

Supporting Information

**Mechanism of Fe(III) Catalyzed Synthesis of Hexahydropyrimidine
with α -Phenylstyrene: A DFT study**

Yaxuan Cheng, Siwei Yang, Chaoyu Zhao, Huiling Liu*

Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry,
College of Chemistry, Jilin University, Liutiao Road 2, Changchun 130023, China

Corresponding author: huiling@jlu.edu.cn (HLL)

Table of Contents

Fig S1. The optimized representative structures in path 1. The important bond distances are shown in Å. The yellow, cyan-blue, green, purple, red, gray and white spheres represent sulfur atoms, iron atoms, fluorine atoms, nitrogen atoms, oxygen atoms, carbon atoms, hydrogen atoms, respectively. pp.1

Fig S2. The optimized representative structures in path 2. The important bond distances are in shown Å. The yellow, cyan-blue, green, purple, red, gray and white spheres represent sulfur atoms, iron atoms, fluorine atoms, nitrogen atoms, oxygen atoms, carbon atoms, hydrogen atoms, respectively. pp.2

Table S1. The Gibbs free energies (in Hartree) and coordinates of all structures, and values of imaginary frequencies (in cm^{-1}) of all transition states. pp.3-58

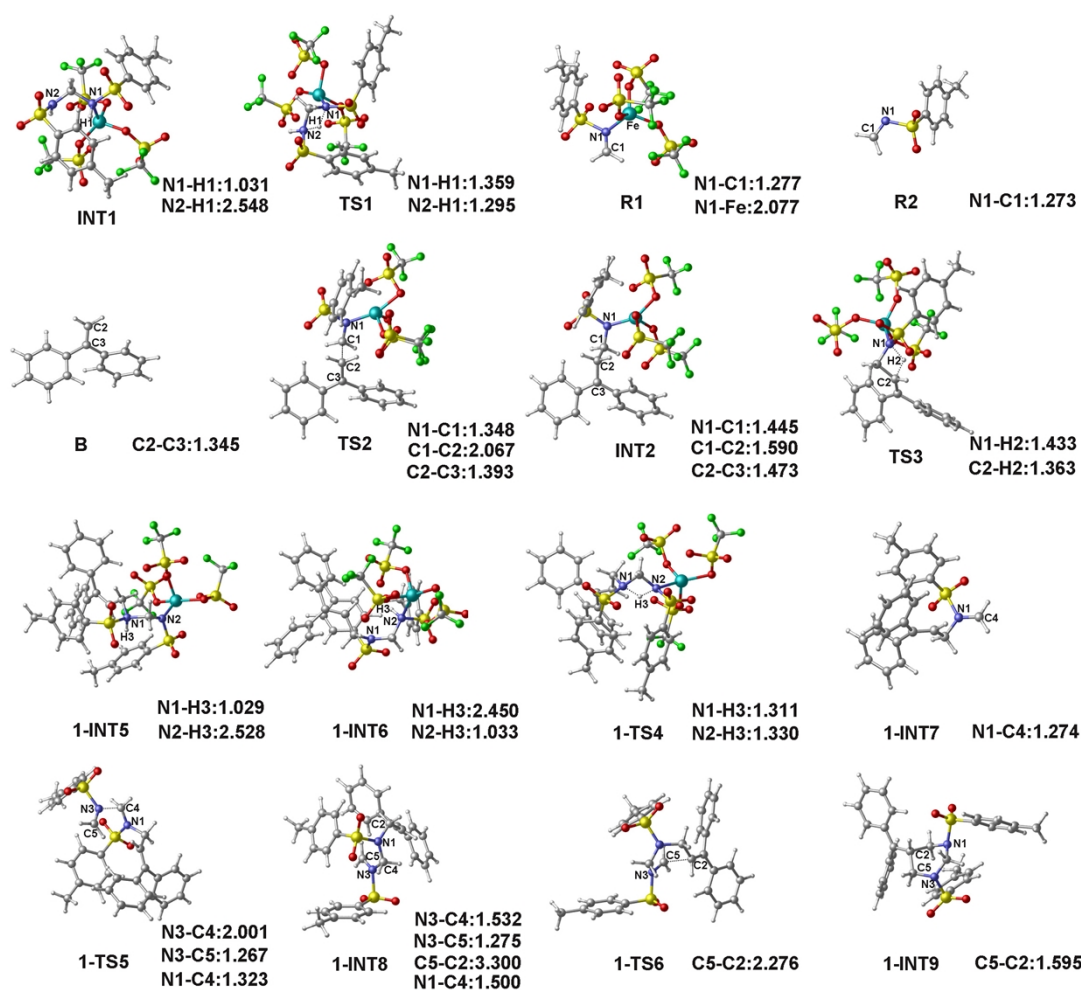


Fig S1. The optimized representative structures in path 1. The important bond distances are shown in Å. The yellow, cyan-blue, green, purple, red, gray and white spheres represent sulfur atoms, iron atoms, fluorine atoms, nitrogen atoms, oxygen atoms, carbon atoms, hydrogen atoms, respectively.

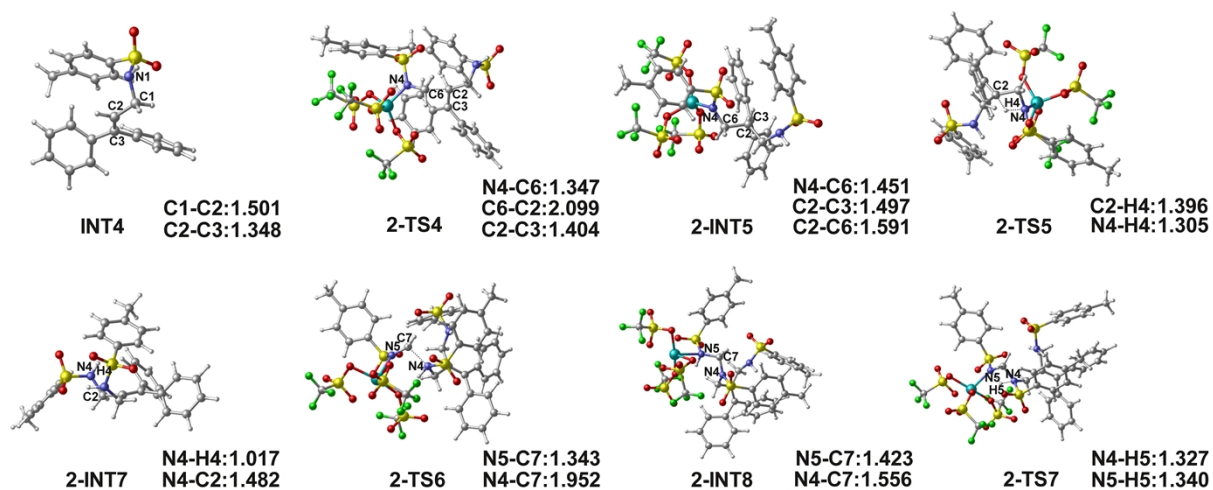


Fig S2. The optimized representative structures in path 2. The important bond distances are in shown Å. The yellow, cyan-blue, green, purple, red, gray and white spheres represent sulfur atoms, iron atoms, fluorine atoms, nitrogen atoms, oxygen atoms, carbon atoms, hydrogen atoms, respectively.

Table S1. The Gibbs free energies (in Hartree) and coordinates of all structures, and values of imaginary frequencies (in cm^{-1}) of all transition states.

	A		
	Energy = -1789.279985		
C	0.00009000	0.00179900	-0.09487800
H	0.71669600	0.52315400	0.54928000
H	-0.71594900	-0.51964100	0.54983700
S	-1.85444000	1.93101600	-0.20332500
O	-2.17162200	2.94558500	-1.21015700
O	-1.36586600	2.30681900	1.12927200
C	-3.24056900	0.83320200	0.01625000
C	-4.01900300	0.48913900	-1.09147500
C	-3.52359500	0.33481100	1.28484500
C	-5.09119000	-0.37530800	-0.91453000
H	-3.78595900	0.90324500	-2.06584800
C	-4.60349000	-0.53375100	1.44175300
H	-2.91110500	0.63452400	2.12724400
C	-5.39786000	-0.90208100	0.35118800
H	-5.70570000	-0.64696900	-1.76813300
H	-4.83244200	-0.92772400	2.42727100
C	-6.56114300	-1.84570200	0.51875200
H	-6.71059700	-2.11472400	1.56689300
H	-7.48873000	-1.39757200	0.14728900
H	-6.40063100	-2.77026000	-0.04684800
N	-0.74136700	0.90438500	-0.97130400
H	-0.13549400	1.47580900	-1.55857600
S	1.85279700	-1.92908500	-0.20490100
O	2.16880800	-2.94327200	-1.21248600
O	1.36393400	-2.30533900	1.12747700
C	3.24017400	-0.83298400	0.01536400
C	4.01785000	-0.48762800	-1.09252900
C	3.52472700	-0.33695100	1.28450600
C	5.09089100	0.37560200	-0.91510000
H	3.78325100	-0.89946000	-2.06749100
C	4.60559900	0.53035700	1.44192800
H	2.91239900	-0.63714500	2.12685100
C	5.39946600	0.89958100	0.35134500
H	5.70452900	0.64865400	-1.76889300
H	4.83553900	0.92280800	2.42781900
C	6.56617600	1.83880700	0.51987500
H	6.69341400	2.13597000	1.56332400
H	7.49847200	1.37233000	0.18397900
H	6.42776400	2.74776300	-0.07575400

N	0.74076200	-0.90071600	-0.97204500
H	0.13429800	-1.47103900	-1.55978100
Fe(OTf) ₃			
Energy = -3008.917228			
Fe	0.27525400	-0.32152300	-0.06670900
O	1.92396200	-0.50626200	-1.29230400
S	2.79114100	-1.16240700	-0.21334200
O	3.48917900	-2.38531800	-0.54262500
O	1.82305600	-1.18284800	0.97616700
O	-1.19642900	-0.93176400	1.24131900
S	-1.64801600	-2.10453200	0.36517900
O	-1.78573600	-3.40634600	0.97925100
O	-0.70484100	-1.96539500	-0.83324200
O	-0.64200300	1.07240700	-1.28409200
S	-0.27514400	2.25900800	-0.39015100
O	0.34712500	3.41290500	-1.00152900
O	0.47108200	1.56046700	0.75044400
C	-1.89839900	2.80553300	0.35962900
C	4.06229500	0.13634200	0.22962100
C	-3.32562700	-1.58769800	-0.27904100
F	-3.23245200	-0.39039200	-0.85100800
F	-4.16802200	-1.53675100	0.74627300
F	-3.72937100	-2.48705100	-1.16692100
F	4.89164600	0.27496300	-0.79734800
F	4.72086700	-0.27745400	1.30526700
F	3.44806300	1.28681400	0.48164200
F	-1.64666000	3.73915600	1.26842300
F	-2.49817500	1.76381100	0.92845200
F	-2.66112600	3.29564300	-0.61043500
INT1			
Energy = -4798.22826			
C	-0.34350700	1.57938200	-2.04254600
H	-1.34591300	1.88976100	-1.76110400
H	-0.25931000	1.53576500	-3.12825000
S	2.10668100	2.71979100	-2.29941500
O	2.72771500	3.81969900	-1.56661000
O	1.80945300	2.75997200	-3.73051100
C	3.03943100	1.23197400	-1.98580300
C	3.91675400	1.18830600	-0.90451700
C	2.77806300	0.09208200	-2.75369000
C	4.52153000	-0.02189600	-0.57570700
H	4.09551700	2.08412700	-0.32198200
C	3.37290600	-1.11480000	-2.39326800
H	2.12457500	0.15307200	-3.61836700

C	4.24845500	-1.19032100	-1.29940300
H	5.19291900	-0.06723000	0.27637200
H	3.14697100	-2.00919100	-2.96489800
C	4.89858900	-2.49807900	-0.92954400
H	5.81962600	-2.64889300	-1.50478200
H	5.16037500	-2.52441300	0.13086600
H	4.23532000	-3.33969700	-1.14154000
N	0.61372100	2.50099900	-1.53774900
H	0.61313400	2.71615300	-0.54732300
S	-0.79684000	-1.13403300	-2.57416800
O	0.10425100	-2.25836900	-2.34982600
O	-0.93553300	-0.49984100	-3.88513100
C	-2.39111900	-1.44456100	-1.88341900
C	-2.56042200	-2.52009700	-1.01117300
C	-3.43982300	-0.57803400	-2.20460900
C	-3.79829000	-2.68351000	-0.39740300
H	-1.74651100	-3.20086000	-0.80463700
C	-4.66692100	-0.76847500	-1.58442800
H	-3.29324900	0.21775400	-2.92535100
C	-4.85647600	-1.80228900	-0.65298800
H	-3.93146300	-3.50293500	0.30154500
H	-5.48871200	-0.09697100	-1.81243700
C	-6.16830600	-1.93279300	0.07305100
H	-7.01620400	-1.81107500	-0.60777100
H	-6.25880100	-2.90053900	0.57107600
H	-6.25009900	-1.15265700	0.83908600
N	-0.14382400	0.16409100	-1.48992700
H	0.86752200	-0.03382600	-1.52759100
O	-0.21849100	-1.87859000	0.67353800
S	0.09662300	-3.15449100	1.54692500
O	0.20147000	-2.81624400	2.95564400
O	-0.74130500	-4.25385500	1.08359700
C	1.82388900	-3.46073200	0.91521300
O	-2.41189000	0.12109500	1.16723000
S	-2.47878500	1.64026100	1.41255200
O	-2.83420500	2.06945300	2.74936000
O	-1.20471400	2.14319300	0.78586800
C	-3.85440600	2.23359800	0.29944600
Fe	-0.44685400	-0.05314100	0.64896100
O	0.28882900	0.40847100	2.68953600
S	1.68406700	0.72343700	2.19847100
O	2.81318200	0.04836200	2.80510200
O	1.53297700	0.60272900	0.67576500
C	1.97170700	2.55579900	2.44456500

F	3.23482100	2.81780400	2.11179200
F	1.75878700	2.86035200	3.71737400
F	1.15484500	3.26445400	1.66497400
F	-4.08194700	3.51405900	0.56216800
F	-4.95173000	1.51670400	0.53166600
F	-3.50183700	2.10595200	-0.98631800
F	1.79673900	-3.68828900	-0.39731100
F	2.33121500	-4.51786800	1.54467300
F	2.57789100	-2.38691200	1.16285600
TS1			
Energy = -4798.178729, Lowest Freq ν = -1676.83			
C	-0.28064600	-0.37040800	-2.12143700
H	0.71849900	-0.71335100	-2.37467200
H	-0.70808100	0.25459400	-2.90484100
S	-2.66042000	-1.80206400	-2.75500500
O	-2.95062200	-3.20340300	-2.47438000
O	-2.37282600	-1.29621800	-4.09358800
C	-3.78880800	-0.73034800	-1.92374100
C	-4.26920300	-1.11237300	-0.66742200
C	-4.11038100	0.49879100	-2.49848600
C	-5.06879700	-0.22074800	0.03207900
H	-4.00911100	-2.07780900	-0.24959900
C	-4.92584200	1.36802600	-1.78143100
H	-3.71533000	0.76787200	-3.46998300
C	-5.39431900	1.03420300	-0.50537100
H	-5.43036300	-0.48944500	1.01954600
H	-5.17489300	2.33453200	-2.20764900
C	-6.18214700	2.02579500	0.30655500
H	-6.71120200	2.73963900	-0.32986100
H	-6.91001200	1.52967200	0.95427800
H	-5.50047300	2.59454600	0.95027600
N	-1.19078600	-1.51130400	-1.77955800
H	-0.70720600	-2.39965500	-1.61826900
S	-1.20516600	1.79826200	-0.70418500
O	-2.32060700	1.56296700	0.21134000
O	-1.43476300	2.19208700	-2.10127300
C	-0.09545400	2.95539200	0.05153100
C	-0.11500900	3.10565400	1.44010500
C	0.76346400	3.70353600	-0.75421500
C	0.79066400	3.98274100	2.02634500
H	-0.81556100	2.54561300	2.04311000
C	1.65529000	4.57855100	-0.14551200
H	0.72601400	3.60079000	-1.83054800
C	1.69804600	4.71599700	1.24929700

H	0.79187600	4.09491500	3.10615900
H	2.33353100	5.16107100	-0.76120200
C	2.71208000	5.61854200	1.90140400
H	3.00586000	6.43714100	1.23900200
H	2.32799600	6.04555400	2.83165800
H	3.61856300	5.05381000	2.15021000
N	-0.34675400	0.26555900	-0.77891400
H	-1.20981200	-0.78214000	-0.70946700
O	0.09132000	0.27709200	2.08772100
S	-0.54583300	-0.34248500	3.38686800
O	0.10686600	-1.58986300	3.75120800
O	-0.77119100	0.72605900	4.34960100
C	-2.22695100	-0.81468900	2.71765300
O	2.55171300	1.11427900	0.34847300
S	3.40928500	0.46885000	-0.75745000
O	4.82428900	0.34424300	-0.46980400
O	2.62317000	-0.72994900	-1.19246100
C	3.26197300	1.64092200	-2.19812500
Fe	1.08524800	-0.26000600	0.60271300
O	2.38657800	-1.67905800	1.57980800
S	1.67088800	-2.91100900	1.06082100
O	1.32808800	-3.97151400	1.98370400
O	0.52016600	-2.30177800	0.24265400
C	2.82058900	-3.67037100	-0.24338300
F	2.95253400	-4.96436400	0.02758600
F	4.00354500	-3.07726300	-0.19750400
F	2.27502200	-3.52730800	-1.45160100
F	4.03303600	1.19204000	-3.18378100
F	3.64607100	2.86402600	-1.84417400
F	1.98935200	1.67672900	-2.62387300
F	-2.99460000	0.25907000	2.56709900
F	-2.80179400	-1.65544200	3.57554700
F	-2.09302700	-1.43600800	1.53122800
R1			
Energy = -3922.626258			
S	2.26760600	-1.49304900	-2.12679200
O	2.51477300	-1.49816900	-3.56806400
O	2.38403300	-2.68796400	-1.30436200
C	2.99811600	-0.10181400	-1.34157900
C	3.48671700	-0.24603500	-0.03990000
C	3.01042600	1.12552200	-2.01453300
C	3.98179800	0.88405000	0.60021900
H	3.45528900	-1.20838700	0.45694200
C	3.50019500	2.23748000	-1.34518500

H	2.63719400	1.20371900	-3.02944100
C	3.97823600	2.13699800	-0.02739400
H	4.34537800	0.79705700	1.61862200
H	3.49002500	3.20430100	-1.83655400
C	4.40999700	3.36733700	0.71875000
H	3.53755300	3.80682300	1.21486900
H	5.14861400	3.13166000	1.48883300
H	4.82744100	4.12163400	0.04700300
N	0.50543300	-1.01665400	-1.96978300
Fe	-0.17834100	-0.26473000	-0.15900900
O	1.27371400	2.24569100	1.65647500
S	0.46473100	2.73854600	0.54957800
O	0.87739500	3.89587700	-0.22968300
O	0.06141100	1.56400600	-0.43314300
C	-1.22122900	3.09330000	1.25887300
F	-1.70719200	1.96556500	1.79490100
F	-2.04446900	3.51966500	0.30406000
F	-1.10492900	4.02106900	2.20312600
C	-0.18354700	-1.09317900	-3.04266700
H	-1.25337400	-0.88850800	-3.00821400
H	0.29986500	-1.39015200	-3.97654900
O	0.79832800	-0.91335800	1.24160700
S	1.01995100	-2.17511700	2.17648600
O	0.55352100	-1.87999200	3.51880200
O	2.34939300	-2.71002200	1.92201700
C	-0.21469500	-3.36576900	1.41673800
F	-0.22592700	-3.20998200	0.07767500
F	0.14442100	-4.60718800	1.70959200
F	-1.42927100	-3.11214500	1.88724500
O	-1.97442400	-0.68516100	0.10276500
S	-3.30417100	-0.90273500	-0.70241200
O	-4.27703300	-1.60618400	0.11021900
O	-3.00336700	-1.34472300	-2.06740600
C	-3.84740100	0.86995700	-0.86399700
F	-2.88923200	1.54945200	-1.51290500
F	-4.03707600	1.40751600	0.33559200
F	-4.97439300	0.91627300	-1.56732300
TsNH ₂			
Energy = -875.6002024			
S	1.89489500	0.02660400	-0.13768800
O	2.33819000	-1.15771100	-0.87902100
O	2.31656000	1.38203500	-0.50742600
C	0.11211100	0.01563900	-0.07609100
C	-0.56309700	-1.20566100	-0.07023200

C	-1.95211300	-1.20613500	-0.02138000
C	-2.67673000	-0.00514600	0.02028500
C	-1.97157500	1.20346100	0.00090900
C	-0.57878600	1.22397200	-0.04767600
H	-0.00370700	-2.13274600	-0.12101200
H	-2.48653900	-2.15188800	-0.02305300
H	-2.51893900	2.14134600	0.01689200
H	-0.02939700	2.15755500	-0.08151000
C	-4.18218500	-0.02408900	0.09674600
H	-4.60839900	0.94743900	-0.16533700
H	-4.60517700	-0.77593900	-0.57631800
H	-4.51835200	-0.27127400	1.11073100
N	2.33640600	-0.25457700	1.47709800
H	3.05597900	-0.97333700	1.48612800
H	2.67762000	0.60838000	1.89301600
R2			
Energy = -913.68023			
S	1.66336900	0.16550100	-0.41408200
O	2.13139200	-1.07764400	-1.04673000
O	2.02447500	1.47271300	-0.96400600
C	-0.10156900	0.07295300	-0.21264900
C	-0.80441200	1.22574100	0.14157700
C	-0.75064300	-1.14278300	-0.41587600
C	-2.18311500	1.14637100	0.30070000
H	-0.27550400	2.16246900	0.27393000
C	-2.13298000	-1.20027000	-0.25535800
H	-0.17710200	-2.01487200	-0.70769400
C	-2.86639600	-0.06405100	0.10882500
H	-2.74195300	2.03755000	0.57128400
H	-2.65158200	-2.14005000	-0.42049700
C	-4.35830800	-0.13904800	0.30979100
H	-4.60299900	-0.22927700	1.37490800
H	-4.85579200	0.76144100	-0.06177400
H	-4.78795700	-1.00403200	-0.20163300
N	2.14865800	0.22531400	1.26336300
C	2.95832900	-0.69579800	1.60380900
H	3.32801300	-0.69358500	2.62978300
H	3.29800000	-1.48410300	0.92443300
B			
Energy = -540.7338557			
C	0.00023700	2.50382100	-0.00014200
H	-0.92119500	3.06931100	0.08529000
H	0.92196100	3.06878700	-0.08583100
C	-0.00004000	1.15921200	0.00024600

C	1.27523500	0.39571800	-0.04053500
C	1.38531100	-0.77650800	-0.80598900
C	2.40404500	0.83988500	0.66517100
C	2.59178100	-1.46851200	-0.88026800
H	0.51935100	-1.13668500	-1.35115600
C	3.61043000	0.14675800	0.59277500
H	2.32139200	1.72374200	1.28933200
C	3.70985700	-1.00921300	-0.18236000
H	2.65946500	-2.36767100	-1.48531000
H	4.47047000	0.50328700	1.15171500
H	4.64837500	-1.55243400	-0.23547900
C	-1.27531900	0.39586600	0.04087100
C	-1.38553300	-0.77633000	0.80641600
C	-2.40389400	0.83997200	-0.66519700
C	-2.59201000	-1.46830300	0.88033400
H	-0.51980600	-1.13600900	1.35234900
C	-3.61030200	0.14681600	-0.59315600
H	-2.32096100	1.72373600	-1.28944900
C	-3.70988400	-1.00910000	0.18195200
H	-2.66005700	-2.36734300	1.48551100
H	-4.47017900	0.50329400	-1.15237600
H	-4.64831000	-1.55251800	0.23468900
TS2			
Energy = -4463.357063, Lowest Freq ν = -312.70			
S	-0.10005100	2.87959300	-1.77794300
O	-1.42920300	3.51232600	-1.75412200
O	0.73282400	2.92993700	-2.97443200
C	0.83251800	3.40882100	-0.36625200
C	2.22494900	3.45870600	-0.45513900
C	0.16333900	3.74488800	0.81502600
C	2.95459700	3.80294100	0.67847900
H	2.71555800	3.21857600	-1.38889000
C	0.91246100	4.09465100	1.92987600
H	-0.91833500	3.73805500	0.85611700
C	2.31453200	4.10511500	1.88622300
H	4.03830100	3.80675600	0.62595400
H	0.40407600	4.33208900	2.85891800
C	3.11203200	4.36520200	3.13403000
H	3.24075800	3.42209300	3.67795500
H	4.10590800	4.75793000	2.90458800
H	2.60310600	5.06704700	3.80064800
N	-0.36735000	1.19559600	-1.39391900
Fe	1.03063100	-0.05869000	-0.67266600
O	1.95691200	1.13915400	2.44467600

S	0.69648800	0.40852500	2.48676100
O	-0.47483500	0.99151700	3.14310800
O	0.27732700	-0.13953500	1.09067500
C	1.04854300	-1.19556100	3.36204900
F	1.92265300	-1.91859300	2.66593200
F	-0.08585300	-1.89275400	3.50929700
F	1.55184800	-0.92267100	4.56621000
C	-1.65231500	0.78902800	-1.43332300
H	-1.80790700	-0.28504100	-1.37956200
H	-2.34332200	1.35722200	-2.04925600
C	-2.54221900	1.30944000	0.35814900
H	-1.74236000	0.91395900	0.96835600
H	-2.56317300	2.38373500	0.22824700
C	-3.73384400	0.59373300	0.25643000
C	-4.91576300	1.21201400	-0.35496700
C	-6.21028100	0.73812900	-0.05328700
C	-4.79255700	2.32718100	-1.21416300
C	-7.33554500	1.34460000	-0.60099700
H	-6.32616800	-0.08883400	0.63689600
C	-5.92088400	2.91745600	-1.77126200
H	-3.81644200	2.73412300	-1.45493900
C	-7.19486100	2.42891400	-1.46938500
H	-8.32338700	0.97400200	-0.34660200
H	-5.80554100	3.76301600	-2.44159300
H	-8.07339100	2.89670900	-1.90279900
C	-3.74987700	-0.81656200	0.66093200
C	-2.96576100	-1.25569900	1.74832600
C	-4.46037200	-1.77338000	-0.09355400
C	-2.90259400	-2.60609900	2.06709000
H	-2.42374100	-0.53630200	2.35189300
C	-4.38066900	-3.12432800	0.22357000
H	-5.02862000	-1.45680700	-0.96023100
C	-3.60253000	-3.54377700	1.30301000
H	-2.29449200	-2.92860700	2.90413400
H	-4.90679300	-3.85170200	-0.38580100
H	-3.53288000	-4.59986100	1.54408800
O	2.55483500	0.74821700	-1.78123800
S	3.70920500	0.20001900	-0.93144300
O	2.98356700	-0.55354500	0.15799800
O	4.75517800	1.13823900	-0.56867000
C	4.48282500	-1.10783200	-2.01542600
F	5.01759600	-0.51778800	-3.08079500
F	5.42938200	-1.72822600	-1.31461500
F	3.55562700	-1.97984400	-2.39607400

O	0.72486200	-1.71815000	-1.51427500
S	-0.33218200	-2.85777700	-1.62965200
O	-0.04460500	-3.70422600	-2.77548600
O	-1.68452700	-2.33750300	-1.41311100
C	0.09021100	-3.84359500	-0.11002600
F	-0.01034600	-3.07228100	0.97633400
F	1.33340200	-4.31095300	-0.20231900
F	-0.76717300	-4.86161400	-0.00379100
INT2			
Energy = -4463.377476			
S	-0.17812300	2.90700700	-1.69478000
O	-1.52695200	3.50585400	-1.61613400
O	0.59586000	3.01799300	-2.92876600
C	0.79400100	3.48559100	-0.32744000
C	2.18481400	3.47206500	-0.43489700
C	0.15732300	3.85835000	0.85950800
C	2.94601600	3.78490300	0.68793500
H	2.65238400	3.20718800	-1.37422500
C	0.93649000	4.18646000	1.96038200
H	-0.92434800	3.89245900	0.91165900
C	2.33659000	4.12525600	1.90085600
H	4.02757400	3.73287000	0.61984800
H	0.45370900	4.46038900	2.89350500
C	3.15959300	4.34911400	3.13964300
H	3.22551100	3.40950600	3.70075800
H	4.17698900	4.66701900	2.89769800
H	2.70662100	5.09702600	3.79695400
N	-0.35069100	1.25788200	-1.29576100
Fe	1.02456800	0.03877200	-0.70344300
O	1.67640200	1.19623000	2.52032800
S	0.53440900	0.29123100	2.47790400
O	-0.73727200	0.70458600	3.09023200
O	0.26239900	-0.30107500	1.08267700
C	1.05086900	-1.25123000	3.37732100
F	2.03959700	-1.85917500	2.72557800
F	0.00712200	-2.09238100	3.47501400
F	1.45789500	-0.92857800	4.60623500
C	-1.71391600	0.78288800	-1.23033300
H	-1.70997300	-0.30457900	-1.30356700
H	-2.30218400	1.17970600	-2.06177000
C	-2.42194000	1.18553600	0.13493600
H	-1.76603500	0.83753800	0.92942100
H	-2.51561500	2.26709500	0.17624000
C	-3.72273900	0.49525100	0.16342500

C	-4.89014800	1.16999200	-0.34508600
C	-6.19427000	0.73265500	0.00280900
C	-4.75297900	2.32008100	-1.16786200
C	-7.31236300	1.39599400	-0.47976900
H	-6.31022900	-0.09689900	0.68954700
C	-5.87962900	2.95961000	-1.66321400
H	-3.77026000	2.69557400	-1.43357100
C	-7.15725400	2.50115400	-1.32337200
H	-8.30453500	1.06479200	-0.19218500
H	-5.76443400	3.82301400	-2.30954300
H	-8.03402700	3.01675200	-1.70296500
C	-3.74360400	-0.88879000	0.55560400
C	-2.84408700	-1.36995900	1.54252300
C	-4.56190200	-1.82165100	-0.13727500
C	-2.77897500	-2.72390800	1.82500700
H	-2.23628200	-0.67717100	2.11190500
C	-4.46189300	-3.17607100	0.13341000
H	-5.19527800	-1.47750700	-0.94572200
C	-3.57051700	-3.62891900	1.11157300
H	-2.08733600	-3.07572500	2.58016100
H	-5.04980700	-3.88577600	-0.43834300
H	-3.48077100	-4.69289700	1.30644800
O	2.54467800	0.74093600	-1.98916000
S	3.69152700	0.37126300	-1.05788500
O	2.97559600	-0.18578400	0.15548700
O	4.73205500	1.36470200	-0.85160100
C	4.50474200	-1.10347300	-1.85884200
F	5.04265600	-0.72311200	-3.01554100
F	5.45743700	-1.55597700	-1.04417400
F	3.60481500	-2.05843700	-2.07118400
O	0.75485300	-1.68898200	-1.49578300
S	-0.27618700	-2.83108300	-1.62330300
O	-0.03538300	-3.62687500	-2.81761400
O	-1.63852500	-2.37438400	-1.32164300
C	0.21384100	-3.89501000	-0.17998200
F	0.19576900	-3.18713500	0.95440100
F	1.43536000	-4.39107800	-0.36438800
F	-0.66505900	-4.90070900	-0.06913200
TS3			
Energy = -4463.323283, Lowest Freq ν = -1674.30			
S	0.05160900	1.87002800	-2.90250400
O	-1.15057900	2.64602300	-3.23139000
O	0.81191900	1.21470100	-3.96782200
C	1.13573400	2.78306900	-1.85138600

C	2.48730400	2.85979700	-2.18793300
C	0.62786600	3.36585800	-0.68662000
C	3.34905600	3.52035300	-1.31993700
H	2.85061600	2.37939100	-3.08842200
C	1.51324600	4.00143400	0.17396100
H	-0.42316000	3.29414400	-0.43725200
C	2.88265800	4.07992500	-0.12124700
H	4.40739100	3.56388200	-1.55399200
H	1.13969600	4.42857200	1.09908900
C	3.84340600	4.69859600	0.85627000
H	4.25016300	3.91319500	1.50306500
H	4.68230500	5.17805100	0.34454300
H	3.35007200	5.44025300	1.48998200
N	-0.48016300	0.61482000	-1.80038900
Fe	0.83096500	-0.22563000	-0.57771400
O	-1.36918700	1.72355200	1.13538000
S	-1.04316600	0.49787400	1.87445700
O	-2.09239400	-0.19938500	2.60788900
O	-0.25249600	-0.50167400	0.98112000
C	0.27406900	0.96756700	3.10589300
F	1.19908300	1.71457300	2.50412200
F	0.83877800	-0.13069800	3.60228400
F	-0.29435400	1.66752600	4.08796600
C	-1.65426600	-0.15794100	-2.40470800
H	-1.56067800	-1.21660200	-2.17855800
H	-1.68504300	-0.03374200	-3.48859100
C	-2.72311900	0.61444600	-1.65478400
H	-1.60045800	1.07889200	-1.03707500
H	-2.90153500	1.59645300	-2.09464400
C	-3.67858700	0.18184700	-0.72983000
C	-4.55792500	1.21151900	-0.15448000
C	-4.83836300	1.18454100	1.22658300
C	-5.08781500	2.25113300	-0.94172400
C	-5.61254900	2.18671200	1.80144100
H	-4.40055400	0.40813300	1.84247500
C	-5.88192600	3.23551500	-0.36373000
H	-4.91112700	2.26186200	-2.01203800
C	-6.13954100	3.20930500	1.00943900
H	-5.80094600	2.17221300	2.87001500
H	-6.30345700	4.02056400	-0.98308300
H	-6.75234100	3.98403100	1.45994500
C	-3.87011000	-1.19515800	-0.26817300
C	-2.81546100	-2.10517600	-0.07738200
C	-5.19151000	-1.63680500	-0.02982900

C	-3.06767800	-3.41075000	0.32393600
H	-1.79343900	-1.78874600	-0.18698900
C	-5.44114100	-2.94984500	0.34962400
H	-6.01686700	-0.95044700	-0.17785700
C	-4.37965800	-3.84012500	0.52992000
H	-2.23523300	-4.08758400	0.47429000
H	-6.46324900	-3.27868200	0.50717400
H	-4.57492200	-4.86366300	0.83433300
O	2.35077000	0.69112100	-0.05910200
S	3.83578500	0.57739000	0.42680100
O	4.03092200	1.43933200	1.58622600
O	4.74905700	0.62451700	-0.70579500
C	3.86278900	-1.17979600	1.07715000
F	4.05066200	-2.03845500	0.08134000
F	4.84772000	-1.29377000	1.96326300
F	2.69299100	-1.45360200	1.68032400
O	1.47592200	-1.86851200	-1.22989200
S	0.86864800	-3.26434800	-1.58526800
O	1.76268000	-4.00692700	-2.45447300
O	-0.55686000	-3.13968100	-1.89996500
C	0.93290600	-4.06302200	0.09513900
F	0.24942800	-3.31191900	0.97033000
F	2.19004300	-4.18701800	0.50852600
F	0.35881500	-5.26610300	0.02163700
INT3			
Energy = -4463.375329			
S	-0.63046800	-0.54085000	-3.40783800
O	0.00402800	-1.55642100	-4.24508100
O	-0.68372700	0.86375200	-3.78896800
C	-2.20370600	-1.09367700	-2.83510800
C	-3.23834600	-0.16383500	-2.70040500
C	-2.38582500	-2.45508200	-2.55998200
C	-4.48055800	-0.61971500	-2.27214100
H	-3.06520900	0.88414600	-2.91453900
C	-3.63085700	-2.87753300	-2.11782300
H	-1.57520100	-3.16129100	-2.70355300
C	-4.69555700	-1.97179700	-1.96994500
H	-5.28917400	0.09148800	-2.14742100
H	-3.78831800	-3.92682700	-1.88916300
C	-6.02914900	-2.43946900	-1.45759400
H	-6.03321000	-2.38322600	-0.36360700
H	-6.84206600	-1.81047900	-1.82906200
H	-6.22735300	-3.47536300	-1.74533300
N	0.30283500	-0.57275900	-1.87018500

Fe	-0.79033500	0.03647300	-0.18286500
O	0.70932600	-2.57261000	0.15117100
S	1.10639300	-1.76473400	1.31954400
O	2.48055100	-1.73589200	1.78430100
O	0.53284300	-0.30983100	1.14196200
C	0.07399800	-2.38933900	2.74780600
F	-1.15227400	-2.68814900	2.32508200
F	0.01207100	-1.45169700	3.69121600
F	0.65726200	-3.48193900	3.23335600
C	1.65967800	0.10056600	-2.07435300
H	1.61032400	1.11239500	-1.67672000
H	1.79768800	0.18956900	-3.15876500
C	2.75235800	-0.73174200	-1.49590900
H	0.47270800	-1.56598500	-1.65686100
H	2.71645400	-1.78893700	-1.74976200
C	3.81271200	-0.28506900	-0.79072100
C	4.91111100	-1.21841300	-0.44006800
C	5.56404800	-1.09336400	0.79722200
C	5.31378900	-2.24024400	-1.31458600
C	6.56981100	-1.98431900	1.16004800
H	5.25899100	-0.30690600	1.47829200
C	6.32637300	-3.12640500	-0.95357200
H	4.84921200	-2.32019700	-2.29235900
C	6.95482000	-3.00395800	0.28674800
H	7.05367900	-1.88424400	2.12686700
H	6.63261100	-3.90508900	-1.64565100
H	7.74539900	-3.69327500	0.56752300
C	3.98317900	1.13210700	-0.36513800
C	3.05526600	1.77824500	0.46156600
C	5.12437800	1.83427700	-0.78620500
C	3.25133400	3.10769000	0.83637600
H	2.19459200	1.23248400	0.82525800
C	5.31326200	3.16323600	-0.41779800
H	5.85724500	1.33011000	-1.40853400
C	4.37456800	3.80434500	0.39445800
H	2.52057600	3.59880200	1.46912800
H	6.19317100	3.69848400	-0.76169100
H	4.52176500	4.84052900	0.68342000
O	-2.32040300	-0.87400700	0.40821900
S	-3.65578400	-0.34843900	1.06083500
O	-4.53283400	-1.48107500	1.32436000
O	-4.14799600	0.85011700	0.39525200
C	-3.00671000	0.23709600	2.71131700
F	-1.88871600	0.96158000	2.51039900

F	-3.92544400	1.00557700	3.28549300
F	-2.71944000	-0.79056100	3.50290100
O	-1.32398500	1.74406600	-0.62262200
S	-0.70263900	3.17923200	-0.84537200
O	-1.67448500	4.03337500	-1.50128100
O	0.67228800	3.07164000	-1.31781700
C	-0.60170700	3.69096000	0.94394600
F	0.08349100	2.75683000	1.62682400
F	-1.81918000	3.80358600	1.46259900
F	0.04228800	4.85246300	1.03311000
INT4			
Energy = -1454.430686			
S	-3.07887300	-0.39909000	0.15105800
O	-3.10576700	0.79410300	-0.70529800
O	-4.27713000	-1.22592400	0.32986500
C	-1.72589000	-1.41741300	-0.40918400
C	-1.54043000	-2.68366500	0.14282200
C	-0.88476900	-0.93140000	-1.40756100
C	-0.47927700	-3.46513100	-0.30766200
H	-2.21892500	-3.04688800	0.90636100
C	0.17174100	-1.72509000	-1.84224700
H	-1.05912900	0.05598700	-1.81664900
C	0.39545200	-2.99612400	-1.29755100
H	-0.32481200	-4.45315900	0.11611700
H	0.83912800	-1.35097800	-2.61340400
C	1.58012700	-3.81409900	-1.73964100
H	2.50203200	-3.40305900	-1.31185000
H	1.49398700	-4.85473200	-1.41697200
H	1.69095100	-3.80066400	-2.82814800
C	-1.66458100	1.13268800	1.87794700
H	-1.86697300	1.56809500	2.86360900
H	-1.85257000	1.90489000	1.12704400
C	-0.25971900	0.60806000	1.81451500
H	-0.07827100	-0.23509700	2.47551000
C	0.73180200	0.99538400	0.98747200
C	0.60664600	2.15740700	0.07055500
C	0.97403100	2.03230100	-1.27976300
C	0.12477600	3.39550400	0.51874500
C	0.82198000	3.09869100	-2.16095500
H	1.37526300	1.08758600	-1.62990900
C	-0.02202800	4.46662000	-0.36209600
H	-0.11404200	3.52116600	1.56984100
C	0.31837000	4.31928600	-1.70587300
H	1.09750500	2.97926200	-3.20438100

H	-0.39655300	5.41751700	0.00421600
H	0.20177900	5.15157400	-2.39289300
C	2.00443800	0.22686800	0.94390000
C	2.01054600	-1.16643800	1.11704000
C	3.22895100	0.87589300	0.71894000
C	3.20399600	-1.88385000	1.08746000
H	1.07023600	-1.68988300	1.24132300
C	4.42273900	0.15796700	0.68746200
H	3.23999000	1.95090800	0.57361100
C	4.41622800	-1.22509400	0.87302900
H	3.18529900	-2.96135200	1.22256100
H	5.35980400	0.68018700	0.51949600
H	5.34591200	-1.78513900	0.84452200
N	-2.61378900	0.00461600	1.73135800
H	-3.47972800	0.12127900	2.25289800
1-INT5			
Energy = -5377.081104			
S	2.05412500	-0.71078100	-3.47170900
O	1.49425600	0.37583100	-4.25766200
O	2.08220500	-2.10185300	-3.91056900
C	3.57900400	-0.24933400	-2.73358200
C	4.38189600	-1.24998900	-2.17542600
C	3.92269800	1.10181200	-2.67589300
C	5.54190400	-0.86884100	-1.51715700
H	4.09442300	-2.29077300	-2.25636500
C	5.09357200	1.45366100	-2.01447300
H	3.28302300	1.85364200	-3.12266900
C	5.90031400	0.48542500	-1.40248900
H	6.17726100	-1.62755000	-1.07037000
H	5.36369000	2.50075500	-1.94525300
C	7.09571700	0.88396200	-0.58265500
H	6.82240900	0.88104600	0.48010400
H	7.92413900	0.18142300	-0.71005500
H	7.44590300	1.88645900	-0.83853900
C	0.98054900	0.39385300	-1.08138000
H	-0.02009100	0.47334400	-0.65728100
H	1.12501000	1.27215000	-1.70963800
C	1.98589200	0.21936800	0.00440500
H	2.04341400	-0.78002100	0.42584400
C	2.67536300	1.20493900	0.61127600
C	2.58681000	2.63087700	0.21520200
C	3.74888800	3.42345800	0.19790800
C	1.36979600	3.22143200	-0.15848000
C	3.70458800	4.74259400	-0.24369400

H	4.68725000	2.99304000	0.53189500
C	1.32500600	4.54356600	-0.60019200
H	0.44837900	2.66999200	-0.04707700
C	2.49243200	5.30351100	-0.65825600
H	4.61303100	5.33780800	-0.25882000
H	0.36973200	4.97331700	-0.88260700
H	2.45824100	6.33262800	-1.00245400
C	3.54405700	0.86321400	1.76646400
C	4.37136600	-0.26918000	1.75079200
C	3.50390100	1.65321600	2.92536200
C	5.14265200	-0.60238700	2.86393300
H	4.41404400	-0.87680200	0.85459500
C	4.26319400	1.31100800	4.04213800
H	2.85080200	2.51871900	2.95084100
C	5.08889000	0.18516400	4.01536900
H	5.79490200	-1.47073500	2.82988800
H	4.20708500	1.92264900	4.93730900
H	5.68750400	-0.07427700	4.88305700
C	-0.52348400	-1.12951500	-2.47203100
H	-0.42570800	-1.86366500	-3.27588500
H	-0.91012600	-0.18270400	-2.84746100
N	-1.27222300	-1.60436600	-1.37183500
S	-1.24929400	-3.21457700	-1.00272000
O	-2.18958400	-3.19538400	0.15681800
O	-1.46252200	-4.07974200	-2.16086100
C	0.39261000	-3.54150600	-0.37410800
C	1.36073800	-4.04234300	-1.25162600
C	0.71323100	-3.18747300	0.93900500
C	2.67348600	-4.16892500	-0.80045800
H	1.08596700	-4.32316700	-2.26197300
C	2.03240900	-3.32198800	1.36647100
H	-0.05016400	-2.79702200	1.59920800
C	3.02898000	-3.80812900	0.50818800
H	3.42863800	-4.56767000	-1.47232700
H	2.29100900	-3.02123500	2.37571500
C	4.44739000	-3.96476400	0.99089600
H	5.16754400	-3.72768500	0.20158600
H	4.64483400	-3.31778600	1.84797900
H	4.63816400	-4.99826800	1.30261800
Fe	-2.45183900	-0.83299300	0.08517800
H	1.25332200	-1.64163400	-1.48116900
N	0.92836500	-0.81031000	-1.99302500
O	-2.39788100	1.03679900	-0.34508400
S	-2.57550500	1.97256000	-1.57197400

O	-1.32202100	2.01982100	-2.33932600
O	-3.83792900	1.78013400	-2.26892600
C	-2.68623600	3.58781200	-0.64957800
O	-4.34114900	-1.19787100	-1.03732100
S	-5.14275500	-1.30569000	0.24186300
O	-6.08276100	-2.40102300	0.38472700
O	-4.08371600	-1.13657000	1.33782300
C	-6.12777600	0.27751700	0.34313000
O	-1.09090500	-0.65926400	1.48025400
S	-0.91827800	0.44723100	2.56324000
O	-0.10836700	1.55785700	2.06329100
O	-2.14833400	0.71340800	3.29607200
C	0.18875600	-0.52403700	3.70083500
F	-2.54633300	4.58837800	-1.52568800
F	-3.86565600	3.68333400	-0.04458700
F	-1.71190300	3.66909900	0.26043100
F	-6.90870400	0.22690200	1.42110400
F	-6.87462900	0.38974600	-0.75172400
F	-5.30684400	1.32243200	0.43968900
F	-0.39712500	-1.67541500	4.04513300
F	0.44639800	0.19043700	4.79482600
F	1.34997700	-0.81050200	3.08595200
1-TS4			
Energy = -5377.033033, Lowest Freq ν = -1665.02			
S	-1.90733000	0.78351600	-2.95229700
O	-2.45655000	-0.17770200	-3.90400400
O	-1.20437600	1.98641200	-3.39948300
C	-3.11648400	1.17724100	-1.72455000
C	-2.78346600	2.06689100	-0.70203200
C	-4.37030300	0.57373100	-1.79859700
C	-3.72907800	2.33598200	0.27900800
H	-1.80788500	2.53181000	-0.66375400
C	-5.30394000	0.86803500	-0.80971600
H	-4.59157000	-0.12575800	-2.59530600
C	-4.99580900	1.73284400	0.24896600
H	-3.46779900	3.00251400	1.09414600
H	-6.28390100	0.40249500	-0.84819800
C	-5.97693400	1.95613300	1.36660600
H	-5.81970400	1.19881100	2.14411500
H	-5.84559400	2.93861300	1.82792200
H	-7.00988400	1.86920900	1.01979900
C	-1.10494200	-1.45468400	-1.55793400
H	-0.18165800	-2.02981100	-1.47944300
H	-1.69353400	-1.87874400	-2.37267000

C	-1.83340200	-1.41555900	-0.25282900
H	-1.31960800	-0.86876900	0.53003400
C	-3.00275900	-2.02373300	0.03260500
C	-3.67168000	-2.91361300	-0.95258200
C	-5.02719500	-2.74296800	-1.27856500
C	-2.95587200	-3.94491400	-1.57947300
C	-5.63527400	-3.55012900	-2.23668200
H	-5.59750900	-1.97317300	-0.77080700
C	-3.56583000	-4.75676900	-2.53594800
H	-1.92465500	-4.12173800	-1.29022400
C	-4.90400900	-4.55589300	-2.87381200
H	-6.68145300	-3.39824700	-2.48540900
H	-2.99628900	-5.54992700	-3.01038300
H	-5.37889800	-5.18568600	-3.61968800
C	-3.64725800	-1.83297800	1.35799900
C	-3.38278500	-0.69127800	2.13348100
C	-4.52567300	-2.79682400	1.87897000
C	-3.96121600	-0.52539700	3.38759500
H	-2.72517200	0.07437400	1.74878200
C	-5.11596300	-2.62578100	3.13094900
H	-4.73712100	-3.69140800	1.30391400
C	-4.83677000	-1.49092700	3.89213400
H	-3.71952600	0.35721000	3.97179000
H	-5.78779900	-3.38748300	3.51506400
H	-5.29139900	-1.36110000	4.86953000
C	0.74049800	0.13363800	-2.45317900
H	0.78795300	0.68150700	-3.39416500
H	1.26224000	-0.82113200	-2.50148600
N	1.17031800	0.95005700	-1.29518700
S	1.77080600	2.52765500	-1.57259900
O	2.82190800	2.54464200	-0.50385500
O	2.10823300	2.72636500	-2.97680500
C	0.52605100	3.67837900	-1.05795700
C	-0.22480200	4.35378000	-2.02150800
C	0.31364500	3.86331800	0.31044500
C	-1.23660400	5.20609900	-1.59224300
H	-0.02805900	4.19486100	-3.07329000
C	-0.70958900	4.71580600	0.71315300
H	0.93291000	3.35254500	1.03617400
C	-1.50592200	5.38568700	-0.22683000
H	-1.83580500	5.73160900	-2.32935700
H	-0.89061500	4.85486600	1.77398500
C	-2.65644500	6.25074700	0.21618900
H	-3.59397300	5.68215300	0.17671500

H	-2.52356200	6.60175300	1.24254900
H	-2.77690100	7.12098100	-0.43466600
Fe	2.58118000	0.40335600	0.24745400
H	-0.11378000	0.70246900	-1.05167900
N	-0.67944200	-0.06246100	-1.95382400
O	2.10213600	-1.43038100	0.40625300
S	2.42515600	-2.77413600	-0.31748500
O	1.82851100	-2.78256400	-1.66064600
O	3.80192100	-3.20283500	-0.13496100
C	1.36080600	-3.88157400	0.73604400
O	4.13463200	-0.10226000	-1.30732600
S	5.23956000	0.38728200	-0.39255400
O	6.14754400	1.40004800	-0.89567800
O	4.48780500	0.70723500	0.91447100
C	6.28704100	-1.10930700	0.06310800
O	1.52614400	1.07879600	1.71688400
S	0.73651700	0.37649400	2.86493500
O	-0.07178800	-0.73600400	2.37181600
O	1.54091200	0.23633600	4.06819700
C	-0.48275400	1.74640400	3.18468900
F	1.55618700	-5.14401600	0.35143200
F	1.68877000	-3.74332700	2.01436900
F	0.07116700	-3.56720400	0.56516800
F	7.50383800	-0.67195400	0.38342400
F	6.35896800	-1.91487500	-0.98885700
F	5.75617000	-1.73760900	1.10223600
F	0.13821100	2.90244900	3.44140000
F	-1.26108000	1.42373600	4.21781400
F	-1.26440500	1.91977500	2.09872100
1-INT6			
Energy = -5377.074616			
S	-1.69677800	0.92164100	-3.14250500
O	-2.39555400	0.18761600	-4.19710700
O	-0.91828400	2.13458900	-3.43544400
C	-2.88747300	1.29768800	-1.87298600
C	-2.58343200	2.26322900	-0.91549900
C	-4.09158000	0.59387700	-1.83520300
C	-3.49768700	2.51886200	0.10193000
H	-1.65308700	2.81001800	-0.96395500
C	-4.99329400	0.86541700	-0.81205900
H	-4.30484400	-0.15621000	-2.58716700
C	-4.70929100	1.82006500	0.17534400
H	-3.25183900	3.25572200	0.86068500
H	-5.92989100	0.31756900	-0.76862100

C	-5.66205200	2.03680100	1.32017000
H	-5.53669600	1.23769600	2.06040300
H	-5.47959300	2.99088700	1.82181400
H	-6.70340100	2.01579600	0.98557800
C	-1.04313000	-1.47312000	-2.01598300
H	-0.16055500	-2.11686400	-2.06443800
H	-1.74062600	-1.82590400	-2.77817900
C	-1.64946000	-1.49798400	-0.64229100
H	-1.12304200	-0.90944800	0.09850900
C	-2.77309900	-2.14280000	-0.27181400
C	-3.50329600	-3.03634600	-1.20615800
C	-4.88953200	-2.89795000	-1.38744800
C	-2.82551300	-4.02720600	-1.93237300
C	-5.57083600	-3.70104800	-2.29836800
H	-5.42375900	-2.15317900	-0.80668600
C	-3.50953800	-4.83614400	-2.84019000
H	-1.76305400	-4.17252400	-1.76198200
C	-4.88131700	-4.67069100	-3.03110700
H	-6.64046900	-3.57356100	-2.43672600
H	-2.97036100	-5.59939400	-3.39307900
H	-5.41309500	-5.29873900	-3.73934900
C	-3.32448500	-1.96898500	1.09591900
C	-3.17161900	-0.75444700	1.78265700
C	-3.99963800	-3.01859200	1.73961000
C	-3.64915700	-0.60327900	3.08160400
H	-2.67960000	0.07466700	1.29318500
C	-4.48977500	-2.86312000	3.03531000
H	-4.12866400	-3.96350700	1.22223000
C	-4.31343500	-1.65625800	3.71426900
H	-3.49190900	0.33820700	3.60035200
H	-5.00266400	-3.68950200	3.51850500
H	-4.68942400	-1.53806900	4.72614400
C	0.78090900	0.25975700	-2.34506000
H	1.07979300	0.87310200	-3.19401400
H	1.39602900	-0.63766700	-2.31241200
N	1.10558000	1.05356300	-1.09257700
S	1.96452800	2.56760100	-1.28772800
O	2.89496100	2.42055500	-0.12390500
O	2.46775100	2.66132600	-2.64779900
C	0.81476800	3.85045400	-0.92753300
C	0.14609800	4.47501300	-1.98422300
C	0.52590400	4.12960600	0.40939000
C	-0.85481800	5.38805600	-1.67409600
H	0.38215300	4.22251600	-3.00922100

C	-0.48834900	5.03688300	0.69025000
H	1.08190200	3.64872000	1.20059800
C	-1.20200300	5.66442100	-0.34204100
H	-1.39428000	5.87518500	-2.48005700
H	-0.73229800	5.25049600	1.72604200
C	-2.35261400	6.58390000	-0.03105200
H	-3.29922800	6.03305100	-0.09282300
H	-2.27477000	6.99961100	0.97651300
H	-2.41005400	7.41000300	-0.74494500
Fe	2.50925300	0.22171100	0.41071500
H	0.25943000	1.20913200	-0.52054800
N	-0.59251200	-0.11561200	-2.39700200
O	1.48104000	-1.36875000	0.28505300
S	1.84610000	-2.89847300	0.29127500
O	1.21713600	-3.54836500	-0.85555000
O	3.26382000	-3.08985700	0.57593200
C	0.92830200	-3.44056100	1.82053700
O	3.74656600	-0.11417000	-1.45961500
S	5.00407300	-0.08878300	-0.62079400
O	6.03050400	0.89065300	-0.91663600
O	4.43207000	-0.04439900	0.82252900
C	5.80076700	-1.80218000	-0.78623400
O	1.69685700	0.88956600	2.05130700
S	0.17979100	0.77248400	2.36482400
O	-0.59612600	1.33087800	1.23774500
O	-0.20646300	-0.50663300	2.93304100
C	0.02794500	2.01812700	3.74032500
F	1.09121000	-4.76033100	1.94160500
F	1.45147800	-2.82957900	2.88078400
F	-0.36391500	-3.15852700	1.71539300
F	6.96672600	-1.63435000	-1.40424000
F	5.01833800	-2.58023700	-1.51692900
F	5.99753100	-2.31256000	0.41800100
F	0.68603100	1.59342300	4.81090800
F	-1.26963900	2.15522600	4.02776100
F	0.51541300	3.20891200	3.36459900
1-INT7			
Energy = -1492.930039			
S	3.08024300	0.10435800	-0.27081700
O	3.01966600	-1.15272200	-0.99339500
O	4.30173300	0.84079000	0.01516200
C	1.77205800	1.17729100	-0.71497100
C	1.80962400	2.50861200	-0.28470100
C	0.74220900	0.67790100	-1.52032000

C	0.77279700	3.35046100	-0.66688100
H	2.63766500	2.87683000	0.30990900
C	-0.27269200	1.54645900	-1.89214400
H	0.74211800	-0.35611700	-1.84187800
C	-0.28357000	2.88523000	-1.46708800
H	0.78536600	4.38748100	-0.34835700
H	-1.07661000	1.18324200	-2.52349900
C	-1.42807700	3.78406300	-1.83725100
H	-1.71394600	3.65167800	-2.88424800
H	-2.30233200	3.53292500	-1.22496200
H	-1.18839000	4.83614400	-1.67179000
C	1.46740800	-1.42951200	1.63702900
H	1.67436900	-2.01825300	2.53832100
H	1.50767400	-2.09570500	0.77448800
C	0.18731600	-0.65566300	1.70787500
H	0.18153500	0.15753300	2.42815400
C	-0.91927600	-0.87775500	0.96111300
C	-1.04057300	-2.03478200	0.04072800
C	-1.55454700	-1.85656700	-1.25586200
C	-0.65457600	-3.32528900	0.43718800
C	-1.62700800	-2.92560700	-2.14410700
H	-1.90197200	-0.87478900	-1.55672500
C	-0.73838300	-4.39815100	-0.44897900
H	-0.33058900	-3.49640200	1.45903600
C	-1.21275600	-4.19848600	-1.74520300
H	-2.01608600	-2.76989000	-3.14505700
H	-0.44630600	-5.39078400	-0.12255600
H	-1.27696100	-5.03276400	-2.43570600
C	-2.06120300	0.06418400	1.04625600
C	-1.84773500	1.43804200	1.24875500
C	-3.38085500	-0.40112100	0.92465700
C	-2.92195200	2.31846200	1.34122500
H	-0.83397600	1.81917900	1.30000800
C	-4.45511600	0.48039700	1.01933300
H	-3.56167200	-1.45893500	0.76944100
C	-4.23030000	1.84167600	1.22806300
H	-2.74006200	3.37715200	1.49828500
H	-5.46882600	0.10324400	0.93408800
H	-5.06803200	2.52761200	1.29939400
C	3.35874800	-0.10677000	2.45575300
H	4.17565200	0.58150100	2.25093700
H	3.18155700	-0.48005700	3.46269100
N	2.61364400	-0.48764800	1.49516400

TsNH[Fe]

Energy = -3884.133749

N	0.37283700	-0.85479100	-1.47005900
S	1.10529100	-2.24712100	-1.08257600
O	0.61073600	-2.38041300	0.33992700
O	0.92245100	-3.35263000	-2.02825800
C	2.85116000	-1.91206500	-0.95549400
C	3.71504000	-2.35661600	-1.95293400
C	3.31208700	-1.15610800	0.12338300
C	5.06780300	-2.02957100	-1.86464800
H	3.32914500	-2.95506500	-2.77054000
C	4.66103700	-0.83411300	0.19009200
H	2.62422700	-0.82861900	0.88936200
C	5.55664900	-1.26086500	-0.80141000
H	5.75311800	-2.37380900	-2.63465100
H	5.01457500	-0.23005300	1.02038000
C	7.01484500	-0.88271500	-0.72211200
H	7.59924500	-1.37158300	-1.50650900
H	7.14437300	0.20025400	-0.83201300
H	7.44555600	-1.16111200	0.24600600
Fe	-0.66467700	-0.48059200	0.15305100
H	0.08775700	-0.69519800	-2.43488300
O	-1.71767700	1.01284700	-0.49970400
S	-2.09408800	1.50157400	-1.91692700
O	-1.57250900	0.63154800	-2.97826200
O	-3.48339800	1.94357800	-1.97636400
C	-1.04304800	3.03125100	-1.98258800
O	-2.35828200	-1.95718300	-0.46040700
S	-2.78715800	-2.07163400	0.97146400
O	-3.03335400	-3.39173400	1.53433100
O	-1.84151500	-1.16000100	1.74818000
C	-4.41482700	-1.17487100	1.06331700
O	0.54105300	0.49095300	1.35598700
S	1.27749600	1.84253900	1.24704500
O	2.29215600	1.85088700	0.19250300
O	0.38859200	2.99061000	1.40540500
C	2.23622000	1.71404100	2.83489100
F	-1.20236400	3.61803500	-3.18014700
F	-1.39794500	3.89012000	-1.02974000
F	0.24278900	2.70254700	-1.83355400
F	-5.31629100	-1.83623600	0.32773500
F	-4.29900900	0.06729200	0.60489200
F	-4.83217500	-1.13991300	2.33501500
F	1.42023000	1.58842600	3.88348600
F	2.98024200	2.81766700	2.99483800

F	3.06244000	0.65100400	2.80504800
1-TS5			
Energy = -2406.602137, Lowest Freq ν = -158.10			
S	-0.60816000	-1.87707800	0.48572900
O	0.29849800	-3.00831600	0.60465700
O	-2.05809700	-1.97969500	0.62743200
C	-0.01015200	-0.51310200	1.43609500
C	-0.88269500	0.53129700	1.75029000
C	1.33042200	-0.49934900	1.82422500
C	-0.37638800	1.63552400	2.43152200
H	-1.93133500	0.46538600	1.48432300
C	1.80764100	0.60890600	2.51177600
H	1.97930400	-1.33309800	1.58693600
C	0.97380800	1.69829400	2.80956900
H	-1.03987900	2.45603900	2.68716700
H	2.84911500	0.63871100	2.81462900
C	1.53561200	2.90565900	3.50850800
H	2.32806800	3.35786800	2.90202100
H	0.76964700	3.66123200	3.69411500
H	1.98272800	2.62985400	4.46878500
C	0.97072600	-1.40444000	-1.81490200
H	0.80385200	-1.60889100	-2.87812500
H	1.43751900	-2.28667500	-1.37833100
C	1.78996400	-0.16912700	-1.59721100
H	1.34776400	0.75281800	-1.96301200
C	3.01410900	-0.09573700	-1.02712800
C	3.80789700	-1.29165100	-0.65248500
C	4.46789300	-1.34001100	0.58802200
C	3.93455400	-2.38645100	-1.52214400
C	5.18411100	-2.47109400	0.96819600
H	4.41975900	-0.48062100	1.24819400
C	4.66184000	-3.51440800	-1.14578900
H	3.49546800	-2.33548400	-2.51334800
C	5.27804000	-3.56448800	0.10425300
H	5.67777500	-2.49742600	1.93419600
H	4.75682400	-4.34805800	-1.83374100
H	5.84299200	-4.44293600	0.39785700
C	3.61049200	1.23405000	-0.74134200
C	2.82448500	2.28452700	-0.24118900
C	4.97927200	1.46358100	-0.95306500
C	3.38180500	3.53504200	0.01611700
H	1.78199300	2.10257800	-0.00621900
C	5.53614100	2.71500400	-0.70087500
H	5.60108300	0.65819700	-1.32868700

C	4.74033100	3.75491900	-0.21695000
H	2.75954300	4.33547200	0.40479900
H	6.59312000	2.87927800	-0.88276500
H	5.17732900	4.72753700	-0.01610000
C	-1.47749400	-0.94325600	-1.86885300
H	-2.43009000	-1.24831000	-1.45532500
H	-1.40007200	-0.82425100	-2.94423000
N	-1.92597100	0.98189600	-1.55701300
S	-3.62907000	1.45899500	-1.87910600
O	-3.70941700	2.88729000	-1.58727100
O	-3.87772400	0.88371900	-3.19436200
C	-4.41811700	0.51046800	-0.61697400
C	-4.91706100	-0.75624600	-0.93109000
C	-4.46072000	1.01745400	0.68521200
C	-5.43838900	-1.53729600	0.09372500
H	-4.90901200	-1.10636300	-1.95740000
C	-4.98447900	0.21557900	1.69217000
H	-4.11252800	2.02328500	0.89362100
C	-5.46285500	-1.07604800	1.41834000
H	-5.83175900	-2.52220200	-0.13589400
H	-5.03062300	0.59647700	2.70745300
C	-5.97286100	-1.95710200	2.52485300
H	-5.17058500	-2.61540300	2.87870000
H	-6.32195500	-1.37098600	3.37786800
H	-6.79155900	-2.59492400	2.18276600
N	-0.39385900	-1.32197900	-1.21107900
C	-1.13568300	1.85663600	-1.08755500
H	-0.10598700	1.57699500	-0.88081000
H	-1.47355700	2.87703500	-0.89435900
1-INT8			
Energy = -2406.614623			
S	1.30524000	-1.64817500	1.99482100
O	0.85472800	-2.45899900	3.11764100
O	2.67515200	-1.15068200	1.84656800
C	0.83823600	-2.44829400	0.47282900
C	1.53291700	-2.13190800	-0.69757200
C	-0.30505600	-3.24889500	0.44349500
C	1.04728700	-2.60256500	-1.91704400
H	2.43801300	-1.53766500	-0.64277200
C	-0.77002500	-3.70996500	-0.78411800
H	-0.81269300	-3.51028500	1.36430700
C	-0.11603300	-3.38347800	-1.98137200
H	1.58369200	-2.36992300	-2.83240600
H	-1.66274000	-4.32383800	-0.81421500

C	-0.65197500	-3.88204100	-3.29657500
H	-1.71910900	-3.65750700	-3.38995900
H	-0.12954300	-3.43224700	-4.14355500
H	-0.54258300	-4.96907000	-3.37386400
C	-1.08646700	-0.36618300	2.51850800
H	-1.04648300	-0.36464800	3.61073100
H	-1.46936900	-1.33341400	2.19986600
C	-1.93485700	0.75552400	1.99634600
H	-1.76651200	1.72807000	2.45063000
C	-2.83095000	0.69379800	0.98391100
C	-3.27283300	-0.58292100	0.35710100
C	-3.31435500	-0.70019800	-1.04342300
C	-3.69775600	-1.67333400	1.13303400
C	-3.73631600	-1.88158400	-1.64855500
H	-3.04197700	0.15456000	-1.65533400
C	-4.12899800	-2.85269200	0.52741600
H	-3.73254600	-1.57634900	2.21318800
C	-4.14558600	-2.96182100	-0.86419700
H	-3.76990500	-1.95015100	-2.73133800
H	-4.47352900	-3.67768000	1.14254900
H	-4.49742200	-3.87455600	-1.33446500
C	-3.39887400	1.94647300	0.42367200
C	-2.59760800	3.09046100	0.26923800
C	-4.74237900	2.00502000	0.01866800
C	-3.12907000	4.26560600	-0.25600800
H	-1.54695100	3.05778400	0.54061400
C	-5.27468800	3.18309300	-0.49789700
H	-5.37065700	1.12719100	0.12535800
C	-4.47049200	4.31591800	-0.63734300
H	-2.49330900	5.13656200	-0.37730300
H	-6.31854800	3.21778600	-0.79207800
H	-4.88520300	5.23041300	-1.04844400
C	0.84543000	0.93334800	1.46407900
H	1.92610300	0.96372600	1.59343100
H	0.39215700	1.82557200	1.89325100
N	0.62359900	1.06739200	-0.04608600
S	1.57779100	2.41367300	-0.89640900
O	1.09539000	2.33391600	-2.26690800
O	1.35438400	3.54432900	-0.01047000
C	3.19331900	1.75025500	-0.72810000
C	3.96661400	2.11841700	0.37850900
C	3.62687500	0.79542100	-1.65511700
C	5.19355600	1.49422000	0.56097900
H	3.61621700	2.88098600	1.06479100

C	4.85862700	0.18892500	-1.44731500
H	3.02051800	0.55313600	-2.52050400
C	5.65146400	0.51311800	-0.33317500
H	5.80749400	1.76946500	1.41206600
H	5.21695900	-0.54654600	-2.16020700
C	6.95648600	-0.19070500	-0.08912800
H	6.80460700	-1.02954300	0.60058100
H	7.37636300	-0.59278700	-1.01361700
H	7.69084800	0.47761200	0.36692200
N	0.31538500	-0.25334100	1.99750300
C	-0.14028600	0.31696700	-0.73840900
H	-0.70691900	-0.47586700	-0.26700100
H	-0.22281500	0.50451000	-1.80501500
1-TS6			
Energy = -2406.60331, Lowest Freq ν = -140.59			
S	-0.24227500	-2.59485700	-1.81124800
O	0.84498200	-3.03158200	-2.67966200
O	-1.63637200	-2.99899000	-1.97889900
C	0.21851900	-2.90842900	-0.11991000
C	-0.78088300	-2.95123200	0.85667100
C	1.56831600	-3.02845500	0.21618500
C	-0.41330500	-3.10553700	2.18890700
H	-1.82342300	-2.88364700	0.56765000
C	1.91114500	-3.19446400	1.55576100
H	2.33018200	-3.00489000	-0.55417000
C	0.93452500	-3.23177500	2.55978100
H	-1.18284200	-3.14611000	2.95393900
H	2.95665000	-3.29849800	1.82256200
C	1.31966100	-3.44167900	4.00033600
H	2.32432000	-3.06351000	4.20564400
H	0.61875500	-2.94941200	4.67941800
H	1.31600100	-4.51000200	4.24570800
C	0.96583400	-0.16235800	-2.33846900
H	0.87891900	0.16109200	-3.38296800
H	1.77591700	-0.88345200	-2.29297900
C	1.24522800	1.07247500	-1.49379400
H	0.61548900	1.92417100	-1.73472700
C	2.36781700	1.33071700	-0.73271700
C	3.34903000	0.26239200	-0.42265400
C	3.64459100	-0.03006500	0.91977700
C	4.00201100	-0.45949000	-1.43498000
C	4.55038400	-1.03797700	1.23999800
H	3.16727300	0.54120300	1.70913000
C	4.91265100	-1.46311200	-1.11148300

H	3.83028900	-0.20611100	-2.47561600
C	5.18282000	-1.75980100	0.22627700
H	4.77011800	-1.25236100	2.28079400
H	5.42012200	-2.00345300	-1.90338600
H	5.89589500	-2.53868800	0.47565200
C	2.59487200	2.65992400	-0.13534200
C	1.55396200	3.59753500	0.02803200
C	3.89581200	3.03070700	0.26001700
C	1.80543300	4.84829900	0.57496900
H	0.53746100	3.35621600	-0.25575300
C	4.14569000	4.29103300	0.79485500
H	4.71547700	2.33600600	0.12404300
C	3.10248400	5.20137100	0.95983000
H	0.98706800	5.54782300	0.70691500
H	5.15662500	4.56150700	1.08041100
H	3.29554800	6.18072100	1.38503700
C	-1.40716600	-0.17668500	-1.53092800
H	-2.26651000	-0.83752300	-1.43012300
H	-1.64753300	0.63919400	-2.22101600
N	-1.13398600	0.50409900	-0.19903300
S	-2.08459000	1.98982100	0.13978900
O	-1.56920200	2.44230700	1.42676200
O	-1.96395300	2.79243100	-1.07611500
C	-3.69778600	1.30369200	0.27890900
C	-4.54901100	1.34340400	-0.82916900
C	-4.07708900	0.70885700	1.48677600
C	-5.80675300	0.76169700	-0.71627400
H	-4.23491700	1.83019200	-1.74514000
C	-5.33908200	0.13580800	1.57129100
H	-3.40316600	0.71011200	2.33588300
C	-6.22093100	0.15127100	0.47744800
H	-6.48118800	0.78583200	-1.56604400
H	-5.65229100	-0.32709800	2.50160700
C	-7.59640200	-0.44595800	0.59540500
H	-7.61179800	-1.27921200	1.30194800
H	-8.30565100	0.30660500	0.95980200
H	-7.96268200	-0.80103100	-0.37057800
N	-0.26691600	-0.89020200	-1.97018800
C	0.06841500	0.41127400	0.33809100
H	0.60198700	-0.52665600	0.26409800
H	0.30567400	1.10031400	1.14188700
1-INT9			
Energy = -2406.616875			
S	-0.48643000	-2.60002000	-1.79194600

O	0.52242700	-3.06754200	-2.73998100
O	-1.89599500	-2.97499300	-1.84971100
C	0.11903100	-2.92204000	-0.14773800
C	-0.76520400	-2.85061000	0.93151500
C	1.48641100	-3.12263500	0.04810900
C	-0.26007800	-2.95937900	2.22205200
H	-1.82474000	-2.70922000	0.75492200
C	1.97149200	-3.23159600	1.34917800
H	2.14918700	-3.19967800	-0.80522300
C	1.11240500	-3.14452500	2.45253900
H	-0.93901500	-2.90373500	3.06766000
H	3.03293100	-3.38950100	1.50942500
C	1.64038000	-3.28146000	3.85639100
H	2.71220900	-3.07336600	3.90391900
H	1.12564600	-2.60485500	4.54424400
H	1.48650900	-4.30093900	4.22814200
C	0.80453500	-0.22731600	-2.15960800
H	0.85039700	0.21069400	-3.16253300
H	1.57639800	-0.98832600	-2.09640100
C	0.99417100	0.89183700	-1.10282900
H	0.43761800	1.76963000	-1.42731100
C	2.35054500	1.28744800	-0.67135400
C	3.36575400	0.26122700	-0.43391600
C	3.87801700	0.11892500	0.87570800
C	3.82384400	-0.60983000	-1.44471700
C	4.78126100	-0.89622600	1.16986700
H	3.52507300	0.77877900	1.66011500
C	4.76424800	-1.58969400	-1.15037700
H	3.50257400	-0.47329500	-2.46993100
C	5.23022900	-1.74771200	0.15855700
H	5.14305500	-1.01505300	2.18548900
H	5.13581200	-2.23015700	-1.94276600
H	5.94986800	-2.52741300	0.38537100
C	2.61320700	2.63417900	-0.26986300
C	1.57060900	3.59493300	-0.10543500
C	3.95878800	3.05039800	-0.04214400
C	1.86792900	4.88143400	0.30422000
H	0.53026100	3.33230600	-0.25823400
C	4.24194000	4.34753000	0.34715800
H	4.76735600	2.35280700	-0.21871900
C	3.19833800	5.26247000	0.52946800
H	1.06482900	5.59483200	0.45038900
H	5.27013600	4.65646000	0.49831900
H	3.42164200	6.27908900	0.83723200

C	-1.54186600	-0.13665900	-1.37753100
H	-2.44364500	-0.74320400	-1.32035700
H	-1.73913900	0.73859600	-2.00890200
N	-1.15344400	0.31448000	0.00219700
S	-1.94217700	1.76841400	0.49386300
O	-1.49059600	2.00806800	1.86624100
O	-1.71332700	2.81084300	-0.52848200
C	-3.62777300	1.24326300	0.43050500
C	-4.48242600	1.80157500	-0.51868100
C	-4.06105900	0.26199200	1.32806800
C	-5.80178600	1.35809400	-0.56797900
H	-4.11550800	2.56267800	-1.19731100
C	-5.37897300	-0.16754900	1.25566600
H	-3.37595200	-0.14969100	2.06051400
C	-6.26893500	0.37237900	0.31093900
H	-6.47878500	1.78350700	-1.30181700
H	-5.73019200	-0.93139300	1.94252400
C	-7.70100300	-0.08908400	0.26568700
H	-7.77150000	-1.17490600	0.37587100
H	-8.27385600	0.35857300	1.08600800
H	-8.18480200	0.19492500	-0.67120300
N	-0.48072800	-0.89899800	-1.96814800
C	0.27790900	0.37287400	0.22472800
H	0.66938300	-0.61873500	0.44926800
H	0.47146800	1.02145700	1.07865200
1-INT10			
Energy = -3281.798029			
S	0.56891500	0.97415800	-3.39188100
O	-0.25219600	2.11190800	-3.80364900
O	1.17369900	0.04394600	-4.34717300
C	1.87926200	1.59920800	-2.34873500
C	2.95504200	0.76313400	-2.03691500
C	1.74847500	2.85387200	-1.75748800
C	3.88258700	1.17999900	-1.09270400
H	3.04426400	-0.20349600	-2.51630300
C	2.69770300	3.26020500	-0.81869300
H	0.91036600	3.48837600	-2.01865200
C	3.76007500	2.42528100	-0.45762600
H	4.70305000	0.52253500	-0.82725600
H	2.60164400	4.23563100	-0.35167300
C	4.75725800	2.83209400	0.59696300
H	4.51235600	3.80494000	1.02989600
H	4.78189000	2.09425000	1.40667000
H	5.76974000	2.89264200	0.18242600

C	-1.36142800	0.69661600	-1.47205600
H	-2.38519300	0.52609500	-1.80071000
H	-1.18752700	1.76943800	-1.53506400
C	-1.12414000	0.19444800	-0.02816500
H	-1.53035200	-0.81108900	0.06392000
C	-1.85306300	1.04862100	1.07668200
C	-1.77323900	2.53766000	0.71948800
C	-0.54695700	3.21193500	0.82339300
C	-2.87731400	3.23226100	0.22093700
C	-0.43679400	4.55047700	0.45476800
H	0.32566400	2.69432400	1.20569800
C	-2.76355300	4.57098500	-0.15871600
H	-3.82273000	2.72159700	0.09734100
C	-1.54626100	5.23749700	-0.04003800
H	0.51720300	5.05815100	0.55778300
H	-3.63294600	5.08774600	-0.55248500
H	-1.45969600	6.27939500	-0.33169100
C	-1.28335600	0.76285300	2.48688600
C	-0.98531800	-0.55601700	2.86335800
C	-1.17647700	1.76860000	3.45257200
C	-0.53265700	-0.84808100	4.14685800
H	-1.08112800	-1.36618800	2.15308500
C	-0.73842500	1.47377700	4.74668100
H	-1.43132800	2.79002300	3.19894800
C	-0.40306700	0.16861000	5.09626600
H	-0.28700300	-1.87455000	4.40073400
H	-0.66159200	2.27253500	5.47800400
H	-0.05462100	-0.05851600	6.09906600
C	0.07592800	-1.25637700	-1.98753700
H	0.71928300	-1.67788900	-2.75515000
H	-0.77642900	-1.92262100	-1.83565100
N	0.85652600	-1.07394800	-0.72539900
S	1.34698600	-2.48465500	0.03174000
O	0.52503500	-2.78143900	1.21697100
O	1.47552700	-3.48296500	-1.03870800
C	2.97393800	-2.02891500	0.60736700
C	4.07338300	-2.29118700	-0.20800800
C	3.11870700	-1.37156600	1.82956200
C	5.33520500	-1.87093900	0.20526500
H	3.93279900	-2.82406300	-1.14151200
C	4.38533800	-0.94186600	2.21613500
H	2.25888600	-1.21648800	2.47201600
C	5.50839800	-1.17609900	1.41037700
H	6.19906700	-2.08064500	-0.41871400

H	4.50705400	-0.42827300	3.16553600
C	6.86667100	-0.66825500	1.82140500
H	6.99256600	0.38102700	1.52755900
H	7.00182400	-0.72012600	2.90534300
H	7.66850400	-1.24008000	1.34764700
N	-0.42770500	0.02416600	-2.40582900
C	0.39415800	0.03202800	0.14121900
H	0.92611500	0.94067600	-0.14319000
H	0.66019500	-0.19527700	1.16803900
S	-4.41284700	-0.06268600	0.21402300
O	-4.52531100	0.69200100	-1.04150300
O	-5.57845000	-0.20961600	1.09235000
C	-3.74525700	-1.66537400	-0.20459300
C	-3.62958200	-2.03137400	-1.54283400
C	-2.98908600	-3.22907800	-1.86148100
C	-2.44865900	-4.05076500	-0.86419500
C	-2.62539100	-3.67787000	0.47841700
C	-3.28167000	-2.50102000	0.81487200
H	-4.00412400	-1.36965000	-2.31477700
H	-2.87799700	-3.51161700	-2.90414300
H	-2.21377800	-4.30444200	1.26258600
H	-3.38750200	-2.20142100	1.85118400
C	-1.63713000	-5.26802400	-1.21830200
H	-0.57157700	-5.00932300	-1.23455100
H	-1.77223000	-6.06597900	-0.48295400
H	-1.90557500	-5.65551400	-2.20455500
N	-3.25775000	0.57835900	1.23629800
H	-3.70174700	0.85393400	2.10334700
P			
Energy = -2406.220137			
S	-0.44566600	-3.31053700	-0.81359400
O	0.40078100	-4.37714300	-0.27678800
O	-1.37168000	-3.51787400	-1.92743800
C	-1.36813700	-2.62617500	0.55236400
C	-2.52697700	-1.89591200	0.28766800
C	-0.86975200	-2.74080400	1.85004700
C	-3.17393600	-1.25565500	1.33570800
H	-2.90279500	-1.83082200	-0.72527000
C	-1.52768000	-2.08343300	2.88912900
H	0.00967200	-3.34591300	2.03703000
C	-2.67804200	-1.32415100	2.64562200
H	-4.06895000	-0.68040700	1.13177800
H	-1.14110800	-2.16129900	3.90109900
C	-3.38872300	-0.59431500	3.75641800

H	-2.80774400	-0.60275500	4.68180700
H	-3.57450500	0.44795600	3.47651200
H	-4.36216200	-1.05156000	3.96826000
C	1.73052300	-1.73470500	-0.41925700
H	2.67956200	-1.98753300	-0.89920600
H	1.65833400	-2.36569800	0.46991500
C	1.67336900	-0.25951400	-0.06975300
C	2.77987200	0.47460800	0.18449800
C	4.13348900	-0.14340000	0.26006600
C	4.38803800	-1.27125000	1.05311700
C	5.20010200	0.43166300	-0.44999200
C	5.66571100	-1.82664800	1.11598300
H	3.58420300	-1.70113800	1.64171400
C	6.47297600	-0.12836300	-0.39661800
H	5.01815200	1.31995000	-1.04621400
C	6.71020000	-1.26064800	0.38637000
H	5.84392500	-2.69782600	1.73876800
H	7.28317500	0.32077500	-0.96279300
H	7.70475000	-1.69327000	0.43229400
C	2.75401400	1.94486200	0.42928900
C	2.16244900	2.83052700	-0.48165200
C	3.37345100	2.46852100	1.57536300
C	2.15593700	4.20285800	-0.23346500
H	1.69446500	2.45031600	-1.38074900
C	3.36763100	3.83880400	1.82167500
H	3.85720400	1.79112500	2.27222800
C	2.75512900	4.71099100	0.91853800
H	1.68189500	4.86873600	-0.94749100
H	3.84292100	4.22734300	2.71738800
H	2.75254200	5.77978900	1.10991700
C	0.10799600	-1.02725100	-2.14009600
H	-0.65425400	-1.39725200	-2.81953800
H	0.95090300	-0.63637300	-2.72237700
N	-0.47299600	0.01954900	-1.26757900
S	-1.32048700	1.25877100	-2.00457200
O	-0.59883000	2.53151800	-1.86335200
O	-1.69501500	0.74756600	-3.32673200
C	-2.80088300	1.41157300	-1.01500500
C	-3.97697800	0.81114900	-1.45919800
C	-2.77049300	2.15228000	0.16696200
C	-5.13636700	0.95053700	-0.69871300
H	-3.97736100	0.26487300	-2.39554200
C	-3.93482600	2.27100500	0.91994800
H	-1.85735900	2.64965700	0.47279100

C	-5.13231400	1.67221800	0.50269800
H	-6.05933000	0.49471800	-1.04490000
H	-3.91976700	2.85155400	1.83804900
C	-6.37719400	1.77904100	1.34588500
H	-6.37028500	1.02814700	2.14556000
H	-6.45350800	2.76014100	1.82308700
H	-7.27903500	1.61578900	0.75066800
N	0.61970000	-2.10088700	-1.32320300
C	0.26647600	0.29394300	-0.01192900
H	-0.27489900	-0.19279300	0.80956300
H	0.28045700	1.36470200	0.17625100
2-TS4			
Energy = -5377.055395, Lowest Freq ν = -237.60			
S	5.71058800	-1.56541000	-1.35859500
O	6.15365400	-0.30968500	-0.73444400
O	6.66477200	-2.44626900	-2.03804300
C	4.79285000	-2.46811700	-0.12447300
C	3.88590100	-3.45760000	-0.51490300
C	4.99593800	-2.16266500	1.21907600
C	3.15154000	-4.11708300	0.46166000
H	3.71582000	-3.65777100	-1.56559500
C	4.25928400	-2.84764200	2.18559000
H	5.69494800	-1.38096200	1.49225000
C	3.31736300	-3.81616400	1.82300600
H	2.40831300	-4.84925400	0.16439200
H	4.39130200	-2.59691900	3.23370700
C	2.44472700	-4.48720000	2.85048300
H	1.39063700	-4.26943400	2.64577400
H	2.56167500	-5.57592600	2.82256700
H	2.67702900	-4.14608400	3.86218600
C	3.74795200	-0.00961500	-2.39496100
H	3.13112900	0.05094400	-3.29820000
H	4.39562400	0.87074000	-2.37800300
C	3.04249700	0.88259400	-0.11208800
C	3.71833800	2.16601100	-0.40399600
C	4.88165100	2.50682100	0.30531800
C	3.24347200	3.02855000	-1.40312200
C	5.55617800	3.68905500	0.01463000
H	5.27083600	1.82143000	1.04922000
C	3.90760400	4.22292500	-1.67001400
H	2.32764000	2.79447600	-1.93242000
C	5.06643200	4.55339400	-0.96631500
H	6.46549100	3.93406700	0.55395600
H	3.51401400	4.89698200	-2.42385900

H	5.58674800	5.48146200	-1.18141100
C	2.51867600	0.65697000	1.22101800
C	1.94003900	-0.58340800	1.58399900
C	2.48243800	1.71017900	2.16944200
C	1.30251200	-0.74349000	2.80776500
H	2.00293200	-1.43820600	0.93166400
C	1.87603600	1.53119200	3.40296100
H	2.87016700	2.68235000	1.90225800
C	1.26569700	0.31291300	3.72034400
H	0.82550200	-1.68731800	3.04098800
H	1.83440700	2.35903700	4.10261400
H	0.74633200	0.18714600	4.66463000
N	4.51298200	-1.26079300	-2.52062100
H	4.93967000	-1.39735100	-3.43317800
C	2.89554800	-0.06458100	-1.13852800
H	2.68708700	-1.08116700	-0.83492500
C	0.88481100	0.05468400	-1.72854500
H	0.74840900	1.12764600	-1.80252300
H	1.13974500	-0.49466500	-2.62980700
S	0.02290200	-2.32300700	-0.96601500
O	0.25532600	-2.85938900	0.37598200
O	0.91501600	-2.67402700	-2.07869300
C	-1.65902700	-2.63223900	-1.41246900
C	-2.56283500	-2.99771800	-0.41395600
C	-2.04191400	-2.51647600	-2.75053300
C	-3.88557500	-3.23766600	-0.77210700
H	-2.23317600	-3.08076700	0.61268900
C	-3.36640600	-2.76468600	-3.08290300
H	-1.32090300	-2.23239400	-3.50617900
C	-4.30637000	-3.11766300	-2.10233400
H	-4.60180200	-3.49974000	-0.00045500
H	-3.68348300	-2.66304200	-4.11596400
C	-5.75367600	-3.29296300	-2.47638300
H	-6.20889400	-2.31125100	-2.64948900
H	-5.86307300	-3.87149500	-3.39846200
H	-6.31886900	-3.79086900	-1.68505400
N	0.09898700	-0.57100100	-0.83065800
Fe	-1.07475800	0.40343600	0.41932400
O	-0.37167700	2.00112700	1.16158800
S	-0.08956200	3.28938500	0.32481100
O	1.02399200	4.04826900	0.87725700
O	-0.09525200	2.94404400	-1.10484200
C	-1.63053700	4.28628800	0.68598900
O	-2.58326500	0.93105700	-0.57920800

S	-2.82848000	1.27870700	-2.08483200
O	-2.92074600	2.71394100	-2.30157500
O	-1.98869400	0.45449200	-2.95546200
C	-4.58653200	0.62432800	-2.20671200
O	-1.64566700	-0.83859900	1.71490500
S	-2.39442800	-0.46588000	3.04116200
O	-1.81090500	-1.17999000	4.17004600
O	-2.64479500	0.97078500	3.10405900
C	-4.02347600	-1.28192400	2.65630600
F	-5.44421300	1.61470700	-1.97913400
F	-4.78460500	0.13709300	-3.43665600
F	-4.79920100	-0.34825400	-1.31689300
F	-1.54987800	4.74695500	1.93329600
F	-1.67673300	5.30457200	-0.16956000
F	-2.71943600	3.53606300	0.56011000
F	-3.84921500	-2.60343500	2.51278000
F	-4.51920200	-0.78450100	1.52157300
F	-4.87446800	-1.05622400	3.65410900
2-INT5			
Energy = -5377.070393			
S	5.59228900	-1.06589300	-1.41641200
O	5.68530500	0.18089000	-0.63681200
O	6.76631900	-1.60984400	-2.10407100
C	4.87699600	-2.28575100	-0.33069700
C	3.95305700	-3.21944600	-0.80600100
C	5.25566900	-2.26213800	1.01227000
C	3.37773400	-4.11188300	0.09159700
H	3.63368400	-3.19664500	-1.83978500
C	4.68168800	-3.17855000	1.89072400
H	5.95726300	-1.51506900	1.36536000
C	3.72472800	-4.10170800	1.44992200
H	2.61321900	-4.79507000	-0.26172800
H	4.95505500	-3.15254200	2.94137700
C	3.03700300	-5.03852300	2.40823800
H	1.95008900	-4.92439900	2.33516900
H	3.26876600	-6.08371900	2.17536200
H	3.33649800	-4.84949400	3.44207000
C	3.49438000	0.25745100	-2.49528300
H	2.91036100	0.26335000	-3.41881000
H	4.04705600	1.19661600	-2.44035900
C	2.82800500	0.98843400	-0.11515600
C	3.33295200	2.32595500	-0.33758000
C	4.28340500	2.87518300	0.55337300
C	2.90759200	3.10013400	-1.44102800

C	4.76915200	4.15996700	0.35870600
H	4.67367700	2.25597500	1.35147600
C	3.36811000	4.39725100	-1.60511000
H	2.15366700	2.71889400	-2.11676500
C	4.30085000	4.92867200	-0.70974600
H	5.51580700	4.56227100	1.03497700
H	2.99259800	4.99931100	-2.42518200
H	4.66807500	5.94047400	-0.84982600
C	2.49223800	0.56471300	1.20582900
C	2.26537500	-0.80501200	1.51813300
C	2.20564800	1.53700900	2.21552400
C	1.75936400	-1.17743100	2.74882800
H	2.49422400	-1.57976700	0.80638200
C	1.70994000	1.14851100	3.44613300
H	2.26010800	2.58870500	1.97261500
C	1.47128400	-0.20551600	3.71282400
H	1.55613100	-2.22290800	2.94299500
H	1.44278600	1.90216600	4.17846000
H	1.01939600	-0.49975000	4.65352500
N	4.40462600	-0.89190900	-2.60633500
H	4.86241400	-0.97617300	-3.50948500
C	2.55338200	0.08473800	-1.27686700
H	2.67812800	-0.94259000	-0.94516100
C	1.02039800	0.13350600	-1.69791900
H	0.66153900	1.16017100	-1.78065500
H	0.96542100	-0.32965400	-2.68479400
S	0.14886800	-2.27946800	-0.93200900
O	0.47638500	-2.86922200	0.37273100
O	0.98517700	-2.59961600	-2.10190200
C	-1.54000900	-2.69097600	-1.28506000
C	-2.38001300	-3.05436400	-0.23163700
C	-1.98812300	-2.66697500	-2.60684800
C	-3.70163100	-3.38465200	-0.51558800
H	-2.00130700	-3.07429500	0.78144300
C	-3.30844000	-3.01022900	-2.86717100
H	-1.31582100	-2.38312600	-3.40602300
C	-4.18430300	-3.36349300	-1.82980300
H	-4.36717300	-3.64747000	0.30031600
H	-3.67333100	-2.98479600	-3.88921600
C	-5.63320800	-3.64585600	-2.12560800
H	-6.17709400	-2.70075400	-2.23729500
H	-5.75224200	-4.20517000	-3.05806600
H	-6.10775500	-4.21040300	-1.31908700
N	0.15997400	-0.57816200	-0.77191700

Fe	-1.08080800	0.35554100	0.33652900
O	-0.33959800	1.99972100	0.97822100
S	-0.19066700	3.36815400	0.25851600
O	0.89680800	4.13787600	0.86163000
O	-0.22424300	3.18653000	-1.19668200
C	-1.76696800	4.22318100	0.77317900
O	-2.62834100	0.85880300	-0.63063400
S	-2.86384000	1.11703900	-2.15184800
O	-3.02297900	2.53425700	-2.44165200
O	-1.96873200	0.29850900	-2.97247700
C	-4.58581500	0.37366000	-2.27426700
O	-1.43710000	-0.78345200	1.82040900
S	-2.21780000	-0.32959100	3.09330900
O	-1.60957800	-0.89401200	4.29370800
O	-2.55493800	1.09038900	3.02239400
C	-3.79930200	-1.26461300	2.79441900
F	-5.49583100	1.33358100	-2.12670000
F	-4.73323600	-0.19506400	-3.47590300
F	-4.77849800	-0.55214600	-1.33019200
F	-1.73207400	4.42591100	2.08965800
F	-1.83012000	5.39559600	0.14061900
F	-2.82646300	3.48585900	0.46308100
F	-3.55495400	-2.58246200	2.75966900
F	-4.32700700	-0.89230400	1.62510700
F	-4.66145700	-1.00404900	3.77520800
2-TS5			
Energy = -5376.997942, Lowest Freq ν = -2232.37			
S	4.18589300	-2.21728400	-1.97245300
O	4.95317200	-1.01777700	-1.58912800
O	4.79951500	-3.25991600	-2.79114000
C	3.59467800	-2.98699600	-0.46819600
C	2.31694000	-3.54383600	-0.37307700
C	4.48518800	-3.04984100	0.60346700
C	1.92590600	-4.13689700	0.82346800
H	1.60547700	-3.47588200	-1.18595900
C	4.08263300	-3.66815100	1.78478000
H	5.46773300	-2.59927600	0.51850400
C	2.79940000	-4.21341800	1.91828500
H	0.91698800	-4.52557300	0.91678300
H	4.76946100	-3.70924100	2.62516000
C	2.34211900	-4.84329300	3.20790600
H	2.15024600	-5.91363200	3.07282100
H	3.09233500	-4.73439000	3.99522500
H	1.40768200	-4.38565000	3.54669900

C	2.55495800	-0.21668700	-2.86973400
H	1.85847300	-0.11238400	-3.70259000
H	3.47294200	0.31914600	-3.11973200
C	2.88438400	0.99862200	-0.63635900
C	3.73339700	2.07204300	-1.14065800
C	5.13295100	2.00822400	-0.96100800
C	3.16948900	3.15957500	-1.84203200
C	5.94341300	3.01398900	-1.47207600
H	5.56116200	1.13014700	-0.49441100
C	3.98891700	4.17827400	-2.31055700
H	2.09503100	3.25228100	-1.93543400
C	5.37401400	4.10377400	-2.13632600
H	7.02020800	2.94526400	-1.35866600
H	3.54591500	5.03469300	-2.80735300
H	6.01006400	4.89412500	-2.52234300
C	2.99214200	0.53882400	0.69541800
C	2.26936800	-0.59844200	1.15866000
C	3.71039300	1.31748600	1.65365900
C	2.26204200	-0.93431200	2.49550100
H	1.72835800	-1.22475000	0.46650400
C	3.71493500	0.95831600	2.98852700
H	4.17775600	2.23964700	1.34499100
C	2.98504100	-0.15632100	3.41107700
H	1.69015500	-1.78710100	2.83477700
H	4.23677200	1.57616100	3.71039600
H	2.95856200	-0.41405700	4.46559800
N	2.84901700	-1.63074000	-2.76663600
H	2.07602400	-2.27026600	-2.91974400
C	1.92416600	0.45173000	-1.62192200
H	1.00266100	-0.44720400	-1.08232100
C	0.57870900	1.17038700	-1.87059500
H	0.37637300	2.05994100	-1.28021300
H	0.35788300	1.35646200	-2.92036700
S	-0.74906700	-1.12641200	-2.57956800
O	-0.00245600	-2.36678900	-2.29849300
O	-0.56585600	-0.45892600	-3.87282900
C	-2.46540600	-1.43244000	-2.31081100
C	-2.84559200	-2.40780800	-1.38803900
C	-3.39032200	-0.78408500	-3.13312300
C	-4.19639100	-2.71771900	-1.27586000
H	-2.10337500	-2.90396500	-0.77782200
C	-4.72928700	-1.12984500	-3.01540700
H	-3.05918600	-0.03138600	-3.83551400
C	-5.15321500	-2.08445200	-2.07941600

H	-4.50902900	-3.45760400	-0.54679700
H	-5.46284500	-0.62949500	-3.63921900
C	-6.61920600	-2.37305000	-1.90106000
H	-7.15856300	-2.31885900	-2.85076100
H	-6.78741900	-3.35889400	-1.46029500
H	-7.06163600	-1.62749300	-1.22913000
N	-0.19885400	0.00206900	-1.32175400
Fe	-0.97328500	0.36912400	0.66843200
O	0.37707900	1.67881800	1.38035000
S	0.62435200	3.18160900	1.23724300
O	1.98654900	3.53953400	1.64935700
O	0.14869100	3.69857500	-0.05630400
C	-0.48541000	3.88239900	2.55414800
O	-2.55348300	1.50992600	0.51963300
S	-3.04118600	2.26273100	-0.72809500
O	-3.13227200	3.70408200	-0.54036400
O	-2.40971600	1.74141200	-1.95389900
C	-4.80298500	1.64849300	-0.74532400
O	-0.82557800	-1.69566400	0.91368500
S	-1.21830800	-1.82192600	2.38676500
O	-0.43445000	-2.79791100	3.14214400
O	-1.36902100	-0.44043400	2.90771200
C	-2.94360400	-2.50928100	2.28867600
F	-5.54250000	2.34693900	0.11556000
F	-5.31740300	1.78459200	-1.97537200
F	-4.85599000	0.35276800	-0.39922800
F	-0.13243100	3.36354800	3.73652500
F	-0.33011200	5.20807200	2.59217500
F	-1.75797600	3.58905800	2.31045900
F	-2.92740000	-3.66815500	1.61199900
F	-3.73464100	-1.64351100	1.65157100
F	-3.41142200	-2.72306200	3.51527700
2-INT6			
Energy = -5377.068391			
S	4.55608100	-2.46667600	-1.35702300
O	5.86646900	-1.82884000	-1.53679400
O	4.33082400	-3.86809400	-1.71765300
C	4.07977600	-2.21486200	0.34395500
C	2.88730500	-2.77127000	0.81671700
C	4.93507100	-1.51129700	1.18709400
C	2.55609300	-2.60616900	2.15815600
H	2.23530500	-3.31709100	0.14469800
C	4.58055600	-1.35188400	2.52652300
H	5.85275700	-1.09377000	0.79224400

C	3.39454500	-1.89502700	3.03317500
H	1.63258400	-3.02984700	2.53582400
H	5.23810200	-0.79495100	3.18805500
C	3.02700100	-1.73574000	4.48572300
H	3.30597100	-2.63009000	5.05596200
H	3.54500400	-0.88413000	4.93491100
H	1.95072800	-1.59373800	4.60447700
C	3.63366400	-0.19356000	-2.52950000
H	3.32530600	-0.03190100	-3.56601800
H	4.70231600	0.00441900	-2.45762300
C	3.34735600	1.40207000	-0.57420200
C	4.78492700	1.73027100	-0.42474000
C	5.37965700	1.73191200	0.84886000
C	5.56777600	2.10883000	-1.52776800
C	6.72873500	2.03782000	1.00351400
H	4.77825300	1.47550600	1.71318100
C	6.91639100	2.42103500	-1.37184600
H	5.10584000	2.18840600	-2.50606400
C	7.50458700	2.37513600	-0.10756800
H	7.17499500	2.01884000	1.99331700
H	7.50482900	2.71022900	-2.23695900
H	8.55594900	2.61664600	0.01389000
C	2.46157200	1.91771600	0.51272300
C	1.94846900	1.02175000	1.46494200
C	2.17729700	3.28092600	0.63810700
C	1.17190500	1.48835500	2.52863700
H	2.21328900	-0.02846800	1.40994800
C	1.36346600	3.73832400	1.67474700
H	2.57015300	3.97703100	-0.09477100
C	0.86369200	2.84583300	2.62331000
H	0.81852600	0.79484600	3.28258300
H	1.11484600	4.79272700	1.73532700
H	0.23656300	3.20473500	3.43278200
N	3.37570300	-1.61396000	-2.21480100
H	3.07999100	-2.18585500	-3.00011700
C	2.82512800	0.66516300	-1.58592100
H	1.15463100	-0.91596300	-0.46352100
C	1.33193300	0.67032300	-1.80442400
H	0.91941700	1.58597300	-1.40414000
H	1.10972300	0.63707400	-2.87195700
S	0.23148800	-1.85654000	-2.28767100
O	0.62409100	-3.04489500	-1.53562600
O	0.83726100	-1.50385700	-3.57457300
C	-1.52205300	-1.83017900	-2.46965800

C	-2.27566100	-2.78787800	-1.79043400
C	-2.10724400	-0.89591900	-3.33171100
C	-3.65378400	-2.79551000	-1.97668600
H	-1.78373200	-3.50437900	-1.14425300
C	-3.48440700	-0.91521900	-3.48546100
H	-1.49790200	-0.17315400	-3.86191400
C	-4.27673800	-1.86203500	-2.81371900
H	-4.25738000	-3.53041600	-1.45421300
H	-3.96083200	-0.17662900	-4.12066200
C	-5.77151100	-1.83700200	-2.97265800
H	-6.05601200	-1.86383700	-4.02949400
H	-6.24486000	-2.68101800	-2.46622900
H	-6.16744000	-0.90901800	-2.54897600
N	0.55688900	-0.46882000	-1.16748800
Fe	-1.14530300	0.15881700	0.11412100
O	-0.79191900	1.97996000	-0.00188200
S	-1.22373800	3.11920900	-1.00299100
O	-0.03129900	3.73512100	-1.57722000
O	-2.28704900	2.64555500	-1.88486200
C	-1.94067300	4.37006700	0.22722700
O	-2.91556400	-0.06578000	-0.45899800
S	-4.18596800	0.85305600	-0.26028400
O	-3.88511700	2.00245400	0.58285700
O	-4.91139600	0.99005900	-1.51410100
C	-5.22631300	-0.27705300	0.79611600
O	-0.44834200	-1.63398800	1.04733700
S	-1.06725400	-1.31426100	2.40154900
O	-0.24047900	-1.47688000	3.58513300
O	-1.69936600	0.04256400	2.16900200
C	-2.44249300	-2.57017500	2.55066500
F	-4.67081200	-0.43358800	1.99893700
F	-6.42671000	0.28405300	0.93596400
F	-5.36693900	-1.47404000	0.21628500
F	-1.12929700	5.43132700	0.24847600
F	-3.14100600	4.73703400	-0.19831800
F	-2.01624800	3.85885800	1.44897500
F	-1.88389000	-3.75186900	2.80191400
F	-3.12054100	-2.63554800	1.40529600
F	-3.25099900	-2.22557200	3.54435400
2-INT7			
Energy = -2368.125159			
S	1.58377100	-3.08450800	-0.29343000
O	2.95382500	-2.99517400	-0.80629700
O	0.92796100	-4.35812700	0.00030900

C	1.54254100	-2.10066200	1.20482800
C	0.45946400	-2.21973000	2.07539000
C	2.55479500	-1.17017100	1.44041800
C	0.36953500	-1.35562900	3.16810500
H	-0.31405500	-2.95596400	1.89090300
C	2.45938400	-0.33148700	2.54566600
H	3.39337000	-1.11095300	0.75773800
C	1.36061500	-0.39702500	3.41527500
H	-0.48961200	-1.42769300	3.82756300
H	3.24233000	0.39833200	2.73199200
C	1.25200900	0.56144500	4.57331700
H	2.10224300	0.45694900	5.25594700
H	1.24905000	1.59809000	4.21789200
H	0.33696500	0.39478900	5.14667100
C	1.02069300	-1.07343300	-2.03647000
H	0.54973700	-1.06665900	-3.02755100
H	2.09503500	-1.14848500	-2.19193200
C	1.55604200	1.15353200	-0.94529600
C	2.98614200	1.11224100	-1.35937500
C	3.99506700	1.34495000	-0.41053600
C	3.36175200	0.90173000	-2.69399800
C	5.33776400	1.31156200	-0.77449200
H	3.71281600	1.55067300	0.61604600
C	4.70641700	0.87812500	-3.06205300
H	2.59275300	0.77406800	-3.44869300
C	5.69859000	1.07256200	-2.10220400
H	6.10423100	1.47645100	-0.02348700
H	4.97680500	0.71186900	-4.10009200
H	6.74563400	1.04877000	-2.38717900
C	1.18993800	2.35101900	-0.13340000
C	0.51521700	2.24473500	1.09211300
C	1.56814500	3.62919900	-0.57720100
C	0.20387400	3.38242100	1.83667800
H	0.25135300	1.27006000	1.47806600
C	1.25207500	4.76525400	0.16244100
H	2.11136600	3.72303100	-1.51203600
C	0.56767000	4.64638500	1.37408700
H	-0.31905200	3.27569500	2.78247700
H	1.54363400	5.74467300	-0.20431000
H	0.32771300	5.53169800	1.95479300
N	0.60557800	-2.31968600	-1.39228100
H	-0.38761200	-2.53529100	-1.30316300
C	0.65406100	0.20263200	-1.29389700
H	-0.61252500	-0.60654700	0.83173900

C	-0.82322900	0.40376300	-1.03569100
H	-1.05229200	1.46837500	-0.96107800
H	-1.38457800	0.00072500	-1.88572600
S	-2.54210600	-1.38442600	0.06843000
O	-2.66243700	-1.98204300	1.40271700
O	-2.34468100	-2.26777800	-1.10155200
C	-3.94411300	-0.35181500	-0.30878300
C	-4.15197000	0.82389000	0.41615500
C	-4.84391000	-0.76789200	-1.28700100
C	-5.27787100	1.59113700	0.14335400
H	-3.42938100	1.13141200	1.16337400
C	-5.96951100	0.01289500	-1.54260000
H	-4.65189800	-1.68086000	-1.83840900
C	-6.20290400	1.19875000	-0.83684500
H	-5.44490400	2.51039000	0.69750200
H	-6.67596000	-0.30312300	-2.30434300
C	-7.40758800	2.05466100	-1.13337200
H	-8.14299700	1.51518000	-1.73487000
H	-7.89585600	2.38498500	-0.21141400
H	-7.11975700	2.95558800	-1.68781000
N	-1.32311000	-0.25296700	0.19518200
2-TS6			
Energy = -6290.743415, Lowest Freq ν = -277.64			
S	0.88826600	-2.24869200	2.03891300
O	1.18603200	-3.51241500	1.37465900
O	-0.19697900	-2.08923200	3.00417500
C	2.37274700	-1.59704100	2.74909100
C	2.28262500	-0.56194500	3.68826300
C	3.59948100	-2.14832300	2.38020900
C	3.45666400	-0.03446000	4.21111000
H	1.31470200	-0.18057000	3.99178900
C	4.76215700	-1.61553500	2.93295700
H	3.62943000	-2.96427500	1.66911600
C	4.71174400	-0.53865500	3.82716800
H	3.40687200	0.79870900	4.90323300
H	5.72435300	-2.02153200	2.63779900
C	5.96553200	0.11696200	4.33393400
H	6.03316700	1.12524200	3.91124700
H	5.94958000	0.21807200	5.42366500
H	6.85857300	-0.44536800	4.05158600
C	1.19356200	-1.21805100	-0.54721300
H	0.63532900	-0.56545200	-1.22269900
H	1.01746600	-2.24194600	-0.86313000
C	3.57451900	-1.75839400	-1.07056600

C	3.22052200	-3.15986000	-1.44240400
C	3.91876700	-4.22097300	-0.84454800
C	2.23715700	-3.45438100	-2.39705200
C	3.59978300	-5.54136200	-1.14745100
H	4.71688000	-4.00167300	-0.14133400
C	1.92018200	-4.77701700	-2.70364500
H	1.70593900	-2.65024200	-2.89461000
C	2.59375700	-5.82268700	-2.07461000
H	4.13500200	-6.35101800	-0.66091000
H	1.13408400	-4.98267600	-3.42206000
H	2.33907700	-6.85206500	-2.30645300
C	5.00995200	-1.42096200	-1.29574900
C	5.78569900	-0.69215800	-0.37933400
C	5.62550500	-1.87248900	-2.47841700
C	7.12396100	-0.40548900	-0.64983500
H	5.33977200	-0.34261700	0.54154200
C	6.95721700	-1.57497200	-2.75095500
H	5.04513300	-2.45363200	-3.18695300
C	7.71452000	-0.83999000	-1.83555100
H	7.70626200	0.15502900	0.07623300
H	7.40672300	-1.92189300	-3.67641700
H	8.75663400	-0.61647800	-2.04344200
C	2.65920900	-0.86300900	-0.60952200
H	3.15140800	0.27117500	1.66560700
C	3.00837800	0.59574500	-0.42028300
H	3.79965400	0.87758100	-1.11768400
H	2.12757800	1.19701100	-0.64349400
S	3.42944800	2.46635300	1.49181300
O	4.30636600	2.55974000	2.66543900
O	2.02222500	2.89955900	1.63934900
C	4.13802000	3.32195200	0.10772900
C	5.52023900	3.25653800	-0.07954300
C	3.30510100	3.96659800	-0.80533800
C	6.07181800	3.85647200	-1.20543400
H	6.14146100	2.74034500	0.64333500
C	3.87946300	4.56475900	-1.92473600
H	2.23231500	3.97535700	-0.65424200
C	5.26274600	4.51986100	-2.14140400
H	7.14468500	3.80695800	-1.36684500
H	3.24073700	5.06400700	-2.64715000
C	5.87691700	5.18535900	-3.34608000
H	5.14997200	5.29780900	-4.15439500
H	6.24419800	6.18661300	-3.09056500
H	6.72841100	4.61350800	-3.72584100

N	3.52001300	0.88522800	0.94568200
N	0.44841300	-1.08156700	0.75762800
H	-0.49171100	-1.42436700	0.50243900
C	-0.25382100	0.63415900	1.36929900
H	-0.58710100	0.19879300	2.30524900
H	0.66335100	1.21941600	1.38045000
S	-1.03629200	2.03802500	-0.75300200
O	-2.11637100	1.52517500	-1.64272900
O	0.35306900	2.05594800	-1.22991900
C	-1.49147400	3.65948300	-0.19989000
C	-2.69947300	4.20263500	-0.63507000
C	-0.62588600	4.35702400	0.64812900
C	-3.04495100	5.47978500	-0.19967100
H	-3.35266900	3.64806700	-1.29524000
C	-0.99967100	5.62745700	1.07032800
H	0.31068000	3.92220100	0.97756100
C	-2.21117800	6.20594500	0.65913400
H	-3.98332100	5.91224900	-0.53329800
H	-0.33877900	6.18041100	1.73157300
C	-2.61580400	7.56952000	1.15673500
H	-1.74704600	8.22052700	1.28990400
H	-3.31050400	8.05660000	0.46762400
H	-3.11727200	7.49134900	2.12891400
N	-1.25409300	1.00461300	0.55413800
Fe	-3.03668800	-0.04274400	-0.01045300
O	-1.91038700	-1.37297000	-0.84799200
S	-2.05143600	-2.54769100	-1.87843000
O	-0.92186200	-3.45614600	-1.69172900
O	-3.41227300	-3.04576900	-1.98144100
C	-1.69000600	-1.60567700	-3.44266600
O	-2.74938900	-0.71056100	2.07783800
S	-3.90216700	-1.70902000	2.07783000
O	-4.81572200	-1.66616100	3.20507500
O	-4.47177100	-1.57948000	0.68172400
C	-3.10732200	-3.39912000	2.10059000
O	-4.36315800	1.51797800	0.36011400
S	-5.22111100	1.39415200	-0.91091600
O	-5.40120100	2.62105500	-1.67528200
O	-4.67492700	0.17894500	-1.60704000
C	-6.91495800	0.94291300	-0.26942500
F	-4.03984700	-4.29965100	1.80264900
F	-2.12759300	-3.45983100	1.19227400
F	-2.61459500	-3.63919400	3.30915200
F	-1.66573600	-2.46624000	-4.46305600

F	-2.61338500	-0.67836100	-3.65911700
F	-0.48331200	-1.01751500	-3.34752600
F	-6.84822000	-0.08806800	0.55964800
F	-7.41308600	2.00266400	0.36977500
F	-7.68804800	0.64098700	-1.31151600
2-INT8			
Energy = -6290.753533			
S	0.84404600	-2.16312600	2.09760400
O	1.07512000	-3.40108300	1.37253400
O	-0.20967800	-1.97201600	3.08155100
C	2.35827500	-1.53376400	2.74362800
C	2.32159400	-0.47792100	3.66460000
C	3.55575600	-2.13699600	2.35499400
C	3.52522800	0.01484100	4.15048900
H	1.37634100	-0.05224800	3.97902500
C	4.74698200	-1.63732300	2.87488600
H	3.54107300	-2.96547200	1.65828300
C	4.75299800	-0.54285300	3.75054000
H	3.52061600	0.86381800	4.82452800
H	5.68740700	-2.08260500	2.56741900
C	6.03890100	0.07718400	4.21708300
H	6.13323100	1.07079100	3.76537400
H	6.04533000	0.20888800	5.30349600
H	6.90532900	-0.52493500	3.93463900
C	1.13823500	-1.13697000	-0.57042100
H	0.60354200	-0.48229600	-1.26110400
H	0.92448300	-2.16271200	-0.85127100
C	3.48944200	-1.79578500	-1.07023500
C	3.08265200	-3.19458800	-1.39587100
C	3.75397000	-4.25894300	-0.77138700
C	2.09181300	-3.48717900	-2.34207300
C	3.39882400	-5.57724800	-1.03872400
H	4.56433000	-4.04410300	-0.08093000
C	1.74084900	-4.80875800	-2.61551500
H	1.58187800	-2.68398400	-2.86200700
C	2.38535500	-5.85517600	-1.95925200
H	3.91368000	-6.38813500	-0.53269800
H	0.94727300	-5.01019600	-3.32633700
H	2.10290800	-6.88283500	-2.16466200
C	4.93597900	-1.53055800	-1.32488600
C	5.76276000	-0.81422800	-0.44413100
C	5.51014700	-2.05245100	-2.50005800
C	7.11140500	-0.61275400	-0.73871400
H	5.35105800	-0.40506000	0.46756000

C	6.85186200	-1.83735300	-2.79832100
H	4.89049600	-2.62390700	-3.18248800
C	7.66129800	-1.11822600	-1.91562600
H	7.73249000	-0.06022000	-0.03939600
H	7.26824500	-2.23713900	-3.71783500
H	8.71128400	-0.96004400	-2.14258900
C	2.61884600	-0.84435200	-0.62831700
H	3.29760000	0.25570300	1.58171100
C	3.04559700	0.60129500	-0.48965400
H	3.83528900	0.82132700	-1.21129800
H	2.19430200	1.24240500	-0.71474800
S	3.48493100	2.46273900	1.45270100
O	4.43378900	2.55055300	2.57033800
O	2.07618300	2.82988500	1.70760600
C	4.07084500	3.38990900	0.05817900
C	5.44403900	3.42057600	-0.19298200
C	3.15627200	4.01410200	-0.78961100
C	5.90315900	4.09842900	-1.31656700
H	6.12998200	2.92185400	0.48223800
C	3.63878800	4.68772300	-1.90894400
H	2.09332400	3.95355600	-0.59141600
C	5.01072400	4.74243500	-2.18781800
H	6.96854800	4.12847400	-1.52541300
H	2.93568700	5.17055200	-2.58092100
C	5.52216500	5.49633100	-3.38829800
H	4.77493900	5.53152400	-4.18531700
H	5.76560500	6.53149900	-3.12000400
H	6.43195100	5.04042600	-3.78861500
N	3.60080900	0.89801800	0.85809700
N	0.35363200	-0.97416900	0.73234100
H	-0.55677500	-1.39767600	0.45244400
C	-0.05747600	0.44850400	1.21087900
H	-0.40025000	0.29790800	2.23349700
H	0.82345600	1.08784100	1.18248400
S	-0.95495900	1.99504400	-0.81267500
O	-2.04776400	1.53145400	-1.72203300
O	0.42744200	2.05049000	-1.32063300
C	-1.41072800	3.60752900	-0.22049800
C	-2.57542600	4.19817600	-0.70752300
C	-0.59706800	4.24639700	0.71924100
C	-2.92740800	5.46088100	-0.23521500
H	-3.19570800	3.68471400	-1.42991300
C	-0.97294400	5.50488700	1.17492700
H	0.30471400	3.77697200	1.09380700

C	-2.14163600	6.12884200	0.71099200
H	-3.83515600	5.92661900	-0.60694200
H	-0.34923100	6.01066900	1.90654600
C	-2.55495600	7.47573200	1.24658700
H	-1.68599300	8.10414900	1.46247800
H	-3.19776200	8.00683200	0.53974800
H	-3.11690000	7.36335000	2.18163900
N	-1.13991100	0.92390200	0.41817800
Fe	-2.92919900	0.00912300	-0.03945200
O	-1.89942900	-1.47773700	-0.80890200
S	-2.08282600	-2.68505800	-1.78413100
O	-0.96441100	-3.60524900	-1.57747600
O	-3.45116800	-3.16706700	-1.85578200
C	-1.72478800	-1.81336800	-3.38904900
O	-2.64262500	-0.63162400	2.07298300
S	-3.84019300	-1.57324400	2.12076500
O	-4.73181100	-1.44764300	3.26071900
O	-4.42266300	-1.48799000	0.73291200
C	-3.11376600	-3.28974200	2.21791300
O	-4.25575200	1.57748100	0.31331600
S	-5.11977400	1.43353100	-0.95017400
O	-5.29102500	2.64373400	-1.74319500
O	-4.59613500	0.19537900	-1.62092700
C	-6.81779900	1.02392800	-0.29188100
F	-4.07363700	-4.17110500	1.95262400
F	-2.12708900	-3.43041800	1.32174000
F	-2.63169500	-3.50139600	3.43904800
F	-1.70199500	-2.71470400	-4.37431400
F	-2.64355300	-0.89178000	-3.64313600
F	-0.51438100	-1.22263800	-3.32348900
F	-6.76561400	0.03168800	0.58405500
F	-7.30971400	2.11606500	0.29727700
F	-7.59297800	0.68190200	-1.32106300
2-TS7			
Energy = -6290.704428, Lowest Freq ν = -1709.63			
S	0.56233600	-1.45331600	2.11275000
O	0.42943100	-2.83115700	1.66472600
O	-0.31035800	-0.83390600	3.10387500
C	2.25068400	-1.17619500	2.59679000
C	2.57568900	-0.05469100	3.35933600
C	3.22275700	-2.08793300	2.17918900
C	3.91511500	0.17774500	3.66988200
H	1.80568200	0.63523100	3.68275500
C	4.55030500	-1.84660100	2.51384800

H	2.93470400	-2.95816900	1.60213200
C	4.91863900	-0.70371000	3.24323300
H	4.17881900	1.06755000	4.23081300
H	5.31736200	-2.54133900	2.18573900
C	6.37165100	-0.42566100	3.52877300
H	6.49128000	0.40584600	4.22731300
H	6.86732500	-1.30419300	3.95302000
H	6.90202700	-0.16945600	2.60410100
C	1.01430700	-0.98871300	-0.59626400
H	0.45740500	-0.54323500	-1.42309600
H	0.78466800	-2.05048700	-0.58647800
C	3.32702600	-1.73246200	-1.17837600
C	2.86130000	-3.13189800	-1.39456200
C	3.53736800	-4.19424000	-0.77063600
C	1.77340300	-3.42606200	-2.22917700
C	3.09844700	-5.50543600	-0.93177100
H	4.40976700	-3.98277000	-0.15940200
C	1.33386900	-4.73861700	-2.39067000
H	1.25682800	-2.62656200	-2.74766600
C	1.98981600	-5.77993700	-1.73683100
H	3.61914600	-6.31421400	-0.42813900
H	0.46404900	-4.93330900	-3.00823500
H	1.64071900	-6.80105400	-1.85258200
C	4.78338400	-1.52998100	-1.42616300
C	5.61422600	-0.83861400	-0.53078000
C	5.36827300	-2.09783700	-2.57157500
C	6.98207300	-0.71720500	-0.77144400
H	5.19588500	-0.41548200	0.37250300
C	6.73030600	-1.95858900	-2.82346000
H	4.74147600	-2.65046900	-3.26347900
C	7.54501100	-1.27264000	-1.91966200
H	7.60319700	-0.18664100	-0.05907000
H	7.15839100	-2.39554500	-3.72041000
H	8.61115700	-1.18192100	-2.10548500
C	2.48599000	-0.72946000	-0.81216300
H	3.44670800	0.62600100	1.20608700
C	2.92732300	0.71372900	-0.83570300
H	3.88582900	0.80656200	-1.35368400
H	2.18589300	1.30793800	-1.37763100
S	3.54374800	2.81545600	0.76696900
O	3.48065300	3.05297500	2.21059100
O	2.79559200	3.63606700	-0.19180400
C	5.25669000	2.80826700	0.27532000
C	6.23506500	2.54384000	1.23416500

C	5.58963600	2.98502500	-1.06908100
C	7.56485500	2.44773100	0.83221900
H	5.95202900	2.43991500	2.27517500
C	6.92254500	2.87342900	-1.45274000
H	4.81580200	3.22172900	-1.79020600
C	7.92594000	2.59545500	-0.51453600
H	8.33531700	2.25687700	1.57397000
H	7.18960800	3.00323800	-2.49732200
C	9.35517700	2.42237200	-0.95767300
H	9.63696600	3.17310300	-1.70164700
H	10.04997700	2.49359000	-0.11722700
H	9.49196700	1.43855100	-1.42310400
N	3.00161100	1.24809300	0.53888300
N	0.31859700	-0.47972500	0.64149700
H	-0.89800300	-0.34404800	0.12877400
C	-0.02675800	0.98232500	0.82213300
H	-0.23550300	1.16198100	1.87461900
H	0.73962800	1.65266900	0.44688000
S	-1.32428800	1.68397100	-1.44614400
O	-2.64937000	1.14911900	-1.90172200
O	-0.12525800	1.43512900	-2.25953200
C	-1.45338100	3.42724700	-1.16387200
C	-2.70747100	4.03875800	-1.15486600
C	-0.27805300	4.14423000	-0.92182200
C	-2.77360700	5.40228800	-0.88267300
H	-3.60323700	3.47100000	-1.36158900
C	-0.37563100	5.50131700	-0.63744200
H	0.69534200	3.67085700	-0.95316100
C	-1.61915200	6.15010800	-0.61412900
H	-3.74349900	5.89052000	-0.87697600
H	0.53259900	6.05985000	-0.43213900
C	-1.70758900	7.62890700	-0.33832600
H	-1.60720400	8.20209400	-1.26806200
H	-2.66940100	7.89480800	0.10807600
H	-0.91122400	7.95675900	0.33541200
N	-1.26955600	0.94041400	0.03850300
Fe	-3.36533500	0.08054500	-0.02467300
O	-2.36299900	-1.46651800	-0.59396700
S	-2.44350600	-2.84990700	-1.30303300
O	-1.25624700	-3.62948300	-0.96344000
O	-3.77292100	-3.43715000	-1.24507200
C	-2.17049100	-2.28467000	-3.05455500
O	-2.91899800	0.07764300	2.03072600
S	-4.07031500	-0.84003400	2.43461100

O	-4.90980300	-0.40918500	3.53735800
O	-4.72225600	-1.14688800	1.10223300
C	-3.28729400	-2.45376400	2.95155100
O	-4.55764700	1.74706600	0.21566100
S	-5.54402900	1.41827500	-0.91259500
O	-5.75237800	2.46829700	-1.89868400
O	-5.11138400	0.05298600	-1.37984400
C	-7.18290300	1.20561000	-0.04246400
F	-4.26211100	-3.34822700	3.10623600
F	-2.44010700	-2.87172000	2.01526900
F	-2.64524300	-2.28208100	4.10245300
F	-2.00941000	-3.35821600	-3.83734000
F	-3.19738100	-1.56395100	-3.48975100
F	-1.05056900	-1.53907200	-3.12267400
F	-7.09108600	0.32884600	0.94572800
F	-7.54692000	2.39392200	0.44289000
F	-8.07763800	0.79102200	-0.93827500
2-INT9			
Energy = -6290.748174			
S	0.67438500	-0.94280800	2.42834900
O	0.47856300	-2.38810200	2.33388800
O	-0.12605100	-0.09538000	3.31207400
C	2.39943900	-0.67619400	2.81138900
C	2.82229300	0.58509700	3.23147400
C	3.30906900	-1.71347200	2.60114000
C	4.18671100	0.81346700	3.41200900
H	2.10379600	1.38028800	3.39220800
C	4.66468000	-1.46974000	2.79819300
H	2.95201400	-2.68430000	2.27919000
C	5.12578000	-0.20323500	3.18962100
H	4.51936300	1.79977100	3.71899200
H	5.38049700	-2.26780000	2.62431400
C	6.60337200	0.05248800	3.34066400
H	6.79975400	1.06417100	3.70414000
H	7.05779200	-0.65436300	4.04247600
H	7.11716200	-0.06884700	2.38040800
C	0.95710200	-1.13050800	-0.26370900
H	0.31451200	-0.90310400	-1.12006000
H	0.74650800	-2.16246900	0.00266300
C	3.23174600	-2.01299800	-0.84668400
C	2.76696000	-3.41990300	-0.69304400
C	3.50374300	-4.31081300	0.10595800
C	1.61005500	-3.89110500	-1.33267400
C	3.06438200	-5.61696200	0.30306800

H	4.42156500	-3.96719700	0.57314400
C	1.16858500	-5.19842100	-1.13382500
H	1.04313100	-3.23564100	-1.98451300
C	1.89078700	-6.06192600	-0.31086100
H	3.63554300	-6.28816100	0.93742000
H	0.25098000	-5.52394900	-1.61103200
H	1.54391500	-7.07790400	-0.14983300
C	4.67761100	-1.87387000	-1.17878300
C	5.52559500	-1.01880800	-0.45878600
C	5.23441500	-2.66790100	-2.19537100
C	6.88830900	-0.95884200	-0.74664300
H	5.12291200	-0.41933800	0.34723600
C	6.59136800	-2.59142100	-2.49794200
H	4.59086700	-3.34776300	-2.74400800
C	7.42523400	-1.73989100	-1.76924700
H	7.52453700	-0.29697300	-0.17124200
H	7.00072200	-3.20474000	-3.29489200
H	8.48716600	-1.69425100	-1.99240900
C	2.39918600	-0.95253800	-0.69262200
H	3.23648900	0.85413200	0.96417200
C	2.81351000	0.45032400	-1.07236800
H	3.76259800	0.42500200	-1.61520900
H	2.05563800	0.88662100	-1.73225200
S	3.54800900	2.84442000	-0.00676100
O	3.44309300	3.42953000	1.33244700
O	2.91171900	3.46020500	-1.17778600
C	5.27969100	2.65334800	-0.39378000
C	6.20790200	2.58098100	0.64537600
C	5.67961500	2.55161800	-1.72736400
C	7.55419800	2.40340100	0.33741900
H	5.87564800	2.68981400	1.67089600
C	7.02816000	2.36308400	-2.01503800
H	4.94466400	2.64354000	-2.51854100
C	7.98258900	2.28328300	-0.99239600
H	8.28510900	2.36163600	1.14002200
H	7.34655400	2.27990500	-3.04995200
C	9.43201500	2.03256800	-1.31879200
H	9.73922900	2.57532400	-2.21722000
H	10.08780600	2.32960000	-0.49645200
H	9.60240400	0.96591600	-1.51119200
N	2.90079100	1.31414100	0.12279200
N	0.51146700	-0.30314300	0.87442600
H	-1.24380900	-0.18739700	-0.62209100
C	-0.14985400	0.96238300	0.68170500

H	-0.51498300	1.32325600	1.64071500
H	0.53194000	1.69509400	0.24184000
S	-1.48523700	1.76443300	-1.60662500
O	-2.89841100	1.42069100	-1.93884400
O	-0.42220800	1.50984900	-2.57877100
C	-1.35238000	3.39560300	-0.95831300
C	-2.43844300	3.96995300	-0.29107900
C	-0.11468100	4.03511100	-1.06121800
C	-2.25865700	5.22064600	0.28935800
H	-3.38752600	3.45363500	-0.22463400
C	0.03848600	5.27838500	-0.45860700
H	0.71860800	3.57240200	-1.57363300
C	-1.02563200	5.88870400	0.22043100
H	-3.09029700	5.68408000	0.81138200
H	1.00648700	5.76604200	-0.51056000
C	-0.85596300	7.24760900	0.84713200
H	-1.11631500	8.03590600	0.13040600
H	-1.50525400	7.36952800	1.71809500
H	0.17840100	7.41516000	1.15820400
N	-1.31837300	0.75811800	-0.22750700
Fe	-3.58294500	0.06117500	-0.13570100
O	-2.62302100	-1.38553400	-0.96493800
S	-2.75906100	-2.70688200	-1.79006500
O	-1.73061100	-3.65101600	-1.36229700
O	-4.14422000	-3.11735000	-1.95011900
C	-2.17071400	-2.02907400	-3.41861200
O	-2.91657200	0.01700100	1.84564600
S	-3.96921200	-0.98123900	2.32569100
O	-4.70702700	-0.65988800	3.53147000
O	-4.75525000	-1.24355600	1.04866900
C	-3.02454100	-2.56286200	2.63815600
O	-4.70396000	1.74921000	0.32183400
S	-5.74988800	1.51979300	-0.77913600
O	-6.01118400	2.63340100	-1.67180000
O	-5.32972500	0.18934300	-1.36740800
C	-7.33551600	1.20018300	0.15547100
F	-3.90825500	-3.53200500	2.86832800
F	-2.29639600	-2.85928700	1.56795600
F	-2.24601000	-2.39372500	3.69828200
F	-2.12491900	-3.00960100	-4.31958900
F	-2.97882000	-1.06316900	-3.84396600
F	-0.93125700	-1.52497400	-3.25881600
F	-7.16166700	0.25487700	1.06735800
F	-7.69979900	2.33763800	0.74736800

F	-8.26498900	0.82600200	-0.72009300
---	-------------	------------	-------------