

Theoretical Study of Reversible Hydrogenation of CO₂ to Formate Catalyzed by Ru(II)–PN⁵P, Fe(II)–PN⁵P, and Mn(I)–PN⁵P Complexes: The Effect of the Transition Metal Center

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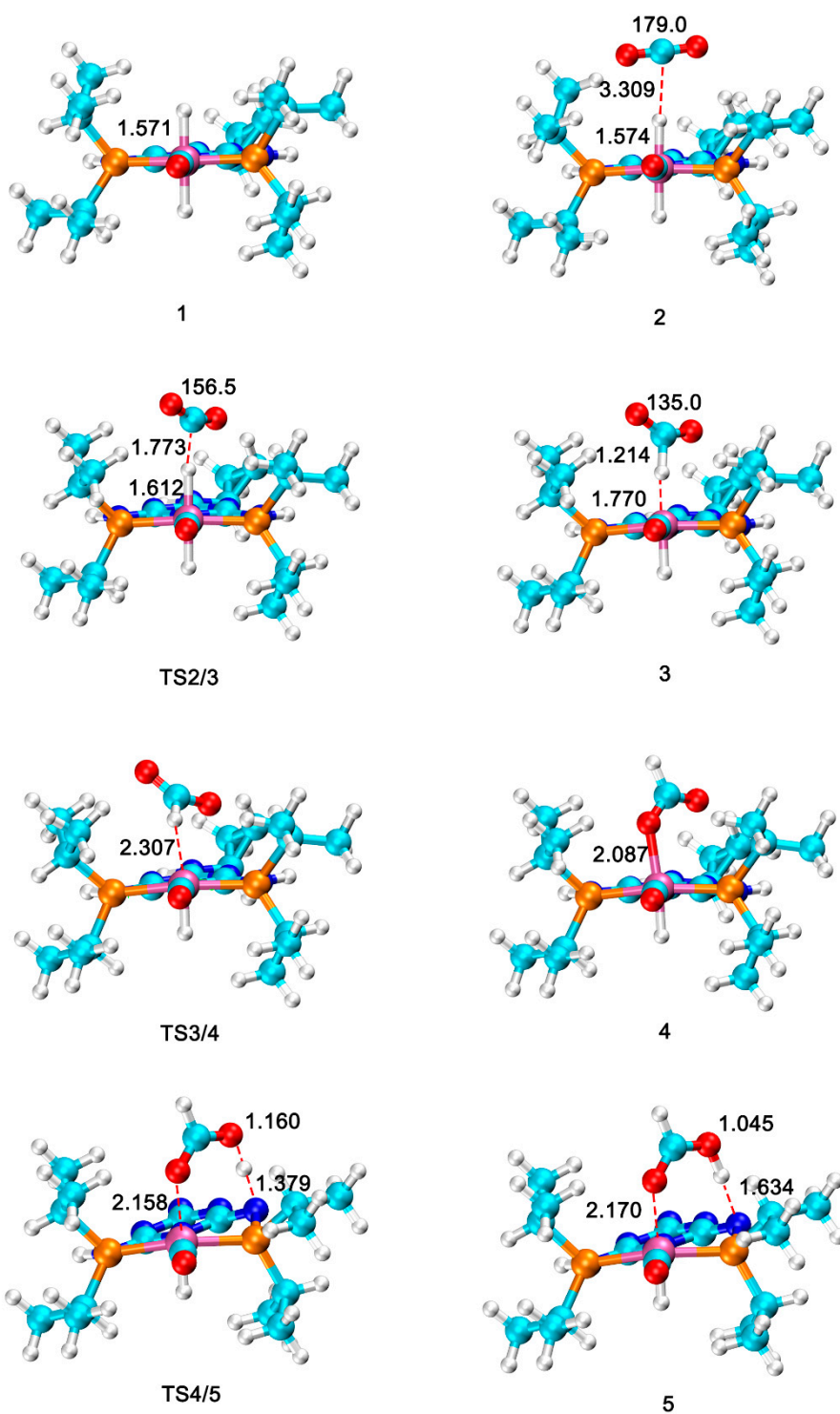


Figure S1. The optimized geometries of all species in CO_2 hydrogenation to formic acid catalyzed by the $\text{Fe(II)}\text{-PN}^5\text{P}$ complex. The R_1 groups in the TS4/5 and complex 5 have been omitted for clarity. The bond distances are in angstrom (Å), and the bond angles are in degree ($^\circ$). (Fe: mauve; C: cyan; P: orange; O: red; N: blue; H: white)

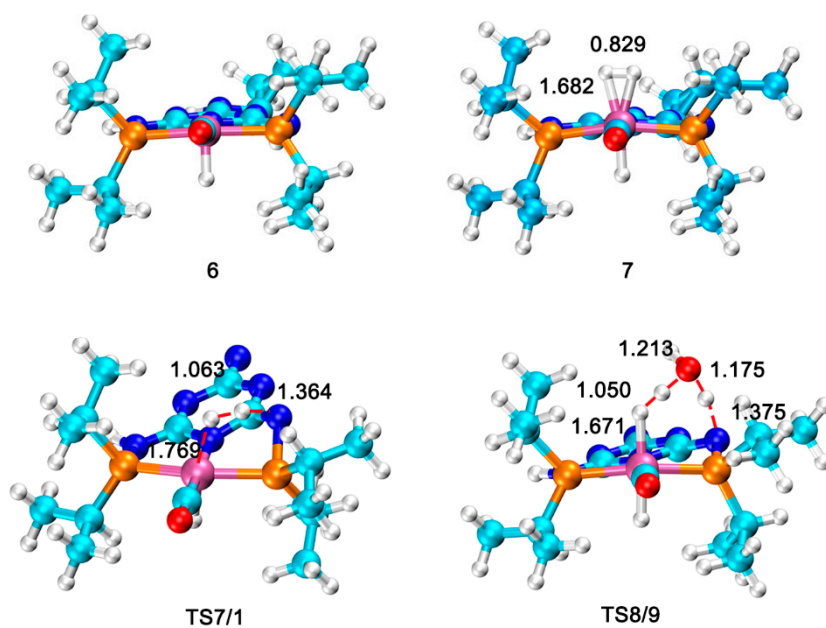


Figure S2. The optimized geometries of selected species in the regeneration of Fe(II)-PN⁵P complexes. The R₁ groups in the TS7/1 and TS8/9 have been omitted for clarity. The distances are in angstrom (Å). (Fe: mauve; C: cyan; P: orange; O: red; N: blue; H: white)

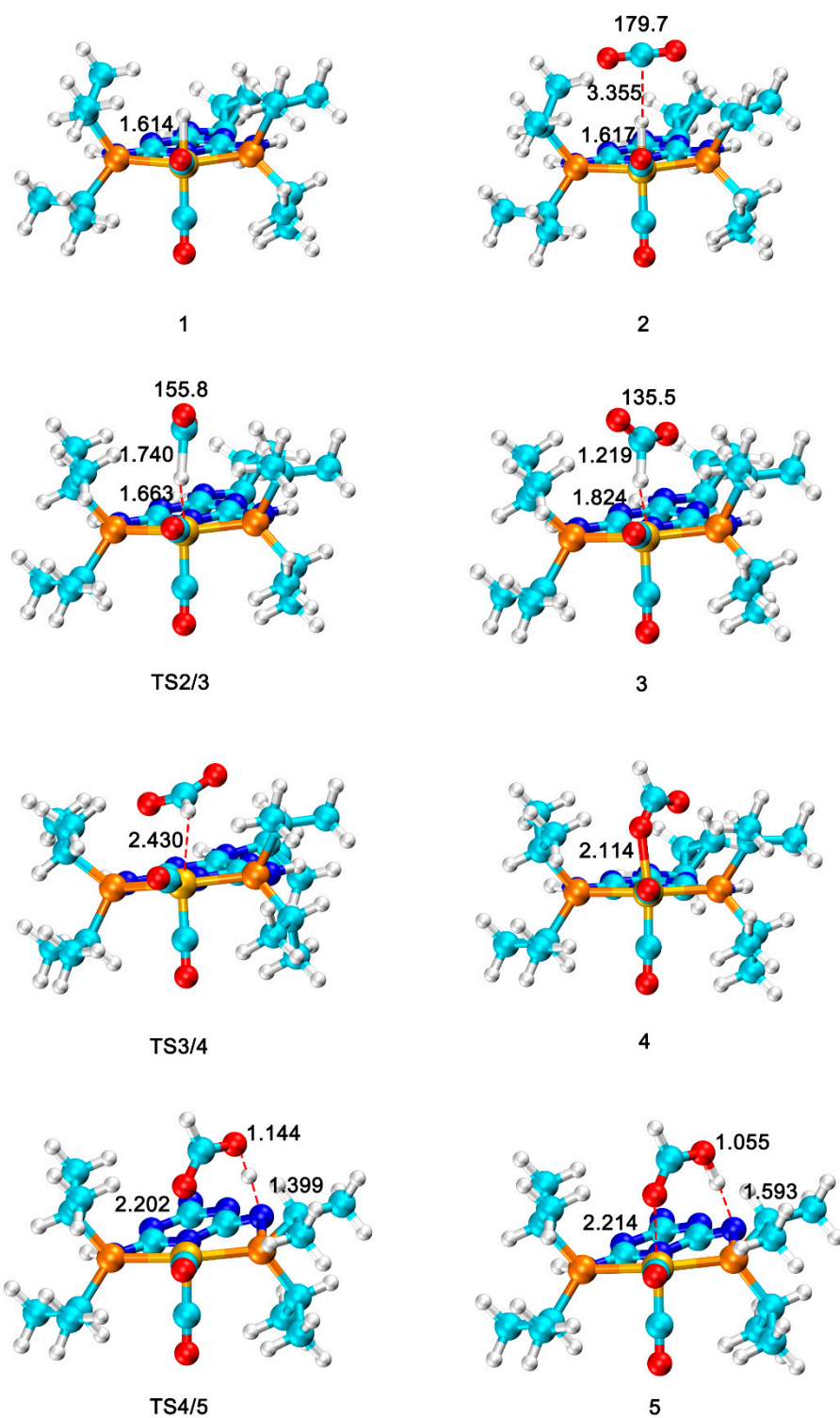


Figure S3. The optimized geometries of all species in CO₂ hydrogenation to formic acid catalyzed by the Mn(I)-PN⁵P complex. The R₁ groups in the TS4/5 and complex 5 have been omitted for clarity. The bond distances are in angstrom (Å), and the bond angles are in degree (°). (Mn: yellow; C: cyan; P: orange; O: red; N: blue; H: white)

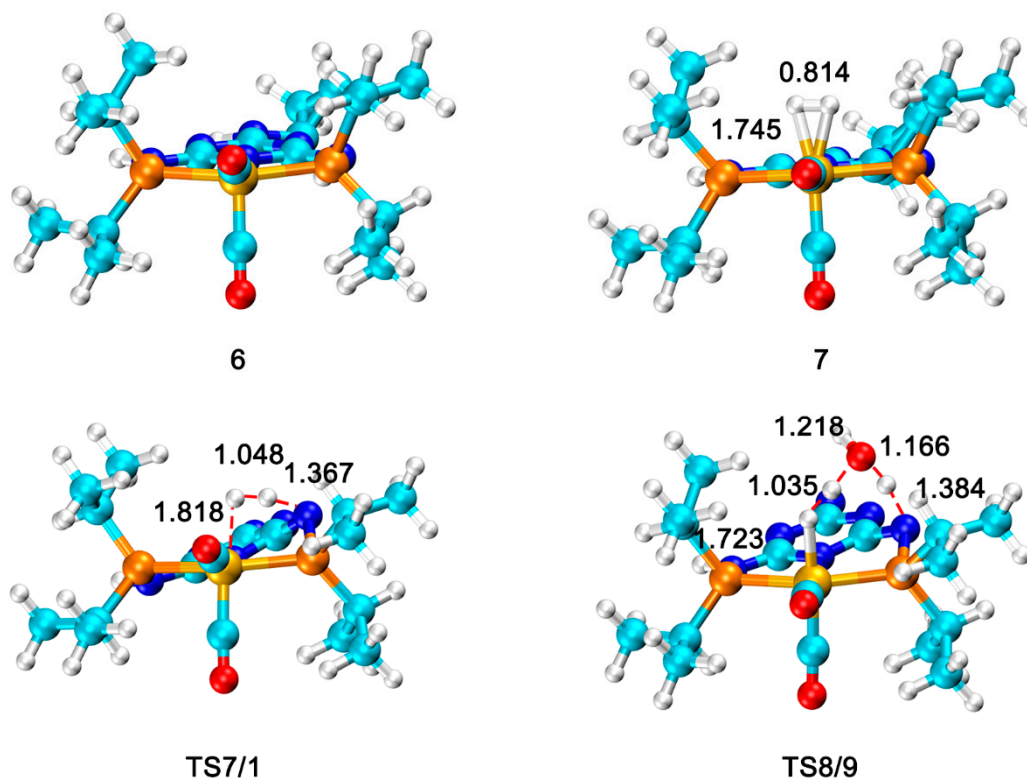


Figure S4. The optimized geometries of selected species in the regeneration of Mn(I)-PN⁵P complexes. The R₁ groups in the **TS7/1** and **TS8/9** have been omitted for clarity. The distances are in angstrom (Å). (Mn: yellow; C: cyan; P: orange; O: red; N: blue; H: white)

Table S1. Cartesian coordinates for optimized geometries of all the species of the three complexes in mixed solution (H₂O : THF = 1 : 1).

Ru-1

P	-0.09328200	2.35037300	-0.00684900
P	1.77843300	-1.85219500	0.00441900
N	-0.76149600	-0.46660100	-0.07724200
C	-1.88624500	0.28607000	-0.09483800
C	-3.19768400	-1.54776100	-0.19887200
C	-0.95399000	-1.80821600	-0.12035300
C	-0.22780000	3.41646900	1.54716800
C	1.11005300	4.05683400	1.94642700
C	-1.36141600	4.44986900	1.54048300
C	-0.16955600	3.54676500	-1.46495900
C	1.20800500	4.17884300	-1.71856300
C	-0.70224700	2.86926000	-2.73349800
C	2.51153700	-2.74823400	1.49543400
C	3.89726200	-2.17967100	1.83951400
C	1.57555300	-2.68921300	2.70889700
C	2.59283200	-2.61918700	-1.51867200
C	3.96932000	-2.01220400	-1.82668700
C	2.63655800	-4.15278500	-1.53482700
H	-0.46440800	2.63509400	2.29007800
H	-0.87584100	4.33965400	-1.16687200
H	2.62586800	-3.80218600	1.19057000
H	1.89090900	-2.27657900	-2.29880600
H	1.03370700	4.45588900	2.97135800
H	1.37131500	4.90151300	1.28938900
H	1.94056000	3.33539500	1.92743500
H	-2.33827300	4.00899500	1.28795500
H	-1.16278100	5.27544000	0.83847300
H	-1.45789800	4.89405800	2.54524600
H	-0.04493500	2.04169700	-3.04476800
H	-0.73740000	3.60517500	-3.55390100
H	-1.71698900	2.46793600	-2.59540500
H	1.60510300	4.70561800	-0.83873500
H	1.94288800	3.41511300	-2.02003900
H	1.13206100	4.91337800	-2.53715000
H	4.28614800	-2.31526000	-2.83838600
H	3.95273700	-0.91270000	-1.79407300
H	4.74135700	-2.36762400	-1.12598500
H	1.65182900	-4.60758600	-1.34451300
H	3.34961700	-4.55285200	-0.79647000

H	2.96633200	-4.50045600	-2.52797500
H	4.61208300	-2.26734000	1.00852100
H	4.31923800	-2.73003300	2.69651700
H	3.83210600	-1.11653000	2.12276600
H	1.39499200	-1.64672200	3.01580300
H	2.03901200	-3.22278000	3.55533300
H	0.60251500	-3.16004800	2.50431200
C	2.87482000	1.15290000	0.09543800
O	3.94442300	1.63019800	0.14666200
N	-2.14620500	-2.40157100	-0.18256400
N	-3.12945400	-0.20094200	-0.15910500
N	0.17087800	-2.57735600	-0.09912400
N	-1.70937300	1.63568800	-0.04325900
H	-2.56563800	2.18257400	-0.08649300
H	0.00582600	-3.58068100	-0.10831500
H	1.02521700	0.36487400	1.69882500
N	-4.42339200	-2.12150900	-0.25753900
H	-4.42199500	-3.12514900	-0.40668100
C	-5.65195700	-1.39868900	-0.42205100
H	-5.72729400	-0.82153500	-1.34962600
C	-6.34986500	-0.83116100	0.79304100
H	-5.86106900	-0.98181700	1.75754800
H	-6.87069500	0.12164700	0.67584800
C	-6.90659600	-2.05163800	0.09535800
H	-7.81299200	-1.94802900	-0.50407500
H	-6.79511400	-3.01455000	0.59990500
H	1.20035400	0.35200400	-1.67683400
Ru	1.19728900	0.40537900	0.01508100

Ru-2

P	-0.09452500	2.22647400	-0.58037200
P	1.46383600	-2.09665900	-0.26312000
N	-0.96175100	-0.51431000	-0.22105500
C	-2.02481200	0.32318800	-0.21254000
C	-3.46787200	-1.39407700	0.03773400
C	-1.25425500	-1.83197000	-0.09076700
C	0.03798800	3.48313300	0.82270200
C	1.45231900	4.06577700	0.96143200
C	-1.02612800	4.58775000	0.82205000
C	-0.26263700	3.23844200	-2.16598400
C	1.11544400	3.70768700	-2.65983000
C	-1.00160800	2.46489000	-3.26509500
C	2.31341200	-2.89606000	1.22129100

C	3.73369800	-2.33416300	1.39421000
C	1.49920300	-2.72514500	2.50980500
C	2.03172200	-3.07988100	-1.77289700
C	3.43216600	-2.66960700	-2.25192000
C	1.90570800	-4.60395100	-1.65192700
H	-0.13694600	2.82210000	1.68792800
H	-0.86339000	4.12370500	-1.89660700
H	2.38202600	-3.97209200	0.98892700
H	1.30012300	-2.72144700	-2.51774700
H	1.55074900	4.55864800	1.94243700
H	1.65860400	4.82683800	0.19226700
H	2.22997900	3.28997500	0.89577000
H	-2.05153800	4.18990200	0.76800600
H	-0.88607700	5.29658700	-0.00965100
H	-0.95379900	5.16642800	1.75808500
H	-0.45730800	1.54595600	-3.53523200
H	-1.07755800	3.09472400	-4.16703800
H	-2.02136700	2.18433800	-2.96277000
H	1.65854500	4.30365200	-1.91209800
H	1.74913500	2.85041800	-2.93895400
H	0.99006100	4.33770700	-3.55584400
H	3.61071200	-3.08000100	-3.25951400
H	3.54886400	-1.57675000	-2.30762400
H	4.22142600	-3.06930600	-1.59547500
H	0.89968900	-4.92372900	-1.33871900
H	2.63776500	-5.02322300	-0.94330900
H	2.10150700	-5.06670900	-2.63351500
H	4.35102300	-2.44456800	0.49079300
H	4.24462600	-2.87004800	2.21114300
H	3.70205300	-1.26646300	1.66094500
H	1.37100400	-1.65935300	2.75605400
H	2.03395800	-3.20531900	3.34618400
H	0.50263700	-3.18477000	2.43785100
C	2.77323300	0.80217600	-0.65221000
O	3.87277600	1.19038500	-0.77545200
N	-2.48526600	-2.32624200	0.04306200
N	-3.29908000	-0.06184700	-0.09048600
N	-0.19368300	-2.68727300	-0.10496000
N	-1.74794200	1.65066300	-0.34056800
H	-2.56384700	2.25682300	-0.36670400
H	-0.43198700	-3.66785300	0.01977500
H	1.08277600	0.37187600	1.23024300
N	-4.73030000	-1.86586800	0.17817000
H	-4.81653100	-2.87638200	0.14355800

C	-5.91489400	-1.06711400	0.04493300
H	-6.05644700	-0.61066100	-0.94048800
C	-6.42419100	-0.28977900	1.23673500
H	-5.83803600	-0.35672400	2.15528100
H	-6.88505400	0.68167200	1.04523600
C	-7.14484900	-1.53682400	0.77677500
H	-8.10471700	-1.43246700	0.26748700
H	-7.04539300	-2.43299100	1.39419700
H	0.83021500	-0.04560900	-2.11527100
Ru	1.04937300	0.19459700	-0.45347700
C	2.13919300	1.39383400	3.78922100
O	1.18967400	2.05755300	3.93638700
O	3.09624200	0.73705600	3.66385300

Ru-3

P	-0.13327500	2.33545000	-0.33914600
P	1.69222500	-1.92811500	-0.25177400
N	-0.82220600	-0.48322700	-0.24140700
C	-1.94012800	0.28664900	-0.30879000
C	-3.27647600	-1.53239700	-0.31339200
C	-1.03671500	-1.82706000	-0.25994000
C	-0.25904500	3.50725800	1.12664400
C	1.09430700	4.13294900	1.49781000
C	-1.35940400	4.56923400	1.00554700
C	-0.10619300	3.37376900	-1.90768000
C	1.30848700	3.91499100	-2.16737000
C	-0.62711700	2.58859700	-3.11850600
C	2.59509500	-2.84604000	1.12741500
C	3.79251000	-2.00596000	1.60691000
C	1.68578500	-3.21165100	2.30802600
C	2.40406900	-2.58863900	-1.86442700
C	3.83981000	-2.09271500	-2.09164400
C	2.29363500	-4.10806500	-2.04104300
H	-0.53189500	2.79136100	1.92075000
H	-0.78553300	4.22220100	-1.71860100
H	2.96633800	-3.77619200	0.66632400
H	1.74648600	-2.09745800	-2.60203800
H	1.00992200	4.61798400	2.48404400
H	1.40348600	4.90898700	0.77976700
H	1.89682800	3.38291900	1.56284600
H	-2.34531100	4.13663100	0.77484600
H	-1.12375500	5.32350800	0.23810900
H	-1.45771500	5.10029800	1.96676300

H	-0.00096600	1.70412600	-3.31845700
H	-0.59467900	3.23526100	-4.01057800
H	-1.66513200	2.25248000	-2.98189300
H	1.70034200	4.50630500	-1.32738500
H	2.01373300	3.09243700	-2.36650300
H	1.29310100	4.56896700	-3.05426100
H	4.15551000	-2.34355500	-3.11739500
H	3.92766300	-1.00251500	-1.97063800
H	4.55194800	-2.57697500	-1.40419000
H	1.26122500	-4.47182300	-1.92685400
H	2.93582200	-4.65539300	-1.33280200
H	2.62377100	-4.38014400	-3.05701500
H	4.44309000	-1.67555200	0.78321600
H	4.40903800	-2.61108800	2.29184700
H	3.43976200	-1.11982200	2.15738700
H	1.29879600	-2.30891500	2.80434800
H	2.27866100	-3.76889700	3.05242900
H	0.83863700	-3.84661300	2.01248100
C	2.82961500	1.07475000	-0.15096200
O	3.90423700	1.52500200	-0.16035100
N	-2.23492300	-2.40075400	-0.28939000
N	-3.18616900	-0.18562700	-0.34303600
N	0.07482400	-2.61846000	-0.25407700
N	-1.74844000	1.63402700	-0.35502500
H	-2.60059100	2.18562700	-0.41797000
H	-0.11340200	-3.61756000	-0.27310400
H	0.96151600	0.33230100	1.71328900
N	-4.50694700	-2.08808400	-0.31546000
H	-4.52462400	-3.09966100	-0.39591100
C	-5.73439300	-1.35699300	-0.45762200
H	-5.85402300	-0.84388500	-1.41731000
C	-6.35208100	-0.69745600	0.75388200
H	-5.81064200	-0.79095400	1.69721500
H	-6.86382800	0.25504100	0.60066000
C	-6.96545800	-1.95170900	0.17415700
H	-7.90310800	-1.87311700	-0.37912900
H	-6.83751100	-2.88017000	0.73609000
C	0.71817800	0.44788200	2.89886600
O	-0.45961800	0.75312900	3.12242500
O	1.71190000	0.22406900	3.59646600
H	1.19194700	0.33197000	-1.75846500
Ru	1.12656400	0.35442600	-0.16670300

Ru-4

P	-0.10514800	2.32587300	-0.28401500
P	1.75098700	-1.91511800	-0.14897000
N	-0.77518600	-0.49490500	-0.22415900
C	-1.88950700	0.26504600	-0.36674800
C	-3.21517600	-1.56194200	-0.37259300
C	-0.97826300	-1.83553000	-0.22111600
C	-0.37274000	3.49236200	1.17028000
C	0.95623400	3.91866800	1.81359900
C	-1.28842600	4.69076200	0.89232500
C	0.01482700	3.40075000	-1.82397400
C	1.38252800	4.09766700	-1.89014400
C	-0.27103800	2.61000900	-3.10625700
C	2.64554100	-2.84121600	1.22984100
C	3.87237500	-2.02825300	1.67712300
C	1.73649200	-3.15967000	2.42455300
C	2.46563800	-2.57749800	-1.76159900
C	3.89490800	-2.06968900	-2.00289600
C	2.36914100	-4.09798100	-1.93629200
H	-0.87539300	2.80228300	1.86680100
H	-0.76792600	4.16981100	-1.70997600
H	2.98810400	-3.78975300	0.78347300
H	1.79917900	-2.09399400	-2.49646700
H	0.75066200	4.44314000	2.76182100
H	1.52847200	4.61228700	1.17659000
H	1.58984500	3.04808700	2.03737400
H	-2.25659500	4.39708300	0.45610400
H	-0.81879400	5.42692200	0.22020000
H	-1.50685900	5.20870400	1.84118200
H	0.48326300	1.82377400	-3.26553200
H	-0.24103300	3.29389000	-3.97057200
H	-1.26270100	2.13442800	-3.08402000
H	1.57752300	4.73330400	-1.01371100
H	2.20034500	3.36328300	-1.96845400
H	1.42473600	4.74385600	-2.78211300
H	4.19986500	-2.30711600	-3.03529300
H	3.97749000	-0.98044500	-1.86988900
H	4.61892300	-2.55714500	-1.33018500
H	1.34209900	-4.47256900	-1.80850600
H	3.02553900	-4.63744900	-1.23486100
H	2.68970200	-4.36929800	-2.95570800
H	4.54212600	-1.77043500	0.84310500
H	4.45821600	-2.61630600	2.40261600

H	3.55510100	-1.09410700	2.16482500
H	1.34243700	-2.23544500	2.87211700
H	2.32470200	-3.68999000	3.19218800
H	0.88904900	-3.80369300	2.14873000
C	2.85792500	1.09765700	-0.05536800
O	3.93141700	1.55798200	-0.09190800
N	-2.17161600	-2.42253500	-0.28545800
N	-3.13264400	-0.21754000	-0.44061500
N	0.13835400	-2.61996700	-0.15422600
N	-1.70404100	1.60878600	-0.46765200
H	-2.55734000	2.15350900	-0.56324900
H	-0.04203800	-3.62039000	-0.17026700
N	-4.44433000	-2.12717900	-0.40169200
H	-4.45203800	-3.13984500	-0.46588900
C	-5.66609100	-1.40853700	-0.62558200
H	-5.74405600	-0.92518900	-1.60514200
C	-6.34373200	-0.71508800	0.53383200
H	-5.84703500	-0.77578200	1.50409200
H	-6.85290200	0.22876300	0.32729500
C	-6.92334800	-1.99062300	-0.03449900
H	-7.83454700	-1.93459400	-0.63299800
H	-6.81787900	-2.90054300	0.56142600
H	0.34121400	0.24994700	4.05256500
C	0.08519500	0.40655300	2.96861100
O	1.09428800	0.26195700	2.19507500
O	-1.08680000	0.68986800	2.67314200
H	1.23381300	0.34500200	-1.65591900
Ru	1.16880100	0.36474800	-0.05844100

Ru-5

P	-0.19590200	2.27863400	-0.26530700
P	1.88520900	-1.84340700	-0.13371900
N	-0.68115200	-0.49398900	-0.27037700
C	-1.83822500	0.26277300	-0.17176200
C	-3.07146100	-1.63810300	-0.46010800
C	-0.82677500	-1.82733700	-0.45370600
C	-0.18064800	3.75852000	0.90154300
C	1.11681500	4.57666000	0.83628100
C	-1.42351200	4.65150100	0.77618400
C	-0.35438000	2.99839400	-2.00599500
C	1.00819900	3.41308400	-2.58046600
C	-1.06866200	2.02312400	-2.95088300
C	2.49311500	-2.92415800	1.28490100

C	3.84856600	-2.42104300	1.80590600
C	1.45611000	-2.98351000	2.41522600
C	2.88007800	-2.33042700	-1.66102200
C	4.22119500	-1.59060600	-1.76401500
C	3.04599500	-3.84174600	-1.86300600
H	-0.21445300	3.26666500	1.88807600
H	-0.98671700	3.89519000	-1.89264300
H	2.62362500	-3.93800300	0.86963100
H	2.21733800	-1.94008300	-2.45288500
H	1.15209200	5.27878900	1.68583800
H	1.17231000	5.18025000	-0.08347900
H	2.01500900	3.94284000	0.88681900
H	-2.35085000	4.06240800	0.81049600
H	-1.41463100	5.22889600	-0.16276400
H	-1.44299100	5.37824100	1.60570700
H	-0.49380100	1.08976500	-3.06900600
H	-1.16793900	2.48241600	-3.94871500
H	-2.07596000	1.76698200	-2.59276300
H	1.54379600	4.12795500	-1.93953300
H	1.65560400	2.53276900	-2.71826200
H	0.86719100	3.88973400	-3.56513500
H	4.65189700	-1.75296600	-2.76583900
H	4.10499300	-0.50710200	-1.61766100
H	4.95510800	-1.96162800	-1.03167200
H	2.08720600	-4.38173600	-1.82105400
H	3.72489400	-4.28394900	-1.11651800
H	3.48352800	-4.03364700	-2.85671200
H	4.63475300	-2.44217200	1.03742000
H	4.18389800	-3.06150900	2.63811100
H	3.77096500	-1.38952000	2.18709400
H	1.27317100	-1.98308200	2.83567600
H	1.83284400	-3.63298200	3.22258700
H	0.49419500	-3.39454700	2.07478300
C	2.84601500	1.24175900	0.26049900
O	3.88338000	1.77110000	0.36709600
N	-1.99278300	-2.45739600	-0.57270100
N	-3.05824400	-0.31107400	-0.26102400
N	0.32561700	-2.56853900	-0.50739200
N	-1.75067000	1.58532400	0.08690800
H	-1.58116700	1.36034900	1.72835600
H	0.18054800	-3.57308800	-0.57615800
N	-4.27635600	-2.25841100	-0.55849800
H	-4.23556000	-3.23188300	-0.84128900
C	-5.53577300	-1.57594000	-0.62382800

H	-5.65353600	-0.89987800	-1.47761000
C	-6.23477500	-1.17965100	0.65631100
H	-5.72298100	-1.41623600	1.59121100
H	-6.79728400	-0.24343000	0.65518300
C	-6.75322500	-2.33703500	-0.16759600
H	-7.67466200	-2.20588400	-0.73816600
H	-6.59249600	-3.34501400	0.22294400
H	-0.27698400	0.44386400	4.16529400
C	-0.33575800	0.64059900	3.07875700
O	0.61400200	0.37290700	2.34471100
O	-1.48724100	1.16776400	2.74323800
H	1.49942500	0.43328500	-1.50979300
Ru	1.21396900	0.41506400	0.03908500

Ru-6

P	0.17817200	2.32219900	0.04906300
P	-1.74147400	-1.89385300	-0.00957300
N	0.76598300	-0.43016400	0.02168500
C	1.90168700	0.40283300	0.11904200
C	3.21339000	-1.48091400	0.15439800
C	0.98194800	-1.76894900	0.05287100
C	0.27459600	3.34631800	-1.53784300
C	-1.08654400	3.78069000	-2.09793500
C	1.26672600	4.51317100	-1.44806300
C	0.08999300	3.52556800	1.48919500
C	-1.22147900	4.32060500	1.53316500
C	0.34069100	2.79295000	2.81410300
C	-2.48033100	-2.70854200	-1.53518100
C	-3.96908500	-2.36743200	-1.69243400
C	-1.67798700	-2.28916900	-2.77577100
C	-2.52312000	-2.67606500	1.51483900
C	-3.81597700	-1.96834700	1.94587300
C	-2.69509300	-4.19795100	1.42588500
H	0.69665100	2.59125500	-2.22606600
H	0.92896600	4.22130400	1.31680800
H	-2.37413900	-3.79794100	-1.39448500
H	-1.74876100	-2.45299500	2.27002900
H	-0.95109400	4.23028800	-3.09622800
H	-1.57568200	4.53718300	-1.46413100
H	-1.77603400	2.92928600	-2.20178400
H	2.23483400	4.18652000	-1.04049100
H	0.87949200	5.32807700	-0.81473100
H	1.44358300	4.93513000	-2.45199100

H	-0.48750100	2.10499900	3.05122800
H	0.41768600	3.52399100	3.63627800
H	1.27329000	2.21053600	2.78346800
H	-1.36577900	4.94959800	0.64243000
H	-2.09386400	3.65270900	1.62411700
H	-1.22236200	4.98911400	2.41052000
H	-4.13493900	-2.35668700	2.92712600
H	-3.67163400	-0.88207400	2.04178500
H	-4.64271300	-2.14465000	1.24026200
H	-1.76028200	-4.71273200	1.15369500
H	-3.46936600	-4.48067900	0.69522100
H	-3.00938300	-4.59137600	2.40661300
H	-4.58230700	-2.75954000	-0.86817000
H	-4.35105600	-2.81077700	-2.62660700
H	-4.12793600	-1.27803600	-1.75081600
H	-1.75487300	-1.20241000	-2.95010800
H	-2.07693600	-2.80088200	-3.66677100
H	-0.61292600	-2.54911600	-2.68429000
C	-2.85324600	1.15800300	-0.10214800
O	-3.91583300	1.64641600	-0.11280100
N	2.17021200	-2.35956100	0.11016100
N	3.14883300	-0.15204400	0.17292900
N	-0.13036500	-2.57636200	0.02356800
N	1.78124700	1.71604400	0.16266900
H	0.06520000	-3.57440600	0.02454200
N	4.44224200	-2.07272200	0.18285800
H	4.42347000	-3.07444500	0.34287500
C	5.66352800	-1.36760000	0.43906500
H	5.69494200	-0.81728300	1.38603900
C	6.43168900	-0.76740800	-0.71630500
H	5.99456600	-0.88246900	-1.71014700
H	6.95543500	0.17509200	-0.54137700
C	6.93998000	-2.01582800	-0.02973100
H	7.81478900	-1.93992000	0.61904700
H	6.84838600	-2.96078800	-0.57103900
H	-1.32883400	0.43505600	1.50694500
Ru	-1.17527200	0.39101400	-0.03965900

Ru-7

P	-0.16643300	2.33603100	-0.01518300
P	1.73223200	-1.89324900	0.00637700
C	-0.25742500	3.55312500	1.42413400
C	1.08102000	4.20760400	1.78986500

C	-1.37745100	4.59111800	1.27081500
C	0.00069500	3.37698200	-1.57853300
C	1.44749600	3.82069100	-1.83617800
C	-0.57469100	2.64229500	-2.79524000
C	2.57753200	-2.88928300	1.36217200
C	3.98535900	-2.33931300	1.64034600
C	1.73841400	-2.93124900	2.64550600
C	2.42919000	-2.48711000	-1.64201100
C	3.76326800	-1.82393300	-2.01127400
C	2.48981700	-4.01237500	-1.79378200
H	-0.53993100	2.86628200	2.24315200
H	-0.61947600	4.26987500	-1.38983900
H	2.66473300	-3.91650700	0.97007100
H	1.65562200	-2.09482000	-2.32537200
H	0.98859700	4.72724700	2.75829400
H	1.38142600	4.96238800	1.04553500
H	1.89560100	3.47246700	1.87972000
H	-2.32675700	4.11559500	0.98527300
H	-1.12550200	5.35118500	0.51315200
H	-1.52837400	5.12124900	2.22625900
H	-0.00858200	1.71951200	-3.00622600
H	-0.50608000	3.28906500	-3.68614200
H	-1.62883500	2.37135300	-2.64275400
H	1.89022100	4.35400100	-0.98225700
H	2.08908700	2.95453600	-2.06377200
H	1.48021200	4.49989100	-2.70458000
H	4.00015600	-2.04480800	-3.06505500
H	3.72650300	-0.73063700	-1.89646400
H	4.59699900	-2.20977700	-1.40419200
H	1.53391400	-4.50110600	-1.54926900
H	3.27690400	-4.45680400	-1.16417200
H	2.72653600	-4.26629900	-2.84011300
H	4.62818300	-2.33898500	0.74830400
H	4.47927500	-2.96178700	2.40396400
H	3.93838600	-1.30811100	2.02750100
H	1.62043100	-1.92743400	3.08655100
H	2.25010900	-3.55897700	3.39316500
H	0.73681600	-3.35143000	2.47531300
C	2.87025100	1.15817200	0.24390500
O	3.93269900	1.63449500	0.21525100
N	-4.45428200	-2.03835300	-0.20275700
H	-4.43987100	-3.03249100	-0.40499000
C	-5.67154900	-1.31854700	-0.43551400
H	-5.70293900	-0.73949500	-1.36537500

C	-6.43320100	-0.74992200	0.73992900
H	-5.99356500	-0.89775800	1.72831600
H	-6.95265300	0.20011900	0.59576900
C	-6.95033700	-1.97397200	0.01714200
H	-7.82676900	-1.87349500	-0.62608300
H	-6.86217700	-2.93561700	0.52881100
C	-0.99355300	-1.74957200	-0.03554800
C	-3.22134200	-1.45418700	-0.15382900
C	-1.89879800	0.41804600	-0.04676500
H	-0.07869000	-3.55540500	-0.10149600
N	0.11874100	-2.56114600	-0.02041700
N	-0.77937700	-0.42105200	0.05879600
N	-1.76547500	1.73353800	-0.07057000
N	-3.14929800	-0.12450500	-0.12793300
N	-2.18243800	-2.33634200	-0.14195300
H	1.16617500	-0.01020300	2.00547800
H	0.83227100	0.76063000	1.97749900
H	1.24474700	0.41976600	-1.37553900
Ru	1.17830600	0.39869800	0.22987900

Ru-8

P	0.38408500	2.21910800	0.01954200
P	-2.19189000	-1.64040400	-0.01026400
C	0.77434400	3.31964500	-1.46539700
C	-0.35321500	4.28964600	-1.83955500
C	2.13189900	4.02870600	-1.35976500
C	0.34362200	3.34762900	1.52671100
C	-1.01566500	4.03946400	1.70021800
C	0.73990200	2.58580200	2.79746600
C	-3.18653000	-2.52189300	-1.34035600
C	-4.57818800	-1.89381500	-1.50616200
C	-2.43168000	-2.56210100	-2.67490500
C	-2.95999200	-2.09050000	1.65160200
C	-4.10631100	-1.15501800	2.06293200
C	-3.34719100	-3.56829200	1.79177900
H	0.85185300	2.55893500	-2.26382200
H	1.11400400	4.11220600	1.32583200
H	-3.30251000	-3.55710300	-0.97638000
H	-2.10405600	-1.88520000	2.31844100
H	-0.15159400	4.73036500	-2.83007500
H	-0.42583700	5.12335500	-1.12298200
H	-1.33453200	3.79209300	-1.88797200
H	2.94284500	3.32239100	-1.13269800

H	2.12246400	4.81210300	-0.58355500
H	2.36253600	4.52519400	-2.31766300
H	0.01284400	1.78799600	3.02347800
H	0.75486800	3.27920100	3.65500700
H	1.73448500	2.12778100	2.70281500
H	-1.32582500	4.60418300	0.80911200
H	-1.80334500	3.30338300	1.92696000
H	-0.96655500	4.74930600	2.54275600
H	-4.37357800	-1.35010100	3.11444800
H	-3.82083900	-0.09635400	1.97814100
H	-5.01341600	-1.31862400	1.46068100
H	-2.52270600	-4.24928400	1.52870100
H	-4.21967800	-3.82523900	1.17040000
H	-3.61910100	-3.77696700	2.83948100
H	-5.18258900	-1.95324500	-0.58988000
H	-5.12848700	-2.42576800	-2.29904200
H	-4.50652100	-0.83436800	-1.80252100
H	-2.33298600	-1.55540100	-3.11284800
H	-2.99579600	-3.17870500	-3.39330800
H	-1.42604800	-2.99504700	-2.57097300
C	-2.80611600	1.55378100	-0.30110800
O	-3.77657400	2.19639800	-0.30490900
N	3.89039600	-2.80848900	0.20675900
H	3.72957900	-3.79724100	0.36677400
C	5.20492400	-2.28078900	0.42842800
H	5.32999600	-1.72037700	1.36143300
C	6.02659900	-1.81280100	-0.75325800
H	5.55891900	-1.88404800	-1.73729300
H	6.67863100	-0.94886700	-0.60588800
C	6.36881700	-3.10729000	-0.04950300
H	7.25788100	-3.14317300	0.58294200
H	6.13703900	-4.03901100	-0.57141400
C	0.51970500	-1.96151100	0.03700600
C	2.76564600	-2.04172300	0.17383700
C	1.76204700	0.02209400	0.11071900
H	-0.68667000	-3.58719100	0.06774100
N	-0.71081400	-2.57266400	-0.00089400
N	0.52803400	-0.61312700	-0.03644000
N	1.84363200	1.34154100	0.18612800
N	2.90835900	-0.71511600	0.18149300
N	1.59599400	-2.73699000	0.14328700
H	-1.28678800	0.10180200	-2.01921600
H	-0.84053600	0.81100100	-1.99227200
O	4.65035400	1.67710600	0.20602600

H	4.56778000	0.72651200	0.00386400
H	3.69410000	1.84714500	0.36363000
H	-1.35101300	0.57371200	1.35866500
Ru	-1.26152000	0.52617600	-0.24422900

Ru-9

P	-0.02844100	2.34836500	-0.13225300
P	1.77530400	-1.88837000	-0.08402200
C	-0.17728700	3.37845300	1.44359700
C	1.17858500	3.90809000	1.93252000
C	-1.23571000	4.48800700	1.40267800
C	-0.04983700	3.56492300	-1.57194700
C	1.33697500	4.20000000	-1.75898200
C	-0.53316500	2.90256100	-2.86790400
C	2.48146900	-2.74739300	1.44384100
C	3.71725500	-1.98511800	1.94691300
C	1.43571200	-2.90296800	2.55647700
C	2.63408600	-2.68735900	-1.56090700
C	4.07554600	-2.18342200	-1.72621800
C	2.56698900	-4.21918100	-1.61113000
H	-0.50977900	2.59468700	2.14595000
H	-0.76738800	4.35392300	-1.29109000
H	2.79368100	-3.75242600	1.11484500
H	2.02971800	-2.27757200	-2.38869900
H	1.07186400	4.29772800	2.95849800
H	1.54742000	4.73730100	1.30784000
H	1.94479300	3.11872000	1.94862600
H	-2.22119600	4.12505700	1.07098500
H	-0.93634900	5.32021900	0.74557700
H	-1.36946900	4.90469000	2.41499700
H	0.13188700	2.07425900	-3.15956500
H	-0.53305300	3.64674800	-3.68150100
H	-1.55401200	2.50404600	-2.77288300
H	1.68699900	4.73041500	-0.86118700
H	2.08928600	3.43840300	-2.02117400
H	1.29964800	4.93288800	-2.58160200
H	4.46677000	-2.50053200	-2.70685400
H	4.14026900	-1.08596100	-1.67676100
H	4.74447100	-2.60459500	-0.95837000
H	1.53900600	-4.60246400	-1.51974300
H	3.18126400	-4.68503000	-0.82429100
H	2.95844700	-4.57090100	-2.58009200
H	4.48227400	-1.85158900	1.16720600

H	4.18304200	-2.54094000	2.77728900
H	3.43206300	-0.98858700	2.31816000
H	0.99320600	-1.93515400	2.84128000
H	1.91753500	-3.33210800	3.45090900
H	0.61691800	-3.57587500	2.26222400
C	2.92364400	1.10441900	-0.07481800
O	4.00056900	1.56452400	-0.05578100
N	-4.42234900	-2.05528900	-0.42882900
H	-4.43392800	-3.05974500	-0.57221800
C	-5.63706100	-1.31511700	-0.61754800
H	-5.68822500	-0.74257300	-1.54959200
C	-6.34570900	-0.73014600	0.58285000
H	-5.87451100	-0.88223000	1.55584000
H	-6.85052400	0.22944500	0.45178800
C	-6.90926500	-1.94648400	-0.11670200
H	-7.80431300	-1.83321200	-0.73124700
H	-6.81992000	-2.90798100	0.39491200
C	-0.95168600	-1.79527800	-0.24627800
C	-3.18911100	-1.50002800	-0.35795900
C	-1.85055900	0.31368000	-0.24577100
H	-0.02427000	-3.58338400	-0.23753200
N	0.16019200	-2.58379900	-0.22249800
N	-0.73827400	-0.45729400	-0.19295100
N	-1.65288400	1.66029200	-0.22159400
N	-3.09968800	-0.15444000	-0.32726900
N	-2.15126900	-2.37004600	-0.32576600
H	1.15955200	0.37870900	1.58491100
H	-0.13173600	0.21074600	2.43092000
O	-0.88665500	0.14362700	3.06524800
H	-0.48440200	0.43064600	3.89970400
H	-2.50097800	2.21963600	-0.26565000
H	1.21683900	0.31821400	-1.79492800
Ru	1.23335300	0.38226000	-0.10870500

Ru-TS2/3

P	-0.08731300	2.30932000	-0.38023800
P	1.63175900	-1.97402100	-0.27202200
N	-0.85223000	-0.48429900	-0.27417700
C	-1.95040300	0.30966100	-0.30087300
C	-3.33074100	-1.47591300	-0.28173000
C	-1.09703600	-1.81919700	-0.28836400
C	-0.14885600	3.47891900	1.10156200
C	1.23009500	4.04742700	1.46808900

C	-1.20853900	4.58511900	1.01341900
C	-0.13883200	3.40113400	-1.91690700
C	1.25837200	3.96107100	-2.22720100
C	-0.71562100	2.65769900	-3.12788800
C	2.43105400	-2.87162700	1.18752300
C	3.65309000	-2.08036000	1.68280200
C	1.44248000	-3.12815400	2.33239300
C	2.39499400	-2.75612200	-1.80755000
C	3.87012300	-2.35723500	-1.96095600
C	2.20339300	-4.27282100	-1.93303500
H	-0.44827300	2.77134000	1.89331800
H	-0.81079700	4.23952500	-1.66763400
H	2.77183000	-3.84436400	0.79524600
H	1.81750900	-2.25901400	-2.60539800
H	1.17086200	4.54165700	2.45180300
H	1.56716800	4.80624300	0.74436700
H	1.99771100	3.26287500	1.53331100
H	-2.21141200	4.19717900	0.77576500
H	-0.94601700	5.34788600	0.26355400
H	-1.28323300	5.09721800	1.98709200
H	-0.09839500	1.78258900	-3.38630000
H	-0.72968000	3.33478100	-3.99792800
H	-1.74512500	2.31257800	-2.95195600
H	1.68685600	4.52791500	-1.38789500
H	1.96037600	3.15254500	-2.48709400
H	1.19743400	4.64379600	-3.09047100
H	4.23169200	-2.65807100	-2.95779100
H	4.01834000	-1.27093800	-1.86355500
H	4.50771100	-2.86189900	-1.21714000
H	1.14365700	-4.56778900	-1.89409500
H	2.74770500	-4.82799600	-1.15215800
H	2.59758000	-4.61072000	-2.90580900
H	4.35569100	-1.82914700	0.87402100
H	4.20338700	-2.68137800	2.42547800
H	3.33843300	-1.14346800	2.16650300
H	0.98243800	-2.19242000	2.68790200
H	1.97989100	-3.58046900	3.18240800
H	0.63434500	-3.81530900	2.04326500
C	2.83997800	1.00018400	-0.29962800
O	3.92525300	1.43645200	-0.31421500
N	-2.31045100	-2.36775600	-0.28743200
N	-3.21055300	-0.13202500	-0.30506600
N	-0.00257200	-2.63223000	-0.31277900
N	-1.72469500	1.65266300	-0.33029300

H	-2.56243400	2.22735200	-0.37480000
H	-0.21003100	-3.62731900	-0.30019200
H	1.06027200	0.35056100	1.45893400
N	-4.57606100	-2.00442400	-0.25188200
H	-4.61799000	-3.01354600	-0.35037200
C	-5.78835300	-1.24569800	-0.37078800
H	-5.92301400	-0.73774000	-1.33162000
C	-6.35845900	-0.56096100	0.84984900
H	-5.79430000	-0.65892800	1.77929900
H	-6.85195900	0.40193500	0.70159300
C	-7.01671300	-1.80510800	0.29842400
H	-7.96676100	-1.70824500	-0.23034400
H	-6.89610600	-2.73168800	0.86507400
C	0.96446700	0.62854800	3.16243000
O	-0.18916900	0.43366800	3.38174900
O	2.08552200	0.90090900	3.44917000
H	1.08961200	0.21310100	-1.93228400
Ru	1.13237400	0.31383500	-0.27390600

Ru-TS3/4

P	-0.17872000	2.37248900	-0.25091300
P	1.71987000	-1.87569100	-0.28631900
N	-0.81602800	-0.46044800	-0.24811600
C	-1.94538400	0.29323100	-0.28977200
C	-3.25415700	-1.54492100	-0.34066300
C	-1.01049600	-1.80494700	-0.30144200
C	-0.32097700	3.50506600	1.24045900
C	0.98491800	4.26348700	1.52163100
C	-1.52993100	4.44833000	1.21298400
C	-0.13895700	3.44730300	-1.79544200
C	1.29390700	3.92618600	-2.08013600
C	-0.72493300	2.72001100	-3.01288500
C	2.65748400	-2.86437700	1.02319900
C	3.78904000	-2.00158100	1.60945400
C	1.75848500	-3.41526800	2.13861900
C	2.43585100	-2.43510600	-1.93503900
C	3.88466400	-1.95418700	-2.10581300
C	2.29985500	-3.93813500	-2.21281800
H	-0.46140000	2.74737500	2.02988900
H	-0.77018300	4.32328600	-1.56843800
H	3.10020600	-3.71217700	0.47460900
H	1.79961600	-1.88601800	-2.64995300
H	0.93234900	4.71358700	2.52644700

H	1.14847100	5.08505800	0.80606300
H	1.86532700	3.60290700	1.49901300
H	-2.48291000	3.91116300	1.09063200
H	-1.45160200	5.20576900	0.41631400
H	-1.58717400	4.98894500	2.17230900
H	-0.15300100	1.80683000	-3.24633200
H	-0.67101600	3.38299500	-3.89182500
H	-1.77718200	2.43822000	-2.86534300
H	1.75145800	4.44423700	-1.22523600
H	1.94299800	3.07947200	-2.35358000
H	1.28219200	4.63035200	-2.92776600
H	4.22154300	-2.16731600	-3.13323800
H	3.98835100	-0.87167900	-1.93725400
H	4.57156700	-2.47860200	-1.42198600
H	1.25652000	-4.28286100	-2.15230800
H	2.90792600	-4.54588700	-1.52391500
H	2.65527800	-4.15024100	-3.23451100
H	4.41681800	-1.53381500	0.83581500
H	4.44530000	-2.63652300	2.22744900
H	3.37020800	-1.21478600	2.25532200
H	1.29577100	-2.59948900	2.71441800
H	2.38341100	-3.99959600	2.83505100
H	0.97264700	-4.08446700	1.75997900
C	2.80852800	1.15370000	-0.13559500
O	3.87637200	1.61606500	-0.19060500
N	-2.19934400	-2.39708800	-0.34557500
N	-3.18447600	-0.19673400	-0.33157900
N	0.11166800	-2.58222300	-0.31543600
N	-1.77747100	1.64413500	-0.30190800
H	-2.63852200	2.18262000	-0.35184200
H	-0.06633700	-3.58188100	-0.36371800
N	-4.47598100	-2.11882700	-0.35557700
H	-4.47963600	-3.12805800	-0.46201500
C	-5.71497600	-1.40162800	-0.46362200
H	-5.83715200	-0.83692000	-1.39335400
C	-6.35144200	-0.82200700	0.77918700
H	-5.81397400	-0.95960800	1.71943400
H	-6.87958900	0.12838100	0.67671500
C	-6.93880000	-2.05206200	0.12503000
H	-7.87448900	-1.95868800	-0.42927700
H	-6.79846000	-3.00840400	0.63492100
H	1.71694400	0.83723200	2.17638500
C	0.97392400	0.31156400	2.87731200
O	-0.24078400	0.53292700	2.61359900

O	1.48079900	-0.39067100	3.77359000
H	1.19437500	0.41545100	-1.68097900
Ru	1.11651800	0.40829400	-0.12256000

Ru-TS4/5

P	-0.18172100	2.27928000	-0.26598300
P	1.88576000	-1.84568100	-0.13510100
N	-0.67723100	-0.49305300	-0.27346100
C	-1.82808600	0.24658400	-0.13274200
C	-3.06969700	-1.63465400	-0.45072600
C	-0.82374000	-1.82668000	-0.47244900
C	-0.14407300	3.78297600	0.86895100
C	1.18646000	4.54773900	0.82553600
C	-1.34735700	4.72028600	0.69131100
C	-0.44892900	2.94078000	-2.01135100
C	0.86346000	3.44049100	-2.63357600
C	-1.11769000	1.89829800	-2.91737100
C	2.46846800	-2.91106400	1.30587000
C	3.77248700	-2.34343200	1.89005200
C	1.38386600	-3.01769200	2.38739200
C	2.90244400	-2.34671400	-1.64181000
C	4.28976200	-1.68978600	-1.67210100
C	2.98759000	-3.85846900	-1.88595800
H	-0.22517100	3.30933200	1.86085100
H	-1.14135000	3.79104100	-1.89467700
H	2.66626900	-3.91634300	0.89674600
H	2.29407000	-1.89347900	-2.44358400
H	1.21949300	5.27195000	1.65639500
H	1.29962100	5.12166300	-0.10766300
H	2.05589700	3.88113700	0.92611700
H	-2.29892700	4.16933000	0.69812600
H	-1.28276800	5.28966500	-0.25007600
H	-1.36879400	5.45338800	1.51499800
H	-0.48373100	1.00435200	-3.03263200
H	-1.27273500	2.33072000	-3.91994200
H	-2.09846600	1.58357900	-2.53278200
H	1.35136700	4.22104800	-2.03239300
H	1.57779900	2.61105900	-2.75726300
H	0.66244900	3.86674400	-3.63061900
H	4.73343800	-1.81944300	-2.67290400
H	4.24353300	-0.61156600	-1.46105000
H	4.97901400	-2.15460200	-0.94989500
H	1.99792900	-4.34038400	-1.90613800

H	3.60439200	-4.36333200	-1.12555400
H	3.45896000	-4.04524200	-2.86508000
H	4.58914100	-2.30624900	1.15478100
H	4.10866500	-2.97895500	2.72564300
H	3.61978400	-1.32474600	2.28222200
H	1.11838900	-2.02310900	2.77709800
H	1.76287000	-3.62664700	3.22479400
H	0.46784700	-3.49743000	2.01233100
C	2.86338100	1.22601700	0.23464400
O	3.90805100	1.74228700	0.33185500
N	-1.99364800	-2.44950700	-0.58860800
N	-3.04712900	-0.30760800	-0.21512200
N	0.32688600	-2.56469700	-0.53839500
N	-1.72229500	1.57413500	0.18643400
H	-1.58858500	1.45736700	1.53979300
H	0.18182000	-3.56890200	-0.61457300
N	-4.27673200	-2.24054000	-0.55885300
H	-4.24778100	-3.21311300	-0.84657500
C	-5.53505500	-1.55139200	-0.57468100
H	-5.66421900	-0.84683200	-1.40285200
C	-6.20718300	-1.19726600	0.73201100
H	-5.67875400	-1.46834900	1.64808100
H	-6.76441700	-0.25888900	0.77377400
C	-6.74650900	-2.32311900	-0.12145600
H	-7.67751700	-2.16874800	-0.67016300
H	-6.58326400	-3.34469600	0.23085400
H	-0.25585700	0.52273600	4.12202700
C	-0.32989000	0.71337500	3.03126300
O	0.62746300	0.38199200	2.31105500
O	-1.43986100	1.27489900	2.68647100
H	1.50278200	0.42442500	-1.52764200
Ru	1.22326800	0.41443900	0.02681400

Ru-TS7/1

P	0.21786500	2.36050800	-0.02377200
P	-1.87639200	-1.76744600	0.08999500
C	0.05233200	3.75809200	-1.27173600
C	-1.26906500	4.53215100	-1.16676800
C	1.26985300	4.69058200	-1.30815700
C	0.93872500	3.09670800	1.54806600
C	-0.10034400	3.98544400	2.25039200
C	1.47349500	2.02144000	2.50382500
C	-2.30676100	-2.83242500	-1.40808400

C	-3.55523900	-2.27550100	-2.10996300
C	-1.12109900	-2.91315300	-2.37879500
C	-3.01225800	-2.29611700	1.49546100
C	-4.40171200	-1.64727100	1.41606500
C	-3.10776100	-3.81216800	1.71050200
H	0.02739000	3.18126000	-2.21275600
H	1.78505700	3.72161400	1.21757600
H	-2.52649900	-3.84460100	-1.02893400
H	-2.47771300	-1.85071900	2.35210700
H	-1.36670800	5.20452900	-2.03524200
H	-1.31236600	5.16062700	-0.26370600
H	-2.14182100	3.86349300	-1.16020000
H	2.21194000	4.12647600	-1.37343400
H	1.31092200	5.34135500	-0.41990100
H	1.20526300	5.34772800	-2.19142800
H	0.67780000	1.32449700	2.81065800
H	1.86441000	2.50831500	3.41263900
H	2.29495900	1.44067600	2.06090100
H	-0.42271600	4.83224800	1.62778900
H	-0.99607300	3.40768000	2.53323600
H	0.33520300	4.40106100	3.17400000
H	-4.93445300	-1.80916600	2.36741700
H	-4.34271500	-0.56278400	1.24308700
H	-5.01823200	-2.09215200	0.61917400
H	-2.12107900	-4.29208700	1.80180800
H	-3.65993000	-4.30853800	0.89693500
H	-3.65405400	-4.01422400	2.64659100
H	-4.43763100	-2.25061000	-1.45429700
H	-3.80522300	-2.90824400	-2.97734500
H	-3.37578600	-1.25254200	-2.47972500
H	-0.82846800	-1.91072600	-2.73201100
H	-1.40693200	-3.51132800	-3.25954400
H	-0.23978300	-3.38793700	-1.92274300
C	-2.86710300	1.26794000	-0.40849300
O	-3.91083000	1.75772200	-0.60343600
N	4.26411400	-2.14355200	0.39278100
H	4.26456100	-3.06551500	0.81634700
C	5.51204600	-1.45727100	0.21919200
H	5.67636200	-0.62167500	0.90725400
C	6.10640900	-1.32840400	-1.16491400
H	5.53234700	-1.75416600	-1.99022800
H	6.64778400	-0.40869100	-1.39703300
C	6.70679900	-2.28996700	-0.16397200
H	7.66414300	-2.04069300	0.29751500

H	6.53871800	-3.35730500	-0.32805100
C	0.80854200	-1.75904400	0.48013100
C	3.04518900	-1.57150400	0.25331300
C	1.76095900	0.23606400	-0.22854400
H	-0.21633800	-3.47321000	0.75962500
N	-0.34809400	-2.46994800	0.64838700
N	0.65152800	-0.44117400	0.20330500
N	1.53349100	1.46032000	-0.81951600
N	2.98815700	-0.29910300	-0.19735200
N	1.98643800	-2.36798800	0.55633200
H	-0.46890700	0.61822300	-1.83245000
H	0.49056900	0.98153600	-1.58877100
H	-1.59461100	0.47756200	1.48751000
Ru	-1.23050700	0.48220200	-0.08279300

Ru-TS8/9

P	0.16625000	2.30323900	0.08181700
P	-1.86433800	-1.82903200	0.06956000
C	0.08270600	3.76433400	-1.10941600
C	-1.29321200	4.44418400	-1.14865600
C	1.21914200	4.78118800	-0.93082200
C	0.50267900	3.04282600	1.78445700
C	-0.76839900	3.64171400	2.40373400
C	1.14067300	2.01882700	2.73256600
C	-2.41801200	-2.89347900	-1.38676000
C	-3.74068900	-2.36585200	-1.96498200
C	-1.33575200	-2.96271600	-2.47231100
C	-2.87838200	-2.38245600	1.56050100
C	-4.26361000	-1.72293600	1.61749400
C	-2.96900200	-3.90091000	1.75757400
H	0.22588300	3.26103900	-2.07946300
H	1.23402400	3.84858200	1.60682100
H	-2.58051300	-3.90843200	-0.98630000
H	-2.26613900	-1.95588100	2.37377000
H	-1.32741700	5.15371200	-1.99226500
H	-1.49740800	5.02056400	-0.23264900
H	-2.10873600	3.71897300	-1.28575300
H	2.20251900	4.29061600	-0.88165500
H	1.08639700	5.38533900	-0.01877500
H	1.22835500	5.47879200	-1.78510800
H	0.47211700	1.15854500	2.89648300
H	1.32774400	2.49256600	3.71090900
H	2.10306000	1.64609600	2.35286800

H	-1.21550600	4.42939300	1.77984900
H	-1.53019800	2.86243100	2.56748100
H	-0.52934900	4.09139700	3.38209200
H	-4.70954300	-1.89370700	2.61117300
H	-4.21252000	-0.63695300	1.45276700
H	-4.95391600	-2.15321500	0.87493300
H	-1.98305500	-4.39123900	1.74740500
H	-3.60022200	-4.37761900	0.99095500
H	-3.42734700	-4.11662400	2.73702500
H	-4.55595800	-2.35714100	-1.22709000
H	-4.06007200	-3.00740900	-2.80266700
H	-3.62076300	-1.34129300	-2.35362800
H	-1.10761200	-1.96066300	-2.86971300
H	-1.69550500	-3.58450000	-3.30863100
H	-0.40046800	-3.40702500	-2.10106200
C	-2.90102000	1.21591700	-0.24534900
O	-3.95572200	1.71969300	-0.30459800
N	4.30678100	-2.16625200	0.46278300
H	4.28476400	-3.12734300	0.78736700
C	5.55630900	-1.46184700	0.48134100
H	5.66745100	-0.73876200	1.29630400
C	6.24201800	-1.12664800	-0.82326000
H	5.72899800	-1.42242600	-1.74046800
H	6.78993100	-0.18338000	-0.87705800
C	6.78223200	-2.22893200	0.05999700
H	7.70433100	-2.05316200	0.61727000
H	6.63451300	-3.25917400	-0.27339000
C	0.84850100	-1.78334000	0.37590000
C	3.09261200	-1.57292500	0.34161400
C	1.83093700	0.28837600	-0.02205300
H	-0.14123900	-3.53059200	0.56042900
N	-0.29497400	-2.52909300	0.46849100
N	0.68840100	-0.45845600	0.14335400
N	1.71083700	1.60242600	-0.38749200
N	3.05713800	-0.25353000	0.07250500
N	2.02520000	-2.39407700	0.50118700
H	-1.03298100	0.34329000	-1.89086100
H	-0.08231700	0.67467200	-2.28550000
O	0.94473100	1.06829100	-2.74365500
H	1.42170500	0.29433500	-3.09084400
H	1.44700700	1.37180700	-1.75549100
H	-1.40642200	0.42761900	1.51471100
Ru	-1.24514600	0.42410700	-0.10913800

Fe-1

P	0.10504400	2.29268300	-0.00750000
P	1.75937200	-1.80726000	0.00700300
N	-0.69196500	-0.41454300	-0.07607000
C	-1.79156200	0.37119300	-0.09483800
C	-3.17068100	-1.41066900	-0.19658900
C	-0.93833400	-1.74532200	-0.12027500
C	0.05366300	3.35977100	1.55235100
C	1.44328800	3.84572200	1.98935200
C	-0.96178900	4.50942200	1.53015700
C	0.11844400	3.50380900	-1.45611100
C	1.53160900	4.06374500	-1.68347600
C	-0.42993800	2.86090900	-2.73638800
C	2.49912800	-2.70233000	1.49689400
C	3.88146500	-2.12774100	1.84444200
C	1.56170600	-2.64988400	2.71009900
C	2.58749600	-2.56937300	-1.51142900
C	3.96209200	-1.95415300	-1.81251400
C	2.64030500	-4.10242000	-1.53198100
H	-0.28373100	2.60483000	2.28360400
H	-0.54909700	4.33356800	-1.16877000
H	2.61994500	-3.75620900	1.19415600
H	1.88846900	-2.23036100	-2.29556600
H	1.38652000	4.25199100	3.01294600
H	1.81886500	4.65356600	1.34135100
H	2.18310400	3.03194200	1.99074800
H	-1.97154000	4.17984700	1.23898500
H	-0.65377400	5.31739200	0.84730400
H	-1.04307100	4.94925200	2.53830700
H	0.18825100	2.00245400	-3.04311600
H	-0.41917100	3.60143600	-3.55355300
H	-1.46484100	2.50916200	-2.61226100
H	1.92709700	4.59131900	-0.80317700
H	2.24000900	3.26166500	-1.94627100
H	1.51528000	4.78326300	-2.51880900
H	4.28298200	-2.24583200	-2.82643800
H	3.94153000	-0.85530900	-1.76880600
H	4.73431800	-2.31282600	-1.11357100
H	1.65644900	-4.56232300	-1.34928500
H	3.34963900	-4.50063200	-0.78884200
H	2.97959500	-4.44694000	-2.52316800
H	4.59979500	-2.21729800	1.01667600
H	4.30274100	-2.67141100	2.70628300

H	3.81228900	-1.06346600	2.12144500
H	1.38403200	-1.60988300	3.02639700
H	2.02075900	-3.19236200	3.55351000
H	0.58689500	-3.11456500	2.49992900
C	2.81293900	0.99941800	0.07259200
O	3.89498400	1.43527100	0.11537300
N	-2.15037300	-2.30036600	-0.18178100
N	-3.05385500	-0.06795900	-0.15800100
N	0.16330600	-2.54599300	-0.10003100
N	-1.55827100	1.71142800	-0.04648600
H	-2.38385800	2.30323900	-0.08416900
H	-0.01836200	-3.54616500	-0.10716500
H	1.08340900	0.35620600	1.57259100
N	-4.41805600	-1.94079100	-0.25092300
H	-4.45167800	-2.94232100	-0.41012400
C	-5.61654500	-1.17263000	-0.42820900
H	-5.67015500	-0.60638300	-1.36428800
C	-6.29039000	-0.55898100	0.77775400
H	-5.80739200	-0.71409800	1.74446400
H	-6.77303700	0.41190900	0.64607600
C	-6.89630600	-1.76679000	0.09908400
H	-7.79848700	-1.63606900	-0.50148400
H	-6.82266700	-2.72558500	0.61816200
H	1.23947300	0.31642800	-1.56514600
Fe	1.20108700	0.35047800	0.00627300

Fe-2

P	0.10506200	2.13097800	-0.61900200
P	1.36033900	-2.09347500	-0.25208800
N	-0.93923000	-0.45631000	-0.20226800
C	-1.95502600	0.43512600	-0.20691600
C	-3.49643900	-1.18679800	0.07635900
C	-1.31324600	-1.74996900	-0.05738600
C	0.36480700	3.42395900	0.73176500
C	1.81891200	3.91337200	0.80351400
C	-0.61914600	4.60060300	0.71974600
C	0.07056100	3.09695400	-2.24313700
C	1.49938100	3.29765800	-2.77330300
C	-0.80826500	2.41067600	-3.29668400
C	2.21510700	-2.91712500	1.21695800
C	3.66278500	-2.41802100	1.35075600
C	1.44061100	-2.69509800	2.52228500
C	1.89068100	-3.08557900	-1.77088100

C	3.26766200	-2.66409500	-2.30422800
C	1.78318700	-4.60931800	-1.63344100
H	0.17305700	2.81193800	1.62884500
H	-0.36525700	4.08350100	-2.01205900
H	2.23078600	-3.99811300	0.99860500
H	1.13060700	-2.74202300	-2.49380800
H	1.98042600	4.45002500	1.75295100
H	2.05403100	4.61731300	-0.01078600
H	2.54059400	3.08388600	0.75865400
H	-1.67026700	4.27299600	0.72517600
H	-0.46609200	5.25845700	-0.15077000
H	-0.46759000	5.21547800	1.62269700
H	-0.43742700	1.39705000	-3.51850600
H	-0.78501500	2.99467200	-4.23196500
H	-1.85707600	2.32955200	-2.97559500
H	2.15497800	3.80777000	-2.05262200
H	1.96138200	2.33058900	-3.02724200
H	1.47263400	3.91162100	-3.68884100
H	3.42043900	-3.08985800	-3.30998800
H	3.36223300	-1.57104900	-2.38307200
H	4.08559300	-3.03774600	-1.66769400
H	0.79475400	-4.93347700	-1.27171800
H	2.54893400	-5.01664700	-0.95392200
H	1.93848600	-5.08059900	-2.61835800
H	4.25322700	-2.56720500	0.43493000
H	4.16930400	-2.96638700	2.16241500
H	3.68711700	-1.34713100	1.60502600
H	1.36841000	-1.62168400	2.75854600
H	1.96842500	-3.19290000	3.35289400
H	0.42084200	-3.10459100	2.47569800
C	2.67041600	0.57913100	-0.64204500
O	3.78456600	0.90042500	-0.77795500
N	-2.57032800	-2.17413000	0.08677200
N	-3.25094700	0.13063000	-0.07306900
N	-0.29882800	-2.65845900	-0.06865900
N	-1.59388600	1.73851600	-0.36528700
H	-2.36009400	2.40553300	-0.40159000
H	-0.57380000	-3.62851500	0.06087200
H	1.10142100	0.31461600	1.11937900
N	-4.78452300	-1.58182300	0.23354900
H	-4.93056300	-2.58557200	0.20837800
C	-5.91957300	-0.71567000	0.09365600
H	-6.02606200	-0.24737300	-0.89065000
C	-6.39433200	0.08613300	1.28422100

H	-5.82131000	-0.01698100	2.20775500
H	-6.79835200	1.08259900	1.09262200
C	-7.18032500	-1.11682600	0.81338600
H	-8.12891000	-0.95708600	0.29728700
H	-7.13641600	-2.01903100	1.42850100
H	0.84136400	-0.11551600	-1.98327000
Fe	1.01131400	0.10268100	-0.43801400
C	2.52808600	1.44879800	3.55080400
O	1.55118800	2.00898600	3.85931900
O	3.51414100	0.89648900	3.25814800

Fe-3

P	0.04289100	2.28437200	-0.32694700
P	1.68267700	-1.88011400	-0.24304000
N	-0.75094200	-0.43199100	-0.21863400
C	-1.84850800	0.36421500	-0.29067300
C	-3.24124700	-1.41028800	-0.29941100
C	-1.01219300	-1.76623600	-0.23793300
C	-0.00797000	3.50751300	1.10117900
C	1.38098300	4.07039400	1.43967500
C	-1.04984100	4.62370600	0.95360600
C	0.17227900	3.28617300	-1.91602900
C	1.63632600	3.65577400	-2.20433300
C	-0.45489500	2.55156000	-3.10815800
C	2.62268600	-2.81011200	1.10313600
C	3.81261400	-1.95764800	1.58019600
C	1.73715400	-3.21166800	2.29037400
C	2.38275400	-2.50381000	-1.87547800
C	3.81719300	-2.00499600	-2.10479400
C	2.26999700	-4.01923200	-2.08233700
H	-0.31500700	2.83542700	1.91976000
H	-0.39906100	4.21160100	-1.73396900
H	3.00308300	-3.72583300	0.62133000
H	1.72040900	-1.99722900	-2.59798100
H	1.33338300	4.59946100	2.40553000
H	1.72731900	4.79723300	0.68771400
H	2.14107600	3.27975000	1.53100600
H	-2.06095700	4.23724500	0.75180900
H	-0.78548700	5.33524500	0.15513200
H	-1.10564800	5.19534000	1.89482700
H	0.06181300	1.59855100	-3.30521200
H	-0.36360700	3.17930300	-4.00981500
H	-1.52207100	2.33825200	-2.95171000

H	2.11207100	4.19713000	-1.37373600
H	2.23601200	2.75632900	-2.41563700
H	1.68137700	4.30705900	-3.09241400
H	4.12564300	-2.23904800	-3.13680900
H	3.90764100	-0.91720400	-1.96742000
H	4.53409400	-2.50085700	-1.43068800
H	1.23727600	-4.38292900	-1.97125100
H	2.91322200	-4.58166300	-1.38683800
H	2.59657200	-4.27187100	-3.10451400
H	4.45122500	-1.61172500	0.75363200
H	4.44383800	-2.55929300	2.25503500
H	3.45081100	-1.08105900	2.14009400
H	1.34262900	-2.32386700	2.80702600
H	2.34920400	-3.77192400	3.01688000
H	0.89611900	-3.85511500	1.99554500
C	2.75319700	0.94876400	-0.12814600
O	3.83222200	1.37126100	-0.17249500
N	-2.22595700	-2.30798700	-0.27084800
N	-3.10960800	-0.06753200	-0.32807500
N	0.07817200	-2.58511300	-0.23093700
N	-1.61117800	1.70322100	-0.34334900
H	-2.43625200	2.29319800	-0.41451500
H	-0.12418000	-3.58099100	-0.25750200
H	0.99465100	0.26147600	1.63053400
N	-4.48884100	-1.92839300	-0.30965100
H	-4.53684700	-2.93841900	-0.39618700
C	-5.68965600	-1.15814600	-0.47035100
H	-5.76994600	-0.62797700	-1.42485000
C	-6.31623100	-0.49589100	0.73529000
H	-5.80092100	-0.61887600	1.68983900
H	-6.79558000	0.47362300	0.58370400
C	-6.95317100	-1.72298800	0.12322100
H	-7.87437700	-1.60807100	-0.45100100
H	-6.86774900	-2.66248500	0.67484400
C	0.76009500	0.42564900	2.81060900
O	-0.40686500	0.76534900	3.03622200
O	1.75402600	0.20080500	3.50875700
Fe	1.11910800	0.30689900	-0.13448900
H	1.21189700	0.30582600	-1.63295200

Fe-4

P	0.07313200	2.28438800	-0.26129700
P	1.74884300	-1.87160000	-0.14350200

N	-0.70096600	-0.44366300	-0.21106800
C	-1.79436500	0.34248800	-0.35644000
C	-3.17543500	-1.44114900	-0.37244700
C	-0.94872600	-1.77435200	-0.21240200
C	-0.12044800	3.48458800	1.17703400
C	1.23165000	3.84291400	1.81489700
C	-0.96481300	4.73159800	0.88569000
C	0.26763400	3.33902100	-1.81003700
C	1.66211100	3.98088100	-1.87520300
C	-0.04110300	2.55203600	-3.08992300
C	2.66643200	-2.79113200	1.22571900
C	3.83691600	-1.92446200	1.72240500
C	1.74971600	-3.19206400	2.38909700
C	2.47603900	-2.51660600	-1.75528200
C	3.92045800	-2.03361500	-1.95621100
C	2.35369000	-4.03211100	-1.95595200
H	-0.66242700	2.83616100	1.88372200
H	-0.48287700	4.14154400	-1.71125400
H	3.07152000	-3.70698700	0.76392200
H	1.83636900	-2.00881700	-2.49731600
H	1.05676600	4.40024100	2.75056700
H	1.84686200	4.48605300	1.16532400
H	1.81334800	2.94285600	2.06249700
H	-1.95079300	4.48905100	0.45749700
H	-0.45598900	5.42902200	0.20082000
H	-1.14807300	5.27589000	1.82733700
H	0.68835700	1.74200500	-3.24401600
H	0.00970200	3.23104400	-3.95731000
H	-1.04670600	2.10662400	-3.06603600
H	1.87601600	4.61981600	-1.00573500
H	2.45326300	3.21718200	-1.94113000
H	1.73444100	4.61432400	-2.77457600
H	4.25130000	-2.27672200	-2.97930400
H	4.01914500	-0.94599400	-1.82185800
H	4.61670700	-2.53229700	-1.26246300
H	1.31379200	-4.38304500	-1.87368500
H	2.96779700	-4.59641400	-1.23569300
H	2.70901600	-4.29814200	-2.96521500
H	4.51139900	-1.61450000	0.90985700
H	4.43659500	-2.49618800	2.44992200
H	3.45547700	-1.01920300	2.21831800
H	1.26950600	-2.30555200	2.82792800
H	2.35197000	-3.68191900	3.17260700
H	0.96421300	-3.89754200	2.08168000

C	2.79321100	0.97724900	-0.07212800
O	3.86688400	1.40702200	-0.18440000
N	-2.15777700	-2.33061900	-0.28142200
N	-3.05273900	-0.10035000	-0.43814800
N	0.14735800	-2.58674100	-0.14835900
N	-1.56323800	1.67871000	-0.45547100
H	-2.39045700	2.26140200	-0.55440200
H	-0.04879800	-3.58375100	-0.17226600
N	-4.42151700	-1.97104600	-0.40828000
H	-4.45702400	-2.98248800	-0.48102900
C	-5.61869500	-1.21681600	-0.64558800
H	-5.67237600	-0.73066500	-1.62554900
C	-6.28768800	-0.50372300	0.50683800
H	-5.80302600	-0.57939600	1.48211700
H	-6.76684700	0.45474200	0.29571500
C	-6.89906500	-1.76140200	-0.06819400
H	-7.80200400	-1.67790200	-0.67598800
H	-6.82712000	-2.67426200	0.52824000
H	0.41514600	0.10480600	3.93539300
C	0.13618700	0.34963800	2.87310400
O	1.10862300	0.18281900	2.05725000
O	-1.01993500	0.73531900	2.64166400
Fe	1.16891800	0.32015500	-0.02407900
H	1.25964700	0.31998900	-1.53734600

Fe-5

P	0.01822400	2.25836900	-0.22868300
P	1.85664400	-1.81407800	-0.15403800
N	-0.60915800	-0.42154600	-0.26736300
C	-1.73280700	0.37155400	-0.14002200
C	-3.05025500	-1.46192600	-0.46845400
C	-0.81639300	-1.73707500	-0.49501600
C	0.15826200	3.73180100	0.94060800
C	1.47157600	4.51130500	0.78381600
C	-1.05899200	4.66742300	0.89742800
C	-0.10976400	3.01228000	-1.95954300
C	1.27359600	3.28492800	-2.56915500
C	-0.95017900	2.12980400	-2.89166300
C	2.45414200	-2.86000600	1.30286700
C	3.52897200	-2.08353200	2.08406500
C	1.30224100	-3.27580300	2.22864300
C	2.92436700	-2.31838600	-1.61933000
C	4.37847800	-1.85007000	-1.46202400

C	2.84963300	-3.80721500	-1.98071600
H	0.17551400	3.24541700	1.93048900
H	-0.63793400	3.97127600	-1.82234600
H	2.90814300	-3.77074800	0.87704100
H	2.45963200	-1.73445400	-2.43170400
H	1.58158500	5.22178600	1.62007100
H	1.48310700	5.10260400	-0.14551600
H	2.35460500	3.85499500	0.78440500
H	-2.00103200	4.11268900	1.00830100
H	-1.10179300	5.23280400	-0.04806000
H	-0.98955100	5.40467400	1.71508400
H	-0.48459700	1.13987400	-3.02800100
H	-1.02443400	2.60501800	-3.88441200
H	-1.96943200	1.98229400	-2.50726700
H	1.90291200	3.92660900	-1.93553900
H	1.81552700	2.34115900	-2.73832300
H	1.15801800	3.79075900	-3.54273600
H	4.91695100	-2.00023000	-2.41212200
H	4.44837400	-0.78334900	-1.20298300
H	4.91162600	-2.42987000	-0.69140800
H	1.81754100	-4.14307000	-2.16249000
H	3.29088900	-4.44550900	-1.19835900
H	3.41914300	-3.98760700	-2.90745300
H	4.37238700	-1.76836400	1.45158100
H	3.93698500	-2.72108900	2.88580600
H	3.09473000	-1.18377400	2.54740500
H	0.77551200	-2.39604300	2.62971300
H	1.70798800	-3.84308400	3.08286900
H	0.56558300	-3.91601000	1.72204800
C	2.81527700	1.07954600	0.15793700
O	3.87061900	1.56908500	0.16493100
N	-2.00690900	-2.31838000	-0.62461900
N	-2.97908700	-0.14413300	-0.22755600
N	0.30913600	-2.51565800	-0.58675800
N	-1.57989600	1.68484700	0.14563400
H	-1.35849900	1.41632700	1.74225200
H	0.13598200	-3.51304700	-0.68141600
N	-4.28117800	-2.03117300	-0.56642400
H	-4.28265000	-2.99409600	-0.88590600
C	-5.51251500	-1.29710500	-0.59250200
H	-5.61465900	-0.58959400	-1.42258700
C	-6.17786400	-0.91405000	0.70951900
H	-5.66317700	-1.20039200	1.62879200
H	-6.70250500	0.04322300	0.74604900

C	-6.75346200	-2.02319100	-0.14229300
H	-7.67670000	-1.83758500	-0.69457700
H	-6.62802500	-3.04862200	0.21425900
H	0.06433700	0.31704600	4.03966300
C	-0.06703500	0.56697600	2.97079500
O	0.80792200	0.27335400	2.15583500
O	-1.20224500	1.17741600	2.74726500
Fe	1.22676600	0.35608200	0.02786500
H	1.47457200	0.37538200	-1.45071400

Fe-6

P	0.01032900	2.28143100	0.04901900
P	-1.75914000	-1.82992300	-0.02094200
N	0.67681300	-0.38555300	0.02509300
C	1.79809800	0.46595500	0.13478100
C	3.15230000	-1.38533600	0.16272900
C	0.92913200	-1.71920100	0.05063500
C	0.07639600	3.31775100	-1.53191300
C	-1.28781600	3.78953800	-2.05189300
C	1.09142000	4.46593000	-1.45812400
C	-0.20896900	3.47176400	1.48936100
C	-1.64701200	3.99419400	1.61191500
C	0.25794800	2.82384200	2.79975600
C	-2.52448200	-2.63286200	-1.53811300
C	-4.01283100	-2.28145700	-1.68007700
C	-1.72986000	-2.21398700	-2.78417000
C	-2.56233200	-2.56392900	1.51319400
C	-3.85546400	-1.83850600	1.91363900
C	-2.74323200	-4.08633200	1.46036700
H	0.46538100	2.56189900	-2.23907600
H	0.46284000	4.31839200	1.26610300
H	-2.42530400	-3.72371800	-1.40313200
H	-1.79438700	-2.32606600	2.27017700
H	-1.17515300	4.20554100	-3.06746500
H	-1.71528700	4.58628700	-1.42240400
H	-2.01850600	2.96865200	-2.10499100
H	2.05837200	4.11919400	-1.06561100
H	0.72801100	5.28545000	-0.81617700
H	1.25784100	4.88806800	-2.46378000
H	-0.37066400	1.95633400	3.06040600
H	0.18446200	3.55408200	3.62331800
H	1.30115300	2.48388600	2.73096700
H	-1.99378800	4.50551600	0.70193700

H	-2.35031400	3.17459600	1.82969800
H	-1.71100800	4.71801100	2.44184800
H	-4.17735700	-2.18961400	2.90791300
H	-3.71091900	-0.74985700	1.97002300
H	-4.68029300	-2.04061900	1.21318200
H	-1.80792600	-4.61257100	1.21377500
H	-3.50925600	-4.38239100	0.72621600
H	-3.07366400	-4.45268700	2.44624700
H	-4.62319700	-2.69608700	-0.86491600
H	-4.39959800	-2.69726500	-2.62488400
H	-4.17168200	-1.19090300	-1.70701600
H	-1.81001500	-1.12785000	-2.96016100
H	-2.13162600	-2.72796200	-3.67259100
H	-0.66373000	-2.47125800	-2.69720800
C	-2.76106600	1.04491400	-0.18837600
O	-3.82609300	1.51196800	-0.22091600
N	2.12784300	-2.28600500	0.10869900
N	3.05785700	-0.05880000	0.19146900
N	-0.16881500	-2.54384700	0.01352100
N	1.64431400	1.77532200	0.18546900
H	0.03077800	-3.54075100	0.00750200
N	4.39282100	-1.95014800	0.19078900
H	4.39780300	-2.95402400	0.33713300
C	5.60024400	-1.21871500	0.43754500
H	5.62652500	-0.66788400	1.38427800
C	6.34521600	-0.60076000	-0.72383200
H	5.90270800	-0.72506600	-1.71417800
H	6.84924400	0.35309000	-0.55253700
C	6.88690000	-1.83789500	-0.04222200
H	7.76518600	-1.74292600	0.59931200
H	6.81196700	-2.78441800	-0.58341500
H	-1.40700900	0.41789900	1.40824100
Fe	-1.16246300	0.34663200	-0.04957900

Fe-7

P	0.03671100	2.27890100	0.01652800
P	1.71288900	-1.84120000	0.03183300
C	0.04910500	3.50749400	1.45264000
C	1.43828200	4.04084400	1.82569600
C	-0.97448700	4.63956500	1.29403300
C	0.27460900	3.30676400	-1.54754100
C	1.74373300	3.66555700	-1.80953900
C	-0.34610800	2.60660400	-2.76254900

C	2.56427700	-2.83661900	1.38719600
C	3.96406700	-2.27395300	1.68014300
C	1.71542200	-2.89100400	2.66439900
C	2.43419100	-2.42380800	-1.61013900
C	3.77579600	-1.76530200	-1.96023700
C	2.49267300	-3.94825800	-1.77106500
H	-0.29777100	2.85164300	2.27266900
H	-0.29292200	4.23400700	-1.35950500
H	2.66565900	-3.86255800	0.99467400
H	1.67108800	-2.02505900	-2.30111800
H	1.38941500	4.57066900	2.79196100
H	1.81209500	4.76153500	1.08078200
H	2.18288500	3.23593900	1.92312300
H	-1.96072100	4.24767700	1.00696500
H	-0.65490200	5.37209700	0.53450500
H	-1.08184100	5.18524700	2.24686200
H	0.17054800	1.65675800	-2.97922800
H	-0.25124000	3.25182500	-3.65248500
H	-1.41127000	2.38951200	-2.60148200
H	2.21956300	4.17542200	-0.95908300
H	2.33537600	2.76486800	-2.03734400
H	1.81425100	4.33877300	-2.68064800
H	4.02185800	-1.97608500	-3.01405800
H	3.74809400	-0.67338300	-1.83513500
H	4.60148100	-2.16338100	-1.34991100
H	1.53141400	-4.43558200	-1.54502400
H	3.26827000	-4.39959300	-1.13177400
H	2.74535300	-4.19773300	-2.81476600
H	4.61710400	-2.27003000	0.79561100
H	4.45626400	-2.88750300	2.45232100
H	3.90513400	-1.24155700	2.06248000
H	1.58314600	-1.88966500	3.10729300
H	2.22509500	-3.51528300	3.41647400
H	0.71837300	-3.31772600	2.48431500
C	2.80301700	1.01021900	0.21454200
O	3.86916200	1.45526300	0.12078800
N	-4.44393400	-1.85135300	-0.19810100
H	-4.46179800	-2.83906300	-0.42936100
C	-5.62442500	-1.07864000	-0.45052100
H	-5.60516800	-0.48016400	-1.36826000
C	-6.39330600	-0.49994500	0.71418000
H	-5.98536800	-0.68204800	1.71027300
H	-6.86799800	0.47369100	0.57382300
C	-6.94082500	-1.68907100	-0.04410900

H	-7.79545800	-1.54223800	-0.70765600
H	-6.90640300	-2.66220200	0.45231800
C	-0.97645700	-1.68686100	-0.01373900
C	-3.18836600	-1.31347600	-0.13716900
C	-1.79645200	0.50215300	-0.01028400
H	-0.09436700	-3.51790200	-0.10119700
N	0.11479900	-2.52800300	-0.00588400
N	-0.70855400	-0.37311900	0.09620800
N	-1.60359000	1.81039500	-0.03212900
N	-3.06748000	0.01081500	-0.09805700
N	-2.18299800	-2.23440400	-0.13077900
H	1.17497500	-0.05300400	1.89218600
H	0.87954900	0.72036300	1.85894400
H	1.25556400	0.36407800	-1.24668900
Fe	1.17812300	0.33677400	0.25580700

Fe-8

P	-0.17378900	2.18497500	0.01437100
P	2.17732200	-1.60074900	0.03479000
C	-0.48146800	3.32241000	1.49183400
C	0.70640100	4.23175800	1.83270300
C	-1.79716700	4.10798600	1.39678100
C	-0.03725000	3.31809800	-1.48777400
C	1.39012300	3.83927100	-1.70680100
C	-0.56887300	2.62774600	-2.75021100
C	3.17835400	-2.46819100	1.37081400
C	4.55777000	-1.81755400	1.55337800
C	2.41144500	-2.52043700	2.69885600
C	2.97049500	-2.03544400	-1.61925800
C	4.11434200	-1.09147300	-2.01785800
C	3.37181500	-3.50943700	-1.76004600
H	-0.59134200	2.58201700	2.30557100
H	-0.69630400	4.17325700	-1.25842200
H	3.31612700	-3.50167600	1.00986600
H	2.12039600	-1.83550800	-2.29492700
H	0.54063200	4.71236600	2.81133200
H	0.82556200	5.03869800	1.09159600
H	1.65639700	3.67728000	1.89078800
H	-2.65047300	3.44589700	1.19287700
H	-1.75659300	4.87660000	0.60676100
H	-1.98344700	4.63260100	2.34933900
H	0.03708000	1.74167100	-3.00377100
H	-0.51611100	3.32483100	-3.60346400

H	-1.61193500	2.30474200	-2.62747300
H	1.80869200	4.33270700	-0.81758900
H	2.06828300	3.01906300	-1.98991700
H	1.39469600	4.57552900	-2.52794600
H	4.39189100	-1.28176700	-3.06764200
H	3.82318000	-0.03468400	-1.93463300
H	5.01753800	-1.25128700	-1.40889700
H	2.55050000	-4.19828700	-1.50813100
H	4.23944600	-3.76097500	-1.12967000
H	3.65724700	-3.71258900	-2.80523200
H	5.17401200	-1.86559600	0.64431000
H	5.10812300	-2.34079400	2.35212400
H	4.46675300	-0.75975400	1.85092000
H	2.30345100	-1.51697000	3.14244100
H	2.97122100	-3.13765200	3.42012200
H	1.40873800	-2.95702000	2.58286700
C	2.76390100	1.38756300	0.30956300
O	3.74575200	2.00119900	0.28014500
N	-3.89527800	-2.65189900	-0.21601200
H	-3.76451400	-3.64353800	-0.38548400
C	-5.18952000	-2.08180700	-0.45024600
H	-5.29208100	-1.52622200	-1.38904800
C	-6.00082800	-1.57723500	0.72303400
H	-5.54009800	-1.65565600	1.70975500
H	-6.62303300	-0.69332200	0.56559500
C	-6.38304400	-2.86521200	0.02811600
H	-7.26986300	-2.87604800	-0.60841200
H	-6.18483800	-3.80008300	0.55813600
C	-0.50043200	-1.91342700	-0.02703700
C	-2.74514200	-1.92232700	-0.17398900
C	-1.66920300	0.10223300	-0.09399600
H	0.68250800	-3.56613200	-0.06106800
N	0.71480300	-2.55258600	0.01247800
N	-0.45918600	-0.56894000	0.05208400
N	-1.69651800	1.42554800	-0.15870700
N	-2.84245900	-0.59134500	-0.17546200
N	-1.59976700	-2.65625500	-0.14050700
H	1.28408300	0.03198300	1.90124600
H	0.86987000	0.74570700	1.87315200
O	-4.47901200	1.87610700	-0.17574100
H	-4.43666200	0.91761400	0.00050200
H	-3.51483300	2.01108300	-0.32138200
H	1.38427500	0.53227000	-1.22935000
Fe	1.27088600	0.45457800	0.26985400

Fe-9

P	0.15145600	2.28730800	-0.14388400
P	1.76310600	-1.83724800	-0.09144100
C	0.08826800	3.34233000	1.42261200
C	1.47753000	3.80968200	1.88065600
C	-0.91432300	4.50273400	1.39067100
C	0.20866800	3.49511100	-1.59184100
C	1.63214100	4.03968400	-1.79113700
C	-0.32036700	2.85633800	-2.88238400
C	2.51555300	-2.68205000	1.42338700
C	3.74495500	-1.89408800	1.90349900
C	1.49428200	-2.85666400	2.55610100
C	2.61152700	-2.62986100	-1.57875100
C	4.04824700	-2.11793900	-1.76119700
C	2.55268000	-4.16172500	-1.63194900
H	-0.26664900	2.58479600	2.14233200
H	-0.45543000	4.33241000	-1.31820400
H	2.84310000	-3.68184600	1.09322900
H	1.99656300	-2.22393400	-2.40045100
H	1.41243000	4.20620800	2.90764400
H	1.87148800	4.61917600	1.24568500
H	2.20764800	2.98687200	1.88411800
H	-1.92349400	4.18404400	1.08555900
H	-0.58966700	5.31007800	0.71467200
H	-1.00484000	4.93966900	2.39935500
H	0.29305600	1.98900200	-3.17353200
H	-0.28209800	3.59508500	-3.70026000
H	-1.36210500	2.51814900	-2.78029400
H	2.01776200	4.55954900	-0.90191800
H	2.33597400	3.23086900	-2.04513800
H	1.63821200	4.76254100	-2.62362700
H	4.43126600	-2.43328900	-2.74583000
H	4.10803100	-1.02034500	-1.71316100
H	4.72808700	-2.53456300	-1.00039000
H	1.52682200	-4.54935600	-1.53540700
H	3.17265900	-4.62621900	-0.84854100
H	2.94096500	-4.51105500	-2.60318400
H	4.49833200	-1.75586000	1.11336600
H	4.23081000	-2.43291600	2.73384100
H	3.45003800	-0.89798200	2.26837900
H	1.04327300	-1.89718800	2.85468400
H	1.99877700	-3.28448000	3.43884500

H	0.67890900	-3.53916200	2.27414700
C	2.84806800	0.96194900	-0.10638600
O	3.93431900	1.38651400	-0.10977900
N	-4.41039000	-1.90169800	-0.40579600
H	-4.45310000	-2.90482400	-0.55246100
C	-5.59774500	-1.12239600	-0.60892700
H	-5.62892400	-0.56328300	-1.55020400
C	-6.28522500	-0.49225000	0.58068800
H	-5.82024300	-0.64487400	1.55657800
H	-6.75509800	0.48263600	0.43330400
C	-6.89240300	-1.69891000	-0.09894300
H	-7.78266300	-1.56338800	-0.71601100
H	-6.83806900	-2.65438500	0.42860100
C	-0.93167500	-1.74288700	-0.23044200
C	-3.15869500	-1.38474600	-0.34060400
C	-1.76236500	0.38368900	-0.23989600
H	-0.03445900	-3.55378300	-0.20930500
N	0.16083400	-2.55646500	-0.20078700
N	-0.67160000	-0.41431300	-0.18716000
N	-1.51510600	1.72165000	-0.21625400
N	-3.02741300	-0.04297400	-0.31783500
N	-2.14801500	-2.28513200	-0.30408800
H	1.19256600	0.33353600	1.45643000
H	-0.01661000	0.20873900	2.38581800
O	-0.65067300	0.20384900	3.14544500
H	-0.08461200	0.50074800	3.87542100
H	-2.33447900	2.32132200	-0.26408300
H	1.24330100	0.29205700	-1.68209000
Fe	1.22738400	0.32869100	-0.11657200

Fe-TS2/3

P	0.08846100	2.26035800	-0.35785800
P	1.66525400	-1.88487200	-0.26299200
N	-0.75684300	-0.43201400	-0.26321000
C	-1.84146300	0.37568400	-0.31009600
C	-3.25717500	-1.38046400	-0.30609400
C	-1.03114400	-1.75893800	-0.26800900
C	0.06152500	3.46534400	1.09629000
C	1.46901900	3.89364800	1.53678900
C	-0.87056700	4.67180400	0.92615800
C	0.15815300	3.32689200	-1.91275200
C	1.59613300	3.80050500	-2.17643700
C	-0.41336900	2.59572300	-3.13401000

C	2.55845700	-2.80223500	1.12885000
C	3.76185700	-1.97188400	1.60721400
C	1.63664700	-3.15238800	2.30360200
C	2.39360900	-2.60288600	-1.84823600
C	3.83832700	-2.12962300	-2.06704100
C	2.26913700	-4.12405200	-1.99696800
H	-0.35478300	2.81042400	1.87937200
H	-0.47310800	4.20779500	-1.70854200
H	2.92862400	-3.74194800	0.68681300
H	1.75493600	-2.11962700	-2.60701300
H	1.40641500	4.42648200	2.50010900
H	1.93635600	4.58208000	0.81491200
H	2.13673000	3.03057100	1.67291500
H	-1.88882700	4.38264900	0.62162300
H	-0.48271300	5.39154900	0.18781000
H	-0.95978500	5.20633600	1.88663900
H	0.17191700	1.69135300	-3.36351200
H	-0.37301700	3.26268000	-4.01128800
H	-1.46149400	2.29704600	-2.98462900
H	2.00970500	4.38914600	-1.34433200
H	2.26723200	2.94567900	-2.35684900
H	1.61632800	4.43995800	-3.07432200
H	4.16756300	-2.40214100	-3.08339300
H	3.93725100	-1.03855700	-1.96333800
H	4.53574100	-2.60889600	-1.36076500
H	1.23008600	-4.47280100	-1.89419500
H	2.89010000	-4.66562700	-1.26525500
H	2.61440700	-4.42425700	-3.00034000
H	4.43369100	-1.68204100	0.78540200
H	4.35403200	-2.56151700	2.32676700
H	3.42246700	-1.05541100	2.11304500
H	1.19584500	-2.24837600	2.75081500
H	2.22409300	-3.65768100	3.08838800
H	0.81790600	-3.82555200	2.01169600
C	2.76924400	0.91294100	-0.21736500
O	3.85776500	1.32812500	-0.23449200
N	-2.25389400	-2.28994900	-0.28477600
N	-3.11181500	-0.04005300	-0.33186600
N	0.05314300	-2.58554100	-0.26324100
N	-1.58336900	1.71190400	-0.34965100
H	-2.39863200	2.31638800	-0.41098700
H	-0.15488500	-3.58026500	-0.27247200
H	1.04657200	0.30935700	1.39073700
N	-4.51454700	-1.88580300	-0.30402400

H	-4.57268700	-2.89307000	-0.41202600
C	-5.70355700	-1.10183400	-0.47841400
H	-5.77601300	-0.57877600	-1.43794600
C	-6.32583800	-0.41971900	0.71828000
H	-5.81499700	-0.54006600	1.67557000
H	-6.79309300	0.55409100	0.55634600
C	-6.97676500	-1.64443900	0.11609500
H	-7.89498600	-1.52270100	-0.46160000
H	-6.90510500	-2.57973300	0.67672200
C	0.66503100	0.47442300	3.11438300
O	-0.51957500	0.55441500	3.10382600
O	1.74979800	0.43852000	3.59496600
Fe	1.14081700	0.29182600	-0.21792500
H	1.16294700	0.24637800	-1.76453800

Fe-TS3/4

P	0.00418200	2.33594200	-0.23055600
P	1.71429100	-1.83126100	-0.28497000
N	-0.73988500	-0.39983200	-0.24559600
C	-1.84974900	0.38356900	-0.26189500
C	-3.21723700	-1.40898900	-0.34960400
C	-0.98349200	-1.73425900	-0.32395700
C	-0.03740200	3.53447500	1.21529200
C	1.34206000	4.14056100	1.51384100
C	-1.12011400	4.61569400	1.11545100
C	0.10906400	3.35800100	-1.80947500
C	1.56734200	3.73681600	-2.11551100
C	-0.53012200	2.63434400	-3.00239100
C	2.64114000	-2.85094100	1.01103200
C	3.75353000	-2.00126400	1.65235800
C	1.72478700	-3.44939600	2.08721800
C	2.46181900	-2.34349500	-1.93460300
C	3.91845500	-1.87309800	-2.06259100
C	2.31684800	-3.83621600	-2.25964700
H	-0.28518400	2.83049900	2.02597800
H	-0.46325900	4.27949800	-1.60978500
H	3.10472100	-3.67522100	0.44415900
H	1.84639500	-1.76721500	-2.64568300
H	1.30611600	4.65870500	2.48624600
H	1.64196600	4.88575300	0.75988400
H	2.12974600	3.37441100	1.57602500
H	-2.12439600	4.19838500	0.94393200
H	-0.90770400	5.34503900	0.31731800

H	-1.16221300	5.17460400	2.06506000
H	-0.01521600	1.68325900	-3.21432700
H	-0.44758100	3.26982700	-3.89945000
H	-1.59562200	2.41935500	-2.83785100
H	2.05722700	4.26240500	-1.28316100
H	2.16463000	2.84294300	-2.35515700
H	1.59580700	4.40539900	-2.99134800
H	4.27811500	-2.07420900	-3.08475900
H	4.02765200	-0.79433000	-1.87718500
H	4.58483200	-2.41311100	-1.37060000
H	1.26865900	-4.17004500	-2.23176900
H	2.90297300	-4.47116800	-1.57609500
H	2.69246000	-4.02204500	-3.27927000
H	4.37015400	-1.47010800	0.91123100
H	4.42514100	-2.65885800	2.22884900
H	3.31980800	-1.26693400	2.34830400
H	1.23136600	-2.65801400	2.67130400
H	2.34159400	-4.04127700	2.78448100
H	0.96180800	-4.12202500	1.66979200
C	2.73909600	1.02963800	-0.11082400
O	3.80922600	1.46742300	-0.19433400
N	-2.18908400	-2.29188900	-0.37720200
N	-3.10485000	-0.06508500	-0.30542500
N	0.11596400	-2.54144300	-0.35436300
N	-1.63700100	1.72645700	-0.24948900
H	-2.47347400	2.30294900	-0.28791400
H	-0.07903800	-3.53660900	-0.42002500
N	-4.45694800	-1.94374400	-0.37904200
H	-4.49216500	-2.94866500	-0.51590300
C	-5.67069400	-1.18323400	-0.47660900
H	-5.75900100	-0.57783600	-1.38426200
C	-6.30852300	-0.63267400	0.77883000
H	-5.79102100	-0.82534400	1.72063400
H	-6.80495700	0.33744900	0.70721400
C	-6.92397500	-1.81624100	0.06679100
H	-7.84709400	-1.67053800	-0.49726100
H	-6.82295300	-2.79623100	0.53976700
H	1.78407600	0.55557800	2.09339600
C	0.96613400	0.23443900	2.83185000
O	-0.19328000	0.63339800	2.53861800
O	1.35522300	-0.45944700	3.79173000
Fe	1.11276800	0.36215200	-0.10478000
H	1.24603100	0.39896000	-1.57823700

Fe-TS4/5

P	0.01374000	2.25870400	-0.23135000
P	1.87327700	-1.80256900	-0.15493900
N	-0.59909000	-0.42550300	-0.27119700
C	-1.72368500	0.34239800	-0.10483200
C	-3.03393700	-1.48215400	-0.46398800
C	-0.79725400	-1.74208600	-0.51528300
C	0.16512600	3.74984100	0.91112800
C	1.48354800	4.51735200	0.73753900
C	-1.04563400	4.69350400	0.85973600
C	-0.22040700	2.96747900	-1.96606400
C	1.12611000	3.29242600	-2.63118500
C	-1.05032800	2.02982300	-2.85310700
C	2.43789600	-2.84432300	1.31735000
C	3.50078600	-2.06684400	2.11391800
C	1.26433700	-3.24489200	2.22258600
C	2.96674400	-2.31380700	-1.59799400
C	4.42190000	-1.86092300	-1.40636600
C	2.88678500	-3.80154800	-1.96353900
H	0.18168400	3.27460300	1.90575800
H	-0.78857400	3.90258300	-1.82601000
H	2.89504500	-3.76022400	0.90614500
H	2.52682900	-1.72398900	-2.41981800
H	1.60000900	5.23952600	1.56275200
H	1.49724700	5.09470400	-0.20041800
H	2.36207000	3.85533500	0.74653300
H	-1.99268400	4.14871500	0.97800400
H	-1.08524200	5.25144100	-0.09010500
H	-0.96940200	5.43687200	1.67109300
H	-0.54516500	1.05979000	-2.98889200
H	-1.17823300	2.48405000	-3.85004500
H	-2.05007900	1.84523400	-2.43480900
H	1.74255500	3.98277200	-2.03735700
H	1.70977000	2.37293900	-2.79602900
H	0.95051000	3.76477700	-3.61237700
H	4.98002000	-2.01671800	-2.34407500
H	4.49822500	-0.79515400	-1.14530000
H	4.93068400	-2.44707800	-0.62422300
H	1.85736500	-4.12656800	-2.17716800
H	3.29789100	-4.44537200	-1.16936400
H	3.48208300	-3.98639500	-2.87298800
H	4.35753600	-1.75955600	1.49562000
H	3.89055900	-2.70078100	2.92754000

H	3.06018000	-1.16255800	2.56174500
H	0.73390900	-2.35706800	2.60040700
H	1.64885300	-3.80381900	3.09198800
H	0.53654100	-3.88837800	1.70718800
C	2.82300800	1.09156900	0.14079500
O	3.87819400	1.58080600	0.14493200
N	-1.98646600	-2.32559700	-0.64381200
N	-2.96443300	-0.16610400	-0.18769200
N	0.33262700	-2.50834200	-0.61796600
N	-1.56439900	1.65866300	0.23550400
H	-1.37793300	1.49125800	1.59201100
H	0.16722500	-3.50690900	-0.71593100
N	-4.26202000	-2.04790200	-0.57253200
H	-4.26595000	-3.00858900	-0.89888500
C	-5.49708000	-1.31847600	-0.55855200
H	-5.61262500	-0.58941100	-1.36756400
C	-6.14454200	-0.97518900	0.76336200
H	-5.61567100	-1.28511100	1.66676700
H	-6.67134100	-0.02106300	0.83381100
C	-6.72827700	-2.06215100	-0.11105500
H	-7.65964000	-1.86495700	-0.64529400
H	-6.59397900	-3.09669400	0.21460300
H	0.08546000	0.39015400	4.01308800
C	-0.06390300	0.63458600	2.94166400
O	0.81929100	0.29978100	2.13445000
O	-1.17176500	1.25653000	2.70944500
Fe	1.23476400	0.36543900	0.01834300
H	1.47869400	0.37524400	-1.46441100

Fe-TS7/1

P	0.02551400	2.33855100	-0.03993000
P	-1.90314000	-1.69778600	0.08722800
C	-0.22351500	3.73756000	-1.27076100
C	-1.46241600	4.59550700	-0.97742200
C	1.02861100	4.59727900	-1.48801200
C	0.69088500	3.12288500	1.53640500
C	-0.47675100	3.62448500	2.40320600
C	1.59618500	2.17937300	2.34017800
C	-2.26194100	-2.81780800	-1.39079600
C	-3.49458100	-2.31222700	-2.15729800
C	-1.03985500	-2.89997600	-2.31631700
C	-3.11253800	-2.17170200	1.44935800
C	-4.48598300	-1.50056300	1.30113300

C	-3.24737300	-3.68072000	1.69118300
H	-0.41749000	3.16676500	-2.19609000
H	1.29276800	3.98638800	1.20817400
H	-2.47244500	-3.82460400	-0.99243900
H	-2.60822700	-1.71857300	2.31994500
H	-1.66063800	5.25977400	-1.83497600
H	-1.31286600	5.24118300	-0.09749800
H	-2.36338400	3.98722300	-0.81036000
H	1.91753300	3.97687100	-1.67038500
H	1.22910600	5.25004200	-0.62270100
H	0.87898000	5.25330100	-2.36191700
H	1.05960700	1.26706500	2.64629900
H	1.93055200	2.69258400	3.25732200
H	2.49217800	1.88112100	1.77779600
H	-1.13741400	4.32254400	1.86847900
H	-1.09040600	2.78061400	2.75759300
H	-0.08112200	4.15229500	3.28685600
H	-5.06506800	-1.65025400	2.22719600
H	-4.40435700	-0.41798500	1.12814500
H	-5.07230200	-1.93848900	0.47820800
H	-2.27495200	-4.17597500	1.83665700
H	-3.77126200	-4.18469600	0.86359900
H	-3.83950100	-3.85270400	2.60517000
H	-4.40297200	-2.28954800	-1.53790900
H	-3.69557300	-2.97588200	-3.01435200
H	-3.32550400	-1.29703700	-2.55295500
H	-0.75925500	-1.90286900	-2.69318100
H	-1.27773200	-3.53519100	-3.18546000
H	-0.16379900	-3.33644500	-1.81396200
C	-2.80141000	1.17153900	-0.48432100
O	-3.83563700	1.65756300	-0.70251000
N	4.19619300	-1.99734600	0.44794300
H	4.21946400	-2.89830000	0.91374900
C	5.42845700	-1.29912200	0.22121500
H	5.59244000	-0.43191900	0.86929600
C	5.99388000	-1.21977400	-1.17873300
H	5.41136700	-1.68981200	-1.97355200
H	6.51510400	-0.30233200	-1.46073900
C	6.62987700	-2.12782400	-0.15016400
H	7.59174100	-1.84360200	0.28076500
H	6.47697500	-3.20379900	-0.26553500
C	0.73438400	-1.67258800	0.55084800
C	2.96447200	-1.45247900	0.30221900
C	1.63818000	0.30328500	-0.23884800

H	-0.27508600	-3.39233100	0.87665100
N	-0.41257500	-2.39264700	0.74225200
N	0.54352900	-0.37477200	0.21508600
N	1.37261400	1.50825200	-0.85769700
N	2.87766700	-0.20278200	-0.20236100
N	1.92470500	-2.25330800	0.65542700
H	-0.61359800	0.55140700	-1.76571700
H	0.34080100	0.97821900	-1.57505100
Fe	-1.24982300	0.44947600	-0.11863800
H	-1.62511300	0.48206900	1.35508700

Fe-TS8/9

P	0.00032200	2.25787500	-0.06168900
P	1.89282900	-1.75484500	-0.04812900
C	0.14570200	3.72645600	1.11422300
C	1.47109900	4.48979700	0.97907500
C	-1.05744300	4.67979200	1.07064600
C	-0.26272900	3.00913800	-1.77549500
C	1.07027400	3.38631100	-2.43975200
C	-1.07339700	2.07484000	-2.68357300
C	2.47442300	-2.83106500	1.38857600
C	3.81568600	-2.32173500	1.93918400
C	1.41700800	-2.90125000	2.49866500
C	2.92545300	-2.26274600	-1.54459700
C	4.25617800	-1.50435100	-1.64586600
C	3.12142000	-3.77509300	-1.71004100
H	0.14851800	3.22447900	2.09582100
H	-0.85378600	3.92503600	-1.60678100
H	2.61895200	-3.84542600	0.97997200
H	2.27096300	-1.90175200	-2.35658800
H	1.57622700	5.19524800	1.82034600
H	1.50636900	5.08541300	0.05310700
H	2.34484300	3.82207700	0.99216400
H	-2.01061400	4.13875500	1.15374800
H	-1.07546700	5.26870900	0.13893800
H	-0.99250100	5.39669000	1.90662300
H	-0.54926400	1.11766200	-2.83752300
H	-1.20843100	2.54667800	-3.67149100
H	-2.07029700	1.86293900	-2.27141300
H	1.66951200	4.08151300	-1.83412700
H	1.67889200	2.48739600	-2.62595600
H	0.87688600	3.87385100	-3.41019800
H	4.71938800	-1.70762300	-2.62568700

H	4.11720400	-0.41766000	-1.55851500
H	4.97519200	-1.82377400	-0.87516200
H	2.17352200	-4.33369600	-1.66023400
H	3.80410800	-4.18685000	-0.94965300
H	3.56874700	-3.98245000	-2.69632100
H	4.61765300	-2.33640400	1.18667800
H	4.13906400	-2.96077100	2.77742900
H	3.72384700	-1.29158600	2.32113500
H	1.22968400	-1.90702500	2.93444500
H	1.77534700	-3.56219700	3.30517800
H	0.45929900	-3.30288900	2.13551900
C	2.81443100	1.12879800	0.30494100
O	3.85968800	1.63779700	0.37311700
N	-4.24987300	-2.06994400	-0.48235200
H	-4.24191600	-3.02519000	-0.82443300
C	-5.48503400	-1.34109400	-0.50981400
H	-5.57872000	-0.61793700	-1.32716500
C	-6.17001500	-0.98813600	0.79022600
H	-5.66700500	-1.29086700	1.71068100
H	-6.69914300	-0.03389500	0.83853500
C	-6.72832500	-2.08214000	-0.09197100
H	-7.64427300	-1.88943300	-0.65382100
H	-6.60274800	-3.11407300	0.24514000
C	-0.78561200	-1.74026600	-0.37591000
C	-3.02517600	-1.49760400	-0.35237500
C	-1.73106200	0.33314900	0.03237200
H	0.20175400	-3.49644700	-0.56219000
N	0.35030900	-2.49551000	-0.45953800
N	-0.59994500	-0.42214500	-0.13110400
N	-1.58462600	1.64686600	0.39986100
N	-2.96783700	-0.18242300	-0.06868400
N	-1.97057300	-2.33305000	-0.51750900
H	1.06030300	0.28688900	1.80593900
H	0.17440200	0.65103700	2.23694400
O	-0.83181000	1.10043500	2.74274700
H	-1.33376500	0.34157100	3.08693300
H	-1.33957000	1.42677300	1.73488800
H	1.45503400	0.40044700	-1.36416400
Fe	1.24469300	0.38231200	0.14830100

Mn-1

P	0.00793100	2.29786000	0.12696200
P	1.72015400	-1.84399400	0.12383300

N	-0.73868500	-0.44031700	-0.11599200
C	-1.84821100	0.33230300	-0.08484900
C	-3.21017400	-1.46080800	-0.22417900
C	-0.97436200	-1.77437800	-0.14934300
C	-0.07013400	3.22582700	1.77261200
C	1.27191100	3.87959900	2.13406100
C	-1.22973500	4.21947500	1.91630400
C	0.00699500	3.65492600	-1.19134000
C	1.45185300	4.07374400	-1.51298100
C	-0.73257300	3.22595800	-2.46630300
C	2.29375600	-2.67402000	1.72175100
C	3.63859100	-2.09340300	2.18613800
C	1.23829100	-2.56000200	2.82906000
C	2.67042400	-2.70226800	-1.26752900
C	4.06359600	-2.09467900	-1.49030700
C	2.72869300	-4.23292700	-1.19085800
H	-0.23829100	2.38459400	2.46640800
H	-0.52270800	4.51899500	-0.75676200
H	2.43138600	-3.74167400	1.48183200
H	2.04217100	-2.42174500	-2.13128900
H	1.24977800	4.21208100	3.18524900
H	1.46772600	4.77166300	1.51725900
H	2.11880200	3.18748600	2.01760500
H	-2.20813100	3.76198500	1.70286400
H	-1.10735100	5.09634400	1.26027600
H	-1.26678600	4.59345000	2.95325300
H	-0.27147500	2.33423500	-2.91894900
H	-0.68361200	4.04010600	-3.20892600
H	-1.79323400	3.00497900	-2.27912400
H	2.01624700	4.37918700	-0.61959800
H	2.00168400	3.24986200	-1.99425800
H	1.44480200	4.92843800	-2.20969500
H	4.47989400	-2.46329700	-2.44263900
H	4.02963900	-0.99627400	-1.54005700
H	4.76956500	-2.38248100	-0.69521500
H	1.73494100	-4.68935500	-1.05942700
H	3.37695700	-4.57932600	-0.37011700
H	3.14786200	-4.63464400	-2.12858000
H	4.43480000	-2.21076600	1.43632200
H	3.96919000	-2.61138700	3.10170100
H	3.54654100	-1.02091900	2.42062600
H	1.04076000	-1.50498600	3.07657300
H	1.60449100	-3.06409300	3.73908200
H	0.28537300	-3.03016100	2.54388200

C	2.79684800	1.02536700	0.35603200
O	3.83826600	1.45907000	0.67171900
N	-2.18158800	-2.34058700	-0.21329400
N	-3.10713000	-0.11894000	-0.14728800
N	0.12899700	-2.57312900	-0.10776400
N	-1.63915700	1.67339600	0.02544700
C	1.45720900	0.42019700	-1.81508600
O	1.69971800	0.46886200	-2.96111200
H	-2.48076300	2.24313900	0.03699700
H	-0.05941200	-3.57213700	-0.08416200
Mn	1.20076900	0.36343500	-0.03938000
H	1.02703900	0.32692100	1.56495700
N	-4.45090800	-2.00234800	-0.30532000
H	-4.47269100	-3.00116800	-0.48222200
C	-5.65832700	-1.24477600	-0.46571000
H	-5.71307300	-0.64866700	-1.38289100
C	-6.34933300	-0.68091200	0.75496300
H	-5.87092600	-0.86160800	1.71951700
H	-6.84474300	0.28702100	0.65214000
C	-6.93336500	-1.87358500	0.03189300
H	-7.83306700	-1.73533300	-0.57068300
H	-6.85019600	-2.84812800	0.51929800

Mn-2

P	-0.00555500	2.15354900	-0.55251300
P	1.36902300	-2.10184600	-0.11156100
N	-0.98351400	-0.50317800	-0.22457300
C	-2.01328700	0.37156900	-0.16793100
C	-3.51618200	-1.28011000	0.15261200
C	-1.32469100	-1.79929800	-0.02431200
C	0.25286400	3.35510400	0.88087600
C	1.65556700	3.98164000	0.86456200
C	-0.83140900	4.42705700	1.04769500
C	-0.11820400	3.26140100	-2.08507800
C	1.28010800	3.46276900	-2.69404100
C	-1.09268300	2.70839800	-3.13427100
C	2.10364800	-2.79547900	1.48415700
C	3.57288600	-2.37473100	1.64007700
C	1.28115100	-2.38846900	2.71281200
C	2.02506600	-3.21813000	-1.49145400
C	3.38255900	-2.74712500	-2.03552500
C	2.03085800	-4.72145600	-1.18738200
H	0.20147500	2.66436000	1.73862900

H	-0.49613000	4.23852500	-1.73984500
H	2.05739700	-3.89290500	1.38446000
H	1.26826000	-3.02435200	-2.27169800
H	1.84714400	4.47659900	1.83068500
H	1.74889900	4.75032900	0.08039700
H	2.44699700	3.23326300	0.70927800
H	-1.84051000	3.99587900	1.13382500
H	-0.83275000	5.15063300	0.21639400
H	-0.64327600	4.99722200	1.97289100
H	-0.78289900	1.71149900	-3.48448800
H	-1.10696100	3.37910100	-4.00993500
H	-2.12090800	2.63319100	-2.75239300
H	2.01334800	3.83583600	-1.96430700
H	1.66672500	2.51979000	-3.11034900
H	1.22537300	4.19718600	-3.51478700
H	3.61411000	-3.28784100	-2.96840000
H	3.38335400	-1.67075100	-2.26074400
H	4.20322300	-2.95202500	-1.33012300
H	1.05980600	-5.08419200	-0.81495200
H	2.80300900	-4.98775800	-0.44801700
H	2.25479900	-5.28436800	-2.10898300
H	4.20045000	-2.70237300	0.79824500
H	3.99084900	-2.82406900	2.55632400
H	3.66481300	-1.28159000	1.73364800
H	1.27968200	-1.29533000	2.84177200
H	1.72302100	-2.83977200	3.61695800
H	0.23676700	-2.72755700	2.64307500
C	2.68179500	0.66825000	-0.45855600
O	3.78587000	1.04490600	-0.35224200
N	-2.56891200	-2.24691600	0.16030200
N	-3.29894400	0.04220100	0.00705800
N	-0.29336200	-2.68999600	-0.01145500
N	-1.68742500	1.68767500	-0.29572900
C	0.99958300	-0.12531400	-2.31245200
O	1.07105600	-0.26573400	-3.47420200
H	-2.47231900	2.33306000	-0.26655700
H	-0.55506700	-3.65260900	0.18651900
Mn	1.00125400	0.10953000	-0.53370900
H	1.05321700	0.35692200	1.06341100
N	-4.79428300	-1.70163600	0.32209300
H	-4.91989400	-2.70823500	0.30076000
C	-5.94827600	-0.85893400	0.19419400
H	-6.07670400	-0.39605300	-0.79007100
C	-6.42415900	-0.06293000	1.38814700

H	-5.83777800	-0.15172100	2.30474000
H	-6.85000300	0.92481600	1.19861500
C	-7.19201600	-1.28258100	0.93063400
H	-8.14969900	-1.14292200	0.42562400
H	-7.12321400	-2.18176600	1.54788400
C	2.54805700	1.60543100	3.79485600
O	3.38515100	0.82272700	3.57348300
O	1.71388500	2.39019400	4.02218000

Mn-3

P	-0.14497300	2.33584700	-0.18098100
P	1.75025200	-1.86506200	-0.13893100
N	-0.75915100	-0.46820600	-0.28616800
C	-1.89786100	0.27320500	-0.31331000
C	-3.20385900	-1.56652200	-0.34039900
C	-0.95998100	-1.81381800	-0.27020100
C	-0.33164900	3.35834200	1.39328400
C	0.99811400	3.97825600	1.84865400
C	-1.45503000	4.40250000	1.35400700
C	-0.10094900	3.58388500	-1.59526500
C	1.34219700	4.04746000	-1.85762000
C	-0.76477000	3.05885400	-2.87632500
C	2.59820500	-2.73843900	1.31000200
C	3.72045700	-1.85063800	1.87510100
C	1.63226600	-3.17495700	2.41905900
C	2.59090400	-2.58829400	-1.66423100
C	4.05673600	-2.13756400	-1.76080900
C	2.45484500	-4.10911900	-1.81255200
H	-0.61451000	2.57041000	2.10947400
H	-0.68514300	4.44820400	-1.24007800
H	3.04707000	-3.64370900	0.86912400
H	2.02905900	-2.11384600	-2.48555900
H	0.87818000	4.39074700	2.86389600
H	1.30987800	4.80969700	1.19611700
H	1.81419700	3.24158600	1.88300900
H	-2.42270300	3.97578300	1.04760400
H	-1.22037000	5.24496300	0.68416500
H	-1.59351900	4.82042600	2.36487800
H	-0.23767100	2.18408100	-3.28482800
H	-0.73823300	3.85058700	-3.64330500
H	-1.81609300	2.78144200	-2.71530500
H	1.83723600	4.43128300	-0.95332600
H	1.95927600	3.23038400	-2.26230200

H	1.33556800	4.86129800	-2.60092700
H	4.46672400	-2.43172200	-2.74060400
H	4.16752900	-1.04631300	-1.66684100
H	4.68152900	-2.61472400	-0.98879900
H	1.40453700	-4.43710300	-1.81128000
H	2.99166500	-4.65686000	-1.02167200
H	2.89149400	-4.41902500	-2.77620900
H	4.40751100	-1.48449800	1.09743800
H	4.31846000	-2.43575400	2.59356700
H	3.29464100	-0.98657500	2.40727400
H	1.15820200	-2.30937300	2.90436300
H	2.20299400	-3.71419700	3.19347300
H	0.84438000	-3.84999700	2.05581300
C	2.72023700	1.10966200	0.17951700
O	3.74895700	1.58695100	0.43171400
N	-2.14681800	-2.41303500	-0.29900500
N	-3.13710700	-0.21934100	-0.34536800
N	0.15878100	-2.59386100	-0.22459500
N	-1.74287900	1.62593000	-0.32063700
C	1.44852900	0.46032200	-1.93256400
O	1.70351800	0.49586300	-3.06854000
H	-2.61002500	2.15710100	-0.33191500
H	-0.01861900	-3.59498300	-0.21845900
Mn	1.12230600	0.37777700	-0.18975300
H	0.89233800	0.25244800	1.61516400
N	-4.42383700	-2.14477800	-0.37708100
H	-4.42193800	-3.15546800	-0.46790900
C	-5.66038700	-1.43249200	-0.53348100
H	-5.74987600	-0.87132800	-1.46901400
C	-6.34482800	-0.85052700	0.68264800
H	-5.84198700	-0.98303900	1.64257600
H	-6.87269800	0.09731600	0.55740900
C	-6.90294200	-2.08516500	0.01148400
H	-7.81773200	-1.99710900	-0.57751800
H	-6.77852700	-3.03931500	0.52957400
C	0.56364800	0.31317200	2.78792500
O	-0.65984300	0.37304000	2.94309100
O	1.54538200	0.29355600	3.53422000

Mn-4

P	-0.15062800	2.34036100	-0.09274600
P	1.84729100	-1.81831500	-0.05420100
N	-0.70009300	-0.47671700	-0.25284700

C	-1.84625000	0.24109400	-0.32918600
C	-3.11259300	-1.62491000	-0.37691500
C	-0.86786300	-1.82016100	-0.23023300
C	-0.44022500	3.33425900	1.48173900
C	0.84912100	4.01182900	1.96849200
C	-1.61265800	4.32163800	1.42154000
C	-0.04793200	3.63402300	-1.46809000
C	1.41685800	4.03778200	-1.70872400
C	-0.72528300	3.19092200	-2.77260900
C	2.69932700	-2.66985600	1.40820500
C	3.73223100	-1.71707700	2.03270900
C	1.72196700	-3.20321900	2.46334500
C	2.71437300	-2.54156000	-1.56288800
C	4.18109300	-2.08591600	-1.62242500
C	2.58694100	-4.06276300	-1.71470200
H	-0.70642100	2.52870200	2.18245800
H	-0.59039300	4.51450300	-1.08715200
H	3.23322100	-3.53026700	0.97156300
H	2.17262500	-2.06705400	-2.39782700
H	0.69298300	4.41424300	2.98325200
H	1.13851400	4.85962600	1.32591000
H	1.69363900	3.30789100	2.01292000
H	-2.55169500	3.84250700	1.10310500
H	-1.41454100	5.17298400	0.75059300
H	-1.78889800	4.73706000	2.42788800
H	-0.25175800	2.29274200	-3.19633200
H	-0.63413700	3.99865900	-3.51816400
H	-1.79547100	2.98066900	-2.63504400
H	1.93125900	4.34298300	-0.78519300
H	1.98993700	3.21176000	-2.15715100
H	1.45513700	4.89062700	-2.40626000
H	4.62176000	-2.38515100	-2.58742900
H	4.28463400	-0.99334800	-1.53232100
H	4.78584600	-2.55423400	-0.82881100
H	1.53709400	-4.39125000	-1.74591800
H	3.09705500	-4.60805300	-0.90418000
H	3.05520000	-4.37640500	-2.66237600
H	4.45371700	-1.33605600	1.29365400
H	4.30464300	-2.25122900	2.80929100
H	3.22383500	-0.85735600	2.49225600
H	1.11827200	-2.39339200	2.89706500
H	2.29577000	-3.67277800	3.27997500
H	1.03839400	-3.96409800	2.05915200
C	2.77034800	1.20053900	0.16529100

O	3.80625800	1.70726800	0.31643500
N	-2.04192000	-2.44893500	-0.28795400
N	-3.07523400	-0.27794500	-0.40413200
N	0.26740400	-2.57690900	-0.14748200
N	-1.71935300	1.59719900	-0.35450900
C	1.39500400	0.47556600	-1.84083000
O	1.56686700	0.47787600	-2.99621200
H	-2.59856800	2.10693700	-0.38389600
H	0.10944400	-3.58108300	-0.14378800
Mn	1.16993200	0.42033500	-0.08304800
N	-4.32191900	-2.23118700	-0.44082900
H	-4.29269600	-3.24108700	-0.53440900
C	-5.56117600	-1.54875900	-0.68099800
H	-5.61955000	-1.02299700	-1.63977500
C	-6.31149800	-0.93600500	0.47952600
H	-5.85115700	-1.02346800	1.46556600
H	-6.84997300	-0.00382500	0.29530500
C	-6.81662700	-2.20484600	-0.16948900
H	-7.70503200	-2.15545200	-0.80189100
H	-6.69926200	-3.13691000	0.38884700
H	0.42982200	-0.07495200	3.89893200
C	0.07979000	0.15715600	2.85553800
O	1.04750900	0.22432700	2.01781800
O	-1.13355500	0.32084400	2.66309400

Mn-5

P	-0.15852200	2.30328500	-0.10305100
P	1.86898000	-1.83170900	-0.06716000
C	-0.06640100	3.63448700	1.23652100
C	1.23908000	4.44358900	1.22619800
C	-1.29836800	4.55061000	1.27973400
C	-0.49768400	3.25708200	-1.70375200
C	0.76917500	3.88847500	-2.30152600
C	-1.22471800	2.38716600	-2.73879900
C	2.33973400	-2.82275200	1.47834100
C	3.31114800	-2.00474900	2.34634300
C	1.11726300	-3.27589200	2.28703000
C	3.05583300	-2.43928800	-1.39628900
C	4.49598300	-1.98598800	-1.11098000
C	2.98338300	-3.94406900	-1.68617400
H	-0.06835100	3.03106300	2.15815300
H	-1.18626300	4.06346300	-1.40125800
H	2.86375900	-3.72123100	1.11229900

H	2.69787500	-1.90203700	-2.28965700
H	1.31940500	5.02218700	2.16174000
H	1.26505200	5.16864700	0.39786100
H	2.13080200	3.80403000	1.15116700
H	-2.23433000	3.97412500	1.25939000
H	-1.30823300	5.25725600	0.43402200
H	-1.28192800	5.15132800	2.20480500
H	-0.59853900	1.54921000	-3.08252400
H	-1.47028000	2.99879100	-3.62353500
H	-2.16391800	1.97837200	-2.33990600
H	1.29029500	4.54939900	-1.59485000
H	1.48183700	3.12006700	-2.63612200
H	0.49921200	4.49563100	-3.18232500
H	5.12743300	-2.19113700	-1.99076200
H	4.55978800	-0.90802700	-0.89693900
H	4.93481500	-2.53250600	-0.26073500
H	1.96852600	-4.26833900	-1.96192800
H	3.32282900	-4.55076100	-0.83129500
H	3.64327800	-4.18312200	-2.53655100
H	4.19595700	-1.66652800	1.78636500
H	3.66776800	-2.62423100	3.18590900
H	2.80883900	-1.11721300	2.75900100
H	0.52178000	-2.41742800	2.63265500
H	1.45586200	-3.82917600	3.17881800
H	0.45691000	-3.94181100	1.71282500
C	2.79276200	1.17167700	0.38444700
O	3.81129900	1.66598700	0.65718100
C	1.63766300	0.51568800	-1.76298300
O	1.92585500	0.56552300	-2.89339100
Mn	1.22435900	0.41299100	-0.05100700
H	-1.51491900	1.24305600	1.80740700
N	-4.24554400	-2.20112700	-0.61393600
H	-4.21193200	-3.15634200	-0.95397200
C	-5.50240800	-1.51132300	-0.61935200
H	-5.62744200	-0.78025500	-1.42540900
C	-6.18358700	-1.19697400	0.69278200
H	-5.66122300	-1.49639700	1.60349700
H	-6.74189100	-0.26065500	0.76026600
C	-6.71764100	-2.29592700	-0.19847900
H	-7.64552300	-2.12429400	-0.74747800
H	-6.55663800	-3.32792500	0.12316100
C	-0.79474500	-1.77851600	-0.53074700
C	-3.03739400	-1.59273400	-0.48643000
C	-1.78854600	0.28102100	-0.11313600

H	0.19006300	-3.53109400	-0.68502100
N	0.35385300	-2.52991400	-0.61018500
N	-0.63409300	-0.45219500	-0.31987900
N	-1.69809200	1.57796000	0.26112900
N	-3.01413300	-0.28296300	-0.19978700
N	-1.96181500	-2.40634200	-0.65028300
H	0.04189200	0.10910300	4.00156000
C	-0.14597600	0.41965400	2.95711300
O	0.72666600	0.26082300	2.10084800
O	-1.33219300	0.94154300	2.80150200

Mn-6

P	-0.14874800	2.28462100	0.06586000
P	1.75615800	-1.85372700	0.11644700
C	-0.20736000	3.07424700	1.78762900
C	1.09542100	3.76005900	2.21938500
C	-1.41901900	3.99629600	1.98186800
C	-0.01783800	3.71524900	-1.15354200
C	1.44210500	4.13439700	-1.38350200
C	-0.71760500	3.38143400	-2.47799200
C	2.38205300	-2.50662300	1.76682100
C	3.85790100	-2.15775900	2.00720000
C	1.49064700	-1.96387100	2.89402000
C	2.68244200	-2.73827300	-1.26147200
C	4.03011600	-2.07917200	-1.59370100
C	2.81459300	-4.25344100	-1.05967800
H	-0.35297500	2.18036300	2.42227000
H	-0.55798800	4.55343700	-0.68077100
H	2.27479200	-3.60416800	1.72735000
H	2.00001500	-2.55719400	-2.11076100
H	1.03619900	4.02942800	3.28761500
H	1.26514200	4.69492400	1.66091200
H	1.97771200	3.11730700	2.08551600
H	-2.34792600	3.51115100	1.65133000
H	-1.30237900	4.93910000	1.42147800
H	-1.52036100	4.26157600	3.04793100
H	-0.23001300	2.53500900	-2.98836800
H	-0.66758800	4.25182100	-3.15409700
H	-1.77311800	3.12189800	-2.31901500
H	1.97333000	4.35706800	-0.44661200
H	2.00329700	3.34539000	-1.90891300
H	1.47688200	5.04186200	-2.00944100
H	4.43336600	-2.52409100	-2.51815800

H	3.93097200	-0.99650600	-1.75895800
H	4.77737500	-2.23746400	-0.80149300
H	1.84475900	-4.73943500	-0.87026000
H	3.49197500	-4.49891800	-0.22648000
H	3.23477500	-4.71003700	-1.97085100
H	4.53003000	-2.64870300	1.28911100
H	4.15321900	-2.49345300	3.01486700
H	4.03267100	-1.07095900	1.95485300
H	1.57420400	-0.86668900	2.97242000
H	1.80794400	-2.39318200	3.85823000
H	0.43141100	-2.22036600	2.74289700
C	2.73381000	1.10188400	0.33856100
O	3.75995400	1.58353100	0.60947800
C	1.50222900	0.49476600	-1.78261000
O	1.70714700	0.56121100	-2.92963800
Mn	1.15054500	0.36560900	-0.06633800
N	-4.39230800	-2.08469000	-0.22478600
H	-4.36859800	-3.08835200	-0.37080400
C	-5.61431700	-1.38439100	-0.49026200
H	-5.63800400	-0.83100800	-1.43549600
C	-6.39585400	-0.79118600	0.65987500
H	-5.96786300	-0.90815000	1.65746000
H	-6.92119700	0.15006300	0.48315700
C	-6.89268400	-2.03900800	-0.03604500
H	-7.76131100	-1.96407400	-0.69316600
H	-6.80299100	-2.98556900	0.50281700
C	-0.93725300	-1.76686800	-0.04768700
C	-3.16850000	-1.48811100	-0.16928200
C	-1.86239400	0.39733200	-0.11482300
H	-0.02180700	-3.57153100	0.06226500
N	0.17280400	-2.57491600	0.00629600
N	-0.71317800	-0.42549500	-0.04603300
N	-1.75509400	1.71205400	-0.11206300
N	-3.10704600	-0.16010300	-0.18603000
N	-2.12210300	-2.36169000	-0.09485400

Mn-7

P	-0.15355800	2.30743600	0.12259500
P	1.76956700	-1.84789600	0.12728800
C	-0.21083200	3.28690700	1.74359400
C	1.11601800	3.96752500	2.10507800
C	-1.39154800	4.26339600	1.82428700
C	-0.02312300	3.63655700	-1.21622200

C	1.43718000	3.98144100	-1.54519400
C	-0.81048400	3.25805200	-2.47765400
C	2.51741200	-2.67803700	1.64950200
C	3.83519200	-1.99567000	2.04893400
C	1.53350300	-2.71478900	2.82624600
C	2.64126200	-2.60415000	-1.36496700
C	4.03144900	-2.00268300	-1.62067100
C	2.67980100	-4.13819600	-1.37131500
H	-0.39581400	2.47706900	2.47346300
H	-0.50100000	4.52744400	-0.77531100
H	2.73100500	-3.71675300	1.34809100
H	1.97179100	-2.27405900	-2.17798500
H	1.06832900	4.35930800	3.13505600
H	1.32515600	4.82344400	1.44280500
H	1.97172900	3.27689100	2.04931300
H	-2.33291200	3.77587900	1.53382400
H	-1.23951200	5.14084000	1.17428600
H	-1.49637000	4.63875100	2.85630300
H	-0.39159300	2.36371500	-2.96517100
H	-0.76297300	4.08624900	-3.20517800
H	-1.86495300	3.05587800	-2.24534900
H	2.02791100	4.22705300	-0.65047600
H	1.93922800	3.14665800	-2.05861400
H	1.47358700	4.85452300	-2.21818000
H	4.38992400	-2.32140700	-2.61315400
H	4.02289500	-0.90243000	-1.60641500
H	4.77014000	-2.35061900	-0.88180000
H	1.68666600	-4.58638700	-1.21421000
H	3.36512200	-4.53665200	-0.60667300
H	3.04355100	-4.48953400	-2.35083100
H	4.57092300	-1.97841600	1.23214100
H	4.29047600	-2.53753500	2.89382200
H	3.66447000	-0.95614700	2.37249900
H	1.28354900	-1.70224300	3.18516700
H	1.99657000	-3.25172300	3.67023500
H	0.59548000	-3.22754400	2.56988200
C	2.80635200	1.13909100	0.26258500
O	3.85378900	1.63554200	0.35736700
C	1.31484300	0.42406500	-1.69122700
O	1.41590300	0.42764000	-2.84792500
Mn	1.18207600	0.38699100	0.09628500
N	-4.39296400	-2.08555400	-0.21578000
H	-4.36441500	-3.07882900	-0.42097700
C	-5.60886900	-1.37611800	-0.48459500

H	-5.62295200	-0.80687200	-1.42105700
C	-6.40024600	-0.79951600	0.66679000
H	-5.98243900	-0.93421400	1.66644000
H	-6.92142800	0.14598400	0.50060600
C	-6.89417600	-2.03413900	-0.05430400
H	-7.75627500	-1.94533400	-0.71831900
H	-6.81232400	-2.98979100	0.46946900
C	-0.93595500	-1.75553500	-0.02474600
C	-3.16567200	-1.48935600	-0.14597300
C	-1.86053100	0.39337100	-0.02834800
H	-0.00315700	-3.55728400	-0.01039000
N	0.18364800	-2.55805900	0.00662600
N	-0.72607800	-0.42597200	0.02907900
N	-1.75005000	1.71252800	-0.00051100
N	-3.10681600	-0.15960700	-0.11683300
N	-2.11893500	-2.36019800	-0.10736800
H	1.14094300	-0.01745200	1.79298900
H	0.87801600	0.75292600	1.76549300

Mn-8

P	-0.31766400	2.20106900	0.09971100
P	2.18915500	-1.63824300	0.12574600
C	-0.63013800	3.09767900	1.73972700
C	0.50382900	4.04965400	2.14226500
C	-2.00345100	3.77982300	1.81167100
C	-0.32769900	3.58052600	-1.19177000
C	1.07858400	4.14923400	-1.43668200
C	-0.98966100	3.13753900	-2.50378300
C	2.98357800	-2.38922600	1.66619700
C	4.15185800	-1.52019700	2.15962700
C	1.95966400	-2.62046600	2.78544000
C	3.22936500	-2.20763700	-1.33944000
C	4.54376600	-1.42432100	-1.47222600
C	3.46247600	-3.72187900	-1.41113000
H	-0.64114400	2.25245300	2.45238100
H	-0.95191800	4.37496600	-0.74871100
H	3.37704200	-3.36966500	1.35097500
H	2.57442900	-1.92072900	-2.17994500
H	0.34828200	4.40002400	3.17633400
H	0.52962300	4.94365900	1.49822600
H	1.49388000	3.56911000	2.09887100
H	-2.81592800	3.08986200	1.54343100
H	-2.05872700	4.65700800	1.14527400

H	-2.17970200	4.14372800	2.83824600
H	-0.41883000	2.33480900	-2.99647300
H	-1.02977900	3.99187400	-3.20069300
H	-2.01333400	2.77459000	-2.33818900
H	1.57937700	4.46147100	-0.50839300
H	1.72656800	3.41245900	-1.93663900
H	1.01362800	5.03299600	-2.09316500
H	4.98996700	-1.62402500	-2.46004800
H	4.39524800	-0.33755100	-1.38551800
H	5.28081800	-1.73267700	-0.71455100
H	2.52434200	-4.29547400	-1.35937500
H	4.13133700	-4.07488300	-0.61036000
H	3.94295300	-3.97108800	-2.37150600
H	4.91684600	-1.35124900	1.38839700
H	4.64450700	-2.01640400	3.01158100
H	3.79830400	-0.53589800	2.50737800
H	1.52744700	-1.67317400	3.14914000
H	2.46179500	-3.09696000	3.64313100
H	1.13375100	-3.27309300	2.46913200
C	2.76827700	1.47202100	0.36149200
O	3.72338000	2.11614500	0.51588000
C	1.48448700	0.59623300	-1.67343800
O	1.63349300	0.65070700	-2.82304800
Mn	1.28206900	0.49202000	0.10647000
N	-3.87125600	-2.76205600	-0.29347600
H	-3.71684100	-3.74850000	-0.47290900
C	-5.18078100	-2.22113200	-0.51130700
H	-5.30252500	-1.65385600	-1.44073400
C	-5.99916300	-1.75530700	0.67360100
H	-5.53256300	-1.83772300	1.65725900
H	-6.64249200	-0.88392900	0.53218700
C	-6.35218100	-3.04124300	-0.04004200
H	-7.24130500	-3.06441700	-0.67300300
H	-6.12859500	-3.97883500	0.47483600
C	-0.49405100	-1.94197500	-0.11440800
C	-2.73977000	-2.00531300	-0.24005800
C	-1.71486800	0.04663400	-0.13453800
H	0.69239200	-3.58620300	-0.08654200
N	0.72993500	-2.57006700	-0.07845900
N	-0.48027800	-0.59497100	-0.05055900
N	-1.79402000	1.37063700	-0.13706800
N	-2.86991100	-0.67778900	-0.21565300
N	-1.57713300	-2.71064700	-0.21156100
H	1.25220500	0.05565500	1.79511700

H	0.84778100	0.76144500	1.76502700
O	-4.58977600	1.69117700	0.09054200
H	-4.48845300	0.72294600	0.16080200
H	-3.64731500	1.89051700	-0.11131000

Mn-9

P	0.02816100	2.31465800	0.00909600
P	1.75296200	-1.84515900	0.02028100
C	-0.10019500	3.22127200	1.66291900
C	1.24522600	3.81797700	2.10084300
C	-1.23001800	4.25389400	1.76313300
C	0.07901900	3.68052100	-1.29650400
C	1.53685400	4.09139400	-1.56432500
C	-0.62462600	3.27475600	-2.59877600
C	2.42113200	-2.65651800	1.59876600
C	3.51787300	-1.77746900	2.21991900
C	1.31837700	-2.96836000	2.61978700
C	2.70463800	-2.69890400	-1.36843100
C	4.18176700	-2.27594000	-1.36605800
C	2.55574800	-4.22433400	-1.43329100
H	-0.33926200	2.37703600	2.33108500
H	-0.45646200	4.54336900	-0.86722000
H	2.87655100	-3.60856200	1.27947500
H	2.22653900	-2.26648000	-2.26390200
H	1.18584900	4.12859100	3.15733700
H	1.50496500	4.71459200	1.51458200
H	2.06991200	3.09589500	2.00813300
H	-2.21082300	3.83680200	1.48612300
H	-1.04143800	5.13954800	1.13516900
H	-1.31215000	4.60720400	2.80481300
H	-0.15086400	2.39256300	-3.05641200
H	-0.55663200	4.10346100	-3.32352800
H	-1.68966300	3.04948000	-2.44451700
H	2.07368000	4.37750500	-0.64766800
H	2.09606600	3.27093300	-2.04094800
H	1.55993800	4.95747000	-2.24627900
H	4.67260200	-2.63374100	-2.28611600
H	4.30026800	-1.18203600	-1.32573800
H	4.72855600	-2.71271200	-0.51447700
H	1.50376200	-4.53987400	-1.50670300
H	3.00693500	-4.72508100	-0.56148900
H	3.07180900	-4.60646900	-2.32996300
H	4.31188200	-1.51953300	1.50310700

H	3.98886100	-2.31238200	3.06139400
H	3.09356700	-0.83752600	2.60441200
H	0.74223900	-2.07013900	2.89239300
H	1.77818600	-3.36847300	3.53937600
H	0.61046500	-3.72399700	2.24813800
C	2.83075800	1.04361300	0.20706000
O	3.87956100	1.48826900	0.47378900
C	1.46196300	0.41230600	-1.91290000
O	1.69577600	0.43727200	-3.06041400
Mn	1.22475200	0.36988600	-0.13574600
N	-4.41829400	-1.99184300	-0.44707900
H	-4.43843700	-2.99409000	-0.60391300
C	-5.62103200	-1.23588800	-0.64722300
H	-5.65694400	-0.66153600	-1.57907200
C	-6.33276400	-0.64201500	0.54681000
H	-5.87268000	-0.80102500	1.52398700
H	-6.82323800	0.32450200	0.41197600
C	-6.90668300	-1.84999700	-0.15872000
H	-7.79454600	-1.72380900	-0.78117900
H	-6.83522400	-2.81299000	0.35286800
C	-0.94530600	-1.76292700	-0.23721700
C	-3.17905300	-1.44988500	-0.35578500
C	-1.81987700	0.34575800	-0.22558900
H	-0.03693700	-3.56194100	-0.16975900
N	0.15677400	-2.56427100	-0.18100300
N	-0.71023900	-0.42874000	-0.21193400
N	-1.61266100	1.68951800	-0.15047700
N	-3.07637700	-0.10664800	-0.30544200
N	-2.15083700	-2.32951700	-0.31317500
H	1.11145800	0.32191600	1.48039900
H	-0.09945100	0.06658100	2.37879300
O	-0.78523700	-0.03195600	3.08563800
H	-0.28172400	0.18390000	3.88625200
H	-2.45540500	2.25772500	-0.15275900

Mn-TS2/3

P	-0.04544700	2.30612800	-0.21303600
P	1.67857800	-1.89996800	-0.15207700
N	-0.78335400	-0.45351300	-0.32465000
C	-1.89256500	0.32335900	-0.30469200
C	-3.26210500	-1.46899100	-0.34629500
C	-1.02608500	-1.78769000	-0.32151600
C	-0.14047700	3.35475100	1.35886000

C	1.23410300	3.87022800	1.80853800
C	-1.18095900	4.48226100	1.33465600
C	-0.05884200	3.55614200	-1.63005300
C	1.36783500	4.05366700	-1.91553900
C	-0.71752600	2.99903100	-2.90000100
C	2.41512400	-2.77822800	1.35868900
C	3.51992100	-1.91449500	1.98846300
C	1.35607100	-3.17843500	2.39446500
C	2.56695600	-2.70547700	-1.60964200
C	4.04697500	-2.29445900	-1.64678200
C	2.39773400	-4.22572200	-1.72422600
H	-0.48024300	2.59540400	2.08223200
H	-0.66395500	4.40746400	-1.27833900
H	2.87617200	-3.70062400	0.96878300
H	2.06088300	-2.23805400	-2.47084100
H	1.15278000	4.29550700	2.82257800
H	1.60381800	4.67209900	1.14948700
H	1.98544400	3.06955600	1.83983300
H	-2.17686300	4.13885600	1.01365600
H	-0.87425000	5.31213700	0.67860100
H	-1.29353300	4.89617300	2.35057200
H	-0.15797100	2.14518600	-3.30946100
H	-0.73626300	3.78605400	-3.67244200
H	-1.75380200	2.67723900	-2.72259900
H	1.85146900	4.48910300	-1.02843800
H	2.00762900	3.23681000	-2.28535700
H	1.33875200	4.83562900	-2.69227600
H	4.50133400	-2.63025200	-2.59340100
H	4.17616900	-1.20294100	-1.58164800
H	4.62022400	-2.75853700	-0.82768900
H	1.33969300	-4.52611100	-1.76667900
H	2.87801600	-4.76511800	-0.89198600
H	2.87250300	-4.57765500	-2.65529600
H	4.26319900	-1.57655600	1.25062700
H	4.05501400	-2.50226400	2.75292100
H	3.09755200	-1.02412700	2.47685300
H	0.75990200	-2.31635100	2.73090000
H	1.85587700	-3.60643700	3.27949500
H	0.65935100	-3.93652400	2.00781100
C	2.75527400	1.00610200	0.10954100
O	3.79959400	1.44364600	0.39464900
N	-2.23476200	-2.35063100	-0.33864200
N	-3.15190000	-0.12579400	-0.32288600
N	0.07135400	-2.59774800	-0.30244900

N	-1.68517700	1.66859300	-0.26647800
C	1.44658700	0.36909500	-2.02511800
O	1.72264100	0.38366300	-3.16205800
H	-2.52912500	2.23576600	-0.26726400
H	-0.13199600	-3.59344700	-0.28257000
Mn	1.14869400	0.33774000	-0.26218500
H	0.96953600	0.30312500	1.39098900
N	-4.50504800	-2.00692400	-0.36972300
H	-4.53705700	-3.01239900	-0.50215900
C	-5.71514900	-1.24953100	-0.51339400
H	-5.80512300	-0.69615300	-1.45419100
C	-6.35118900	-0.62526200	0.70760600
H	-5.83427500	-0.76449100	1.65906200
H	-6.84447000	0.34079700	0.58011900
C	-6.97140900	-1.84566000	0.06563500
H	-7.89460200	-1.72907700	-0.50513500
H	-6.87279000	-2.79702800	0.59416500
C	0.56608200	0.39070800	3.08137900
O	1.58256400	0.78486200	3.55309500
O	-0.56345200	0.01971400	3.09441000

Mn-TS3/4

P	-0.24824300	2.37953100	-0.07768000
P	1.88836200	-1.75397500	-0.14139800
N	-0.69963300	-0.47079000	-0.13870200
C	-1.87716400	0.20778300	-0.08576400
C	-3.07703200	-1.69955100	0.01733300
C	-0.82233100	-1.82853600	-0.08166100
C	-0.38584400	3.43869300	1.47466700
C	0.89581900	4.24445200	1.73892400
C	-1.63089000	4.33440300	1.52502300
C	-0.35441700	3.58694300	-1.52556500
C	1.04388200	4.10847000	-1.89932000
C	-1.08165000	3.00056100	-2.74384200
C	2.96487500	-2.63423500	1.15154600
C	3.77521300	-1.61598500	1.96781200
C	2.19609900	-3.60588300	2.05595900
C	2.61399100	-2.37910800	-1.76736000
C	4.02704700	-1.81271300	-1.98000900
C	2.58023900	-3.90366900	-1.93853500
H	-0.48180200	2.66796200	2.25957700
H	-0.95104400	4.43314200	-1.14758800
H	3.67172400	-3.21896500	0.54028400

H	1.94577400	-1.93758200	-2.52422600
H	0.85746400	4.65930100	2.75958000
H	1.00154000	5.09556300	1.04705800
H	1.80411100	3.62710300	1.66746700
H	-2.56597600	3.76919200	1.38963700
H	-1.60069800	5.14158400	0.77570800
H	-1.68730800	4.81374900	2.51651500
H	-0.55410200	2.12919500	-3.15919100
H	-1.12931400	3.76736100	-3.53476600
H	-2.11157900	2.69802800	-2.50765900
H	1.58798400	4.52162200	-1.03783400
H	1.66381100	3.31584100	-2.34479000
H	0.94521500	4.91390800	-2.64519100
H	4.38794700	-2.08621200	-2.98490900
H	4.05522200	-0.71491400	-1.90314900
H	4.74674300	-2.22331900	-1.25279900
H	1.56116900	-4.30921100	-1.84756900
H	3.22547200	-4.42028800	-1.20995300
H	2.94903600	-4.16685100	-2.94370400
H	4.36336200	-0.94145300	1.32626300
H	4.48358200	-2.15359700	2.62021400
H	3.10351700	-1.01299200	2.59412600
H	1.43006500	-3.07337800	2.63452600
H	2.90816100	-4.07237200	2.75783200
H	1.72017700	-4.42349800	1.49229300
C	2.70630700	1.27969000	0.16518000
O	3.72653500	1.80399500	0.34212700
N	-1.97541300	-2.48656600	-0.00148500
N	-3.08523500	-0.35034700	-0.01426100
N	0.32972200	-2.55189600	-0.12432100
N	-1.80168400	1.56883600	-0.10493000
C	1.37358800	0.59740900	-1.86971700
O	1.55264100	0.65496500	-3.01859300
H	-2.69847800	2.04596400	-0.05622500
H	0.20048700	-3.55785200	-0.06261400
Mn	1.12379800	0.46835900	-0.13121600
H	1.12575700	1.02776800	2.23356000
N	-4.26344500	-2.34131700	0.07657100
H	-4.20593600	-3.34658200	0.20328400
C	-5.53564200	-1.69227800	0.22461400
H	-5.65411400	-1.12359000	1.15236200
C	-6.74268100	-2.41627300	-0.31043100
H	-6.56933900	-3.37037700	-0.81441200
H	-7.66091500	-2.36646400	0.27764700

C	-6.24852700	-1.16433500	-0.99930100
H	-6.82427800	-0.24310300	-0.88752500
H	-5.73887600	-1.28438300	-1.95727900
C	0.40857600	0.29010500	2.74495100
O	0.67930100	-0.92194600	2.54368700
O	-0.52200300	0.80502200	3.39564000

Mn-TS4/5

P	-0.15087300	2.30219300	-0.10413000
P	1.86919700	-1.83131400	-0.06450300
N	-0.63091900	-0.45172300	-0.32461300
C	-1.78154300	0.26702900	-0.09511800
C	-3.03332100	-1.59315000	-0.49352700
C	-0.78989800	-1.77761700	-0.55121300
C	-0.04709000	3.65600200	1.21026300
C	1.26721200	4.45034500	1.18236400
C	-1.26982300	4.58500700	1.23912300
C	-0.54567700	3.21393900	-1.71433600
C	0.69493500	3.86910800	-2.34076700
C	-1.26362000	2.30646800	-2.72353300
C	2.31096300	-2.82899100	1.48464500
C	3.28046500	-2.01996800	2.36326000
C	1.07296900	-3.26439600	2.27931300
C	3.07035400	-2.43799300	-1.38087000
C	4.50796400	-1.98849300	-1.07723200
C	2.99870000	-3.94175300	-1.67616500
H	-0.05410000	3.06743400	2.14102600
H	-1.25206600	4.00604600	-1.41560100
H	2.82869700	-3.73373700	1.12514800
H	2.72432600	-1.89714100	-2.27680500
H	1.35055700	5.05132800	2.10336500
H	1.30514100	5.15373600	0.33604500
H	2.15173000	3.79909300	1.12740900
H	-2.21247000	4.01889000	1.23522500
H	-1.27681200	5.27530000	0.38006600
H	-1.24332200	5.20310800	2.15238000
H	-0.62199300	1.47774500	-3.06083000
H	-1.53505700	2.89633200	-3.61535200
H	-2.18916300	1.88354400	-2.30742400
H	1.19705400	4.56768400	-1.65698500
H	1.43120400	3.11575400	-2.65823400
H	0.39804900	4.44093700	-3.23625500
H	5.14886000	-2.19138500	-1.95066000

H	4.57117900	-0.91152500	-0.85831300
H	4.93591000	-2.53935700	-0.22432100
H	1.98719100	-4.26354800	-1.96664900
H	3.32543000	-4.55156700	-0.81858300
H	3.66948400	-4.17949400	-2.51833600
H	4.17412100	-1.68904800	1.81307000
H	3.62273800	-2.64323000	3.20601300
H	2.78009000	-1.12884900	2.77043400
H	0.48496200	-2.39620100	2.61321000
H	1.39353300	-3.81826200	3.17740900
H	0.41235500	-3.92497600	1.69924100
C	2.79840900	1.16485200	0.39795500
O	3.81770300	1.65209500	0.67945400
N	-1.95855000	-2.40118100	-0.67578800
N	-3.00537700	-0.28576500	-0.17871800
N	0.35870600	-2.52489800	-0.63489100
N	-1.67999400	1.56458300	0.31809300
C	1.65230100	0.51775900	-1.75736200
O	1.94870100	0.57271500	-2.88543600
H	-1.52393700	1.31929400	1.68633800
H	0.19761700	-3.52584000	-0.72018100
Mn	1.22894300	0.41364300	-0.04676800
N	-4.24191100	-2.19282000	-0.62968400
H	-4.21469100	-3.14672700	-0.97406100
C	-5.49960500	-1.50443800	-0.59472500
H	-5.63757300	-0.75333300	-1.37961200
C	-6.15843500	-1.22578600	0.73682000
H	-5.62061500	-1.54865300	1.63035100
H	-6.71564000	-0.29192500	0.83817600
C	-6.70672700	-2.30124000	-0.17412100
H	-7.64353300	-2.11619300	-0.70316900
H	-6.53988000	-3.34124700	0.11736600
H	0.03092000	0.16252100	3.98716200
C	-0.16029600	0.47019000	2.93968300
O	0.72445100	0.26849300	2.09215400
O	-1.31858600	1.01802300	2.77046200

Mn-TS7/1

P	0.14999900	2.34357900	-0.16172100
P	-1.82880500	-1.76939500	-0.01538400
C	-0.06949000	3.64969100	-1.50058700
C	-1.33925200	4.49771700	-1.34087900
C	1.17649900	4.51444700	-1.73013800

C	0.90730500	3.21441700	1.32532600
C	-0.16209500	4.02158400	2.08068900
C	1.62217000	2.24123200	2.27423200
C	-2.03267900	-2.85005300	-1.54950200
C	-3.24740900	-2.39234400	-2.37219700
C	-0.75860200	-2.84598300	-2.40557200
C	-3.12306900	-2.34914500	1.22598900
C	-4.48835900	-1.67408100	1.02152600
C	-3.26116100	-3.87183300	1.35651500
H	-0.20963300	3.00383000	-2.38527500
H	1.65704900	3.90825100	0.91062900
H	-2.20958500	-3.87670300	-1.18796900
H	-2.69200400	-1.95832800	2.16382100
H	-1.51017300	5.07765600	-2.26319700
H	-1.25079600	5.22288300	-0.51684100
H	-2.23211100	3.88109500	-1.16306700
H	2.08299400	3.89886800	-1.82415800
H	1.32742100	5.23762400	-0.91208300
H	1.05785400	5.09540900	-2.66018000
H	0.93061800	1.48499200	2.67863700
H	2.03304000	2.80561800	3.12811000
H	2.45868400	1.72089800	1.78700200
H	-0.65646100	4.77114000	1.44667800
H	-0.93841100	3.36045800	2.49734000
H	0.30776800	4.55810100	2.92178900
H	-5.13597300	-1.89222600	1.88649200
H	-4.40377600	-0.58106900	0.93322800
H	-5.00501500	-2.05116800	0.12528900
H	-2.29714300	-4.37218100	1.53781300
H	-3.71967400	-4.32093100	0.46120500
H	-3.91552500	-4.10789200	2.21190000
H	-4.19195600	-2.46821100	-1.81410300
H	-3.34362200	-3.02303700	-3.27117200
H	-3.13017400	-1.34830800	-2.70590500
H	-0.51716600	-1.83036800	-2.75819700
H	-0.91196900	-3.48377500	-3.29163300
H	0.11291000	-3.23843500	-1.86070300
C	-2.74019300	1.13665100	-0.75760800
O	-3.71711300	1.56654300	-1.22765300
C	-1.76203200	0.67550300	1.59442900
O	-2.10736300	0.85961700	2.69421600
Mn	-1.22714200	0.45853600	-0.08856300
N	4.24625400	-2.06008800	0.50327000
H	4.25814500	-2.95230500	0.98601200

C	5.48514000	-1.37269900	0.27997500
H	5.64409800	-0.49278700	0.91194400
C	6.07129500	-1.32622700	-1.11288100
H	5.49797400	-1.81050500	-1.90581200
H	6.60121800	-0.41757300	-1.40683600
C	6.68763300	-2.21493700	-0.05588500
H	7.64453100	-1.92608000	0.38294300
H	6.53097400	-3.29244500	-0.15018400
C	0.78648000	-1.70993100	0.56096900
C	3.01976400	-1.51341600	0.32621600
C	1.70856100	0.24123100	-0.25862700
H	-0.21396100	-3.43353700	0.85363900
N	-0.36475600	-2.43336800	0.73328000
N	0.60763700	-0.40785000	0.22917800
N	1.46241000	1.41958700	-0.93071100
N	2.94388200	-0.27688300	-0.20921500
N	1.96995500	-2.30264900	0.67459400
H	-0.55061800	0.48513700	-1.77568300
H	0.40619800	0.87826000	-1.60805500

Mn-TS8/9

P	-0.10767700	2.29428900	0.05014100
P	1.84021500	-1.82152200	0.03556100
C	0.03991300	3.61490400	1.39564600
C	1.37825500	4.36828600	1.38434400
C	-1.15236500	4.58078300	1.45224200
C	-0.52242200	3.25097000	-1.52917900
C	0.72025600	3.89927000	-2.15808400
C	-1.26281400	2.37354500	-2.54832300
C	2.21539200	-2.79639200	1.61074400
C	3.42247400	-2.18750300	2.34125100
C	0.99407800	-2.87259800	2.53622300
C	3.01034800	-2.49438300	-1.28223000
C	4.42052700	-1.89318800	-1.18449400
C	3.05777300	-4.02390700	-1.39264400
H	0.01991200	2.99860600	2.30866200
H	-1.21372700	4.04592300	-1.20422000
H	2.47003200	-3.81914800	1.28690500
H	2.53692900	-2.09672500	-2.19602000
H	1.47457300	4.95628000	2.31266300
H	1.44468300	5.07946200	0.54612700
H	2.24133200	3.68937900	1.32795200
H	-2.11269300	4.04537200	1.43147900

H	-1.13684200	5.29619400	0.61390400
H	-1.10810300	5.17101200	2.38323800
H	-0.63449600	1.54279800	-2.90550500
H	-1.53393800	2.98266100	-3.42733000
H	-2.19037200	1.95491200	-2.13212600
H	1.23734300	4.58172500	-1.46886600
H	1.44348400	3.13920000	-2.49032800
H	0.42450900	4.48677400	-3.04382900
H	4.98618800	-2.13308800	-2.09979200
H	4.40011200	-0.79834100	-1.07941200
H	4.98521000	-2.30998000	-0.33575600
H	2.05808200	-4.47329600	-1.49865500
H	3.55332200	-4.48436300	-0.52318800
H	3.63693000	-4.30911600	-2.28662800
H	4.32804400	-2.15986200	1.71780400
H	3.65600800	-2.78712900	3.23654500
H	3.20522300	-1.15910200	2.67165300
H	0.68577200	-1.87075700	2.87359900
H	1.24919800	-3.46295600	3.43181700
H	0.13185700	-3.35424100	2.05195600
C	2.82538200	1.13034900	0.46238400
O	3.84792900	1.60642600	0.76334900
C	1.63705200	0.50146700	-1.70589300
O	1.94742300	0.55537900	-2.83133900
Mn	1.25574800	0.40200600	0.03020800
N	-4.27960100	-2.11783400	-0.53673400
H	-4.26576100	-3.06595900	-0.89765000
C	-5.52226200	-1.40159300	-0.52604800
H	-5.62630100	-0.64355200	-1.30962200
C	-6.20522100	-1.11471300	0.79150600
H	-5.69538800	-1.45371900	1.69543700
H	-6.74403200	-0.16929000	0.88503100
C	-6.75594000	-2.17353000	-0.13727400
H	-7.67617900	-1.96536100	-0.68642900
H	-6.61860300	-3.21829200	0.15255600
C	-0.81926600	-1.75950500	-0.43469000
C	-3.06039300	-1.54149400	-0.38523400
C	-1.77944800	0.29194000	0.03887300
H	0.15272400	-3.51971600	-0.58870500
N	0.31916100	-2.51846500	-0.51496300
N	-0.64098900	-0.43763800	-0.20025600
N	-1.65320000	1.57897900	0.49200400
N	-3.01206300	-0.23732200	-0.05628900
N	-1.99857500	-2.36508300	-0.56452600

H	1.03788000	0.27994900	1.73516700
H	0.15303400	0.51793800	2.21565100
O	-0.87032500	0.86315200	2.77811200
H	-1.33626800	0.05458500	3.05249700
H	-1.39271300	1.25518800	1.81232400