.287514000	H	-4.343921000	2.640350000	-1.931477000
H	3.086588000	-0.154189000	0.644168000	H	2.644771000	4.414097000	-0.375211000
H	2.789044000	2.053660000	1.711022000	H	-2.585855000	4.444037000	-0.929843000
H	2.424362000	1.276693000	3.275299000	C	3.405254000	0.077297000	-1.818629000
H	4.795766000	2.023801000	3.231356000	C	-3.291807000	-0.068348000	-1.778350000
H	5.087373000	1.095381000	1.745530000	C	0.002126000	3.239104000	-0.387754000
H	5.913839000	-0.186159000	3.714306000	C	0.150637000	-3.240662000	-0.409749000
H	4.320452000	-0.077245000	4.482258000	C	4.814500000	0.145027000	-2.297049000
H	4.571629000	-2.307889000	3.417803000	C	5.109701000	0.562305000	-3.603829000
H	4.975992000	-1.551844000	1.865336000	C	5.917390000	-0.151308000	-1.487057000
Li	-0.312772000	-1.351384000	2.276789000	C	6.409004000	0.654643000	-4.093368000
Br	0.029717000	0.034784000	4.305091000	C	7.233040000	-0.064480000	-1.927728000
Li	-0.231601000	1.385858000	2.253439000	C	7.471759000	0.337878000	-3.244123000
Br	-2.976132000	-1.447336000	2.212346000	H	6.568809000	0.976228000	-5.125654000

H	8.501467000	0.410313000	-3.599910000	C	4.444203000	-1.464096000	2.784328000
H	8.041911000	-0.306280000	-1.239692000	H	2.626490000	-2.269004000	1.846820000
C	0.183265000	-4.527658000	0.335314000	H	2.365354000	-1.371240000	3.374274000
C	0.217610000	-5.800739000	-0.246942000	H	0.984703000	-0.051931000	1.126843000
C	0.173836000	-4.507304000	1.728049000	H	2.987482000	-0.149502000	0.621476000
C	0.253422000	-6.969854000	0.505765000	H	2.847661000	2.026326000	1.729874000
C	0.200178000	-5.633127000	2.532627000	H	2.469947000	1.241518000	3.292205000
C	0.256689000	-6.878322000	1.901867000	H	4.838341000	1.992775000	3.300372000
H	0.292137000	-7.931066000	-0.012116000	H	5.143448000	1.123449000	1.771004000
H	0.309393000	-7.792488000	2.500275000	H	5.974626000	-0.227158000	3.697131000
H	0.187108000	-5.514089000	3.619106000	H	4.373977000	-0.139408000	4.472860000
C	-4.712813000	-0.124835000	-2.211213000	H	4.639536000	-2.345107000	3.418043000
C	-5.773675000	0.290508000	-1.389890000	H	5.025449000	-1.592554000	1.865858000
C	-5.062818000	-0.655679000	-3.459455000	Li	-0.360584000	-1.392831000	2.307991000
C	-7.106757000	0.199841000	-1.785819000	Br	0.050836000	-0.003351000	4.319909000
C	-6.378481000	-0.734451000	-3.904950000	Li	-0.303244000	1.392653000	2.315431000
C	-7.400085000	-0.310149000	-3.051957000	Br	-2.973980000	-1.440319000	2.205615000
H	-7.894203000	0.540440000	-1.108527000	Li	-1.816645000	0.019643000	0.564318000
H	-8.437865000	-0.362346000	-3.380107000	Br	-2.882517000	1.608824000	2.212010000
H	-6.583834000	-1.140500000	-4.897287000	RC HBr adds to CHA			
C	-0.011253000	4.531332000	0.345769000	C	1.101080000	0.429298000	1.409434000
C	0.156910000	4.530720000	1.735658000	C	1.142180000	-0.892802000	1.154743000
C	-0.186869000	5.784381000	-0.245855000	C	1.666371000	-1.470328000	-0.134486000
C	0.170862000	5.672822000	2.522658000	C	2.466987000	-0.443554000	-0.947415000
C	-0.187389000	6.964814000	0.492293000	C	1.745803000	0.908672000	-0.987092000
C	-0.011147000	6.902430000	1.877507000	C	1.556836000	1.477214000	0.426508000
H	0.293643000	5.600387000	3.604735000	H	0.729280000	0.778221000	2.379851000
H	-0.328798000	7.910743000	-0.037081000	H	0.777453000	-1.597093000	1.911366000
H	-0.011653000	7.823457000	2.468865000	H	2.279799000	-2.361118000	0.085819000
F	0.224149000	-5.876307000	-1.583138000	H	0.810078000	-1.845846000	-0.728728000
F	0.147284000	-3.281529000	2.344399000	H	2.642166000	-0.821960000	-1.967593000
F	4.083841000	0.884521000	-4.412048000	H	3.460379000	-0.308478000	-0.482513000
F	-0.369486000	5.840558000	-1.572695000	H	2.297320000	1.628247000	-1.613551000
F	5.685023000	-0.523290000	-0.215027000	H	0.755287000	0.773485000	-1.457109000
F	0.313803000	3.306540000	2.341311000	H	0.831926000	2.310220000	0.416607000
F	-4.073737000	-1.090981000	-4.256451000	H	2.503435000	1.917845000	0.794917000
F	-5.477666000	0.774680000	-0.168693000	H	-0.834115000	-0.107660000	0.519933000
Cl	0.046898000	-0.006921000	-3.400139000	Br	-2.123673000	-0.011911000	-0.153976000
O	0.018577000	-0.027841000	0.901467000	TS HBr adds to CHA			
C	2.940700000	-1.388557000	2.432496000	C	-0.628018000	-0.071161000	1.301514000
C	2.727175000	-0.119353000	1.674801000	C	-0.924444000	1.201566000	0.740818000
C	3.059874000	1.156655000	2.366290000	C	-1.954512000	1.329650000	-0.388277000
C	4.566413000	1.097617000	2.713669000				
C	4.892033000	-0.179583000	3.497964000				

C	-2.690841000	0.014804000	-0.687559000	C	0.775489000	-1.268487000	0.833503000
C	-1.740571000	-1.187345000	-0.650837000	C	1.572728000	-1.264549000	-0.473517000
C	-1.121788000	-1.330927000	0.738822000	C	2.425458000	0.003438000	-0.604727000
H	-0.011647000	-0.112699000	2.205276000	C	1.569735000	1.270099000	-0.469030000
H	-0.841616000	2.040732000	1.446521000	C	0.764118000	1.266649000	0.835177000
H	-2.674324000	2.118124000	-0.119143000	H	-0.569470000	0.003852000	2.001306000
H	-1.438623000	1.681457000	-1.297318000	H	0.149613000	-2.168592000	0.913504000
H	-3.190183000	0.084436000	-1.666473000	H	1.470434000	-1.301336000	1.693142000
H	-3.484656000	-0.140834000	0.064891000	H	2.203208000	-2.167267000	-0.519316000
H	-2.266887000	-2.116156000	-0.917713000	H	0.871287000	-1.331177000	-1.321085000
H	-0.920725000	-1.047808000	-1.376591000	H	2.959326000	0.006437000	-1.569855000
H	-0.355912000	-2.116222000	0.815257000	H	3.198783000	0.002899000	0.185755000
H	-1.902035000	-1.616163000	1.486179000	H	2.203218000	2.171519000	-0.507127000
H	0.158052000	1.152989000	0.285081000	H	0.873686000	1.336022000	-1.323614000
Br	2.036846000	0.009503000	-0.207224000	H	0.119809000	2.155683000	0.915030000
PC HBr adds to CHA				H	1.460784000	1.302275000	1.694229000
C	-0.053711000	-0.003926000	1.032112000	Br	-1.636102000	-0.000847000	-0.259517000