

SUPPORTING INFORMATION

**Mechanistic Studies on the pH-Controllable Interconversion
between Hydrogen and Formic Acid in Water: DFT Insights**

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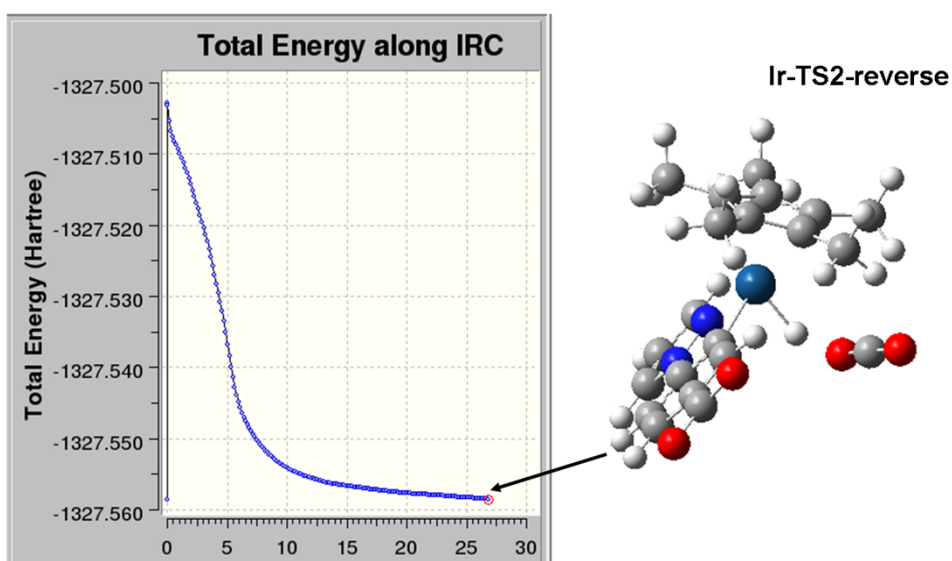


Figure S1. The reverse IRC plot of transtions state **Ir-TS2** at M06/BSI level.

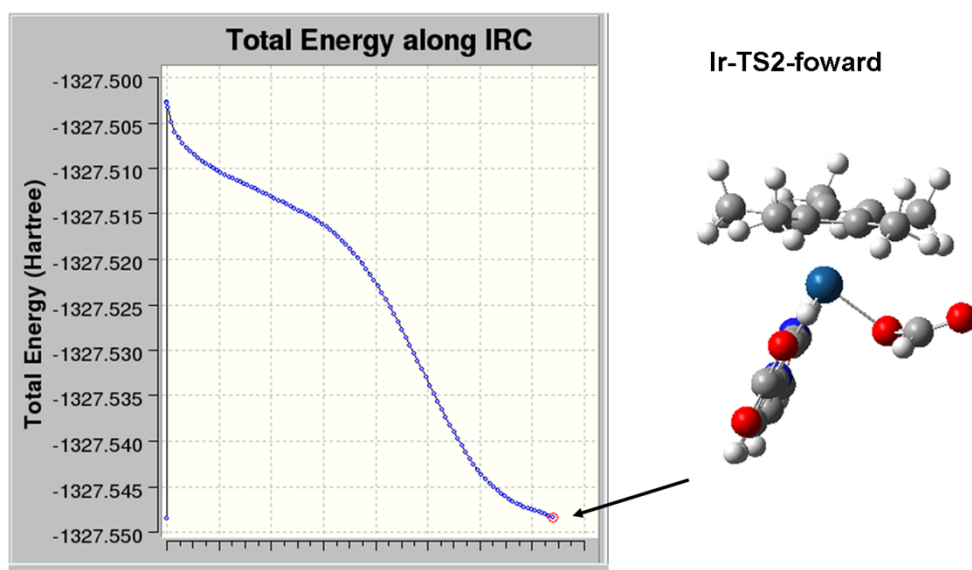


Figure S2. The forward IRC plot of transtions state **Ir-TS2** at M06/BSI level.

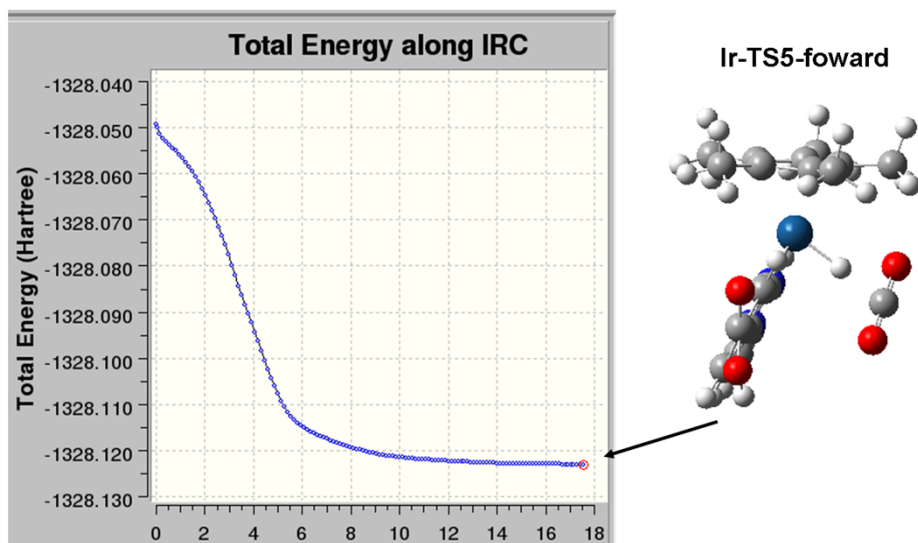


Figure S3. The forward IRC plot of transtions state **Ir-TS5** at M06/BSI level.

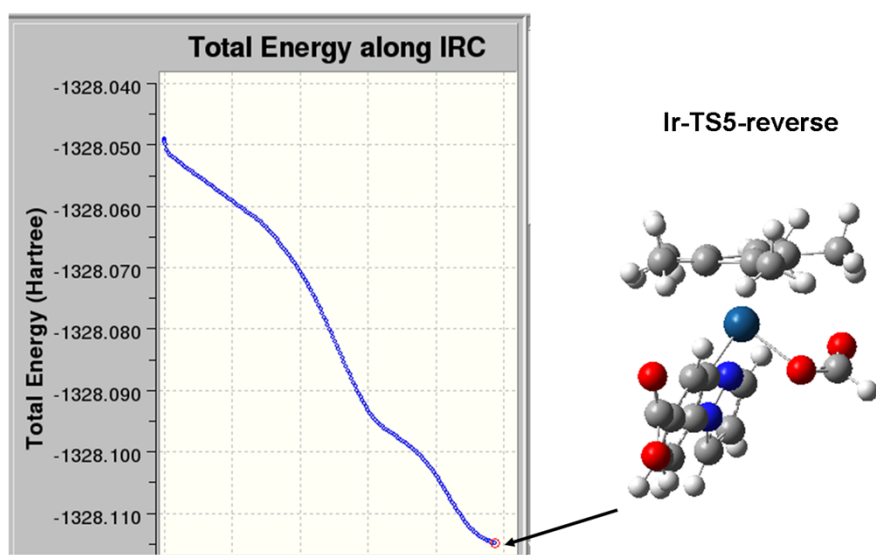


Figure S4. The reverse IRC plot of transtions state **Ir-TS5** at M06/BSI level.

Cartesian coordinates, imaginary vibrational modes, the solvent corrected absolute electronic energies (E) and free energies (G) of each species [in Hartree and at the M06/BSII (SMD, water) level of theory] for the key structures involved in this study.

Ir-2

E= -1215.13962(au) G= -1214.803055 (au)

C	-0.69308800	-1.95735000	-1.02480800
C	-1.12841100	-1.26500200	-2.23729700
C	-2.19972700	-0.41950100	-1.90059600
C	-1.61693500	-1.60700600	0.03624600
C	-2.47063600	-0.58059400	-0.47074100
Ir	-0.40102000	0.09547900	-0.56904400
C	-0.48315500	-1.43298400	-3.56551900
H	-0.83029200	-2.36161900	-4.03690600
H	-0.71729100	-0.60408700	-4.24085500
H	0.60610300	-1.50647500	-3.47152500
C	0.34335700	-3.02318300	-0.96601700
H	0.72953800	-3.14086200	0.05240800
H	-0.06833300	-3.98960200	-1.28614200
H	1.18982500	-2.78754800	-1.62102800
C	-1.67960800	-2.25310900	1.37186800
H	-2.19774000	-1.63051400	2.10773900
H	-2.23531800	-3.19642100	1.28925600
H	-0.68345100	-2.49158700	1.75923600
C	-3.55170600	0.12645200	0.26633500
H	-3.66585200	1.15534100	-0.09370500
H	-4.51631100	-0.37842900	0.12362900
H	-3.34510300	0.16228200	1.34152000
C	-2.94070100	0.51050000	-2.79271000
H	-2.42214700	0.65884600	-3.74512500
H	-3.94135900	0.11557600	-3.01234900
H	-3.07976100	1.49198900	-2.32386700
C	3.63874900	1.21942200	-0.96516000
C	3.40908600	1.30978700	-2.32343400
C	2.05880300	0.98042000	-2.49327900
N	1.50311000	0.70657800	-1.31264400

H	4.53364000	1.39170900	-0.38265600
H	4.12344700	1.57653200	-3.08881600
H	1.46493900	0.93437200	-3.39798400
N	2.47530200	0.85429800	-0.38057800
C	0.73793100	0.29880200	1.14612400
C	2.08139400	0.67096000	0.96839300
C	0.30208700	0.20190200	2.46917100
C	2.96412000	0.88552700	2.02118200
C	1.15191200	0.42007700	3.55959100
H	-0.73815000	-0.04703500	2.67621000
C	2.48826100	0.74866700	3.31872700
H	3.99968600	1.16467300	1.83780900
H	3.15457000	0.91272000	4.16122500
C	0.63223000	0.31168200	4.98232100
O	-0.59506800	0.06678200	5.13324700
O	1.46851200	0.47704600	5.90988600
O	-0.73321000	2.39410000	-0.27416500
H	0.07489500	2.78441400	0.09341300
H	-1.35510200	2.39309600	0.46932800

Ir-3**E= -1139.877487(au) G= -1139.547511(au)**

C	-0.60204500	-1.85831700	-1.05977200
C	-1.03068200	-1.22424100	-2.30589400
C	-2.17580800	-0.44973100	-2.03492000
C	-1.59257300	-1.56001900	-0.05663400
C	-2.50115500	-0.61248000	-0.62134400
C	-0.35383600	-1.39703200	-3.61693400
H	-0.69592000	-2.32745100	-4.08865000
H	-0.57686600	-0.57272300	-4.30174900
H	0.73315300	-1.47226500	-3.50536300
C	0.52970700	-2.81525000	-0.91878900
H	0.88737800	-2.84962000	0.11633400
H	0.22707200	-3.83106900	-1.20405000
H	1.37421100	-2.52881500	-1.55640000
C	-1.67171900	-2.16385900	1.29687600
H	-2.19176900	-1.51589400	2.00888900
H	-2.23515800	-3.10409700	1.23467000
H	-0.68224000	-2.39893900	1.70156700
C	-3.69108200	-0.02470200	0.05198600
H	-3.92017600	0.96881600	-0.34694000
H	-4.57417800	-0.65797600	-0.10291500
H	-3.53153800	0.07367400	1.13081000
C	-2.95716500	0.37876900	-2.99098300
H	-2.37453000	0.62586400	-3.88383800
H	-3.85759900	-0.16004700	-3.31355800
H	-3.28607100	1.31581400	-2.52925700
C	3.70731800	0.72896700	-0.88471100
C	3.54490200	0.80336300	-2.25361300
C	2.16174600	0.75552800	-2.46752400
N	1.52587800	0.66218600	-1.30015700
H	4.59856800	0.73464700	-0.27175400
H	4.32289400	0.88541600	-2.99887400
H	1.59781500	0.78788900	-3.39173700
N	2.47461400	0.64253300	-0.33499400
C	0.61464300	0.41368900	1.12316500
C	2.00414900	0.55481500	0.99532100
C	0.11167500	0.38137400	2.42246200
C	2.86589700	0.63218500	2.08430300
C	0.94285500	0.45819600	3.54497700
H	-0.96241100	0.29899900	2.58330700
C	2.32273000	0.57760400	3.36021600
H	3.93877800	0.74050600	1.94031900
H	2.96819800	0.63795200	4.23236300

C	0.35685600	0.42427800	4.94574500
O	-0.89140300	0.28242000	5.04705900
O	1.16627200	0.54068100	5.90344700
H	-0.84607500	1.89899400	-0.09303800
H	-0.64248600	2.01540700	-0.91728900
Ir	-0.45668600	0.26888300	-0.65273200

Ir-TS1

E= -1215.811854(au) -167.45 *i* cm⁻¹

G=-1215.47406(au)

C	-0.70160800	-1.90653200	-1.26992800
C	-1.38759900	-1.09418600	-2.26741900
C	-2.43686100	-0.40621400	-1.60636400
C	-1.37996100	-1.75454200	-0.02054800
C	-2.40668300	-0.75839500	-0.19745500
Ir	-0.46117100	0.21092100	-0.62519000
C	-1.05671600	-1.05825900	-3.71841400
H	-1.51334000	-1.90656000	-4.24479300
H	-1.42080900	-0.13943700	-4.18949200
H	0.02486700	-1.11487300	-3.88546600
C	0.45208400	-2.80502400	-1.54172500
H	1.05186500	-2.96035900	-0.63824800
H	0.10880000	-3.78628100	-1.89327700
H	1.10896800	-2.38653100	-2.31290300
C	-1.08728600	-2.49896800	1.23169100
H	-1.34167500	-1.91659700	2.12322600
H	-1.68121800	-3.42159800	1.25788000
H	-0.03159400	-2.78194400	1.29864100
C	-3.42050900	-0.33713800	0.80915500
H	-3.65331400	0.72946000	0.71664500
H	-4.35653800	-0.89493800	0.67447800
H	-3.07061400	-0.51567900	1.83104400
C	-3.40062100	0.55547600	-2.20392300
H	-3.04367500	0.94704600	-3.16157100
H	-4.36753800	0.06547300	-2.37695600
H	-3.57978100	1.40173500	-1.53161900
C	3.70640600	0.67305000	-0.70970300
C	3.60701500	0.62121600	-2.08510900
C	2.23722600	0.50490800	-2.35571500
N	1.55066900	0.48727900	-1.21455900
H	4.56573800	0.76500400	-0.05911300
H	4.41719900	0.66363500	-2.79877000
H	1.71603200	0.43592500	-3.30346900
N	2.45226100	0.58799900	-0.20899400

C	0.52838700	0.49246600	1.17611700
C	1.92381900	0.60674200	1.10325600
C	-0.03626100	0.54932800	2.44858100
C	2.73512300	0.74721200	2.22440700
C	0.74379800	0.68275200	3.60198000
H	-1.11866900	0.49530200	2.56190200
C	2.13193200	0.78025800	3.47467000
H	3.81537400	0.83050900	2.12556200
H	2.73792900	0.88524300	4.37059000
C	0.09491200	0.72141800	4.97400900
O	-1.15501200	0.56629400	5.02572900
O	0.85586000	0.90335700	5.96107000
H	-0.81790300	1.86187100	-0.22042200
H	-0.52354400	1.88530100	-1.04748700
O	0.09474000	3.63596900	0.01479400
H	0.26651500	4.55068400	0.26415300

Ir-4

E=-1139.431888(au) G=-1139.113713(au)

C	-0.78715400	-2.16386200	-1.41643200
C	-1.26802000	-1.23650200	-2.42957800
C	-2.22651900	-0.38312000	-1.82789800
C	-1.45913200	-1.87694500	-0.20013100
C	-2.30805100	-0.72032600	-0.41720800
Ir	-0.26441500	-0.02128100	-0.75718400
C	-0.87087900	-1.27126300	-3.86559800
H	-1.46644400	-2.00733000	-4.42292900
H	-1.00965100	-0.29810200	-4.34956200
H	0.18156600	-1.55542500	-3.98396100
C	0.20581000	-3.24610700	-1.66794900
H	0.62161600	-3.63322600	-0.73148400
H	-0.24703100	-4.08974700	-2.20634900
H	1.04235100	-2.88573600	-2.28074200
C	-1.33542900	-2.61633400	1.08553500
H	-1.33905400	-1.93492400	1.94483800
H	-2.17671200	-3.30945300	1.21825700
H	-0.41078500	-3.20297700	1.12635100
C	-3.31703400	-0.19573900	0.54789600
H	-3.53603500	0.86226300	0.36391800
H	-4.26433700	-0.74831300	0.47460400
H	-2.96491200	-0.28816800	1.58205400
C	-3.04985800	0.65873300	-2.50366700
H	-2.55764500	1.04997000	-3.40033300
H	-4.01927300	0.24393900	-2.81183000

H	-3.25310600	1.50221400	-1.83508200
C	3.84842400	0.81546000	-0.88373200
C	3.77795300	0.58696400	-2.24185300
C	2.43872400	0.25647300	-2.49470700
N	1.73943600	0.28123200	-1.35986900
H	4.67900000	1.09802900	-0.25106200
H	4.58607100	0.65339800	-2.95641000
H	1.94658600	0.01179600	-3.42906700
N	2.60557400	0.62248900	-0.37587200
C	0.69243400	0.39635300	1.01583800
C	2.07018600	0.67852100	0.93337100
C	0.15151500	0.44968000	2.30651800
C	2.86647200	0.98447400	2.03194100
C	0.91432700	0.74901000	3.44025200
H	-0.91317600	0.26168400	2.44817100
C	2.27811200	1.01779900	3.28907900
H	3.92820800	1.19280600	1.91288400
H	2.87536000	1.25578000	4.16532500
C	0.27416000	0.79447800	4.81581300
O	1.02033700	1.09185500	5.78732600
O	-0.95737800	0.53374300	4.89291700
H	-0.33061100	1.60629200	-0.78163400

Ir-5

E= -1327.996621(au) G=-1327.669147

C	-0.86474400	-2.10389300	-1.36874100
C	-1.41369400	-1.04599100	-2.20461200
C	-2.34231800	-0.30918200	-1.42807700
C	-1.45987400	-2.00694300	-0.08425500
C	-2.33138200	-0.84598300	-0.07999800
Ir	-0.31800500	-0.06881400	-0.43279500
C	-1.09900000	-0.86628800	-3.65062100
H	-1.69347700	-1.55045200	-4.27183000
H	-1.30760000	0.15336800	-3.99324900
H	-0.04341800	-1.08020600	-3.85943100
C	0.10787900	-3.12730100	-1.84458500
H	0.57001300	-3.66459600	-1.00966200
H	-0.37995500	-3.87035600	-2.49013200
H	0.91390700	-2.67203400	-2.43486400
C	-1.25594900	-2.91973100	1.07346700
H	-1.27656600	-2.37154100	2.02290600
H	-2.05270600	-3.67403100	1.11771400
H	-0.29804700	-3.44778600	1.01238300
C	-3.28804600	-0.47777100	1.00302400

H	-3.51704200	0.59401800	0.98488400
H	-4.23808000	-1.02086500	0.89942900
H	-2.88229400	-0.71369400	1.99370300
C	-3.24295900	0.78161300	-1.89681700
H	-2.87225200	1.26050400	-2.80995400
H	-4.23897800	0.37651100	-2.12249800
H	-3.37496400	1.55616400	-1.13295500
C	3.79323000	0.73488400	-0.70193800
C	3.63138300	0.71417800	-2.07130800
C	2.26915200	0.45261200	-2.28148400
N	1.64316000	0.32226200	-1.11151400
H	4.66849600	0.90395900	-0.08969300
H	4.39557500	0.86833400	-2.81987600
H	1.71236200	0.36691300	-3.20736800
N	2.57953600	0.49319000	-0.14799200
C	0.75373100	0.09379600	1.31968700
C	2.13030900	0.36148700	1.18701600
C	0.29858500	-0.03995000	2.63802500
C	3.00546400	0.47925600	2.26164900
C	1.14280600	0.06812400	3.74892600
H	-0.75843400	-0.23525900	2.82339700
C	2.50137000	0.32928400	3.54624700
H	4.06316800	0.68149900	2.10277700
H	3.16236900	0.41436000	4.40441800
C	0.59840300	-0.08925500	5.15694900
O	1.42461800	0.00566400	6.10422700
O	-0.63813700	-0.30241300	5.28339900
H	-0.40940700	1.53913200	-0.23786500
C	-0.72127700	3.11020500	-2.33680600
O	0.01785800	2.58019800	-3.06567400
O	-1.46315200	3.67100000	-1.63455400

Ir-TS2

E=-1327.996833 (au) -103.74 *i* cm⁻¹

G=-1327.665249(au)

C	-0.84114100	-1.98778300	-1.21105100
C	-1.16365500	-1.09887300	-2.32445700
C	-2.04040600	-0.11163300	-1.84321400
C	-1.64544300	-1.58759200	-0.06458600
C	-2.31338100	-0.38184200	-0.42533400
Ir	-0.13663100	-0.10821100	-0.54497700
C	-0.58267200	-1.21656900	-3.68814000
H	-1.11703300	-1.97835800	-4.27012300
H	-0.64171200	-0.27030600	-4.23585000

H	0.46931600	-1.52223700	-3.64417600
C	-0.03271900	-3.22849700	-1.31630700
H	0.33474700	-3.54872900	-0.33596900
H	-0.64124600	-4.04253400	-1.73276900
H	0.82823800	-3.08367500	-1.97789800
C	-1.77186000	-2.35752200	1.19961300
H	-2.16768500	-1.74519800	2.01558600
H	-2.46286800	-3.19690600	1.04836300
H	-0.81009300	-2.77441000	1.51713300
C	-3.23571900	0.42246000	0.41840300
H	-3.09168200	1.49592100	0.24839600
H	-4.28076200	0.18491500	0.17859900
H	-3.07989400	0.22340000	1.48385000
C	-2.60146200	1.03906200	-2.59503600
H	-2.01055300	1.27174000	-3.48693800
H	-3.62429100	0.80751000	-2.92132000
H	-2.65543500	1.93791500	-1.97141900
C	3.92863000	0.88499700	-0.81126600
C	3.74561700	0.94503900	-2.17961300
C	2.41087800	0.58315000	-2.38959800
N	1.82275700	0.31414800	-1.22302800
H	4.79887400	1.08672400	-0.20129100
H	4.48238100	1.21164100	-2.92332800
H	1.84339200	0.50695600	-3.30956100
N	2.75580500	0.50378100	-0.26036500
C	0.95753400	0.00399100	1.21507500
C	2.31534700	0.33968700	1.07688100
C	0.48798600	-0.11473400	2.52567400
C	3.17457300	0.52311400	2.15345000
C	1.31333200	0.07159800	3.63974600
H	-0.56085000	-0.35030500	2.70316900
C	2.66051200	0.38182400	3.43603400
H	4.22178300	0.77588000	2.00122800
H	3.30793800	0.52087400	4.29757100
C	0.75974700	-0.05630600	5.04795300
O	1.57590800	0.08802400	5.99640500
O	-0.47200300	-0.29553700	5.16618300
H	-0.59404200	2.25504700	0.49792400
C	-0.78886900	3.03015500	-0.30272200
O	0.13127800	3.17231100	-1.15088500
O	-1.88993400	3.62146000	-0.26021700

Ir-6

E= -1328.005971(au) G=-1327.673406(au)

C	-0.72223700	-2.10237900	-1.36781100
C	-1.27366000	-1.22750200	-2.39834500
C	-2.23442600	-0.40118100	-1.78221200
C	-1.44100500	-1.86248100	-0.14342000
C	-2.32790000	-0.74973400	-0.36951700
Ir	-0.26469000	-0.11197600	-0.65832800
C	-0.86333200	-1.22917700	-3.82874000
H	-1.40194700	-2.00675300	-4.38644600
H	-1.07042100	-0.26866700	-4.31247200
H	0.20672300	-1.43777400	-3.93958700
C	0.27826800	-3.17894700	-1.60563600
H	0.80852300	-3.43978700	-0.68350500
H	-0.20896000	-4.08801600	-1.98222300
H	1.02484700	-2.87417100	-2.34805000
C	-1.33924100	-2.66480000	1.10334600
H	-1.57859600	-2.07085300	1.99130200
H	-2.05177200	-3.49898300	1.06287900
H	-0.33793600	-3.08839000	1.23558600
C	-3.34350900	-0.22055200	0.58261700
H	-3.59695500	0.82176200	0.35828200
H	-4.27242900	-0.80441200	0.52847600
H	-2.98642200	-0.26451800	1.61785400
C	-3.01110300	0.69442200	-2.41833500
H	-2.59314400	0.97927800	-3.38887700
H	-4.05157300	0.38240300	-2.57675700
H	-3.03708600	1.58652100	-1.78126200
C	3.87890500	0.59283600	-0.76304800
C	3.79787200	0.46243900	-2.13409700
C	2.44967100	0.18648300	-2.40070900
N	1.75712500	0.15046700	-1.26319400
H	4.71969300	0.80811300	-0.11743200
H	4.60496100	0.55416400	-2.84677400
H	1.95049700	0.01630100	-3.34788000
N	2.63534300	0.40067600	-0.26341800
C	0.72807800	0.14296100	1.13431400
C	2.10502800	0.40892300	1.05065800
C	0.18229100	0.16586100	2.41955200
C	2.90694200	0.66774300	2.15737400
C	0.95027200	0.42210000	3.56118200
H	-0.88484500	-0.01093600	2.55665900
C	2.31758600	0.66989900	3.41467300
H	3.97057400	0.86823500	2.04486900
H	2.91904500	0.87182400	4.29706200
C	0.30972800	0.44088900	4.93748500

O	1.06056800	0.69920300	5.91567100
O	-0.92599800	0.19948300	5.00478500
H	-1.61678000	2.11254900	0.75434900
C	-1.00435100	2.73962600	0.06678400
O	-0.20534800	2.09010200	-0.70328700
O	-1.12456700	3.96703900	0.08109200

Ir-2'

E= -1214.668042(au) G=-1214.344145(au)

C	-1.16937100	-2.12886700	-0.46534200
C	-0.97708100	-1.59860100	-1.78537700
C	-1.97450100	-0.55392400	-2.00417600
C	-2.18879500	-1.33321400	0.18244300
C	-2.70788800	-0.40262000	-0.81023700
Ir	-0.48193500	-0.07427100	-0.30198000
C	-0.04933800	-2.12945700	-2.82342400
H	-0.54004700	-2.89718300	-3.43650300
H	0.29041800	-1.33785800	-3.50165800
H	0.83880100	-2.58187500	-2.36858000
C	-0.49396600	-3.32279800	0.11025800
H	-0.38845800	-3.24616300	1.19773900
H	-1.08057000	-4.22600500	-0.10250300
H	0.50533700	-3.46786200	-0.31465900
C	-2.78908900	-1.56787500	1.52579600
H	-2.99563900	-0.62146700	2.04051500
H	-3.73896000	-2.11461900	1.44922600
H	-2.12077800	-2.15612500	2.16405300
C	-3.79129300	0.57718400	-0.53643000
H	-3.67820000	1.02423500	0.45821300
H	-3.80982600	1.38520600	-1.27471500
H	-4.77016100	0.08031200	-0.55633100
C	-2.15534900	0.19327400	-3.27929300
H	-1.19521000	0.38323000	-3.77281700
H	-2.77120300	-0.38088800	-3.98441700
H	-2.64644200	1.15889400	-3.11869400
C	3.26620800	1.59140600	-1.24224600
C	2.68878500	2.06469700	-2.40211400
C	1.35466100	1.63470800	-2.35314500
N	1.13736300	0.94135600	-1.23705200
H	4.27297900	1.68188500	-0.85721100
H	3.16783000	2.64137600	-3.18044500
H	0.54832900	1.79045800	-3.06059400
N	2.30859900	0.91952000	-0.55973600
C	1.07720300	-0.37298800	1.00883200

C	2.30541800	0.22302600	0.67326800
C	1.03774500	-1.02978800	2.24182400
C	3.44078500	0.15047100	1.47403100
C	2.15568700	-1.13060900	3.07799700
H	0.10563900	-1.48525700	2.57850400
C	3.35659500	-0.53924900	2.67633700
H	4.37236300	0.62492700	1.17114300
H	4.22611400	-0.61651000	3.32328600
C	2.07177500	-1.87037800	4.40103700
O	3.14304300	-2.00509800	5.05076500
O	0.93971200	-2.29741800	4.75477000
O	-0.73115100	1.75162100	0.77977400
H	-0.03300000	1.76304000	1.44530000

OH-TS1

E= -1215.803358(au) -1175.79 *i* cm⁻¹

G=-1215.464375(au)

C	-0.55448000	-2.26813300	-0.88194200
C	-1.78635200	-2.04630700	-1.63351400
C	-2.64860100	-1.28053800	-0.82396600
C	-0.72720500	-1.71263400	0.43639200
C	-1.99247600	-1.03323800	0.45630900
Ir	-0.69651700	-0.11440600	-1.04023200
C	-2.02750800	-2.54596800	-3.01437400
H	-2.26864200	-3.61712700	-3.00205500
H	-2.85802400	-2.02199200	-3.49773500
H	-1.13840800	-2.42089700	-3.64273400
C	0.58348400	-3.10809400	-1.34561800
H	1.50727200	-2.86537300	-0.80863700
H	0.36658500	-4.17318300	-1.18544700
H	0.76909100	-2.96600800	-2.41660500
C	0.21727900	-1.84938200	1.57764900
H	0.15018200	-0.99811900	2.26427100
H	-0.01706700	-2.75663700	2.14930300
H	1.25591100	-1.92551700	1.23754400
C	-2.63434900	-0.35563500	1.61585800
H	-3.17779900	0.54342900	1.29959300
H	-3.35944600	-1.02131200	2.10332700
H	-1.89862600	-0.05550300	2.36908100
C	-3.98884200	-0.74540800	-1.17721500
H	-4.16976500	-0.77425300	-2.25611100
H	-4.77799200	-1.32848000	-0.68446800
H	-4.10024800	0.29185600	-0.83898400
C	2.85035100	-0.03010700	-2.06562200

C	3.64503100	-1.07613600	-2.48494700
C	3.98430000	-1.74864800	-1.29846100
N	3.44863400	-1.16994000	-0.22427500
H	2.37885600	0.77987900	-2.60668900
H	3.94644600	-1.30666300	-3.49757500
H	4.59987600	-2.63301800	-1.17928100
N	2.74932100	-0.11934300	-0.71616100
C	0.67662600	0.98030900	0.07167300
C	2.06213700	0.76948700	0.17238400
C	0.14118200	1.88807700	1.00228200
C	2.83856400	1.36830900	1.16799000
C	0.88782100	2.49445100	2.01371300
H	-0.92784200	2.10140700	0.98216400
C	2.25428400	2.21784500	2.09380700
H	3.90509100	1.15328000	1.20292000
H	2.84961500	2.67831700	2.87827600
C	0.21961300	3.41100800	3.02350400
O	0.96236800	3.95435900	3.88370400
O	-1.02910400	3.55912000	2.93067300
O	-1.36665300	1.89132100	-1.90274400
H	-0.86133000	2.53644800	-1.38859800
H	0.16404800	0.31483500	-2.57537000
H	-0.40740700	1.04709500	-2.46040300

H₂O-TS1

E= -1216.288362 (au) -1449.72 i cm⁻¹

G=-1215.938195 (au)

C	-0.60850800	-2.04293400	-1.33812300
C	-1.22522100	-1.10983400	-2.27856200
C	-2.23085000	-0.40230400	-1.58949500
C	-1.31437800	-1.94774700	-0.09245200
C	-2.26764700	-0.87504200	-0.20970800
Ir	-0.25859000	-0.04395100	-0.48617900
C	-0.85244500	-0.97032100	-3.71307600
H	-1.47413400	-1.62451100	-4.33853000
H	-0.98868000	0.05632400	-4.07006000
H	0.19119100	-1.25352700	-3.88727100
C	0.45414700	-3.02261800	-1.69424100
H	0.91720400	-3.45333200	-0.80042900
H	0.04181100	-3.84705200	-2.29040200
H	1.24704600	-2.55299700	-2.28887500
C	-1.11075300	-2.79137900	1.11424100
H	-1.27887700	-2.22304800	2.03596300
H	-1.81770900	-3.63101100	1.11126100

H	-0.09818100	-3.20581900	1.15259400
C	-3.28950300	-0.50009100	0.80609900
H	-3.62011900	0.53604800	0.68067600
H	-4.17608700	-1.14246900	0.71778600
H	-2.90247500	-0.61079100	1.82543300
C	-3.12133000	0.65660100	-2.13673100
H	-2.72027900	1.08712900	-3.05987000
H	-4.11240000	0.24157500	-2.36266400
H	-3.26579600	1.46875100	-1.41527300
C	3.91531600	0.51437600	-0.73549200
C	3.76371500	0.47959000	-2.10687900
C	2.38433700	0.35716500	-2.32458400
N	1.73680100	0.32232400	-1.15975500
H	4.79574100	0.59766900	-0.11217700
H	4.54510000	0.53360600	-2.85134100
H	1.83120400	0.30183800	-3.25455500
N	2.68153000	0.41465600	-0.19082600
C	0.83496500	0.11961500	1.24685500
C	2.19776300	0.42779000	1.13888300
C	0.26123600	0.29136200	2.49816300
C	2.97355900	0.84209900	2.21828700
C	0.96222400	0.86802500	3.55559700
H	-0.80684800	0.11263000	2.62609400
C	2.33851700	1.07508500	3.43585000
H	4.03229300	1.06072100	2.09116800
H	2.89434400	1.49855800	4.26981600
C	0.15975600	1.49403300	4.66400000
O	0.63681200	1.55653300	5.81838300
O	-0.95829700	1.97728600	4.28796800
H	-0.40869800	1.68602600	-0.30205900
H	-1.18227600	2.22450200	2.51111600
O	-1.44441200	2.44462400	1.56861600
H	-1.26548800	3.38956300	1.44943700
H	-0.84891500	1.82658500	0.58617300

N-TS1

E=-1139.828338 (au) -975.45 *i* cm⁻¹

G=-1139.504906

C	0.80584700	-2.61914100	-0.63372700
C	0.57702100	-2.35788600	-2.05206300
C	-0.78708600	-2.05076300	-2.22922300
C	-0.42573400	-2.49778900	0.05477100
C	-1.41725800	-2.04715800	-0.91234600
Ir	0.05194200	-0.49740000	-0.81532700

C	1.64174000	-2.41805500	-3.08848300
H	1.90159700	-3.45968200	-3.31818800
H	1.32787700	-1.93564900	-4.01925100
H	2.55601700	-1.92264100	-2.74010200
C	2.12385800	-2.99772300	-0.06063600
H	2.14045500	-2.87809300	1.02681200
H	2.35453400	-4.04640000	-0.29004900
H	2.93093000	-2.38758900	-0.48387800
C	-0.69661500	-2.78796400	1.48578700
H	-1.42875700	-2.09050400	1.90833000
H	-1.11001600	-3.79922700	1.59169000
H	0.21386100	-2.73062400	2.09096700
C	-2.87495000	-1.90484500	-0.66005300
H	-3.32585300	-1.17345000	-1.33911700
H	-3.38387100	-2.86578000	-0.81592500
H	-3.07631800	-1.58777600	0.36895700
C	-1.49128200	-1.74838900	-3.50393900
H	-0.79965000	-1.40119400	-4.27788600
H	-1.99565100	-2.64730100	-3.88128400
H	-2.25725100	-0.97818200	-3.36360700
C	3.14005900	2.28963900	0.43681200
C	3.83690900	2.05488000	-0.74299600
C	2.96939800	1.34318300	-1.55511500
N	1.81014000	1.15140600	-0.89682800
H	3.44734400	2.79428900	1.34348200
H	4.84818400	2.36058100	-0.96813900
H	3.08779100	0.96237700	-2.56156900
N	1.91787100	1.74656400	0.31980700
C	-0.17761100	0.68801500	0.87632000
C	0.82132400	1.61550500	1.22438500
C	-1.25277400	0.61592700	1.76906000
C	0.78730200	2.39357800	2.37919700
C	-1.32325000	1.36605300	2.94438000
H	-2.08513700	-0.05198700	1.55349300
C	-0.28706300	2.25385000	3.24400700
H	1.58137200	3.10386400	2.59936700
H	-0.33477900	2.84406900	4.15474600
C	-2.51021900	1.21855300	3.88237800
O	-3.40166700	0.39017400	3.55580800
O	-2.51231800	1.93469300	4.91809800
H	-0.51118800	0.88038200	-1.62390900
H	0.65344100	1.12954700	-1.42475300

Ir-TS3

E=-1403.879025 (au) -249.12 *i* cm⁻¹

G=-1403.533415(au)

C	-0.54035500	-1.63860000	-1.42142600
C	-1.42887000	-0.96660400	-2.37799900
C	-2.45596300	-0.35328300	-1.64375200
C	-1.14203800	-1.54191100	-0.09689700
C	-2.24482100	-0.64946300	-0.21594100
Ir	-0.42297400	0.37806100	-0.83723200
C	-1.18896000	-0.76610700	-3.83613900
H	-1.97515900	-1.24358500	-4.44007900
H	-1.17491700	0.32176300	-4.03465100
H	-0.22406700	-1.18740400	-4.13994700
C	0.64416500	-2.47045000	-1.77236200
H	1.35445000	-2.51723400	-0.93866500
H	0.34646000	-3.49795800	-2.03382800
H	1.18547300	-2.03923800	-2.62219300
C	-0.64407600	-2.19908300	1.14515900
H	-0.90830800	-1.62127600	2.03824900
H	-1.06070000	-3.21191500	1.24684800
H	0.45000200	-2.27657100	1.14000900
C	-3.11930100	-0.16525100	0.89220700
H	-3.44529900	0.86358500	0.69480000
H	-4.02104100	-0.78840300	0.98808800
H	-2.60270400	-0.14881800	1.86069400
C	-3.47157300	0.57120100	-2.21599200
H	-2.93389700	1.42499800	-2.68679600
H	-4.06108400	0.06978400	-2.99734100
H	-4.16587600	0.93354000	-1.44951600
C	2.95200400	0.25105800	-1.43521100
C	3.84471500	-0.49450300	-2.18416200
C	4.28939800	-1.49714500	-1.30645100
N	3.72307100	-1.39662800	-0.10559900
H	2.32294000	1.10755900	-1.68428700
H	4.12222200	-0.32434800	-3.21632400
H	4.99903600	-2.29864800	-1.49156400
N	2.90994100	-0.31827000	-0.20482000
C	0.83309200	0.59861100	0.78034600
C	2.14208400	0.11240800	0.93010000
C	0.16940800	0.92151800	1.97808000
C	2.73218600	-0.04701400	2.18970100
C	0.69498200	0.69249100	3.24737200
H	-0.86152200	1.27641800	1.95439600
C	2.00802500	0.22759400	3.34029400
H	3.74891300	-0.43458700	2.23609200

H	2.42045500	0.07091200	4.33586600
C	-0.20213300	0.80215500	4.49647800
O	0.39572100	0.81593100	5.59545900
O	-1.43624600	0.82218200	4.26312300
C	-0.57093900	2.59721600	-2.27170200
H	-1.20328100	2.55299300	-1.27592900
O	0.53362700	1.76430500	-2.01940500
O	-0.07137100	3.95221400	-2.28617600
H	-0.44647100	4.23364100	-3.12879600
O	-1.30019700	2.33513800	-3.31844900

Ir-TS4

E= -1403.8924291 (au) -152.40 i cm-1

G=-1403.547382(au)

C	-0.47309000	-1.75339800	-1.41129700
C	-1.57331500	-1.12912900	-2.14142100
C	-2.48871700	-0.67929700	-1.18134900
C	-0.83798900	-1.87953000	-0.01591900
C	-2.03554800	-1.11210800	0.15225500
Ir	-0.47033000	0.19011600	-0.53110500
C	-1.58700200	-0.90420200	-3.60722800
H	-2.50055500	-0.38614500	-3.91679100
H	-0.69648800	-0.26310200	-3.85015400
H	-1.52263200	-1.86480000	-4.14228000
C	0.74678900	-2.28916400	-2.07835600
H	1.59755000	-2.33752700	-1.38673600
H	0.56213100	-3.29882200	-2.47762600
H	1.01655800	-1.61843600	-2.90607600
C	-0.08863600	-2.60657800	1.04849400
H	-0.16623100	-2.08926000	2.01209200
H	-0.47492200	-3.62874800	1.17298000
H	0.97868500	-2.67066200	0.80803200
C	-2.80526000	-0.94265400	1.41767500
H	-3.36125200	0.00207200	1.41575700
H	-3.53358000	-1.75848800	1.53948600
H	-2.16637600	-0.91186800	2.30810000
C	-3.68524000	0.16268700	-1.46461800
H	-3.36980800	1.03596600	-2.04977100
H	-4.43820900	-0.40223900	-2.03296700
H	-4.15422400	0.51349800	-0.53894800
C	2.93155500	0.53139200	-0.92389100
C	3.84854800	-0.13530300	-1.71237900
C	4.25310900	-1.22443000	-0.92396200
N	3.63922600	-1.24400500	0.25969600

H	2.31776900	1.40882000	-1.10219100
H	4.13531800	0.12490500	-2.72217300
H	4.96533500	-2.00829900	-1.16361400
N	2.83350400	-0.15894100	0.23859000
C	0.65014200	0.50127200	1.17797900
C	1.99834100	0.15625700	1.36086100
C	-0.07020200	0.76860200	2.35580000
C	2.57131700	0.04449300	2.63154300
C	0.45460500	0.61100500	3.63800800
H	-1.12472900	1.03815200	2.30974000
C	1.79937900	0.25702300	3.76343900
H	3.62042400	-0.24163000	2.70068500
H	2.20099400	0.14929800	4.76962900
C	-0.45460800	0.72440600	4.88145600
O	0.14019500	0.74292800	5.98241100
O	-1.68492900	0.75303100	4.64060900
C	-0.37029000	2.30552500	-2.45344700
H	0.30442600	3.01921200	-2.95647600
O	0.13007900	1.95279200	-1.24890500
O	0.78190500	0.81354200	-3.60037600
H	1.25442300	0.50709500	-2.82094100
O	-1.55078400	2.18911000	-2.76491500

Ir-1

E= -1215.589672 (au) G=-1215.240457 (au)

C	0.69700500	-2.46751600	-0.52530000
C	0.52723600	-2.19017800	-1.95072600
C	-0.81695900	-1.83666800	-2.16373000
C	-0.60816200	-2.39485900	0.10098900
C	-1.52883000	-1.91988000	-0.88565900
Ir	0.03989200	-0.43536300	-0.57501900
C	1.62393300	-2.24832600	-2.95199800
H	1.79830100	-3.28635000	-3.26352700
H	1.38957900	-1.66368800	-3.84727900
H	2.56596700	-1.87412500	-2.53511000
C	1.95282600	-2.95295900	0.10616000
H	1.94619900	-2.77676900	1.18684000
H	2.08291500	-4.03008400	-0.06203500
H	2.82657000	-2.44183200	-0.31391200
C	-0.91829200	-2.78927000	1.49929700
H	-1.81385000	-2.28664900	1.87764000
H	-1.10381400	-3.87028900	1.53993300
H	-0.08705900	-2.57092900	2.17797600
C	-2.98951100	-1.69535000	-0.71634300

H	-3.33242200	-0.85054000	-1.32468100
H	-3.55935900	-2.57989300	-1.03031900
H	-3.24355400	-1.48501500	0.32761800
C	-1.44929800	-1.39435100	-3.43247300
H	-0.70406600	-1.13894200	-4.19163100
H	-2.08787600	-2.18988700	-3.83793000
H	-2.08949900	-0.51997400	-3.26690100
C	3.18856900	2.24372700	0.20008300
C	3.67290300	1.91361900	-1.04720700
C	2.75971200	0.98584900	-1.56729200
N	1.78278400	0.76518600	-0.69068000
H	3.56914500	2.92170000	0.95184500
H	4.56877900	2.29082700	-1.51883700
H	2.76220700	0.46884500	-2.51951300
N	2.04930600	1.53600500	0.39307700
C	0.03929100	0.58659400	1.22816000
C	1.10218800	1.48534400	1.43900600
C	-0.94413200	0.56681100	2.21417400
C	1.22729000	2.28213800	2.57117800
C	-0.87096000	1.38233800	3.35189700
H	-1.81081100	-0.08342200	2.10086300
C	0.22959800	2.22611000	3.53343300
H	2.07977000	2.94292300	2.70571700
H	0.33845100	2.83088500	4.43088300
C	-1.97308000	1.28983700	4.33575500
O	-2.74039800	0.34611600	4.39928900
O	-2.13300500	2.30426900	5.20393600
H	-1.56618800	3.06046300	4.98878600
O	-1.00281100	1.53059800	-1.30579400
H	-0.36902200	1.97406900	-1.88935300
H	-1.08899400	2.12004000	-0.54098300

Ir-7

E= -1328.454128 (au) G=-1328.110381(au)

C	0.72237600	-2.32714000	-0.51526400
C	0.51501300	-2.16070300	-1.95367700
C	-0.85217200	-1.90318900	-2.16458500
C	-0.56789300	-2.26901000	0.12649100
C	-1.53514100	-1.91188300	-0.87325600
Ir	-0.03590700	-0.31901000	-0.69924700
C	1.59690000	-2.23400400	-2.97215300
H	1.80980900	-3.27874200	-3.23376500
H	1.32693600	-1.70566000	-3.89237800
H	2.52906000	-1.79917900	-2.59304800

C	2.01180900	-2.69787500	0.12988300
H	2.01474100	-2.42906300	1.19201400
H	2.19250600	-3.77839000	0.05631800
H	2.85603500	-2.18752700	-0.34835900
C	-0.84248400	-2.58713800	1.55157900
H	-1.74268400	-2.08548600	1.92073300
H	-1.00210800	-3.66817900	1.65601700
H	-0.00485200	-2.31271700	2.20094700
C	-3.00557400	-1.76570000	-0.69454400
H	-3.39887600	-0.95976600	-1.32549200
H	-3.53219200	-2.68812200	-0.97394900
H	-3.26017300	-1.53536200	0.34502000
C	-1.53135400	-1.59757500	-3.45046900
H	-0.81795300	-1.36198500	-4.24606700
H	-2.13156000	-2.45634100	-3.77844400
H	-2.21864300	-0.75011900	-3.34142600
C	3.29204000	2.05027400	0.28202500
C	3.77651900	1.76477300	-0.97609500
C	2.78133600	0.99042900	-1.59154200
N	1.75617300	0.81866200	-0.76119300
H	3.72014500	2.61911200	1.09604800
H	4.72251500	2.07590000	-1.39545100
H	2.75476500	0.55455600	-2.58344000
N	2.07325100	1.46601700	0.38833500
C	-0.05347100	0.68501600	1.09562000
C	1.09870400	1.43178400	1.40998000
C	-1.05646900	0.68619500	2.06197600
C	1.27777000	2.11002700	2.60995700
C	-0.91728500	1.36931600	3.27744400
H	-1.98763700	0.15281100	1.87525600
C	0.25977700	2.07295900	3.55258100
H	2.19360100	2.65794800	2.81767600
H	0.41274200	2.57396300	4.50617500
C	-2.02995000	1.26864000	4.24769900
O	-2.86079400	0.37743400	4.22694000
O	-2.12829100	2.21083600	5.20152900
H	-1.49584400	2.93231300	5.06599700
C	-1.04763700	2.59737700	-1.27172000
H	-0.57859500	2.77214700	-0.27845300
O	-1.57271900	3.53909600	-1.87231100
O	-1.00129300	1.38960700	-1.70677800

Ir-TS5

E= -1328.42525 (au) -167.02 i cm⁻¹

G=-1328.079566(au)

C	-0.71860400	-2.13834900	-1.19108100
C	-1.23358800	-1.24925700	-2.21185600
C	-2.17983900	-0.40068900	-1.59308800
C	-1.44770200	-1.88149500	0.04965400
C	-2.30621700	-0.76118600	-0.18612300
Ir	-0.20989600	-0.20652100	-0.45652500
C	-0.81931400	-1.20493100	-3.63972400
H	-1.45864200	-1.85413400	-4.25200400
H	-0.89810300	-0.18828800	-4.04067600
H	0.21433200	-1.54296600	-3.77248700
C	0.27093500	-3.22295400	-1.40953200
H	0.78707800	-3.48569100	-0.48058100
H	-0.23268500	-4.12456100	-1.78223800
H	1.02403100	-2.92898200	-2.14893500
C	-1.35408000	-2.69446700	1.28823300
H	-1.63757000	-2.11876800	2.17481900
H	-2.03385400	-3.55321300	1.21517300
H	-0.34197500	-3.08364200	1.44069400
C	-3.25821000	-0.14301300	0.77595800
H	-3.26428500	0.94866700	0.67716900
H	-4.28147200	-0.50011100	0.60217600
H	-2.99022900	-0.38524600	1.80954600
C	-2.91928200	0.69523700	-2.26779700
H	-2.24725100	1.33993600	-2.84796900
H	-3.64850800	0.26467100	-2.96673200
H	-3.46809700	1.31440200	-1.55203700
C	3.81949000	0.90653400	-0.58054900
C	3.74017900	0.74173200	-1.94851500
C	2.44246900	0.27546700	-2.19129600
N	1.77725500	0.15979800	-1.04325600
H	4.63322300	1.24401500	0.04750600
H	4.51991700	0.92755900	-2.67273100
H	1.95602300	0.02115300	-3.12636600
N	2.62524700	0.54579700	-0.05727300
C	0.73205000	0.20622400	1.33686100
C	2.09231700	0.56066000	1.25161100
C	0.18043800	0.21521100	2.61588200
C	2.87374400	0.89457300	2.35057000
C	0.93075400	0.56402900	3.74673700
H	-0.86938800	-0.04101100	2.75767800
C	2.28258500	0.89465200	3.60625100
H	3.92616900	1.14343200	2.24116600
H	2.90247300	1.12828800	4.46926200

C	0.24728600	0.51626600	5.06011700
O	-0.80268100	-0.07238300	5.24637500
O	0.81833200	1.14795900	6.09992000
H	1.58250000	1.68046600	5.83309300
C	-0.16953000	2.79932300	-1.65580200
H	-1.12993000	2.55692500	-1.11388900
O	-0.16849600	2.60239100	-2.89455000
O	0.76943500	3.22392900	-0.93816500

Ir-8

E= -1328.456893 (au) G=-1328.115877(au)

C	-0.80752200	-2.29410500	-1.33725700
C	-1.31960800	-1.30994700	-2.28117200
C	-2.31847500	-0.54692400	-1.62614200
C	-1.50145200	-2.13181700	-0.11017500
C	-2.39686900	-0.99839400	-0.24647000
Ir	-0.39177500	-0.17865600	-0.51504400
C	-0.89957600	-1.22100800	-3.70820100
H	-1.39890500	-1.99160600	-4.31156600
H	-1.14570100	-0.24835700	-4.14790300
H	0.18004800	-1.37943400	-3.81817200
C	0.22667200	-3.31184000	-1.67589800
H	0.63766400	-3.78645500	-0.77864000
H	-0.18925100	-4.10484200	-2.31222700
H	1.06074300	-2.86159600	-2.23030100
C	-1.36055400	-2.95459500	1.12203000
H	-1.38678300	-2.33575600	2.02760600
H	-2.18555500	-3.67491600	1.20177100
H	-0.42208700	-3.51937800	1.12818500
C	-3.42907300	-0.58903900	0.74936200
H	-3.66948500	0.47651900	0.66375800
H	-4.36274700	-1.15200400	0.61164300
H	-3.08640800	-0.77057300	1.77478500
C	-3.16781100	0.51820900	-2.22947900
H	-2.66223400	1.01602500	-3.06400500
H	-4.10625900	0.09527800	-2.61258700
H	-3.43081500	1.28437000	-1.49222400
C	3.64508700	0.97508900	-0.58426500
C	3.58637600	0.82730700	-1.95235300
C	2.28014400	0.39195900	-2.22585200
N	1.58805000	0.28122300	-1.09204600
H	4.45237000	1.28850400	0.06363400
H	4.38112800	1.00832300	-2.66185900
H	1.80565000	0.16667400	-3.17441400
N	2.42916500	0.63009900	-0.08783400

C	0.53378600	0.20030200	1.27558300
C	1.89070400	0.58601700	1.21580200
C	-0.00875500	0.14940500	2.56196300
C	2.66651500	0.89026400	2.32901700
C	0.73769400	0.46103500	3.70564800
H	-1.05719100	-0.11831600	2.69476900
C	2.08329800	0.82766300	3.58585200
H	3.71371100	1.16467200	2.22606600
H	2.69751100	1.03662400	4.45905800
C	0.05765900	0.35914900	5.01546000
O	-0.96884600	-0.27183700	5.19725200
O	0.60766600	0.99699900	6.06533800
H	1.34403700	1.56688700	5.79710000
C	0.60429600	2.96133800	-2.16632000
H	-0.60391200	1.43076800	-0.43509300
O	-0.05450600	2.57153700	-3.04588500
O	1.26834000	3.39070600	-1.30953200

Ir-9

E= -1139.884317 (au) G=-1139.55203(au)

C	-0.97303100	-1.91376200	-1.35203100
C	-1.41674800	-0.76444200	-2.12643400
C	-2.29580100	0.00032700	-1.31856400
C	-1.57910800	-1.84325300	-0.07085400
C	-2.35153800	-0.61612800	-0.00462500
Ir	-0.27011500	0.00288300	-0.29244800
C	-1.05213700	-0.52029900	-3.55076600
H	-1.67467900	-1.12293100	-4.22614000
H	-1.18148800	0.53148900	-3.82847600
H	-0.00786400	-0.79374200	-3.74661200
C	-0.08294100	-2.98638100	-1.87775800
H	0.32058300	-3.60758600	-1.07140600
H	-0.62333100	-3.64650700	-2.56970900
H	0.76582100	-2.56757900	-2.43345700
C	-1.46653200	-2.85044400	1.01946000
H	-1.53064500	-2.38834800	2.01145600
H	-2.28049400	-3.58426200	0.95222100
H	-0.52005400	-3.40012500	0.96751500
C	-3.28485900	-0.23593100	1.09475900
H	-3.43476000	0.84885800	1.13563300
H	-4.27144500	-0.70096400	0.95895500
H	-2.90499200	-0.55497900	2.07208100
C	-3.05432700	1.21695000	-1.72486600
H	-2.56093700	1.74782300	-2.54589500

H	-4.06457800	0.94783900	-2.06156300
H	-3.16376200	1.91758600	-0.89017100
C	3.89392900	0.48798000	-0.49337300
C	3.73487700	0.62102700	-1.85488900
C	2.35667900	0.48193100	-2.08563300
N	1.71868000	0.27482600	-0.93600500
H	4.77821200	0.52495600	0.12830500
H	4.51008600	0.79655200	-2.58702200
H	1.79564800	0.53120900	-3.01164400
N	2.66241000	0.27823700	0.03851100
C	0.79995500	-0.09993200	1.45593900
C	2.19908100	0.04927000	1.35085000
C	0.32804000	-0.34643900	2.74726800
C	3.07791200	-0.03638800	2.42506200
C	1.18185400	-0.44338700	3.85331600
H	-0.74279600	-0.45554700	2.91973700
C	2.56270500	-0.28449300	3.68912800
H	4.15049300	0.07373800	2.28391400
H	3.25023000	-0.38889700	4.52585000
C	0.57106200	-0.76266100	5.16209500
O	1.26795600	-0.46620500	6.27381400
O	-0.52400700	-1.28310200	5.28601200
H	-0.20719700	1.60289700	0.00511600
H	2.07065300	0.03668500	6.06868100

Ir-TS6

E= -1216.746082 (au) -1326.13 *i* cm⁻¹

G=-1216.384421 (au)

C	0.92380700	-2.31021700	-0.71321300
C	0.64623500	-1.99493400	-2.10738900
C	-0.74915200	-1.77620700	-2.22514600
C	-0.31040500	-2.30898700	0.00365900
C	-1.35323300	-1.90782800	-0.91290500
Ir	0.06975900	-0.23876200	-0.75501400
C	1.66150000	-1.98064900	-3.19735700
H	1.34735500	-1.35206300	-4.03802600
H	2.62722500	-1.60524600	-2.83977700
H	1.83248600	-2.99279300	-3.58758400
C	2.26819300	-2.64824200	-0.17282700
H	2.31071600	-2.50880300	0.91233400
H	2.52222300	-3.69414000	-0.38849100
H	3.04710500	-2.02278700	-0.62485500
C	-0.50822400	-2.67044600	1.43235200
H	0.39359100	-2.48767900	2.02612700

H	-1.33032500	-2.10187500	1.88125800
H	-0.75698800	-3.73561200	1.52200200
C	-2.81752000	-1.89782400	-0.63736100
H	-3.32579800	-1.11254800	-1.20783800
H	-3.27353800	-2.85742100	-0.91603500
H	-3.02542900	-1.73050500	0.42515200
C	-1.50850100	-1.46182900	-3.46564400
H	-0.85514000	-1.11417100	-4.27215900
H	-2.02817100	-2.36094400	-3.82210500
H	-2.27145800	-0.69650200	-3.28564700
C	3.06280900	2.36676100	0.64796200
C	3.77841600	2.02948600	-0.48005900
C	2.96343100	1.12969900	-1.18428500
N	1.82597000	0.93347200	-0.52355200
H	3.29902100	3.03010500	1.46890100
H	4.75955800	2.38562300	-0.75938500
H	3.13726600	0.62299900	-2.12677300
N	1.88759600	1.69108900	0.59864200
C	-0.26094600	0.77245000	1.01433500
C	0.77079400	1.62060900	1.45855000
C	-1.38206600	0.70415700	1.83914300
C	0.72421300	2.34153500	2.64665000
C	-1.47139100	1.42716000	3.03609000
H	-2.23235600	0.08677700	1.55046700
C	-0.40781300	2.24016800	3.44144500
H	1.55631000	2.96853300	2.95706200
H	-0.42877900	2.78005700	4.38544500
C	-2.70652800	1.26841200	3.83696200
O	-3.50070500	0.35906900	3.67384200
O	-2.96355000	2.17601000	4.79515200
H	-2.33865300	2.91631300	4.77289000
H	0.39422100	0.86776700	-3.89469100
H	-0.72613600	1.14872600	-1.33652300
O	0.28713200	1.64871100	-3.32518100
H	-0.15070500	1.21332000	-2.21611400
H	-0.40280000	2.19145400	-3.74264200

Ir-10

E= -1216.765093 (au) G=-1216.400737

C	0.63240000	-2.22216200	-0.30240800
C	0.67675700	-2.14165900	-1.76283900
C	-0.64468400	-2.00417700	-2.23485500
C	-0.75803600	-2.25163900	0.09018400
C	-1.53916000	-2.00948300	-1.08148700

Ir	-0.17590300	-0.27857200	-0.75973200
C	1.92136100	-2.20253400	-2.57079100
H	2.23404200	-3.24741000	-2.69414400
H	1.78241700	-1.77211500	-3.56767700
H	2.74535400	-1.67432200	-2.07916600
C	1.80246400	-2.46939400	0.58454200
H	1.60876900	-2.11237700	1.60211700
H	2.03074500	-3.54149900	0.64198800
H	2.69797300	-1.95825300	0.21244000
C	-1.26399500	-2.52536300	1.45845400
H	-2.26220400	-2.10832300	1.62328900
H	-1.33316800	-3.61182200	1.60031800
H	-0.59133400	-2.13698400	2.22965300
C	-3.02296700	-1.94718400	-1.16185100
H	-3.34738700	-1.25425100	-1.94525000
H	-3.43667600	-2.93550600	-1.40072500
H	-3.46297900	-1.61810800	-0.21495000
C	-1.09224000	-1.89074400	-3.64795500
H	-0.26990800	-1.60315300	-4.30975900
H	-1.48387700	-2.85515000	-3.99691400
H	-1.89516200	-1.15457600	-3.75938700
C	3.07123800	2.22147800	0.14643700
C	3.52467300	1.96311500	-1.12940200
C	2.55424100	1.13319000	-1.71023000
N	1.57556800	0.90205100	-0.83886300
H	3.49421400	2.81568900	0.94499700
H	4.43547400	2.32605300	-1.58323100
H	2.51334000	0.70105000	-2.70289300
N	1.89673900	1.56318100	0.30001200
C	-0.19410100	0.73475200	1.05225200
C	0.93853200	1.51666500	1.33386800
C	-1.19049300	0.71975100	2.02152300
C	1.10934400	2.21841000	2.52227500
C	-1.06193700	1.43315000	3.22032300
H	-2.10495700	0.15497900	1.84712100
C	0.09887900	2.17206000	3.47106200
H	2.01164300	2.79393100	2.71221200
H	0.24404100	2.69874000	4.41175100
C	-2.17403700	1.33808500	4.19325200
O	-2.99212100	0.43561400	4.18998900
O	-2.28601800	2.29986600	5.12472400
H	-1.66384200	3.02758300	4.97560500
H	-0.04822300	4.50539700	-1.89710400
H	-1.30270500	1.10335100	-1.02791500

O	0.12840200	3.58968900	-1.65331300
H	1.03693500	3.44803100	-1.94484800
H	-0.90547600	1.04260900	-1.77273400

Co-2

E= -1256.604273 (au) G=-1256.26505(au)

C	-0.47420000	-1.80387300	-1.15482200
C	-1.08846000	-1.04877500	-2.22972300
C	-2.15694100	-0.32446300	-1.67858700
C	-1.25623300	-1.61559400	0.02942400
C	-2.24057500	-0.62506100	-0.26326600
C	-0.67509400	-1.03846100	-3.65924300
H	-1.36871300	-1.64355100	-4.25736700
H	-0.68912300	-0.02515100	-4.07881200
H	0.32605200	-1.45765300	-3.79972800
C	0.70541700	-2.70144800	-1.27425000
H	1.25472300	-2.76019600	-0.32753300
H	0.39554900	-3.72071000	-1.53895100
H	1.40074000	-2.35474700	-2.04661100
C	-1.07053200	-2.35765700	1.30278700
H	-1.49046400	-1.82655500	2.16169300
H	-1.58170400	-3.32644600	1.22674400
H	-0.01453500	-2.56011100	1.50933400
C	-3.25967000	-0.05772400	0.66193600
H	-3.24480500	1.03997600	0.65168300
H	-4.26983700	-0.36833600	0.36567000
H	-3.09959300	-0.38759700	1.69296700
C	-3.02875200	0.63640200	-2.40164200
H	-2.48046400	1.16951500	-3.18647500
H	-3.85627300	0.10167000	-2.88593700
H	-3.46879700	1.37416200	-1.72304800
C	3.60033200	0.59595400	-0.87946200
C	3.44739700	0.61769100	-2.25170000
C	2.06581800	0.54352400	-2.46971300
N	1.41574700	0.48066200	-1.30756500
H	4.48487000	0.63984400	-0.25801700
H	4.22898300	0.68241200	-2.99501100
H	1.51765100	0.53727800	-3.40351900
N	2.36526600	0.51207700	-0.33997900
C	0.48623700	0.37741400	1.08172400
C	1.87417700	0.52458800	0.98744100
C	-0.06614500	0.48955700	2.35366400
C	2.70151300	0.72152100	2.08795300
C	0.72594500	0.69000600	3.49072900

H	-1.14396200	0.41621400	2.49567900
C	2.11115100	0.79375700	3.34370300
H	3.77795100	0.82990600	1.96994700
H	2.72479900	0.94475800	4.22806200
C	0.08882000	0.78242400	4.86487200
O	-1.15890700	0.61602900	4.93369000
O	0.85545300	1.01699400	5.83647300
O	-0.83820400	2.12732400	-0.67133100
H	-0.00411600	2.61786600	-0.60926200
H	-1.29862900	2.32926800	0.15870300
Co	-0.38784400	0.14244100	-0.62541500

Co-3

E= -1181.336577 (au) G=-1181.004442(au)

C	-0.41174600	-1.84174600	-1.18276500
C	-0.96923500	-1.12152600	-2.31027000
C	-2.08507000	-0.39886700	-1.84246700
C	-1.25864700	-1.62728100	-0.04990600
C	-2.24195400	-0.66386700	-0.42731700
C	-0.48411400	-1.15724200	-3.71568100
H	-1.13258800	-1.80841900	-4.31578100
H	-0.50605000	-0.16411800	-4.17905900
H	0.53316100	-1.55245000	-3.78999700
C	0.78639300	-2.72028700	-1.20289100
H	1.30503900	-2.70239800	-0.23754100
H	0.49664300	-3.75981800	-1.40310600
H	1.49852400	-2.41685700	-1.97757700
C	-1.12906100	-2.32299600	1.25468700
H	-1.63385600	-1.79076400	2.06584900
H	-1.58759900	-3.31697700	1.16872300
H	-0.08168900	-2.46928200	1.53786200
C	-3.33395800	-0.10740100	0.41583200
H	-3.42083000	0.97796900	0.28910800
H	-4.29775100	-0.54773500	0.12923900
H	-3.17605300	-0.31602900	1.47804500
C	-2.95946000	0.49866400	-2.64107700
H	-2.45042700	0.86489000	-3.53800200
H	-3.85513900	-0.04809500	-2.96382300
H	-3.29602400	1.36003100	-2.05487600
C	3.60702200	0.56037800	-0.80030900
C	3.51728700	0.57355800	-2.17792800
C	2.14761600	0.49890200	-2.46000800
N	1.44585900	0.44213500	-1.32878600
H	4.46161600	0.61143000	-0.13880800

H	4.33220800	0.63462300	-2.88477600
H	1.64325700	0.49074100	-3.41787700
N	2.34794800	0.47854400	-0.31792900
C	0.40362300	0.41378800	1.01990900
C	1.79869100	0.50086100	0.98325800
C	-0.20236300	0.52527300	2.26544200
C	2.58251800	0.64036000	2.12365900
C	0.54784900	0.66446400	3.43887400
H	-1.28728600	0.49835000	2.35717200
C	1.94102300	0.71428400	3.35331500
H	3.66679200	0.69826400	2.05458700
H	2.52129400	0.82161300	4.26599700
C	-0.14698500	0.74807600	4.78554500
O	-1.39843500	0.59931200	4.79467500
O	0.57948200	0.95633100	5.79294700
H	-0.78012300	1.67086100	-0.33703200
H	-0.75855300	1.68079900	-1.16411200
Co	-0.39293200	0.13913400	-0.73915200

Co-TS1

E= -1257.272296 (au) -188.31 *i* cm⁻¹

G=-1256.932689(au)

C	-0.51994300	-1.78381800	-1.12384200
C	-1.17516500	-1.00819800	-2.15771500
C	-2.25645900	-0.32926300	-1.56038100
C	-1.26390600	-1.63858000	0.08599200
C	-2.29133000	-0.67254500	-0.15465400
C	-0.80886300	-0.95368700	-3.59871700
H	-1.52031900	-1.54636200	-4.18805900
H	-0.84294200	0.07127600	-3.98738200
H	0.18896700	-1.36274600	-3.78361700
C	0.68568700	-2.63610900	-1.29550700
H	1.26499000	-2.69240600	-0.36675200
H	0.40079500	-3.66005100	-1.56923100
H	1.34541000	-2.25279600	-2.08170800
C	-1.00368900	-2.38264500	1.34524500
H	-1.44693000	-1.89218100	2.21682700
H	-1.43988700	-3.38686000	1.26520900
H	0.06868500	-2.50457200	1.53330600
C	-3.32037300	-0.18535600	0.80490500
H	-3.38590900	0.90915400	0.79997500
H	-4.31029400	-0.57261400	0.53136600
H	-3.10862200	-0.50768700	1.82875600
C	-3.19721200	0.60250800	-2.23599400

H	-2.72519300	1.10914600	-3.08424100
H	-4.06419000	0.04784100	-2.61788800
H	-3.57291000	1.36378800	-1.54441500
C	3.49520100	0.51360400	-0.86359500
C	3.32414100	0.59353900	-2.23095300
C	1.93751500	0.57912400	-2.43208100
N	1.30383100	0.49289800	-1.26403900
H	4.38900900	0.50494200	-0.25409700
H	4.09716000	0.66043800	-2.98296600
H	1.37619300	0.63587600	-3.35618000
N	2.26417900	0.45260000	-0.30934000
C	0.39763700	0.40326100	1.13438800
C	1.79079900	0.44430500	1.02215200
C	-0.13442200	0.49027900	2.41514500
C	2.64040100	0.51845300	2.12078200
C	0.68322000	0.56274800	3.54879200
H	-1.21340100	0.49567100	2.56477800
C	2.07072200	0.56911600	3.38672200
H	3.72061200	0.54451300	1.99248900
H	2.70447400	0.62330600	4.26803900
C	0.06996700	0.61634100	4.93606900
O	-1.18373900	0.51042300	5.01633200
O	0.86221000	0.75534200	5.90548900
H	-0.94231800	1.63311600	-0.09386200
H	-0.85372300	1.71581500	-0.92118400
O	0.06718900	3.56236700	-0.39429300
H	0.36459600	4.47787800	-0.41769300
Co	-0.49466600	0.18484200	-0.57609500

Co-4

E= -1180.885972 (au)

G=-1180.56574(au)

C	-0.59925600	-2.06260300	-1.38012600
C	-1.13734200	-1.14553000	-2.36159400
C	-2.11852200	-0.34985900	-1.72623000
C	-1.26412400	-1.83371100	-0.14975600
C	-2.17019700	-0.72976000	-0.33958800
C	-0.78445200	-1.09502000	-3.80992200
H	-1.57498300	-1.55204700	-4.42050400
H	-0.66087000	-0.06419200	-4.16535500
H	0.14080400	-1.64117200	-4.02322500
C	0.46978600	-3.06617900	-1.64255600
H	0.94259400	-3.39998800	-0.71211600
H	0.07081000	-3.95507300	-2.14890100

H	1.25752400	-2.65473600	-2.28633300
C	-1.05869800	-2.58440500	1.11962000
H	-1.22599000	-1.95030400	1.99727300
H	-1.75303100	-3.43200700	1.18969700
H	-0.04124500	-2.98574400	1.19138000
C	-3.14272800	-0.18566300	0.65209300
H	-3.11334400	0.91039500	0.69227800
H	-4.17021000	-0.47160300	0.38816500
H	-2.95095600	-0.56449900	1.66143200
C	-2.97912600	0.67860700	-2.37593600
H	-2.47157800	1.15836600	-3.22024700
H	-3.90085300	0.22192300	-2.76229900
H	-3.27380800	1.46209100	-1.66944700
C	3.66768500	0.57178300	-0.95473200
C	3.57524300	0.34456100	-2.31236700
C	2.21842800	0.08070400	-2.55119000
N	1.52603300	0.14207300	-1.41323800
H	4.51347900	0.81530600	-0.32578000
H	4.37879600	0.36866300	-3.03474500
H	1.71683700	-0.13656300	-3.48606200
N	2.42156500	0.43981100	-0.44188300
C	0.49897200	0.35738700	0.92798000
C	1.88713600	0.55557000	0.86261500
C	-0.06247400	0.49682400	2.20000700
C	2.68903600	0.84468600	1.96221600
C	0.70097000	0.78237700	3.33782900
H	-1.13716700	0.38349700	2.33631000
C	2.08198000	0.95353600	3.20645900
H	3.76360100	0.98138200	1.85391700
H	2.67511700	1.17456700	4.09015400
C	0.04360600	0.90048400	4.69945100
O	0.78772800	1.19666400	5.67325800
O	-1.19873300	0.69284100	4.76509300
H	-0.53146400	1.39389500	-0.82297900
Co	-0.29500100	-0.07678400	-0.76935100

Co-5

E= -1369.449672 (au) G=-1369.121827(au)

C	-0.68371400	-2.03771600	-1.33898800
C	-1.27523700	-0.99988700	-2.15641900
C	-2.21381900	-0.30147600	-1.36260800
C	-1.27478900	-1.97944500	-0.05241100
C	-2.18387800	-0.86207100	-0.03804300
C	-1.01244700	-0.76197800	-3.60563300

H	-1.83058700	-1.16188200	-4.21990200
H	-0.92730700	0.30660700	-3.84007400
H	-0.09335000	-1.25689500	-3.93762300
C	0.36260800	-2.99701200	-1.79035200
H	0.93389100	-3.39363400	-0.94325700
H	-0.07659800	-3.85217600	-2.32096400
H	1.07448900	-2.52227900	-2.47658500
C	-0.99646200	-2.89824300	1.08564800
H	-1.14224800	-2.40460600	2.05267700
H	-1.66606600	-3.76798300	1.05690000
H	0.03247900	-3.27542100	1.05835900
C	-3.09909100	-0.45694100	1.06836800
H	-3.06182000	0.62434400	1.25130400
H	-4.14068000	-0.70729400	0.82387500
H	-2.85694700	-0.96597300	2.00711200
C	-3.12605500	0.78478000	-1.81824400
H	-2.72871400	1.30745600	-2.69610700
H	-4.10122000	0.36728900	-2.10545600
H	-3.30960400	1.52240100	-1.02895500
C	3.62151800	0.49979100	-0.81348600
C	3.44377300	0.47918100	-2.18145000
C	2.07202300	0.25726900	-2.37262100
N	1.45091200	0.14851700	-1.19767400
H	4.50698800	0.64367800	-0.20920100
H	4.20217700	0.60819600	-2.94060400
H	1.51270700	0.18173900	-3.29731100
N	2.40723000	0.29541700	-0.25042900
C	0.56809800	0.03007700	1.20899600
C	1.95241500	0.22856100	1.08699300
C	0.08531100	0.00108600	2.52027600
C	2.82191700	0.36265500	2.16486000
C	0.91774900	0.13273800	3.63815100
H	-0.98068200	-0.12466400	2.70454000
C	2.29141000	0.30858400	3.44674500
H	3.88975500	0.50705500	2.00997500
H	2.93996800	0.40878600	4.31301200
C	0.34263300	0.08979500	5.04173300
O	1.15150900	0.24014400	5.99733200
O	-0.90020200	-0.09228500	5.15695400
H	-0.54884500	1.30720800	-0.30493400
C	-0.80529400	3.23744600	-2.00956900
O	-0.23567500	2.70725500	-2.87774300
O	-1.37805300	3.79584200	-1.16221700
Co	-0.33056100	-0.15585700	-0.48187500

Co-TS2**E= -1369.445928 (au) -119.11 *i* cm⁻¹****G=-1369.115431(au)**

C	-0.59055500	-1.82069900	-1.19577000
C	-1.03965600	-0.92675100	-2.24409600
C	-1.98622900	-0.06298400	-1.67470200
C	-1.38300000	-1.57025400	-0.01470400
C	-2.17048900	-0.42310500	-0.27848600
C	-0.57590700	-0.91323600	-3.65675500
H	-1.29011800	-1.45395400	-4.29075300
H	-0.50304800	0.10842400	-4.04816900
H	0.39741700	-1.39937300	-3.77498100
C	0.43959000	-2.88223400	-1.31754200
H	1.02432800	-2.97017100	-0.39415300
H	-0.03433500	-3.85599900	-1.50016800
H	1.13034300	-2.68273200	-2.14293900
C	-1.36496600	-2.41414300	1.20571700
H	-1.78250400	-1.90173600	2.07649000
H	-1.97612900	-3.30750000	1.01997700
H	-0.35519700	-2.75586800	1.45392900
C	-3.08521200	0.29176200	0.65105200
H	-2.87037500	1.36869400	0.66401400
H	-4.12820000	0.17521700	0.32895000
H	-3.00332000	-0.08905500	1.67363200
C	-2.69596100	1.04929600	-2.35400700
H	-2.15184500	1.40613900	-3.23370100
H	-3.67999800	0.69604400	-2.69175100
H	-2.86826600	1.89376800	-1.67900300
C	3.78960800	0.38261600	-0.85045400
C	3.59965700	0.54577100	-2.20954000
C	2.21483600	0.48149200	-2.39848300
N	1.59815300	0.28863600	-1.23149200
H	4.69129100	0.37237700	-0.25259800
H	4.36085900	0.69413200	-2.96175100
H	1.64139200	0.57390500	-3.31245900
N	2.57170400	0.22869900	-0.29021100
C	0.71350000	0.05600800	1.15319800
C	2.10764700	0.14261700	1.04415200
C	0.19192000	0.06986200	2.44422500
C	2.96407300	0.19473500	2.13677500
C	1.01357200	0.13199500	3.57583500
H	-0.88444800	0.03491800	2.60553000
C	2.39905700	0.18020200	3.40670200

H	4.04257100	0.25559500	2.00592600
H	3.03488600	0.21703800	4.28754700
C	0.41072100	0.13110000	4.96904200
O	1.21136000	0.23260900	5.93609600
O	-0.84231600	0.02463800	5.05535800
H	-0.32060400	2.40342800	0.06805700
C	-0.75821300	3.11744000	-0.70069200
O	-0.15256800	3.17446200	-1.79714800
O	-1.78294300	3.73689400	-0.34003600
Co	-0.18693000	0.00369900	-0.55163500

Co-6

E= -1369.469999 (au)

G=-1369.138788(au)

C	-0.54150200	-1.97096100	-1.32947400
C	-1.13769400	-1.08863100	-2.30751700
C	-2.14370000	-0.35147800	-1.64846700
C	-1.22145500	-1.79463700	-0.08920000
C	-2.18180300	-0.74463300	-0.26424700
C	-0.77813500	-0.95746600	-3.74766900
H	-1.58284300	-1.34148100	-4.38764400
H	-0.61785000	0.09207000	-4.02770100
H	0.12988300	-1.51669800	-3.99479700
C	0.55998200	-2.94410300	-1.55929200
H	1.24937700	-2.97107000	-0.70643700
H	0.15635400	-3.95748800	-1.68329600
H	1.14048700	-2.70370400	-2.45546500
C	-0.99151300	-2.60939300	1.13294700
H	-1.31754200	-2.09419600	2.04159100
H	-1.55457300	-3.54941000	1.06121100
H	0.06627000	-2.86897700	1.25210400
C	-3.18587100	-0.26679800	0.72670200
H	-3.24755900	0.82776500	0.75411700
H	-4.18592200	-0.63739100	0.46497800
H	-2.96190200	-0.61931600	1.73841800
C	-2.98933000	0.70677100	-2.25646600
H	-2.49323600	1.18256000	-3.10935500
H	-3.92947600	0.27165200	-2.62048700
H	-3.25200400	1.48557000	-1.53213900
C	3.71995600	0.25483200	-0.79731500
C	3.61860000	0.19844100	-2.17252500
C	2.24623100	0.08306600	-2.43656100
N	1.55795200	0.06546300	-1.29735500

H	4.57903100	0.35312400	-0.14725200
H	4.42660100	0.23637600	-2.88913100
H	1.73363500	0.01271300	-3.38826300
N	2.46505100	0.17170900	-0.30019500
C	0.52830500	0.17913800	1.05778900
C	1.92610400	0.24364600	1.00672600
C	-0.04187900	0.29453500	2.32351000
C	2.73501600	0.39253100	2.12914000
C	0.72942800	0.44142500	3.48263400
H	-1.12424700	0.27064300	2.44371400
C	2.12116300	0.48805800	3.37102400
H	3.81859600	0.43657300	2.03822800
H	2.72081800	0.60180700	4.27043200
C	0.06343000	0.53466000	4.84245400
O	0.81157600	0.74045300	5.83538900
O	-1.18930200	0.39570400	4.88212400
H	-1.41774500	2.19607700	0.75779900
C	-1.08852900	2.65990500	-0.19876900
O	-0.43167300	1.88823000	-0.98746800
O	-1.35354400	3.84198800	-0.43398200
Co	-0.29608300	-0.04401900	-0.67979900

Co-1

E= -1257.055722 (au)

G=-1256.700766(au)

C	0.78120800	-2.17337600	-0.45492300
C	0.56019600	-1.98702000	-1.87579800
C	-0.80348500	-1.71198900	-2.06026100
C	-0.49106100	-2.14074400	0.20206400
C	-1.46110300	-1.75410200	-0.76801900
C	1.58277400	-2.07926000	-2.95082200
H	1.49699300	-3.04825700	-3.45982700
H	1.44543100	-1.30451400	-3.71459700
H	2.60168600	-2.00799000	-2.55848600
C	2.08448100	-2.46946700	0.19674700
H	2.08991500	-2.13938600	1.24167300
H	2.28705200	-3.54836900	0.19025200
H	2.91505200	-1.97420500	-0.31908100
C	-0.72385300	-2.49507100	1.62540800
H	-1.66653100	-2.09832400	2.01392200
H	-0.76884200	-3.58903900	1.70945200
H	0.08835900	-2.15266000	2.27482600
C	-2.91832200	-1.54401300	-0.55280600
H	-3.26598000	-0.61001600	-1.01157800

H	-3.49558700	-2.35690300	-1.01212200
H	-3.17287800	-1.51549400	0.51077000
C	-1.45894000	-1.38000900	-3.35079300
H	-0.80175200	-0.78443300	-3.99479200
H	-1.70636100	-2.29977600	-3.89657800
H	-2.39172800	-0.82730900	-3.20173200
C	3.29313000	1.79384700	0.23532600
C	3.73848500	1.52945300	-1.04241200
C	2.70182900	0.81024400	-1.65479400
N	1.68941800	0.64403700	-0.80746600
H	3.75447600	2.32531500	1.05681500
H	4.68387400	1.81990900	-1.47755100
H	2.64457500	0.41554900	-2.66169600
N	2.06055300	1.24825200	0.34984500
C	-0.08481300	0.55354800	1.03577200
C	1.08028900	1.25974800	1.36350600
C	-1.11944300	0.61075400	1.95816600
C	1.25774800	1.94705000	2.55895200
C	-0.98395600	1.29757100	3.17364800
H	-2.06704600	0.11279600	1.75655900
C	0.21435900	1.95309400	3.47435100
H	2.18667900	2.46743000	2.77942200
H	0.36247800	2.45557100	4.42811000
C	-2.11974100	1.23043500	4.11971000
O	-2.98227000	0.37118000	4.06814800
O	-2.20073600	2.16141700	5.08507700
H	-1.53760400	2.85902800	4.97385100
O	-0.99096800	1.21704800	-1.54994200
H	-0.53924400	2.03734300	-1.29731500
H	-1.85735000	1.28135500	-1.11855800
Co	-0.00297900	-0.32906300	-0.68011600

Co-7

E= -1369.92063 (au)

G=-1369.572178 (au)

C	0.76405400	-2.15471600	-0.42876700
C	0.54571700	-1.98376100	-1.85219600
C	-0.82397800	-1.74254400	-2.04744500
C	-0.50785400	-2.13165600	0.22180800
C	-1.48230000	-1.77472800	-0.75731800
C	1.59028700	-2.06427200	-2.90751400
H	1.63586800	-3.08304500	-3.31425500
H	1.38033500	-1.38940100	-3.74518100
H	2.58596100	-1.82855600	-2.51783400

C	2.07268300	-2.42844800	0.22478800
H	2.07349500	-2.10076400	1.27054500
H	2.29884200	-3.50275500	0.21623300
H	2.89498400	-1.91580900	-0.28794900
C	-0.74679300	-2.46412400	1.65023000
H	-1.66862700	-2.02204000	2.04095700
H	-0.83711000	-3.55403700	1.74883600
H	0.08172400	-2.14630300	2.29185500
C	-2.94332400	-1.58044400	-0.55008400
H	-3.27854100	-0.61707000	-0.95382800
H	-3.51704300	-2.36352500	-1.06253200
H	-3.21054900	-1.61355900	0.51068900
C	-1.50136900	-1.46548600	-3.33987300
H	-0.82452200	-0.99797200	-4.06325400
H	-1.86371800	-2.40177600	-3.78426100
H	-2.36895200	-0.81181100	-3.20704700
C	3.23455000	1.81904800	0.21812100
C	3.64128100	1.61793200	-1.08308800
C	2.60476000	0.88812800	-1.68702800
N	1.63418700	0.65228200	-0.81093400
H	3.70444800	2.33917300	1.04216000
H	4.56047900	1.95601600	-1.53959100
H	2.52204200	0.53311500	-2.70681300
N	2.02648000	1.22258700	0.35597800
C	-0.13194700	0.55831400	1.02770600
C	1.05435300	1.21778600	1.37858800
C	-1.16504800	0.62058700	1.95097300
C	1.25416200	1.85670600	2.59712500
C	-1.00782400	1.25910400	3.19001700
H	-2.12825600	0.16187800	1.72995600
C	0.21155700	1.86386000	3.51354900
H	2.19975700	2.33846800	2.83439200
H	0.37460100	2.32717000	4.48452900
C	-2.14116500	1.19007300	4.13839100
O	-3.02880400	0.35860300	4.05951100
O	-2.18674700	2.08057300	5.14429500
H	-1.51298700	2.77059900	5.04981400
C	-0.87618600	2.34062900	-1.50819700
H	0.00031000	2.63873000	-0.89156600
O	-1.53663300	3.21182200	-2.08229400
O	-1.12232100	1.08391500	-1.57196200
Co	-0.05506700	-0.31150400	-0.68886500

Co-TS5

E= -1369.896129 (au) -107.32 *i* cm⁻¹

G=-1369.54954 (au)

C	-0.54835900	-2.03489900	-1.12249100
C	-1.08985200	-1.18328500	-2.15145000
C	-2.08661200	-0.39054000	-1.55152500
C	-1.29305000	-1.80827100	0.09678200
C	-2.19349000	-0.73862900	-0.15001500
C	-0.69002900	-1.10558400	-3.58191400
H	-1.49115800	-1.50137900	-4.21922100
H	-0.51587900	-0.06726900	-3.89266600
H	0.21343100	-1.68625700	-3.79049300
C	0.54901300	-3.02337600	-1.25941800
H	1.23673500	-2.96656600	-0.40678100
H	0.13842900	-4.04166100	-1.27827000
H	1.12424800	-2.87116000	-2.17742200
C	-1.12577000	-2.60368200	1.33770800
H	-1.53640900	-2.09946900	2.21690400
H	-1.65427100	-3.55910900	1.22038600
H	-0.07293300	-2.83466900	1.53016600
C	-3.14099300	-0.10149900	0.80383200
H	-2.98653900	0.98387600	0.85307000
H	-4.17757600	-0.26909700	0.48611300
H	-3.03429300	-0.50714300	1.81417800
C	-2.84967200	0.68066600	-2.23681900
H	-2.17423900	1.40330900	-2.71327400
H	-3.46904700	0.24034200	-3.02920700
H	-3.50683200	1.21740600	-1.54668800
C	3.68272000	0.54412700	-0.71133300
C	3.54707500	0.48159000	-2.08296300
C	2.18694700	0.23373800	-2.30958400
N	1.53338100	0.14973100	-1.15198800
H	4.54765300	0.72178800	-0.08603500
H	4.32606300	0.59909700	-2.82225800
H	1.65865000	0.12274300	-3.24871000
N	2.45904400	0.33577800	-0.17768300
C	0.56499100	0.14866200	1.21303100
C	1.94768300	0.37514000	1.13557500
C	0.00033100	0.23948700	2.47899300
C	2.75437100	0.64259700	2.23365300
C	0.77366000	0.53961800	3.61039200
H	-1.06931900	0.09395100	2.61973700
C	2.15373300	0.72289100	3.48275700
H	3.82598700	0.79020500	2.12656800
H	2.78307400	0.90336000	4.35164100

C	0.08136000	0.60172100	4.91712500
O	-0.98803400	0.06118100	5.13512000
O	0.66989900	1.28696300	5.91274600
H	1.43658600	1.79243500	5.60249000
C	-0.29147900	2.85300900	-1.32935300
H	-1.29176700	2.59487300	-0.87333800
O	-0.19317900	2.68705100	-2.56907600
O	0.59054100	3.25152800	-0.53132000
Co	-0.25599100	-0.16787900	-0.50299400

Co-8

E= -1369.90525 (au)

G=-1369.562065 (au)

C	-0.63474900	-2.18203900	-1.29229300
C	-1.20548300	-1.22202300	-2.21244900
C	-2.21605200	-0.50666100	-1.52863000
C	-1.30315800	-2.05569100	-0.04908000
C	-2.25166000	-0.97644900	-0.16897600
C	-0.85290200	-1.06065200	-3.65260400
H	-1.65222800	-1.45149500	-4.29643400
H	-0.70998400	-0.00700100	-3.92343900
H	0.06227200	-1.60446300	-3.91091400
C	0.46619700	-3.12842500	-1.62296300
H	0.89294900	-3.57955800	-0.72063500
H	0.10884500	-3.94536300	-2.26358100
H	1.27881000	-2.62656000	-2.16366800
C	-1.05299600	-2.87156600	1.17173600
H	-1.31774500	-2.32866900	2.08603800
H	-1.64956700	-3.79310300	1.15647500
H	0.00033300	-3.16338900	1.25414000
C	-3.24397600	-0.53071400	0.85198500
H	-3.22478100	0.55711700	0.99348200
H	-4.26434200	-0.79884900	0.54607400
H	-3.06813500	-1.00026800	1.82552000
C	-3.11290900	0.52932100	-2.11214700
H	-2.62741700	1.06829200	-2.93302400
H	-4.02407500	0.06658600	-2.51595200
H	-3.42384100	1.26192700	-1.35974600
C	3.51148500	0.66831100	-0.69197200
C	3.43673500	0.48515800	-2.05532800
C	2.10055500	0.13667600	-2.31125800
N	1.40299200	0.10729900	-1.17603500
H	4.33931100	0.94330100	-0.05217500
H	4.23725100	0.59181400	-2.77349300

H	1.61946500	-0.08631500	-3.25619000
N	2.27628200	0.42573400	-0.18820900
C	0.35738300	0.16609600	1.15864000
C	1.73024700	0.46780100	1.11109500
C	-0.20911400	0.20002300	2.43148700
C	2.50971300	0.77134100	2.22233000
C	0.53782800	0.50168500	3.57922500
H	-1.27063700	-0.00184700	2.56370000
C	1.90416200	0.78533500	3.47034200
H	3.57249100	0.98076900	2.12565500
H	2.51762200	0.98762800	4.34583900
C	-0.16601500	0.45442000	4.87944500
O	-1.23030100	-0.11520100	5.04878700
O	0.40229400	1.06580800	5.93554900
H	1.17855300	1.58580500	5.67926100
C	0.50663500	2.99660500	-1.95143700
H	-0.70895100	1.22745000	-0.53750400
O	-0.12864500	2.70009100	-2.88282900
O	1.15108200	3.33243200	-1.03957100
Co	-0.40567100	-0.22698200	-0.55549600

Co-9

E= -1181.339804 (au)

G=-1181.005032 (au)

C	-0.80552800	-1.84581600	-1.39485100
C	-1.30168500	-0.65977300	-2.05915300
C	-2.16658400	0.01234100	-1.16340200
C	-1.37197400	-1.89748000	-0.09675400
C	-2.17886000	-0.71476700	0.07631500
C	-1.02079200	-0.24520700	-3.46428500
H	-1.90629500	-0.38654800	-4.09824300
H	-0.74435700	0.81483000	-3.52986000
H	-0.21077000	-0.83487500	-3.90629100
C	0.14413200	-2.82565200	-1.99073100
H	0.65581600	-3.41040000	-1.21855000
H	-0.37406900	-3.53203800	-2.65237200
H	0.91350200	-2.32510500	-2.59153500
C	-1.16817500	-2.97032200	0.91544900
H	-1.19387200	-2.57864500	1.93851600
H	-1.95486100	-3.73252100	0.83976900
H	-0.20634300	-3.47755300	0.77862400
C	-3.04830400	-0.38084900	1.24134800
H	-2.93246700	0.66590900	1.54931300
H	-4.10743100	-0.52770500	0.98934100

H	-2.83473800	-1.01356200	2.10910400
C	-2.95360900	1.24167900	-1.45892300
H	-2.44496700	1.87976600	-2.18986700
H	-3.93428400	0.97780700	-1.87841200
H	-3.13182300	1.83405000	-0.55519100
C	3.72481200	0.18728200	-0.57785600
C	3.56349300	0.24229600	-1.94443200
C	2.17719400	0.16744200	-2.15852400
N	1.53252600	0.07286100	-0.99745900
H	4.61316500	0.21297500	0.03859300
H	4.34039900	0.32896700	-2.69066100
H	1.62648400	0.18978900	-3.09091000
N	2.48671100	0.08476200	-0.03372200
C	0.61378600	-0.14550500	1.38239200
C	2.01267500	-0.03258400	1.28867400
C	0.11959400	-0.25776000	2.68061100
C	2.87943000	-0.03843500	2.37660000
C	0.95529200	-0.26686400	3.80671200
H	-0.95245700	-0.33136100	2.85451000
C	2.34202800	-0.15897200	3.64988800
H	3.95569500	0.03760800	2.24073500
H	3.02094100	-0.19719600	4.49971900
C	0.30929600	-0.42468500	5.12760400
O	1.02374000	-0.11673100	6.22538600
O	-0.83442300	-0.81885800	5.27784700
H	-0.35705800	1.34441600	-0.05895500
H	1.87748800	0.28059700	5.99866500
Co	-0.27576900	-0.11926100	-0.31944400

Co-10

E=-1258.2267871 (au)

G=-1257.853717 (au)

C	-0.42366300	-1.83430900	-1.15200500
C	-1.03969300	-1.10220400	-2.24560300
C	-2.14833300	-0.35094600	-1.71334100
C	-1.07447200	-1.46174100	0.03330900
C	-2.12037900	-0.51220600	-0.30448200
C	-0.69812300	-1.23217200	-3.68478100
H	-1.35317700	-1.97444400	-4.16027100
H	-0.83377700	-0.28385400	-4.21644300
H	0.33411600	-1.56616500	-3.82816700
C	0.73646500	-2.75324900	-1.27710500
H	1.24955100	-2.88355300	-0.31811200
H	0.40311800	-3.74274800	-1.61471900

H	1.46449800	-2.39071500	-2.01173000
C	-0.79706800	-1.96314800	1.40397600
H	-0.96440800	-1.19421000	2.16661500
H	-1.47576300	-2.79508700	1.63410000
H	0.22681200	-2.33735600	1.50644100
C	-3.08485900	0.06176900	0.67061300
H	-3.55668100	0.97355900	0.29239800
H	-3.88351100	-0.66640100	0.86664800
H	-2.61352200	0.28606700	1.63435200
C	-3.15053000	0.41217800	-2.50375800
H	-2.74389600	0.73216300	-3.46792000
H	-4.02189500	-0.22446200	-2.70428200
H	-3.50187100	1.29991500	-1.96889400
C	3.69136400	0.26470700	-0.86905900
C	3.64628800	0.17643500	-2.24062300
C	2.28510500	0.25848900	-2.57642800
N	1.54375600	0.38612500	-1.48228200
H	4.52054800	0.27918000	-0.17403900
H	4.48381700	0.07968900	-2.91603000
H	1.81352700	0.22693100	-3.55129300
N	2.41068100	0.38964500	-0.43540500
C	0.60695300	1.16891300	0.93008300
C	1.87219300	0.57191300	0.84885300
C	-0.00399600	1.30726500	2.16513800
C	2.53099300	0.12734600	1.98791400
C	0.64455900	0.86737100	3.31987900
H	-0.98362200	1.77366200	2.24285900
C	1.91172100	0.28439400	3.22147000
H	3.49572000	-0.36644800	1.91150500
H	2.41660700	-0.10159900	4.10408700
C	-0.10886900	0.95928700	4.59405300
O	-1.32436300	0.99767900	4.62876000
O	0.58075700	0.98381100	5.74130700
H	0.17464700	1.72727900	0.06737700
H	-0.57637400	1.47780200	-1.85741100
H	1.53536300	1.07362100	5.59724100
O	-2.17150000	3.17312700	-0.31419500
H	-1.75651700	2.43207900	-0.78496700
H	-2.31496800	2.82360700	0.57331600
Co	-0.33774200	0.27849600	-1.00510700

Co-11

E= -1181.787102 (au)

G=-1181.43948(au)

C	-0.40513300	-1.91151400	-1.16729900
C	-1.09792500	-1.18281900	-2.21591500
C	-2.21548100	-0.50340700	-1.61879600
C	-1.03449300	-1.61841100	0.05474800
C	-2.13531500	-0.70982100	-0.21624800
C	-0.80554400	-1.23863600	-3.67096400
H	-1.45811000	-1.97474600	-4.15890400
H	-0.98503700	-0.27009600	-4.15095700
H	0.22900700	-1.53570100	-3.86782600
C	0.80865500	-2.74731200	-1.35090700
H	1.45067100	-2.72412200	-0.46265500
H	0.53134800	-3.79371400	-1.53086000
H	1.40320200	-2.41503100	-2.20906000
C	-0.63295300	-2.14240800	1.38804200
H	-1.04706700	-1.54789600	2.20911900
H	-0.99549100	-3.17104100	1.51075200
H	0.45712000	-2.16662100	1.50354400
C	-3.09562600	-0.15156600	0.77389200
H	-3.26212700	0.91931100	0.60599900
H	-4.06949700	-0.64820700	0.67184300
H	-2.75891900	-0.28964900	1.80581600
C	-3.28237800	0.24708000	-2.33223900
H	-2.93634000	0.62225700	-3.30033500
H	-4.13810700	-0.41578300	-2.51602900
H	-3.64114100	1.09527300	-1.74064100
C	3.59267500	0.51557400	-0.81801300
C	3.55394100	0.39877700	-2.18714600
C	2.19022700	0.34613800	-2.52017900
N	1.44148100	0.42404600	-1.42706900
H	4.41794500	0.61516800	-0.12539000
H	4.39628600	0.36861700	-2.86287600
H	1.72252600	0.25315000	-3.49324300
N	2.30624600	0.53009600	-0.38220000
C	0.41382600	1.06233000	0.97656400
C	1.75087500	0.64519400	0.90147100
C	-0.22640000	1.07592400	2.20446900
C	2.45502400	0.28734700	2.04399100
C	0.45894300	0.69778600	3.35916600
H	-1.26524400	1.38807000	2.26940100
C	1.80384100	0.32446900	3.27141000
H	3.48280400	-0.05797700	1.97649400
H	2.35033700	0.00272400	4.15531000
C	-0.33738100	0.60001700	4.60682300
O	-1.54247600	0.42975100	4.59165900

O	0.29454700	0.67915600	5.78409400
H	-0.08379800	1.60628600	0.12777600
H	-0.78667100	1.41586700	-1.67972900
H	1.22618500	0.93055600	5.69218000
Co	-0.42356900	0.18067900	-0.93180600

Co-TS7

E= -1181.773922 (au) -1050.53 *i* cm⁻¹

G=-1181.430352 (au)

C	-1.00002500	-1.83733800	2.45355200
C	-1.62116300	-1.07721800	1.38190700
C	-2.71293800	-0.36141600	1.93269600
C	-1.72507800	-1.59505800	3.64622700
C	-2.75080700	-0.62892900	3.34534400
C	-1.24469100	-1.09263500	-0.05657000
H	-1.98129600	-1.67157600	-0.62846800
H	-1.22795100	-0.08105000	-0.47907500
H	-0.26600900	-1.55306700	-0.22057900
C	0.19512700	-2.71319100	2.33817600
H	0.81955600	-2.64847700	3.23751300
H	-0.10650800	-3.76208900	2.22332900
H	0.81473700	-2.44892600	1.47489400
C	-1.42730000	-2.20468900	4.96884700
H	-1.92973900	-1.68217200	5.78947500
H	-1.76636500	-3.24822500	4.97865100
H	-0.35015500	-2.20875200	5.17651300
C	-3.76929400	-0.07575700	4.27891200
H	-3.83118900	1.01631000	4.20158400
H	-4.76172900	-0.47582100	4.03472400
H	-3.55582800	-0.33471300	5.32087000
C	-3.65835800	0.51150100	1.18894200
H	-3.17073100	1.00696000	0.34317100
H	-4.48507900	-0.09072400	0.78996000
H	-4.09014900	1.27910300	1.83876100
C	3.05140000	0.62487900	2.75742700
C	2.96306600	0.54966400	1.38674800
C	1.59122600	0.44792400	1.10436100
N	0.88467900	0.45719800	2.22883400
H	3.90188200	0.72638200	3.41824200
H	3.77841300	0.57282100	0.67826400
H	1.09382400	0.37235200	0.14540400
N	1.78601700	0.56417900	3.24213300
C	-0.14979000	0.72134900	4.59383800
C	1.25110800	0.65064700	4.53576900

C	-0.74673100	0.82035000	5.84035500
C	2.03966800	0.63268200	5.67837400
C	0.02346000	0.80545400	7.00734400
H	-1.82757200	0.90570600	5.92280900
C	1.41521000	0.70653400	6.91674900
H	3.12033400	0.54308400	5.61093100
H	2.03426400	0.65471000	7.80927700
C	-0.70889700	0.81340000	8.29571300
O	-1.87410100	0.47284600	8.39036200
O	-0.05620200	1.19561800	9.40315700
H	-0.87387900	1.51961500	3.61906600
H	-1.30616600	1.64691600	2.59297200
H	0.81362100	1.57790900	9.21164400
Co	-0.95014900	0.18602400	2.85345300

Co-12

E= -1181.787376 (au)

G=-1181.441623(au)

C	-0.44225400	-1.82956200	-1.19181900
C	-0.99941100	-1.09844100	-2.31150500
C	-2.10219400	-0.36263800	-1.83077000
C	-1.26829800	-1.59929400	-0.04677300
C	-2.24392000	-0.62236200	-0.41319000
C	-0.52251300	-1.13344700	-3.71915000
H	-1.17089400	-1.78649000	-4.31716000
H	-0.54845100	-0.13993700	-4.18111900
H	0.49651100	-1.52328600	-3.79794800
C	0.73567300	-2.73408800	-1.23062900
H	1.25924600	-2.74873800	-0.26820100
H	0.41787000	-3.76198800	-1.44791600
H	1.45231700	-2.43837800	-2.00382700
C	-1.11986100	-2.29091300	1.25852400
H	-1.64747600	-1.77833100	2.06803800
H	-1.53895800	-3.30168500	1.16946000
H	-0.06841700	-2.39717700	1.54655100
C	-3.32023000	-0.04802800	0.43714900
H	-3.38694700	1.03895100	0.31123500
H	-4.29276500	-0.46923600	0.15146600
H	-3.16416200	-0.26203400	1.49853600
C	-2.98069300	0.53999000	-2.61807100
H	-2.48441600	0.90181200	-3.52355700
H	-3.88343100	-0.00403600	-2.92551300
H	-3.30491300	1.40336500	-2.02781400
C	3.62835300	0.40642200	-0.78961800

C	3.54520900	0.44999900	-2.16465800
C	2.17332100	0.44573000	-2.45475000
N	1.46370000	0.40130000	-1.33064800
H	4.48090900	0.40605000	-0.12327100
H	4.36511100	0.48789200	-2.86726900
H	1.67548400	0.48128500	-3.41564900
N	2.36212200	0.37354200	-0.31326500
C	0.40868700	0.41697800	1.00405300
C	1.80867000	0.40923500	0.98175800
C	-0.19703700	0.56479500	2.24187700
C	2.59380600	0.46105500	2.12778100
C	0.56216400	0.64884600	3.41701500
H	-1.28119900	0.62017700	2.32608500
C	1.95677400	0.57266400	3.35569600
H	3.67831000	0.41800600	2.06882700
H	2.56267600	0.57853800	4.25910500
C	-0.17404300	0.77163700	4.69463900
O	-1.34406700	0.45924500	4.82518300
O	0.48706700	1.25143200	5.76132600
H	-0.69722700	1.71148700	-0.37551600
H	-0.75132200	1.68845500	-1.20057800
H	1.36873000	1.57805000	5.52543200
Co	-0.38812600	0.15412600	-0.74927100

Fe-2

E= -1312.638025 (au)

G=-1312.2552(au)

C	3.56993900	0.35808600	-0.82454600
C	3.44482900	0.63343200	-2.17180800
C	2.07366700	0.83410300	-2.37983600
N	1.40269300	0.68449000	-1.23705100
H	4.43947800	0.15219400	-0.21432700
H	4.23755200	0.68625100	-2.90425900
H	1.54597100	1.06939900	-3.29659100
N	2.32936000	0.39621300	-0.29029000
C	0.43751700	0.49034700	1.11113400
C	1.82872900	0.33444200	1.03254100
C	-0.08036500	0.58709600	2.40131500
C	2.66160200	0.19076800	2.13647800
C	0.71127600	0.43973400	3.54774000
H	-1.14288800	0.76863000	2.55115400
C	2.08379800	0.22761300	3.40042500
H	3.73614600	0.06375300	2.01826100
H	2.70181900	0.10702600	4.28642500

C	0.07857900	0.48712000	4.92573200
O	-1.17348600	0.63174200	4.98096800
O	0.84842300	0.36957400	5.91633400
O	-0.44673300	2.61186800	-0.45945600
H	0.47407300	2.89044800	-0.58202200
H	-0.64484500	2.83091800	0.46473500
C	-2.23405200	0.75046000	-1.94170200
C	-1.30324100	-0.10141600	-2.55839400
C	-0.70422900	-1.16104300	-1.79002300
C	-1.16791100	-1.43604500	-0.48079800
C	-2.13819300	-0.57783000	0.12882800
C	-2.58467900	0.56910000	-0.56001000
C	-2.68391400	-0.94737500	1.47362600
C	-3.43778400	1.59240200	0.13205200
C	-2.81202600	1.90970800	-2.69649000
C	-0.65387000	-2.61002800	0.30157500
C	0.40264600	-2.00507000	-2.35341200
C	-0.93364100	0.15050900	-3.99232400
H	-2.81752800	1.72962500	-3.77309700
H	-3.84419800	2.10174000	-2.39042400
H	-2.23963500	2.82979900	-2.51795600
H	-3.14866600	1.70711400	1.18109400
H	-3.34728200	2.57631500	-0.33382600
H	-4.49864600	1.31118000	0.11015400
H	-1.91882000	-1.31663700	2.16143600
H	-3.21302000	-0.12869800	1.96393000
H	-3.40789100	-1.76170900	1.33098500
H	-0.09783500	-3.31397100	-0.31856300
H	-0.00114300	-2.29316200	1.12628500
H	-1.48979100	-3.16120900	0.74553100
H	1.15473800	-2.22911700	-1.59009200
H	0.00931500	-2.96088000	-2.72239900
H	0.92622100	-1.52219000	-3.17934300
H	-0.15072800	-0.51449800	-4.35663300
H	-1.80799500	-0.00320800	-4.63679800
H	-0.59976100	1.18316400	-4.14864400
Fe	-0.46682700	0.56943400	-0.62172800

Fe-3

E= -1237.374421 (au)

G=-1236.99729 (au)

C	5.08067000	-3.28790600	-2.68459700
C	5.53078200	-2.70891300	-1.51475900
C	4.54341000	-1.78110400	-1.15783300

N	3.55920400	-1.78635400	-2.05602100
H	5.50477000	-4.06259400	-3.30951100
H	6.44610400	-2.93233100	-0.98574100
H	4.49544800	-1.12331100	-0.29862200
N	3.89459500	-2.71314200	-2.98458100
C	1.76590000	-2.15339200	-3.82249700
C	2.90951500	-2.95021000	-3.96833000
C	0.71945800	-2.43268400	-4.69920700
C	3.06059000	-3.91780900	-4.95580900
C	0.81916500	-3.40204500	-5.70484000
H	-0.21891300	-1.88657200	-4.62707600
C	2.00382800	-4.13015000	-5.83213600
H	3.97701800	-4.49976000	-5.03475900
H	2.08596000	-4.87533700	-6.61886700
C	-0.34817600	-3.65386000	-6.64126500
O	-1.39137400	-2.97035100	-6.45708900
O	-0.19090200	-4.52967700	-7.53342700
H	0.92557000	-1.94009600	-1.84884900
H	1.33081100	-1.66316200	-1.16869400
Fe	1.90952900	-0.78356300	-2.40856100
C	0.41811400	0.59308200	-3.09228700
C	0.62005300	0.69899800	-1.68672700
C	1.90181900	1.04227900	-1.15911300
C	3.01091600	1.07250200	-2.02725300
C	2.84019300	0.81411500	-3.42711500
C	1.52991300	0.73535500	-3.96954400
C	4.03990500	0.68932300	-4.31937500
C	1.33196100	0.74143600	-5.45399800
C	-0.97002800	0.35396200	-3.61389000
C	4.37133800	1.38670600	-1.48878500
C	2.07730200	1.31766400	0.30741000
C	-0.52717300	0.47961100	-0.74738000
H	-1.00029600	0.24958900	-4.69951700
H	-1.40392700	-0.55832800	-3.18991900
H	-1.63043600	1.18514100	-3.33725400
H	0.42961100	1.30213400	-5.71301500
H	2.17001700	1.22241500	-5.96208400
H	1.22076000	-0.27011400	-5.86465600
H	4.44409900	1.67244100	-4.59343200
H	4.84282000	0.13186000	-3.82623500
H	3.80148700	0.15206500	-5.24042600
H	4.46996600	1.15777100	-0.42619900
H	5.17229400	0.87064000	-2.02094900
H	4.54813800	2.46441400	-1.61082900

H	2.48233600	0.44910100	0.84243900
H	2.76819600	2.15146800	0.46292100
H	1.13220500	1.59005900	0.78090600
H	-1.00534200	1.43643300	-0.50045100
H	-1.29086700	-0.16897700	-1.18045200
H	-0.19507800	0.02005200	0.18762100

Fe-TS1

E= -1313.310724 (au)

G=-1312.924838 (au)

C	3.16306600	0.80336200	-1.26647900
C	2.79485300	1.21241100	-2.53224300
C	1.39290600	1.19378200	-2.53352600
N	0.93624900	0.78331200	-1.35176600
H	4.13526700	0.68522700	-0.80667100
H	3.45008400	1.49047800	-3.34523200
H	0.70126400	1.45851600	-3.32419100
N	2.02504000	0.55026400	-0.58084100
C	0.37527300	0.34906500	1.08746200
C	1.74170100	0.30035800	0.78097400
C	0.05385400	0.23055800	2.43694100
C	2.73991300	0.07565300	1.72289800
C	1.01855400	-0.01069200	3.42086800
H	-0.98121500	0.30612200	2.76387400
C	2.36306800	-0.08970700	3.05029500
H	3.78728300	0.03361900	1.43010200
H	3.11544900	-0.27776700	3.81202500
C	0.59243100	-0.21871300	4.86072200
O	-0.64538600	-0.32460700	5.08014700
O	1.50278100	-0.28455000	5.72915800
H	-0.77592900	1.90393200	0.26512900
H	-0.87235000	2.09756000	-0.55267600
O	0.23403300	3.78465200	0.12542900
H	0.68130900	4.63154800	0.22530500
Fe	-0.79507300	0.50749800	-0.48338600
C	-1.11300300	-1.55452700	-0.99301600
C	-1.79180600	-1.28603400	0.22810500
C	-2.66051400	-0.16342000	0.32353900
C	-2.85378900	0.66507100	-0.82076300
C	-2.27568900	0.33174400	-2.08084300
C	-1.37985500	-0.76028500	-2.14981500
C	-2.58697700	1.16010300	-3.29615300
C	-0.65778300	-1.06972200	-3.42561900
C	-0.14234800	-2.69950600	-1.06194100

C	-3.65906800	1.92330100	-0.68818400
C	-3.39002500	0.18676100	1.59028000
C	-1.53488700	-2.19312300	1.39265900
H	0.82798100	-2.43130800	-0.62077300
H	-0.51920400	-3.56748600	-0.51332800
H	0.03845500	-3.02446100	-2.08760900
H	0.39306500	-1.31428900	-3.24640400
H	-1.11950900	-1.94006500	-3.91018700
H	-0.68599900	-0.24190600	-4.13564200
H	-3.57913900	1.61128900	-3.21928700
H	-1.86218600	1.97251400	-3.43859400
H	-2.58513700	0.54785900	-4.20164900
H	-3.60165300	2.33119600	0.32369400
H	-3.30656500	2.69713100	-1.37516600
H	-4.71681100	1.73091800	-0.91087300
H	-4.44703600	0.37962700	1.37585700
H	-3.35192100	-0.61472800	2.32944700
H	-2.98434000	1.09274400	2.05790200
H	-1.80340500	-1.75805600	2.35593200
H	-2.12004200	-3.11346800	1.26205700
H	-0.48170300	-2.48125600	1.45252900

Fe-4

E= -1236.911968 (au)

G=-1236.546257(au)

C	3.65759800	1.03551400	-1.09931400
C	3.44775800	1.13914900	-2.45867100
C	2.08976300	0.84046800	-2.64613600
N	1.50514400	0.56567000	-1.47774200
H	4.54392900	1.18383600	-0.49737000
H	4.17611500	1.39698400	-3.21446000
H	1.51329500	0.82405800	-3.56294400
N	2.47405500	0.68608500	-0.53915800
C	0.66296700	0.27947500	0.91747300
C	2.04272700	0.52146600	0.79644700
C	0.20904500	0.19357800	2.24170500
C	2.92763700	0.62668600	1.86498800
C	1.05343800	0.29576800	3.35376300
H	-0.85106500	0.03825400	2.43973500
C	2.42156900	0.50494700	3.15210200
H	3.98911000	0.80497800	1.69939700
H	3.08369400	0.58002900	4.01045000
C	0.49906400	0.18360600	4.76130800
O	1.32308900	0.27157600	5.71227500

O	-0.74435700	0.00965400	4.88763700
H	-0.43279300	1.65213300	-0.53662200
C	-0.59376800	-1.25272900	-2.38604500
C	-0.53982300	-1.94835600	-1.14634600
C	-1.40934400	-1.56382900	-0.08811000
C	-2.23649500	-0.41191600	-0.21992100
C	-2.23834500	0.30825300	-1.45832000
C	-1.47394900	-0.15003700	-2.56815800
C	-3.08987500	1.53810800	-1.60119000
C	-1.56055000	0.54823000	-3.89922400
C	0.30537400	-1.71013900	-3.49883500
C	-3.10829000	0.08791100	0.90013100
C	-1.39620800	-2.40550000	1.15553600
C	0.42361000	-3.08212100	-0.94794600
H	1.35846100	-1.70777600	-3.19749200
H	0.05631600	-2.74163500	-3.77918900
H	0.22435400	-1.09227000	-4.39443300
H	-0.71413400	1.22682500	-4.07297900
H	-1.57372800	-0.17302200	-4.72239100
H	-2.47523700	1.13825000	-3.98614900
H	-3.27508200	2.02001400	-0.63934800
H	-2.61672500	2.28203500	-2.24778400
H	-4.06622000	1.28605200	-2.03766700
H	-3.04551000	-0.52696700	1.79900000
H	-2.83596100	1.10831500	1.19554100
H	-4.16178100	0.11081900	0.59383600
H	-0.47502800	-2.26747300	1.73448200
H	-2.23464200	-2.19764100	1.82115400
H	-1.45286100	-3.46516600	0.88234300
H	-0.03423800	-4.05206500	-1.18916800
H	1.30970600	-2.97700800	-1.57936900
H	0.77142800	-3.13615100	0.08816500
Fe	-0.28376500	0.14880700	-0.78646400

Fe-5

E= -1425.47514 (au)

G=-1425.101381 (au)

C	3.49785100	1.26294900	-1.28060000
C	3.01599800	1.88998200	-2.41060600
C	1.62251300	1.72936200	-2.35614600
N	1.27244300	1.04150700	-1.26645200
H	4.50397600	1.14542900	-0.90085400
H	3.59134600	2.39762400	-3.17193400
H	0.86431600	2.08770600	-3.04239600

N	2.42838100	0.76044800	-0.61668500
C	0.93002900	-0.09934200	0.98812100
C	2.27236200	0.13507100	0.64127900
C	0.75157100	-0.60386700	2.28279200
C	3.36431400	-0.16042800	1.45180800
C	1.81217000	-0.92944400	3.13580200
H	-0.25595200	-0.76018600	2.66723300
C	3.12450500	-0.71213100	2.70385500
H	4.38109100	0.03814600	1.11631800
H	3.95223800	-0.96677500	3.36086500
C	1.54084300	-1.52200200	4.50475800
O	2.53700800	-1.75094500	5.24356300
O	0.33779700	-1.75401200	4.80645100
H	-0.37457600	1.64000900	0.43194100
C	-0.74487200	4.10430200	0.20912100
O	-0.25147900	4.16453700	-0.84595800
O	-1.24238000	4.09256000	1.26321500
Fe	-0.35428700	0.36443300	-0.40416300
C	-0.93486000	-0.64416700	-2.22397700
C	-0.82898900	-1.57330000	-1.16129600
C	-1.58297600	-1.36054500	0.03639500
C	-2.29612000	-0.15062800	0.22752300
C	-2.35758700	0.80885300	-0.84049800
C	-1.70800900	0.54960700	-2.07039000
C	-3.18370300	2.05276100	-0.68901900
C	-1.81684400	1.55261700	-3.18607000
C	-0.22556700	-0.90038400	-3.52285900
C	-2.97623900	0.17362500	1.52867700
C	-1.60417400	-2.46616600	1.05481100
C	0.08838700	-2.75946400	-1.26837300
H	0.59711300	-0.19490000	-3.69677200
H	0.18472300	-1.90976000	-3.57634200
H	-0.92336700	-0.79461200	-4.36076900
H	-1.46606600	2.54548800	-2.87811400
H	-1.23851800	1.26547200	-4.06603800
H	-2.86114300	1.66928600	-3.50392100
H	-3.28135000	2.37111900	0.35081600
H	-2.77938000	2.89307900	-1.26059700
H	-4.19928400	1.87054200	-1.06820500
H	-2.72851700	-0.53323500	2.32218700
H	-2.67693100	1.16454100	1.88963900
H	-4.06863100	0.18288800	1.41765700
H	-0.65277700	-2.58150200	1.58677200
H	-2.38647100	-2.33210600	1.80370200

H	-1.80600700	-3.41588300	0.54583200
H	-0.36300400	-3.58898600	-1.82964100
H	1.02224400	-2.48856300	-1.77313800
H	0.36427200	-3.14269200	-0.28288800

Fe-TS2

E= -1425.479525 (au) -177.36 i cm⁻¹

G=-1425.103319(au)

C	3.49986100	1.17584800	-1.37518500
C	3.01755700	1.79827100	-2.51072300
C	1.62602800	1.65960100	-2.44426400
N	1.28030700	0.99151100	-1.34237000
H	4.50878500	1.04692700	-1.00620200
H	3.59480300	2.28608300	-3.28286000
H	0.86700800	2.00507100	-3.13596200
N	2.43485200	0.70024000	-0.69484800
C	0.92454100	-0.11012700	0.92319900
C	2.26643400	0.11469700	0.58289400
C	0.70033700	-0.56152900	2.22350500
C	3.33849400	-0.14552600	1.42717100
C	1.74519800	-0.84156700	3.11299300
H	-0.31545100	-0.70897400	2.58810900
C	3.06284700	-0.64214600	2.69609600
H	4.36294700	0.04233600	1.11176200
H	3.87511900	-0.86717900	3.38229100
C	1.44705400	-1.37405000	4.50217100
O	2.43182700	-1.59090800	5.25759000
O	0.23641200	-1.56921400	4.79358800
H	-0.08246900	2.28776000	0.93329400
C	-0.62845500	3.27404800	0.77431600
O	-0.37482900	3.86752200	-0.30009200
O	-1.39607200	3.61372700	1.70004400
Fe	-0.35045400	0.35399200	-0.48693000
C	-0.90776600	-0.63399600	-2.26409600
C	-0.77155500	-1.53898600	-1.16926700
C	-1.58526400	-1.38824900	-0.00143800
C	-2.30995300	-0.19044700	0.17555800
C	-2.39817300	0.74405300	-0.91088400
C	-1.77586100	0.48939000	-2.15557400
C	-3.18915200	2.00441500	-0.73102100
C	-1.98859900	1.45650200	-3.28527800
C	-0.09250900	-0.89193400	-3.49529000
C	-2.96777900	0.16245400	1.47808400
C	-1.59720900	-2.49726200	1.00582500

C	0.18254600	-2.69220100	-1.26552700
H	0.96631300	-1.03325700	-3.25696700
H	-0.43954200	-1.81570400	-3.97536500
H	-0.15184400	-0.08737100	-4.22827500
H	-1.44108200	2.39553700	-3.12927400
H	-1.68213300	1.04563300	-4.24798400
H	-3.04992800	1.71236800	-3.36864300
H	-3.16086200	2.36926900	0.29722800
H	-2.83387900	2.80912000	-1.37724800
H	-4.24090500	1.81191200	-0.98505900
H	-2.80978700	-0.59127100	2.25013200
H	-2.57002000	1.10795100	1.86781200
H	-4.04901900	0.29360900	1.34990400
H	-0.64871300	-2.60324400	1.54291800
H	-2.38945600	-2.37885700	1.74618300
H	-1.77595000	-3.44296800	0.48115900
H	-0.25969100	-3.51964400	-1.83663200
H	1.10950700	-2.40595200	-1.77068600
H	0.45618000	-3.07526200	-0.28022200

Fe-6

E= -1425.502852 (au)

G=-1425.12564 (au)

C	3.53765900	1.14260100	-1.45374000
C	3.07064600	1.75182200	-2.60058400
C	1.67288400	1.66212500	-2.52110000
N	1.31118200	1.03143900	-1.40486200
H	4.54280800	0.99018300	-1.08391000
H	3.65869200	2.20082600	-3.38828500
H	0.92226300	2.01592900	-3.21796100
N	2.45705800	0.72002500	-0.75747900
C	0.94166000	0.01504300	0.90971700
C	2.28431800	0.16175000	0.53200700
C	0.74812200	-0.44184300	2.21517000
C	3.37051500	-0.16029400	1.33970000
C	1.80265400	-0.79635000	3.06541500
H	-0.26068100	-0.54405100	2.61444500
C	3.11666500	-0.65519300	2.61243400
H	4.39172300	-0.02805500	0.98650600
H	3.93862800	-0.93067900	3.26815200
C	1.51944100	-1.35226700	4.44729300
O	2.51243800	-1.59980800	5.18329700
O	0.31097100	-1.54018300	4.75604100
H	-0.68286300	1.88296600	2.10608400

C	-0.69920500	2.71552500	1.36747500
O	-0.37753000	2.39565900	0.16925100
O	-1.01175500	3.85414500	1.73501400
Fe	-0.34801300	0.51010400	-0.48698300
C	-0.88790300	-0.58422000	-2.25481300
C	-0.77735300	-1.46001000	-1.14420400
C	-1.56354200	-1.23587600	0.02428500
C	-2.33178300	-0.05418100	0.13428600
C	-2.45003300	0.81643900	-0.99584600
C	-1.72309300	0.57425500	-2.18324100
C	-3.32483000	2.02875700	-0.88686100
C	-1.80667700	1.58101800	-3.29639200
C	-0.10387100	-0.92997600	-3.48712800
C	-3.05639800	0.28003900	1.40727300
C	-1.58799000	-2.29301800	1.08710000
C	0.15252600	-2.63481000	-1.21096100
H	0.97735800	-0.85177900	-3.32275600
H	-0.31026900	-1.96835100	-3.77085100
H	-0.35509000	-0.30238500	-4.34229500
H	-1.64657200	2.59539700	-2.91090000
H	-1.06637800	1.41429100	-4.08008200
H	-2.79387900	1.56592900	-3.77510900
H	-2.81258700	2.85035000	-0.36885900
H	-3.63297300	2.39663400	-1.86712400
H	-4.23338300	1.80073300	-0.32206200
H	-2.53399200	-0.10714100	2.28620500
H	-3.15419200	1.36045300	1.54511800
H	-4.07085300	-0.14125900	1.40978900
H	-0.61408400	-2.45609700	1.55955000
H	-2.31038300	-2.07805100	1.87608100
H	-1.87972500	-3.24184600	0.61963600
H	-0.31410000	-3.48529600	-1.72657800
H	1.06836900	-2.38728200	-1.75699100
H	0.44878900	-2.97434900	-0.21563600

Fe-1

E= -1313.090153 (au)

G=-1312.691391 (au)

C	3.23481900	1.85823900	0.19903900
C	3.54677200	1.73130100	-1.13710900
C	2.47731700	1.01681400	-1.70096100
N	1.57807500	0.71631900	-0.76701400
H	3.75749000	2.34468000	1.01158500
H	4.42774100	2.10331700	-1.64024100

H	2.32145700	0.71138600	-2.72927500
N	2.04647000	1.23794100	0.39388500
C	-0.07975300	0.56358100	1.15481400
C	1.13591700	1.19345100	1.47187100
C	-1.04441200	0.60500200	2.15736100
C	1.42850500	1.76959900	2.70346300
C	-0.80176900	1.18838400	3.41000100
H	-2.03247800	0.17940300	1.98725500
C	0.44676100	1.75673200	3.68400700
H	2.39711500	2.22373600	2.89976400
H	0.67672600	2.17515100	4.66179100
C	-1.88666300	1.11916600	4.41367000
O	-2.80975200	0.32589300	4.34905900
O	-1.84726300	1.96890700	5.45558800
H	-1.15473200	2.63904400	5.35404800
O	-1.00087400	1.59858900	-1.24404800
H	-0.69681000	1.76209200	-2.15151900
H	-0.62651200	2.32556700	-0.72284700
C	-0.28224000	-1.28865500	-2.51985000
C	0.71100800	-1.89266600	-1.70754400
C	0.43499800	-2.18197100	-0.34076200
C	-0.88466300	-2.03456900	0.17374400
C	-1.89240300	-1.44293200	-0.63521700
C	-1.58829100	-1.10411900	-1.98507100
C	-3.26569200	-1.14272700	-0.10920900
C	-2.65739900	-0.49971300	-2.84442100
C	0.02099200	-0.77835600	-3.89879000
C	-1.16219000	-2.53707300	1.55803300
C	1.53331500	-2.67699200	0.55229300
C	2.07810500	-2.20687600	-2.23537200
H	1.09305600	-0.66134800	-4.06925100
H	-0.36900300	-1.44677700	-4.67707900
H	-0.43553600	0.20605200	-4.05364000
H	-2.70023700	0.59161400	-2.73664700
H	-2.48768700	-0.72144200	-3.90037900
H	-3.64140400	-0.89218700	-2.57642100
H	-3.32068900	-1.19976100	0.97886600
H	-3.58444000	-0.13393400	-0.39575300
H	-4.00646800	-1.84558500	-0.51180200
H	-0.65557500	-1.94652900	2.32889300
H	-2.22677400	-2.55070400	1.79410000
H	-0.79033600	-3.56474000	1.64303200
H	1.36172100	-2.39254500	1.59396000
H	1.61063400	-3.77230900	0.51889000

H	2.50467300	-2.27170900	0.25458200
H	2.36029800	-3.21980600	-1.92789700
H	2.12000900	-2.17009700	-3.32480100
H	2.84603500	-1.52994700	-1.84258800
Fe	-0.15918200	-0.17838500	-0.65877500

Fe-7

E= -1425.952177 (au)

G=-1425.557095(au)

C	3.61633700	0.73550200	-0.88706700
C	3.43200700	1.01492400	-2.22324700
C	2.05824000	0.82724700	-2.45276100
N	1.45161800	0.44433200	-1.33437200
H	4.50242800	0.75975400	-0.26668300
H	4.18408200	1.31668400	-2.93814200
H	1.48841100	0.96350200	-3.36480800
N	2.40917200	0.38150600	-0.38157900
C	0.51587900	0.23035500	1.00744100
C	1.91992800	0.25614500	0.93449600
C	0.00179200	0.23678400	2.29947700
C	2.77182400	0.21643400	2.03128000
C	0.82018500	0.20863700	3.44013700
H	-1.07502400	0.25871500	2.46057800
C	2.21107300	0.18196200	3.30188500
H	3.85205800	0.20962500	1.90447500
H	2.86820400	0.10760000	4.16572800
C	0.14502900	0.12087000	4.75136600
O	-0.99610300	-0.28652900	4.89088100
O	0.82652800	0.49533500	5.84984300
H	1.66475400	0.92848600	5.62799200
C	0.04207000	3.12272500	-0.55076700
H	-0.48736400	4.08995900	-0.72077300
O	-0.71779600	2.11696800	-0.76283900
O	1.22521600	3.15638300	-0.19843500
C	-1.64660400	-0.19583100	-2.48635400
C	-0.68280800	-1.22376700	-2.44280200
C	-0.42346300	-1.91661700	-1.21771500
C	-1.26807400	-1.71393000	-0.09837600
C	-2.28149700	-0.70931000	-0.15067800
C	-2.46989100	0.03139900	-1.33915700
C	-1.15557200	-2.58083600	1.11959300
C	-3.16859000	-0.44081400	1.03055100
C	-3.53985300	1.07851400	-1.37655200
C	-1.79130500	0.68247600	-3.69518000

C	0.10614400	-1.60919300	-3.65823500
C	0.74656600	-2.85448900	-1.14014000
H	-0.89172300	-2.02071400	2.02421900
H	-2.12821400	-3.05244600	1.30523900
H	-0.42425000	-3.38027100	0.99335800
H	1.54262100	-2.54794300	-1.82485500
H	1.17802000	-2.87332700	-0.13469300
H	0.46396500	-3.88322200	-1.40027300
H	1.14858700	-1.27325300	-3.61503500
H	0.13020600	-2.70151900	-3.74059900
H	-0.33658400	-1.21933000	-4.57643600
H	-0.86848300	0.72039200	-4.27961800
H	-2.59263900	0.33514900	-4.36066100
H	-2.02896200	1.71115700	-3.40767000
H	-3.19117600	2.01303300	-0.91969600
H	-3.85197800	1.30200300	-2.39858800
H	-4.42533100	0.74945600	-0.82539400
H	-3.24435700	0.63378500	1.23409700
H	-4.18687600	-0.80619200	0.84225300
H	-2.81344000	-0.92696000	1.94177400
Fe	-0.37631200	0.14966800	-0.73019300

Fe-TS5

E= -1425.930062 (au) -214.32 *i* cm⁻¹

G=-1425.536805(au)

C	3.74656600	0.47050100	-0.51246300
C	3.73567100	0.51392900	-1.89181400
C	2.39938300	0.30466500	-2.25732000
N	1.64465200	0.13640500	-1.17255600
H	4.55188600	0.59096300	0.19997300
H	4.57930200	0.67529300	-2.54712000
H	1.95052700	0.28115900	-3.24373900
N	2.47844500	0.23119000	-0.10881500
C	0.43181800	0.26765500	1.05306500
C	1.83341400	0.28714800	1.14372100
C	-0.23930100	0.42975800	2.26060100
C	2.54843500	0.39078500	2.33034400
C	0.43929900	0.56097000	3.48106600
H	-1.32643900	0.46872200	2.29184000
C	1.83593800	0.52093700	3.51425200
H	3.63545100	0.36898400	2.33805100
H	2.38256200	0.56656600	4.45375900
C	-0.38370200	0.68239900	4.70294000
O	-1.54749300	0.32621000	4.76570700

O	0.18447300	1.20910400	5.80213000
H	1.06275100	1.57553500	5.61790100
C	0.26808300	2.88131700	-0.82532100
H	-0.59424000	2.56240100	-0.16387700
O	0.07038100	2.74903700	-2.06159400
O	1.29134900	3.30786500	-0.24998700
Fe	-0.25289500	0.01931400	-0.76920800
C	-1.33357500	-0.36621700	-2.64030800
C	-0.53830800	-1.49020000	-2.34885600
C	-0.51499600	-2.01655100	-1.01741900
C	-1.45904900	-1.56503700	-0.04774200
C	-2.30772000	-0.46282900	-0.35270500
C	-2.18328800	0.16896300	-1.61981900
C	-1.51552700	-2.28278400	1.26483800
C	-3.30002400	0.08240400	0.63520200
C	-2.94098900	1.43180500	-1.89885500
C	-1.24015300	0.28303600	-3.99131700
C	0.34524300	-2.10305500	-3.39110700
C	0.45756400	-3.09535600	-0.64112700
H	-0.51962300	-2.51976000	1.64662200
H	-2.04100400	-1.73321400	2.04588100
H	-2.03949700	-3.23638800	1.11506900
H	1.19566800	-3.28403500	-1.42159300
H	1.00722500	-2.82908700	0.26874900
H	-0.06515700	-4.03916500	-0.44065800
H	1.40833400	-2.02555100	-3.13887400
H	0.11669700	-3.17263800	-3.47022300
H	0.20222800	-1.65714000	-4.37604800
H	-0.20140600	0.52757800	-4.24261600
H	-1.61680000	-0.39386600	-4.76756000
H	-1.82013200	1.20400100	-4.05126800
H	-2.26536300	2.20396000	-2.27763100
H	-3.70893300	1.25153000	-2.66161900
H	-3.43677900	1.82826000	-1.01304400
H	-3.02921700	1.09244100	0.96741600
H	-4.29256100	0.14877100	0.17580300
H	-3.39720300	-0.54335900	1.52291100

Fe-8

E= -1425.932706 (au)

G=-1425.542495(au)

C	3.68358800	0.71601600	-0.50183200
C	3.66510900	0.61320700	-1.87523700
C	2.35646600	0.21961800	-2.20120600
N	1.62118400	0.08296400	-1.09665400

H	4.47244400	0.99385400	0.18383600
H	4.48500200	0.79774300	-2.55488100
H	1.91701800	0.03674600	-3.17479200
N	2.44461700	0.37989100	-0.06045700
C	0.44162900	0.14060500	1.15617900
C	1.82183200	0.42519400	1.20244100
C	-0.20474100	0.25033300	2.39146600
C	2.53421400	0.74712400	2.35289800
C	0.46927600	0.58123300	3.57493200
H	-1.28086000	0.09500400	2.46211000
C	1.84774900	0.82302500	3.55642500
H	3.60554000	0.93290100	2.31958300
H	2.40053400	1.03847200	4.46850700
C	-0.32226600	0.62073000	4.82142500
O	-1.37551900	0.02563900	4.97308300
O	0.14947800	1.35677000	5.84607500
H	0.91929100	1.88294200	5.58082300
C	0.77890100	3.09581300	-1.89862200
H	-0.44308200	1.22261100	-0.59760400
O	0.08085500	2.92171900	-2.81613300
O	1.48986000	3.30878200	-0.99975300
C	-1.07299100	-0.93330500	-2.49943500
C	-0.26371400	-1.96869300	-1.94354500
C	-0.47657700	-2.41752600	-0.61111000
C	-1.52518300	-1.84571700	0.16717300
C	-2.27345300	-0.74615700	-0.33413600
C	-2.02343000	-0.28274200	-1.66748300
C	-1.77999300	-2.43924600	1.52341300
C	-3.32166000	-0.04111400	0.48165600
C	-2.81126100	0.87240600	-2.21444500
C	-0.91999500	-0.47668000	-3.92562100
C	0.84433000	-2.60406200	-2.73349800
C	0.38505000	-3.49317000	-0.01578100
H	-0.97875000	-2.20794000	2.23598600
H	-2.71912200	-2.10507800	1.96644000
H	-1.83004400	-3.53071000	1.43903500
H	1.37392300	-3.53003500	-0.47962500
H	0.53691400	-3.33803200	1.05676700
H	-0.06787200	-4.48714900	-0.14055200
H	1.80346900	-2.52846000	-2.21010800
H	0.63976800	-3.67244700	-2.87757100
H	0.98375600	-2.15522300	-3.71748900
H	-0.43966000	-1.23099300	-4.55164500
H	-1.89940700	-0.27608400	-4.37213900

H	-0.33072400	0.44627000	-4.00780800
H	-2.23977100	1.43956400	-2.95432200
H	-3.72591200	0.51292400	-2.70662700
H	-3.11447900	1.56924000	-1.43004900
H	-3.08462500	1.02267200	0.60298300
H	-4.30214600	-0.09980700	-0.00803200
H	-3.43281100	-0.45732700	1.48347500
Fe	-0.23485400	-0.28815800	-0.61307000

Fe-9

E= -1237.367349 (au)

G=-1236.987109(au)

C	3.89703300	0.41947000	-0.49041700
C	3.76063500	0.70078200	-1.83120300
C	2.38258900	0.61495500	-2.08914500
N	1.71529700	0.29443100	-0.98057600
H	4.77004900	0.38013100	0.14718500
H	4.54783000	0.93823400	-2.53262800
H	1.85333700	0.78274000	-3.01863700
N	2.65310100	0.17464100	-0.00643300
C	0.74151600	-0.10046900	1.34047500
C	2.14833500	-0.05239900	1.28882300
C	0.22697900	-0.24377900	2.63188300
C	2.99526500	-0.18258800	2.38539400
C	1.03754600	-0.37861900	3.76665000
H	-0.84915900	-0.24139700	2.79381100
C	2.43191500	-0.35470800	3.64138400
H	4.07630300	-0.15807500	2.26758000
H	3.08726100	-0.49568200	4.49875400
C	0.35797200	-0.58124300	5.06205200
O	1.05414100	-0.33396600	6.18737500
O	-0.79616400	-0.96092800	5.16988000
H	-0.11486800	1.52313600	-0.01218300
H	1.91781700	0.05820000	5.98941600
C	-1.35600900	0.13859400	-2.16985800
C	-0.60845100	-1.06852500	-2.17127500
C	-0.64178800	-1.95878500	-1.06060100
C	-1.40632700	-1.61729000	0.08690300
C	-2.14329300	-0.39403500	0.12229500
C	-2.07816100	0.49325200	-0.99440700
C	-3.00007200	-0.00163900	1.29562000
C	-2.79474700	1.81160500	-0.93228700
C	-1.36857100	1.03444900	-3.37915800
C	-1.40117000	-2.57750100	1.24219300

C	0.15667700	-3.23284600	-1.10392600
C	0.23576600	-1.43805600	-3.35608600
H	-1.35944600	0.44922700	-4.30365000
H	-2.26933400	1.65255600	-3.40801800
H	-0.50335100	1.71058600	-3.40879100
H	-2.87166600	2.18411600	0.09179700
H	-2.27680500	2.57677700	-1.51670300
H	-3.81546800	1.72051600	-1.32888300
H	-3.11438300	-0.80647100	2.02326000
H	-2.59827500	0.86986700	1.82799000
H	-4.00817700	0.26725400	0.95804000
H	-0.38720600	-2.92899300	1.45812900
H	-1.79654700	-2.15870800	2.16861200
H	-2.00770000	-3.45886400	0.99546900
H	1.19995500	-3.06985700	-0.79536300
H	-0.26078900	-4.00041200	-0.44856500
H	0.18127400	-3.65436900	-2.11301800
H	-0.27294100	-2.21136500	-3.94758800
H	0.42776500	-0.59502000	-4.02187500
H	1.20472700	-1.84955500	-3.05575600
Fe	-0.14309000	0.04470300	-0.38620500

Fe-10

E= -1314.25964 (au)

G=-1313.845139(au)

C	3.74508300	0.56496400	-0.20377100
C	3.94277800	0.34667400	-1.54654200
C	2.65644600	0.20714300	-2.09599000
N	1.72990400	0.32100800	-1.15058200
H	4.43648000	0.74954200	0.60783600
H	4.88721200	0.30355700	-2.06935200
H	2.36511800	0.03851500	-3.12600200
N	2.40272100	0.53880300	0.00947100
C	0.32163900	1.25423100	0.93483700
C	1.63754100	0.82015400	1.14935300
C	-0.48559000	1.51728300	2.03031800
C	2.13736900	0.63428500	2.43223300
C	0.00047300	1.33927100	3.32573500
H	-1.49903600	1.88243900	1.88654100
C	1.31412700	0.90068600	3.51854600
H	3.14589900	0.25812000	2.58008200
H	1.70155200	0.71829300	4.51899700
C	-0.95443800	1.55327400	4.43880000
O	-2.15903200	1.45414000	4.29576000
O	-0.46194400	1.85010000	5.64838500

H	-0.00538700	1.71565900	-0.04831600
H	-0.20674100	1.54136000	-1.88564400
H	0.48990900	2.03226400	5.62150600
C	-1.13579600	-0.59157600	-2.69608800
C	-0.29177800	-1.56264300	-2.10425700
C	-0.41816000	-1.89305500	-0.71626000
C	-1.36307900	-1.21854900	0.08101100
C	-2.24481000	-0.25266900	-0.51918200
C	-2.15920300	0.02628600	-1.90228100
C	-3.27749700	0.48196000	0.28916400
C	-3.10413900	0.99440000	-2.55429100
C	-0.96002500	-0.19976900	-4.13359700
C	-1.41696700	-1.53319000	1.54678900
C	0.50881100	-2.90550800	-0.10979400
C	0.74915200	-2.27282700	-2.91292200
H	0.09747100	-0.09049700	-4.39069000
H	-1.38844100	-0.95888500	-4.80057800
H	-1.44371300	0.75321800	-4.35536000
H	-2.60690900	1.93444300	-2.81820000
H	-3.49990200	0.56272200	-3.48000400
H	-3.95678500	1.23701700	-1.91988400
H	-3.21422700	0.28014000	1.35826700
H	-3.19780500	1.56568100	0.14774800
H	-4.28329900	0.18523300	-0.03240500
H	-0.41751200	-1.70876700	1.95627800
H	-1.88003000	-0.74792000	2.14539500
H	-1.99758400	-2.45179000	1.70422900
H	1.42917800	-2.43200500	0.26126300
H	0.04105400	-3.42544000	0.72920200
H	0.80294400	-3.66344300	-0.83936600
H	0.41204500	-3.30267400	-3.09029100
H	0.91731000	-1.81584200	-3.88828200
H	1.71017100	-2.33465000	-2.39367600
Fe	-0.22300500	0.27676500	-1.04221200
O	1.74980500	3.45427600	-1.50905900
H	1.09816700	2.79487300	-1.79369300
H	2.58680600	3.09094000	-1.82278700

Fe-11

E= -1237.821155 (au)

G=-1237.426889 (au)

C	3.82106900	0.32843100	-0.26836200
C	4.00437300	0.06456400	-1.60414800
C	2.71247600	0.00889200	-2.15525100

N	1.79415800	0.21617900	-1.21823800
H	4.52357200	0.48282800	0.53975000
H	4.94455000	-0.06157500	-2.12124200
H	2.41417000	-0.16685300	-3.18193900
N	2.48038200	0.41637400	-0.06116400
C	0.43359200	1.22905500	0.85097800
C	1.73296100	0.75243300	1.07428800
C	-0.36096100	1.54817800	1.94079600
C	2.23039600	0.57934900	2.35980100
C	0.12139700	1.38222300	3.23943300
H	-1.36214100	1.94399400	1.79100100
C	1.41841300	0.89971800	3.43961800
H	3.22511400	0.17098500	2.51572400
H	1.80066700	0.72868800	4.44394900
C	-0.82028100	1.65669800	4.34999500
O	-2.02862100	1.63695200	4.20547400
O	-0.31078800	1.92006100	5.56053400
H	0.13162200	1.67857100	-0.14852800
H	-0.09875500	1.48082300	-1.93489500
H	0.65224600	2.02810300	5.53486100
C	-1.11410100	-0.64023300	-2.72120200
C	-0.30291400	-1.62928400	-2.11287600
C	-0.43353400	-1.92851600	-0.71841500
C	-1.34635800	-1.20097100	0.06970400
C	-2.19428500	-0.21455400	-0.54599400
C	-2.10773800	0.03296200	-1.93536800
C	-3.19022600	0.57777000	0.25448500
C	-3.02134200	1.02186400	-2.60145200
C	-0.93693400	-0.29076200	-4.16923300
C	-1.40207400	-1.47751700	1.54310200
C	0.46165000	-2.96162500	-0.09810400
C	0.70393900	-2.39413400	-2.91581900
H	0.12105000	-0.21751000	-4.43603900
H	-1.39023900	-1.05561800	-4.81289000
H	-1.39615200	0.66858100	-4.41344100
H	-2.49452900	1.94066900	-2.88212100
H	-3.43407400	0.58888500	-3.51910800
H	-3.86458400	1.30249300	-1.96998900
H	-3.11796800	0.40447400	1.32812300
H	-3.07548400	1.65383600	0.08236700
H	-4.21082700	0.30826100	-0.04387200
H	-0.40925200	-1.69830600	1.94646100
H	-1.81186700	-0.65161200	2.12626100
H	-2.03311000	-2.35627600	1.73058600

H	1.40561100	-2.51526600	0.24693400
H	-0.01149400	-3.44290900	0.76081500
H	0.71366300	-3.74999200	-0.81122300
H	0.32134100	-3.41054700	-3.07860200
H	0.88667400	-1.95689400	-3.89783300
H	1.66484200	-2.49193500	-2.40195100
Fe	-0.16357600	0.22757000	-1.08822400

Fe-TS7

E= -1237.813408 (au) -723.53 i cm⁻¹

G=-1237.423576(au)

C	3.00388500	1.52134700	2.48927800
C	2.76164500	1.75470600	1.15519800
C	1.40161500	1.45865100	0.96304500
N	0.84857300	1.06103800	2.10477900
H	3.89933200	1.62851000	3.08613800
H	3.46862800	2.10131600	0.41538100
H	0.80548900	1.51300500	0.05974800
N	1.83564800	1.10142400	3.03832700
C	0.05335100	0.62113700	4.50724800
C	1.43971900	0.80093600	4.34898500
C	-0.40623900	0.36037100	5.79310400
C	2.34268700	0.66989900	5.39550700
C	0.47884100	0.21925700	6.86666400
H	-1.47390500	0.26668400	5.98078800
C	1.85298700	0.37242400	6.66018500
H	3.41112600	0.77927200	5.22886700
H	2.56092700	0.23345100	7.47406900
C	-0.10161900	-0.15683700	8.17621700
O	-1.18605900	-0.69941100	8.28734400
O	0.60699400	0.10897600	9.28397300
H	-0.79114800	1.53421400	3.83730200
H	-1.27630200	1.92837800	2.82262300
H	1.39804400	0.63551100	9.09263200
Fe	-0.89513800	0.45274000	2.74510000
C	-1.93782200	-0.01477800	0.93296000
C	-0.95153500	-1.02003300	1.13108600
C	-0.83314300	-1.67028100	2.39214800
C	-1.81166300	-1.45117200	3.39986200
C	-2.78359100	-0.42734200	3.23013900
C	-2.83472700	0.29710100	2.00000400
C	-1.75713600	-2.30811300	4.62901000
C	-3.74940700	-0.05623200	4.31959600
C	-3.86437300	1.36841300	1.80864700

C	-2.04696100	0.76965400	-0.34372900
C	0.03039600	-1.40299100	0.06625800
C	0.31165600	-2.60252900	2.65399700
H	-0.92257800	-2.04524900	5.29045800
H	-2.67423600	-2.25922000	5.21668100
H	-1.61181600	-3.35206300	4.33148200
H	1.21105300	-2.29358500	2.11364000
H	0.56484300	-2.63105100	3.71739000
H	0.07559700	-3.62882900	2.34185200
H	1.04952500	-1.08218000	0.31107300
H	0.05519500	-2.49482400	-0.02143600
H	-0.21836900	-0.99844400	-0.91420500
H	-1.34607900	0.43856200	-1.10930700
H	-3.05638500	0.68175400	-0.76238400
H	-1.85868300	1.83553000	-0.17004400
H	-4.14731400	1.84441500	2.74894600
H	-3.52081600	2.15297900	1.13194500
H	-4.77269800	0.92995400	1.37355800
H	-3.65267200	1.00311300	4.58338000
H	-4.78315100	-0.21556600	3.99014800
H	-3.59952600	-0.62740700	5.23632000

Fe-12

E= -1237.826119 (au)

G=-1237.433178 (au)

C	3.30089600	1.47228400	-1.15861200
C	2.84092000	1.85803300	-2.39903600
C	1.47478700	1.53815700	-2.40502000
N	1.12527200	0.98313800	-1.24685400
H	4.28055000	1.54113200	-0.70473500
H	3.41154400	2.31538800	-3.19435100
H	0.73702200	1.68883300	-3.18377100
N	2.24830600	0.94910900	-0.48733800
C	0.72469800	0.18875200	1.13535600
C	2.05597000	0.51657000	0.83837500
C	0.46921500	-0.13710700	2.46246100
C	3.09884600	0.46354000	1.75653300
C	1.48787400	-0.19187400	3.42313300
H	-0.54284900	-0.36422800	2.79165100
C	2.80774600	0.09609400	3.06255600
H	4.11918700	0.69943500	1.46383200
H	3.62232700	0.01135700	3.77875900
C	1.10667700	-0.61691700	4.78761100
O	0.10278700	-1.26345200	5.03058000

O	1.91271300	-0.27436300	5.80741100
H	-0.77601900	1.57125100	0.45807900
H	-0.93524600	1.79756000	-0.33223500
H	2.61060800	0.33741400	5.52692100
Fe	-0.48712100	0.23371800	-0.41502900
C	-1.01112000	-1.82144000	0.07602400
C	-2.12341700	-0.96286500	0.31085600
C	-2.54856000	-0.07240900	-0.71691100
C	-1.95870900	-0.11014800	-2.01501200
C	-0.83934800	-0.94269600	-2.22636600
C	-0.33212400	-1.76395800	-1.17305800
C	-2.49574200	0.73349000	-3.13586100
C	-0.14880300	-0.95635100	-3.55357000
C	0.88758200	-2.59877500	-1.43660000
C	-0.50686200	-2.76659300	1.12332100
C	-2.88072500	-0.95945200	1.60889200
C	-3.62196000	0.93068100	-0.41799800
H	-1.87203800	1.61703300	-3.32145700
H	-2.53020900	0.15454900	-4.06394200
H	-3.51197500	1.07602700	-2.93361100
H	-3.62647400	1.21198800	0.63743000
H	-3.48873700	1.84500500	-1.00169500
H	-4.61033900	0.51719200	-0.65701900
H	-2.68092100	-0.05617200	2.19871400
H	-3.95814000	-0.98357500	1.41359200
H	-2.64667700	-1.82379200	2.23129100
H	-0.90356000	-2.56802000	2.11909500
H	-0.79375000	-3.78972900	0.84735400
H	0.58365700	-2.74229700	1.19773100
H	1.80048800	-1.98818100	-1.42571000
H	1.01465400	-3.39639500	-0.70446400
H	0.82560800	-3.07344100	-2.42078700
H	0.93721100	-1.03153100	-3.45348500
H	-0.48433800	-1.83585900	-4.11993000
H	-0.37568200	-0.07288600	-4.15238600

5-Co-2

E= -1256. 5819004 (au)

G=-1256.250781 (au)

C	-0.41029800	-1.72517000	-1.19311800
C	-1.09229300	-0.93601600	-2.16951700
C	-2.22187100	-0.33826200	-1.52913100
C	-1.11558000	-1.62003700	0.03803100
C	-2.22625300	-0.75647200	-0.16043700

C	-0.74563100	-0.75980300	-3.60810700
H	-1.49419100	-1.23446500	-4.25646800
H	-0.71683000	0.30377800	-3.88354600
H	0.22897200	-1.19542800	-3.85014300
C	0.83584500	-2.51548300	-1.37688200
H	1.61540200	-2.21152900	-0.66301400
H	0.64810300	-3.58272500	-1.19792700
H	1.24518800	-2.41465100	-2.38685100
C	-0.70354200	-2.29566100	1.29593100
H	-1.26587800	-1.93612000	2.16376000
H	-0.86091000	-3.38073700	1.22372600
H	0.36496200	-2.14226500	1.50130400
C	-3.21630500	-0.29284400	0.84809200
H	-3.23950500	0.80588800	0.89944200
H	-4.23236000	-0.61437200	0.58250900
H	-2.99461700	-0.67149900	1.85068300
C	-3.27573200	0.47963700	-2.19379000
H	-2.88452400	1.01519100	-3.06602400
H	-4.09815800	-0.15758700	-2.54707900
H	-3.71401700	1.21553800	-1.50873700
C	3.67290500	0.20408800	-0.69722200
C	3.69157000	0.19138500	-2.07797200
C	2.36620800	0.43051900	-2.45750700
N	1.59020400	0.58316500	-1.38476700
H	4.47010300	0.06657700	0.02090500
H	4.54768200	0.03456700	-2.71839800
H	1.93900300	0.50371300	-3.45059900
N	2.40051000	0.44409800	-0.30865500
C	0.43030200	0.72620000	1.03834100
C	1.81508200	0.53473800	0.99067600
C	-0.13909900	0.81163800	2.30825600
C	2.60858600	0.41784900	2.13040500
C	0.61385600	0.69523200	3.48105000
H	-1.21680200	0.94127700	2.41341900
C	1.99275300	0.49692600	3.37285100
H	3.68360600	0.26393500	2.06248400
H	2.58583300	0.39844100	4.27861900
C	-0.05615500	0.74648000	4.84065400
O	-1.30986900	0.87964300	4.85806200
O	0.68746200	0.64473500	5.85271900
O	-1.07435000	2.61024900	-1.42933000
H	-0.49752000	3.25794600	-0.99683000
H	-1.94689500	2.74495300	-1.02837200
Co	-0.44292900	0.67986700	-0.79358400

5-Fe-1**E=-1313.15251 (au)****G=-1312.757847 (au)**

C	3.75205700	1.90977700	0.59362800
C	4.33669100	1.92632400	-0.65344500
C	3.29958900	1.60003900	-1.53819700
N	2.15823500	1.40444400	-0.88391000
H	4.17557000	2.09312300	1.57163800
H	5.36880100	2.14352400	-0.88855200
H	3.32266400	1.49865100	-2.61686500
N	2.44347300	1.59564200	0.43041200
C	0.13791100	1.07638300	0.92669700
C	1.40768900	1.43161300	1.40251200
C	-0.84441900	0.90787400	1.90087700
C	1.70286200	1.61611900	2.75374700
C	-0.59647200	1.08965000	3.26737400
H	-1.85543300	0.62463100	1.60470500
C	0.69083600	1.44274700	3.68626600
H	2.70137900	1.88059100	3.09193700
H	0.93273300	1.55472600	4.74129600
C	-1.71142400	0.85771500	4.20971500
O	-2.69122400	0.18329800	3.94098700
O	-1.64003300	1.42089000	5.42864000
H	-0.89596000	2.03789800	5.49919400
O	-0.79111800	2.04431000	-2.54584900
H	-0.33438200	1.97233000	-3.39730900
H	-0.70995600	2.97352800	-2.28625800
C	-0.61583500	-1.34723100	-2.37777700
C	0.43417400	-1.81377500	-1.55328300
C	0.17077900	-2.15756400	-0.21066300
C	-1.14622000	-2.13591400	0.27202300
C	-2.19466900	-1.67405900	-0.54670300
C	-1.94046000	-1.31107000	-1.88072700
C	-3.58007400	-1.54096900	0.02444500
C	-3.06865500	-0.92537700	-2.79616800
C	-0.31518300	-0.94602300	-3.79889400
C	-1.43485400	-2.59125000	1.67443500
C	1.30636700	-2.47377300	0.72176000
C	1.81607900	-2.01002000	-2.12227500
H	0.64670000	-0.42345400	-3.87321400
H	-0.25469400	-1.81908800	-4.46396200
H	-1.07802900	-0.28164900	-4.21197500
H	-3.18992900	0.16439200	-2.87360500
H	-2.90315400	-1.30228300	-3.81025800

H	-4.02289300	-1.33550800	-2.45686900
H	-3.55549700	-1.34365600	1.10099600
H	-4.12846500	-0.71575800	-0.43961900
H	-4.17939300	-2.45078200	-0.12160600
H	-1.45922900	-1.74943900	2.38431300
H	-2.40465800	-3.09376500	1.74270200
H	-0.68121500	-3.29631500	2.03597100
H	1.12669600	-2.04487600	1.71523700
H	1.45942400	-3.55324700	0.85907900
H	2.25231900	-2.05720300	0.36163300
H	2.31335500	-2.86660500	-1.65668600
H	1.78342400	-2.20597000	-3.19750700
H	2.46853000	-1.13824200	-1.96998300
Fe	0.07397400	0.78215100	-1.11075000

5-Fe-2

E=-1312.402279 (au)

G=-1312.026652(au)

C	4.02731100	0.45194900	-0.97537700
C	4.01484700	0.89030200	-2.28264400
C	2.75306100	1.47719700	-2.44810300
N	2.04476300	1.41453800	-1.32260200
H	4.79158400	-0.06901000	-0.41486700
H	4.80733600	0.79649900	-3.01153000
H	2.32962500	1.95045300	-3.32607900
N	2.83691100	0.78406800	-0.42031400
C	0.95930400	0.75592600	1.10330800
C	2.31060700	0.46998800	0.87547300
C	0.45770100	0.37313700	2.35030200
C	3.13721100	-0.12399700	1.82888400
C	1.23368700	-0.26158800	3.32486800
H	-0.59529600	0.54661000	2.57920800
C	2.58496500	-0.48684700	3.05106400
H	4.19009000	-0.31485800	1.63249400
H	3.20453100	-0.96605400	3.80529500
C	0.61561800	-0.73531000	4.62451500
O	-0.63929800	-0.65072400	4.73021400
O	1.39728000	-1.18857900	5.50261200
O	-0.69146700	3.41326600	-1.14344200
H	-0.25319600	4.07786700	-0.59196000
H	-1.63790300	3.50930000	-0.95767800
C	-2.42470800	0.67162100	-1.92002800
C	-1.27010400	-0.09821000	-2.19166600
C	-0.83852500	-1.07193500	-1.26053300

C	-1.58556400	-1.29133600	-0.08592800
C	-2.68232100	-0.46432700	0.21823800
C	-3.12873700	0.48951200	-0.71415700
C	-3.35204500	-0.59172300	1.56032500
C	-4.36581500	1.30421200	-0.45485200
C	-2.90735500	1.68108600	-2.92374400
C	-1.20438000	-2.39189300	0.86406700
C	0.42792400	-1.85172200	-1.50080300
C	-0.57638700	0.07921900	-3.51869400
H	-2.10592600	2.02985600	-3.57976300
H	-3.68691000	1.25450000	-3.57144100
H	-3.34242700	2.56304100	-2.44272000
H	-4.12395900	2.31144400	-0.08483900
H	-4.95389500	1.43623700	-1.36875300
H	-5.02281400	0.83534900	0.28143600
H	-2.64131500	-0.89288200	2.33781200
H	-3.79015100	0.35670000	1.88383400
H	-4.16009700	-1.33687000	1.55634900
H	-0.71409300	-3.22259200	0.34938100
H	-0.51697200	-2.03887700	1.65031900
H	-2.08308900	-2.80307000	1.36984800
H	0.87709100	-2.18809200	-0.56146600
H	0.25683300	-2.74493700	-2.11735800
H	1.18667900	-1.24697900	-2.01041600
H	0.21838800	-0.65139200	-3.67969300
H	-1.28889300	-0.03400700	-4.34517100
H	-0.13011700	1.07838700	-3.62319700
Fe	-0.04283900	1.49725500	-0.52413100

5-Co-1

E=-1257.033763 (au)

G=-1256.686324 (au)

C	0.83267300	-2.08413100	-0.45396600
C	0.51919200	-1.87808500	-1.83041900
C	-0.90003800	-1.72932400	-1.93565000
C	-0.38184100	-2.08278900	0.28498600
C	-1.45238700	-1.84507100	-0.62100500
C	1.45484100	-1.87926300	-2.98888500
H	1.27236200	-2.74897600	-3.63408100
H	1.32217800	-0.98621400	-3.61485200
H	2.50037300	-1.91555400	-2.66814900
C	2.18064600	-2.23919900	0.15235400
H	2.34274900	-1.51056500	0.96005200
H	2.29660300	-3.23421200	0.60280900
H	2.98196500	-2.11135000	-0.58251700

C	-0.46755600	-2.27705700	1.75507500
H	-1.44762500	-2.00066500	2.15982500
H	-0.28875600	-3.32996000	2.01450400
H	0.29605000	-1.68955500	2.28298800
C	-2.89563500	-1.68023500	-0.30353800
H	-3.27708300	-0.72634900	-0.69698800
H	-3.49739900	-2.47223200	-0.76918800
H	-3.08756200	-1.70178200	0.77390900
C	-1.67388000	-1.59367800	-3.20192200
H	-1.07690600	-1.11831900	-3.98842600
H	-1.98527500	-2.57746800	-3.57954900
H	-2.58417100	-0.99974600	-3.05854700
C	3.43471900	1.43689000	0.50073100
C	4.03995100	1.21378000	-0.71735700
C	3.00006100	0.81952400	-1.56948000
N	1.83749900	0.80330500	-0.92140700
H	3.84988500	1.75540100	1.44735700
H	5.08819300	1.32322500	-0.95588400
H	3.03748700	0.55126600	-2.61798900
N	2.11210000	1.19030400	0.34991100
C	-0.20474700	0.80878000	0.82691200
C	1.04479200	1.23361100	1.29001100
C	-1.24681500	0.84642600	1.74542900
C	1.27493700	1.66275100	2.59612300
C	-1.05975000	1.26882200	3.06756000
H	-2.24409700	0.51656500	1.45249400
C	0.21134100	1.67472000	3.48758500
H	2.26124900	1.97492500	2.92999300
H	0.39972300	1.96704300	4.51846400
C	-2.21517100	1.17537500	3.98550600
O	-3.15352400	0.42004700	3.80063800
O	-2.22289900	1.95352700	5.08166300
H	-1.50403000	2.60374300	5.06853800
O	-1.21003900	1.54205600	-2.29947300
H	-1.21341600	2.38467700	-1.82128200
H	-2.13509800	1.25133000	-2.30929100
Co	-0.17740000	0.11486900	-1.08526700

3-Co-1

E=-1257.024264 (au)

G= -1256.676769 (au)

C	0.96148100	-2.26748900	-0.77443800
C	0.45733500	-1.90175400	-2.06442500
C	-0.95945500	-1.70611800	-1.96375400

C	-0.10202900	-2.15069600	0.14582300
C	-1.31608300	-1.81005700	-0.60019500
C	1.22832300	-1.81403200	-3.33268800
H	0.98309200	-2.65511400	-3.99493300
H	0.98427500	-0.89625700	-3.88255600
H	2.30885700	-1.83042700	-3.15871700
C	2.36506300	-2.59741500	-0.40562400
H	2.70143000	-2.01627400	0.46422300
H	2.45444500	-3.65718100	-0.13327400
H	3.06200000	-2.40946800	-1.22810000
C	-0.02005000	-2.45717500	1.59751100
H	-0.84894700	-2.01657000	2.15974800
H	-0.05060000	-3.54370500	1.75564000
H	0.92069500	-2.09430600	2.02993300
C	-2.69331000	-1.71061000	-0.04581800
H	-3.23070400	-0.84867100	-0.46269800
H	-3.27768300	-2.60571900	-0.29649700
H	-2.69071500	-1.61714700	1.04479500
C	-1.87080400	-1.40668800	-3.10077300
H	-1.38616400	-0.77448300	-3.85565900
H	-2.17357900	-2.33060800	-3.61140300
H	-2.78699400	-0.90717900	-2.76526700
C	3.43480300	1.40863000	0.81739500
C	4.07658700	1.07004000	-0.35700500
C	3.07494900	0.55436400	-1.18718700
N	1.89592200	0.58070800	-0.56787700
H	3.81405400	1.83900600	1.73455400
H	5.12739700	1.18415700	-0.58113500
H	3.14761100	0.17289800	-2.19875000
N	2.12738100	1.10323200	0.66522000
C	-0.19820600	0.73826000	0.98838700
C	0.99873400	1.25298500	1.50305100
C	-1.34193500	0.92042300	1.74876800
C	1.08474600	1.88349900	2.73979100
C	-1.29746400	1.56927500	2.99311900
H	-2.30644800	0.55836000	1.39336600
C	-0.07460400	2.03224900	3.48798600
H	2.03219200	2.25613100	3.12100000
H	0.00589700	2.49725700	4.46824900
C	-2.56950300	1.68837900	3.74266300
O	-3.56637300	1.04250600	3.47253200
O	-2.62735500	2.54840400	4.77292800
H	-1.82913500	3.09218300	4.84539200
O	-0.97462700	1.41126300	-1.73272500

H	-1.70492700	1.72072300	-1.17668200
H	-1.38111000	1.15404900	-2.57294100
Co	0.01999800	-0.17265400	-0.73064600
3-Co-2			
E= -1256.599341 (au)			
G= -1256.268312 (au)			
C	-0.46368200	-1.82214000	-1.47844100
C	-1.18437600	-0.90031500	-2.30162400
C	-2.25322000	-0.33649100	-1.53199000
C	-0.98053100	-1.71619600	-0.16854900
C	-2.11909000	-0.79848400	-0.20140300
C	-0.93867200	-0.59557800	-3.73746200
H	-1.75718300	-0.97295600	-4.36469400
H	-0.88431200	0.48846400	-3.90529700
H	-0.00760100	-1.04282100	-4.09917300
C	0.69839800	-2.66964600	-1.86217000
H	1.54944400	-2.52653900	-1.18227700
H	0.43210200	-3.73397400	-1.81782800
H	1.04289000	-2.45896400	-2.87941400
C	-0.51865500	-2.51037900	1.00054900
H	-0.81821600	-2.05858000	1.95115300
H	-0.93980200	-3.52426400	0.96434300
H	0.57358700	-2.61335800	1.00340300
C	-3.04438600	-0.49849200	0.92549100
H	-3.31027100	0.56596200	0.95346000
H	-3.98055400	-1.06240500	0.81842500
H	-2.61066500	-0.76497100	1.89418800
C	-3.28925500	0.59658900	-2.05364600
H	-2.87318400	1.29496800	-2.79011500
H	-4.09331300	0.04407600	-2.55806900
H	-3.74823000	1.18171000	-1.24960400
C	3.68552900	0.06494800	-0.48843300
C	3.68710200	-0.03941100	-1.86732700
C	2.35296600	0.13244800	-2.24841900
N	1.58471800	0.33736100	-1.17723200
H	4.49127500	-0.00523400	0.23054400
H	4.54008200	-0.21756700	-2.50620900
H	1.91049500	0.11737100	-3.23772300
N	2.41283800	0.29138700	-0.10211300
C	0.41483700	0.61597700	1.14551400
C	1.81015500	0.51917300	1.16111000
C	-0.22064100	0.91662400	2.34234900
C	2.56116500	0.67517100	2.32148500
C	0.50004700	1.08689100	3.53229800

H	-1.30470300	1.02409500	2.38016300
C	1.88930000	0.94910600	3.50667200
H	3.64645800	0.59794500	2.30491400
H	2.44731300	1.07440300	4.43075800
C	-0.21745800	1.41761300	4.82907400
O	-1.46821400	1.55735200	4.77315500
O	0.49314100	1.53050000	5.86295400
O	-1.01856600	2.32945000	-0.73025400
H	-1.15025100	2.57923600	-1.65689000
H	-0.31643400	2.90957300	-0.40093200
Co	-0.37035900	0.31749400	-0.61679900

3-Co-3

E= -1181.332291 (au)

G=-1181.010454 (au)

C	-0.85113600	-2.42007700	-1.26635800
C	-0.96774400	-1.46889500	-2.31874100
C	-1.81186900	-0.39427000	-1.87921900
C	-1.54295400	-1.90314300	-0.13397200
C	-2.15617500	-0.63909900	-0.52180900
C	-0.36002900	-1.60253800	-3.66751700
H	-0.98352400	-2.24553900	-4.30303100
H	-0.26933800	-0.63418300	-4.17108600
H	0.63255200	-2.06510400	-3.61530400
C	-0.05043900	-3.67209600	-1.31665300
H	0.10177800	-4.09130300	-0.31716600
H	-0.55619100	-4.43329900	-1.92500800
H	0.93397900	-3.50279200	-1.77061200
C	-1.75227900	-2.61409600	1.15500900
H	-2.22705800	-1.97133400	1.90198700
H	-2.41219300	-3.47699100	0.99711800
H	-0.81362200	-2.99660700	1.57180400
C	-3.04365400	0.17462100	0.35128300
H	-3.20271600	1.17701600	-0.05752200
H	-4.02581900	-0.30517900	0.45310300
H	-2.62947500	0.28113700	1.36077500
C	-2.15811200	0.78961900	-2.71223400
H	-1.25626900	1.26086700	-3.12568700
H	-2.78579900	0.49333900	-3.56220200
H	-2.70264700	1.54662700	-2.14096900
C	3.34273800	1.59940800	-0.85058000
C	3.28358400	1.41105900	-2.21966100
C	2.15349900	0.61811400	-2.43366700
N	1.56413400	0.33528600	-1.26923700
H	4.04582700	2.14925100	-0.23918200

H	3.96850000	1.79754500	-2.96033600
H	1.74077600	0.24096800	-3.36170600
N	2.29912400	0.94235900	-0.30582300
C	0.61008500	0.10158100	1.14765900
C	1.81785300	0.80541600	1.02148200
C	0.09678600	-0.02965300	2.43372800
C	2.50413200	1.34310500	2.10284000
C	0.75300800	0.50020300	3.55171100
H	-0.84197900	-0.55313300	2.60729800
C	1.95731800	1.18159300	3.37018300
H	3.44161300	1.87797500	1.96528400
H	2.46636300	1.59121200	4.23872600
C	0.16084600	0.33800000	4.94043200
O	-0.95123400	-0.24732000	5.02383900
O	0.82697100	0.80224100	5.90288500
H	-0.68715700	2.06502400	-0.37670900
H	-0.70704500	2.73484500	-0.70882400
Co	-0.06909000	-0.48228300	-0.59045400

3-Fe-1

E= -1313.11403 (au)

G=-1312.721088 (au)

C	3.27136200	1.91531900	0.01254700
C	3.52765500	1.80616100	-1.33832500
C	2.38334000	1.20438800	-1.87897700
N	1.48233300	0.96010900	-0.92818200
H	3.86933400	2.31980900	0.81813900
H	4.42021100	2.11852100	-1.86129100
H	2.17169800	0.94304800	-2.90899200
N	2.04123200	1.39793600	0.23078500
C	-0.01828200	0.70030100	1.17511900
C	1.23184500	1.30485700	1.38438300
C	-0.88664800	0.69803600	2.26163900
C	1.64620200	1.81765200	2.60903600
C	-0.50188500	1.19686400	3.51452500
H	-1.89310200	0.29017200	2.15921600
C	0.77248300	1.74709200	3.68502500
H	2.62240700	2.28164400	2.72758900
H	1.08219100	2.17259400	4.63739500
C	-1.49243600	1.14979700	4.61149300
O	-2.69375600	1.05378600	4.43444700
O	-1.03235100	1.21611100	5.87364700
H	-0.06534300	1.15719900	5.90592300
O	-1.63128900	1.72647300	-0.91152800

H	-1.65548500	1.99447100	-1.84129000
H	-1.28765600	2.49252000	-0.43012700
C	-0.14275600	-1.28657300	-2.45607900
C	0.73355100	-1.94400100	-1.54967500
C	0.31671000	-2.11846700	-0.21627400
C	-1.08063100	-1.96768800	0.11809100
C	-2.00922000	-1.59532800	-0.87993700
C	-1.52197200	-1.11349500	-2.12086300
C	-3.47315300	-1.55277800	-0.56036500
C	-2.45569100	-0.49075000	-3.11584500
C	0.32691800	-0.84132500	-3.81130500
C	-1.56910800	-2.38871900	1.47045900
C	1.29800300	-2.52997200	0.84083100
C	2.13346300	-2.29621400	-1.95125100
H	1.40173500	-0.97351600	-3.94880100
H	-0.18514700	-1.39412900	-4.60921500
H	0.10947600	0.22181900	-3.97097200
H	-3.30413600	-0.00237300	-2.62958100
H	-1.95100200	0.26468800	-3.72414300
H	-2.85678500	-1.24525600	-3.80589100
H	-3.74066000	-0.64618700	0.00170000
H	-4.08476300	-1.57417900	-1.46461300
H	-3.76549300	-2.41209300	0.05006600
H	-0.84231700	-2.19549600	2.26141000
H	-2.49977100	-1.88884100	1.74848700
H	-1.76363300	-3.47037700	1.46646300
H	1.07835800	-2.05031100	1.79919000
H	1.28232700	-3.61528500	1.00842700
H	2.31872100	-2.24522100	0.57105700
H	2.51533000	-3.12640400	-1.35213500
H	2.17374900	-2.60778700	-2.99818800
H	2.82818900	-1.45182200	-1.83044300
Fe	-0.35211600	0.01112100	-0.60669400

3-Fe-2

E=-1312.658238 (au)

G= -1312.280636 (au)

C	3.66439400	0.02792800	-0.64893300
C	3.62129300	0.14240500	-2.02511000
C	2.28954900	0.45599500	-2.32165000
N	1.56088800	0.53070700	-1.20609500
H	4.48387900	-0.19772400	0.02040700
H	4.44188900	0.01674700	-2.71692900
H	1.82835300	0.63112200	-3.28641400
N	2.41780600	0.26280900	-0.18692800

C	0.49997400	0.60893600	1.16477100
C	1.87577000	0.34839000	1.11964100
C	-0.05547700	0.79457700	2.42807300
C	2.66440600	0.21713300	2.25831000
C	0.69878400	0.67285200	3.60104000
H	-1.11487100	1.03338500	2.52635100
C	2.06005200	0.37307700	3.50042300
H	3.72970400	0.00682500	2.18318100
H	2.64861500	0.27180700	4.40880300
C	0.04050900	0.84704800	4.95632000
O	-1.21052800	1.00503500	4.97073300
O	0.79005600	0.81574400	5.96856400
O	-0.42333900	2.85962000	-0.29482600
H	-0.36762000	3.31143900	-1.14868800
H	0.36875700	3.12998800	0.19127600
C	-2.23296700	0.85150900	-1.81894800
C	-1.30001700	0.02684200	-2.52178900
C	-0.87238400	-1.20371100	-1.95466000
C	-1.12256100	-1.44294600	-0.58923400
C	-2.08900900	-0.62984100	0.11225700
C	-2.73378200	0.43250200	-0.56018400
C	-2.53195900	-1.03335600	1.48623900
C	-3.81665500	1.21046800	0.12671100
C	-2.73932200	2.11350100	-2.45336200
C	-0.45273600	-2.58878000	0.11037800
C	-0.02487800	-2.16298400	-2.73445100
C	-0.86428600	0.44784200	-3.89596900
H	-1.98551500	2.57374500	-3.09739500
H	-3.61976600	1.91361600	-3.07914300
H	-3.02783300	2.85656500	-1.70562900
H	-3.40265000	1.95135400	0.82587900
H	-4.44278800	1.74553600	-0.59045700
H	-4.47164900	0.54970500	0.70139100
H	-1.70979900	-1.41078900	2.09750800
H	-2.99125500	-0.20925200	2.03645100
H	-3.27614300	-1.83850800	1.41056200
H	0.52635100	-2.80429000	-0.32812800
H	-0.28855800	-2.37577100	1.16974900
H	-1.05423100	-3.50616800	0.05130900
H	1.04652200	-1.92485300	-2.65991000
H	-0.15895300	-3.18580700	-2.37329800
H	-0.29008300	-2.15719600	-3.79460100
H	-0.10454700	-0.21246500	-4.31728600
H	-1.71371800	0.46889600	-4.59080400

H	-0.44091900	1.45925100	-3.88091900
Fe	-0.42000200	0.70125200	-0.53869400
3-Fe-3			
E= -1237.3957253 (au)			
G=-1312.280636(au)			
C	5.06146000	-3.53431100	-3.24399900
C	5.99335600	-2.62350500	-2.78181600
C	5.29458500	-1.42084000	-2.64571400
N	4.01747400	-1.58295900	-3.00264500
H	5.15358400	-4.58407200	-3.48966100
H	7.03767800	-2.80651000	-2.57433000
H	5.65191700	-0.45474100	-2.31123900
N	3.88799900	-2.88268900	-3.36807700
C	1.62951800	-2.25334100	-3.73894200
C	2.59196000	-3.27557400	-3.78556700
C	0.35070100	-2.61206300	-4.16196200
C	2.32724300	-4.57299900	-4.20542400
C	0.03166900	-3.90694500	-4.58963200
H	-0.45200700	-1.87909700	-4.17673200
C	1.03146600	-4.88041800	-4.60285800
H	3.10796000	-5.33074500	-4.22352000
H	0.78696700	-5.88713600	-4.93170100
C	-1.38271700	-4.24481100	-5.02516500
O	-2.22634500	-3.30832800	-5.01835100
O	-1.61023800	-5.43824600	-5.35776000
H	2.13897200	-2.16233300	-0.96001400
H	2.43270300	-2.48129500	-0.35018400
Fe	2.34964700	-0.53924300	-3.05019900
C	0.81034800	0.84606400	-3.68400400
C	0.59379400	0.46734500	-2.30632600
C	1.57246600	0.79776600	-1.33408100
C	2.87017300	1.17717100	-1.75336600
C	3.10540200	1.51062100	-3.13440200
C	2.02599900	1.47696100	-4.05256000
C	4.44834800	1.96038500	-3.62996800
C	2.24204800	1.90231800	-5.47346200
C	-0.26715700	0.70725700	-4.71767400
C	3.94737500	1.27584800	-0.71369300
C	1.28843000	0.57923600	0.12099700
C	-0.69180400	-0.15315600	-1.84616000
H	0.10175800	0.20541200	-5.61915900
H	-1.14013500	0.16063600	-4.36102600
H	-0.61683800	1.70224500	-5.02096200
H	1.31035000	2.23457700	-5.93706700

H	2.95839700	2.72494000	-5.53771900
H	2.63391100	1.07513600	-6.08184900
H	4.45496400	3.04595100	-3.79242600
H	5.26014200	1.73156100	-2.93926100
H	4.69068000	1.48722100	-4.58752400
H	3.96361900	0.38201000	-0.07877700
H	4.94455500	1.39913000	-1.13615300
H	3.76752600	2.13726000	-0.05783500
H	0.23586900	0.76863700	0.34663500
H	1.51484100	-0.44784100	0.43653900
H	1.88620500	1.25056800	0.74240700
H	-1.36896200	0.61144600	-1.44299600
H	-1.22513000	-0.67163700	-2.64360100
H	-0.50946800	-0.88399400	-1.05169600

CO₂

E= -188.5554294 (au)

G=-188.5650394 (au)

C	1.57421700	-0.48874900	2.67950700
O	2.73832500	-0.48874900	2.67950700
O	0.41010800	-0.48874900	2.67950700

H₂

E= -1.1677429 (au)

G=-1.1691369(au)

H	2.89352000	-0.62348200	-1.72757400
H	2.15261700	-0.62348200	-1.72757400

H₂O

E= -76.4318392 (au)

G=-76.4286682(au)

O	-2.30362400	-1.80475300	0.00000000
H	-1.34422300	-1.76003800	0.00000000
H	-2.58176600	-0.88541300	0.00000000

H₃O⁺

E= -76.8456809 (au)

G=-76.8291223(au)

O	0.11438700	-0.36130000	0.41342600
H	1.02707100	-0.44554300	0.07085300
H	-0.26881000	0.47134400	0.07095200
H	-0.41433900	-1.11111900	0.07171700

HCO₃⁻

E= -264.5374665 (au)

G=-264.5414162(au)

C	-1.98424700	-1.43523800	-0.22787900
O	-1.42822900	-0.47092400	-0.79626200
O	-1.52084100	-2.54431100	0.09917200
O	-3.33291100	-1.26218300	0.10295500
H	-3.56641700	-0.37334400	-0.19860700

HCOO⁻

E= -189.2853509 (au)

G=-189.2884069(au)

C	-0.81172900	-2.01721800	0.21375400
H	-0.27432600	-1.24774300	0.83813200
O	-0.14478000	-3.03154300	-0.10051400
O	-2.00194500	-1.75151100	-0.07772000

OH⁻

E= -75.9363997 (au)

G=-75.9437947 (au)

O	0.21776400	0.10874400	3.69029900
H	-0.10320100	1.01512300	3.69029900