

Electronic Supplementary Information

Cobalt-Catalysed Unactivated C(sp³)-H Amination: Two-State Reactivity and Multi-reference Electronic Character

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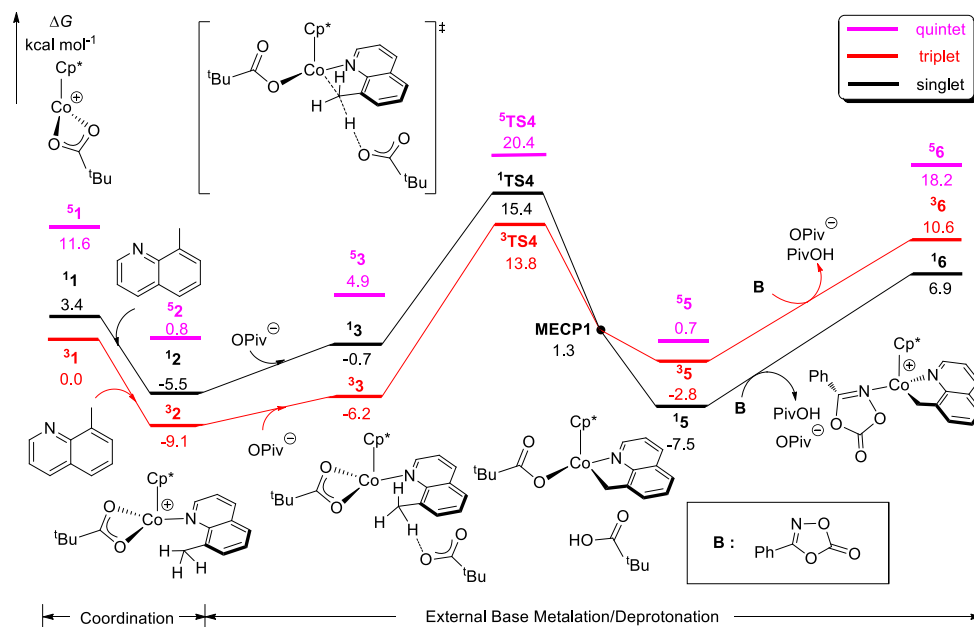


Fig. S1 The whole calculated free energy profiles for C(sp³)–H activation by Co(III) catalyst via external base metalation/deprotonation (energies in kcal mol⁻¹). The left-superscript denotes the spin state of corresponding species.

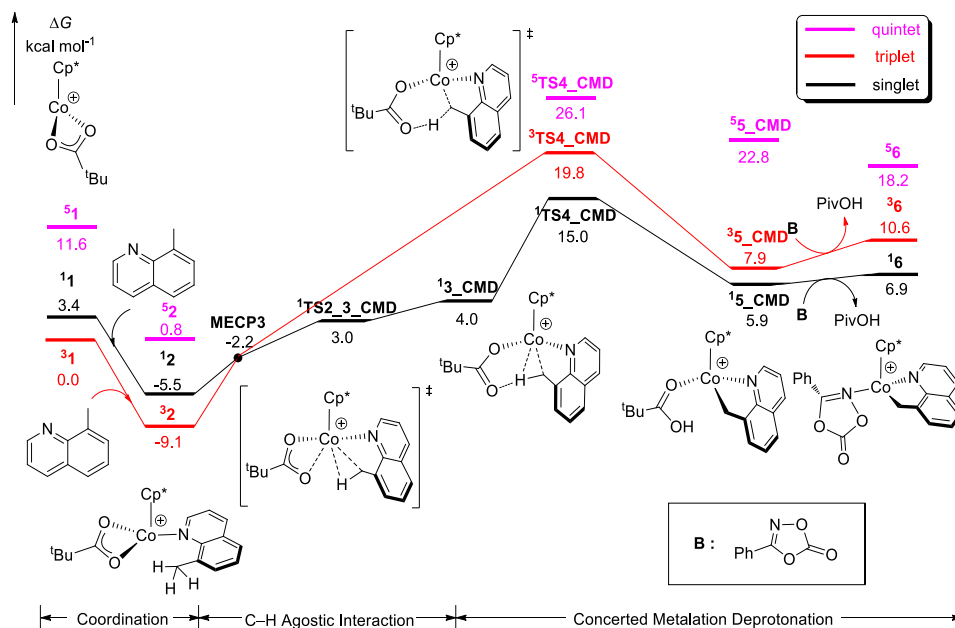


Fig. S2 The whole calculated free energy profiles (kcal mol⁻¹) for C(sp³)–H activation by Co(III) catalyst via intramolecular concert-metalation deprotonation (CMD). The left-superscript denotes the spin state of corresponding species.

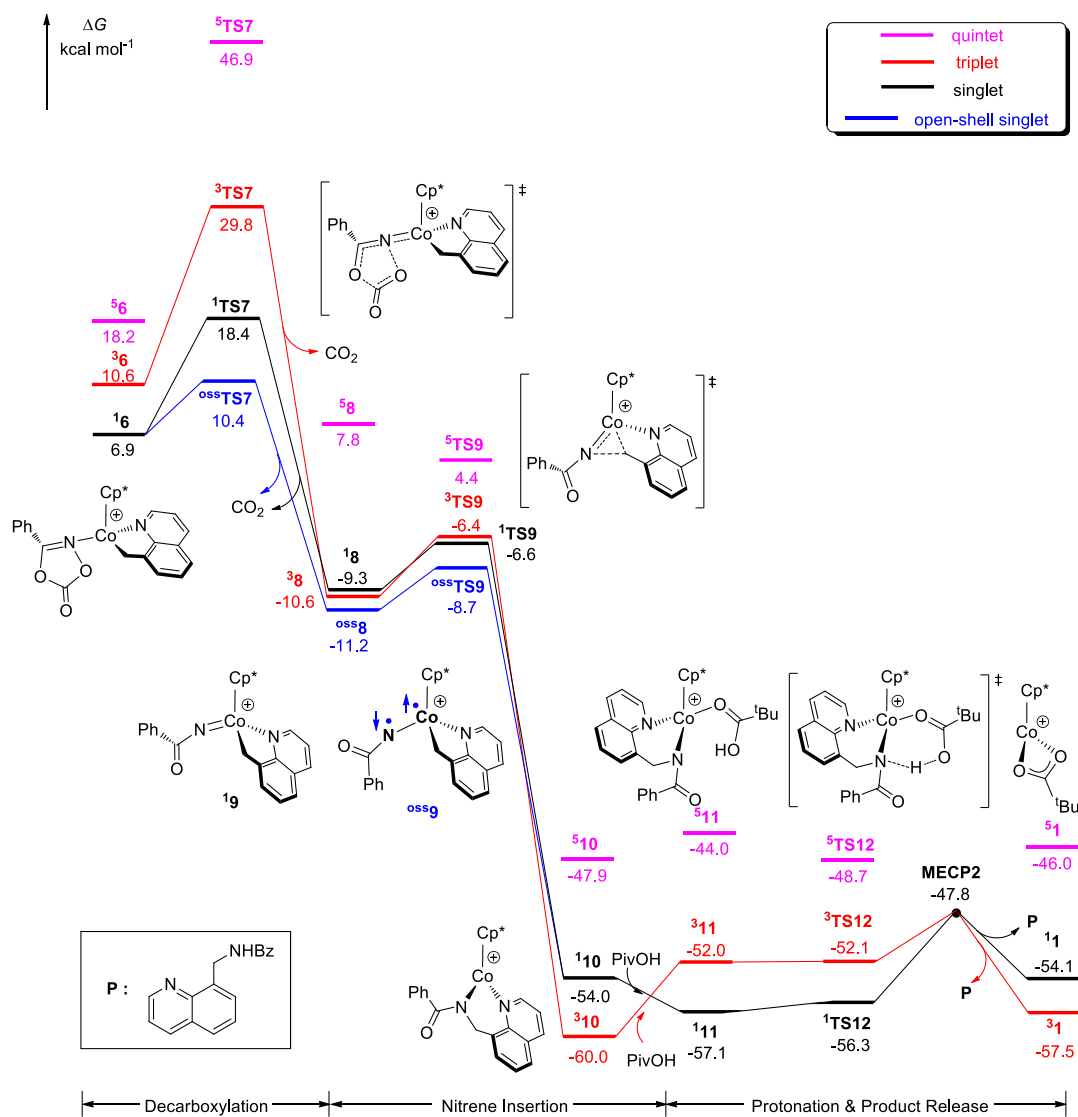


Fig. S3 The whole calculated free energy profiles for C–N bond formation by Co(III) catalyst (energies in kcal mol⁻¹). The left-superscript denotes the spin state of corresponding species.

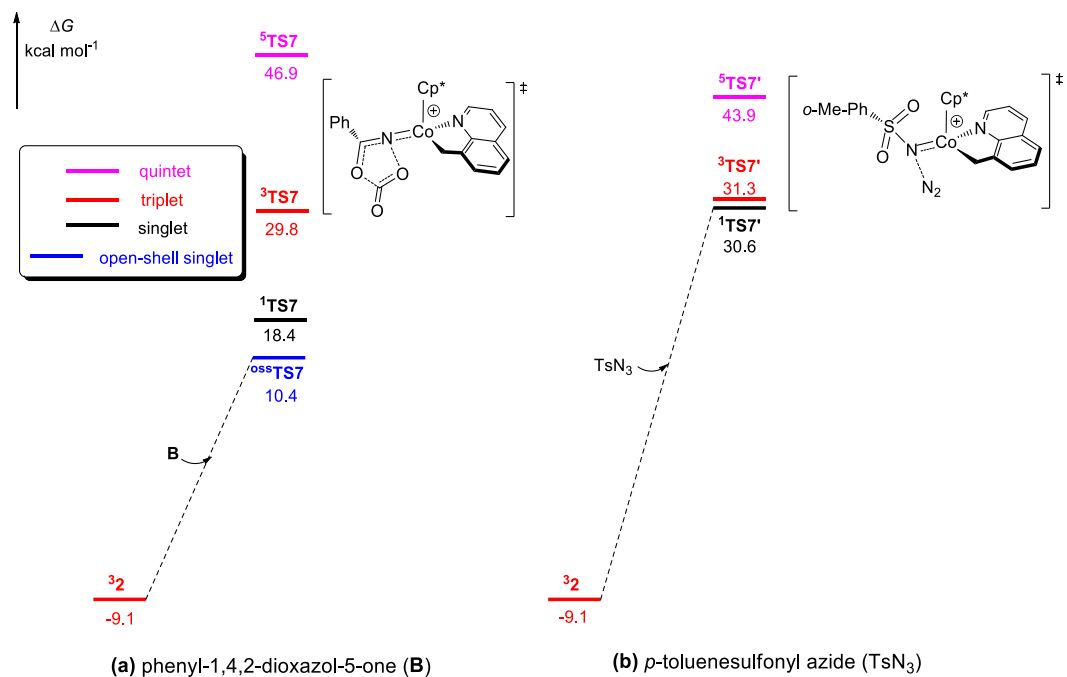


Fig. S4 The whole calculated free energy profiles (energies in kcal mol⁻¹) for generation of Co nitrenoid intermediates using (a) phenyl-1,4,2-dioxazol-5-one, (b) TsN₃. The left-superscript denotes the spin state of corresponding species.

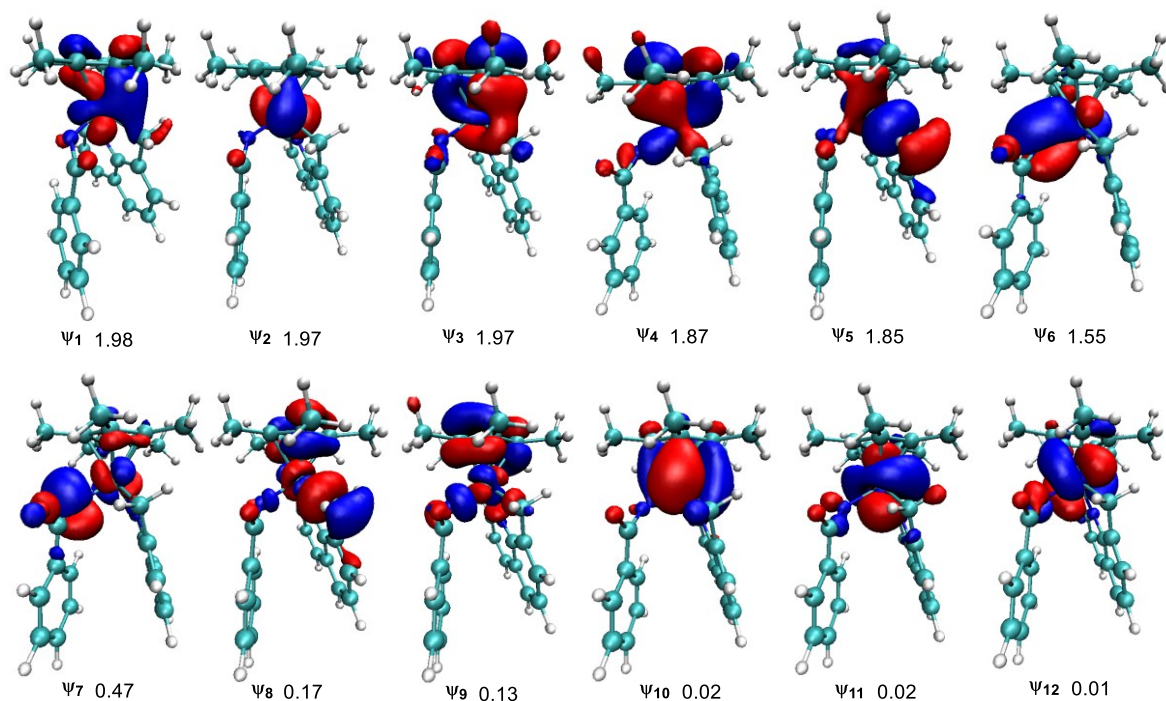


Fig. S5 Active space orbitals of ^{1oss8} calculated at the CASSCF(12,12) level of theory, the corresponding occupation numbers are given below each molecular orbital.

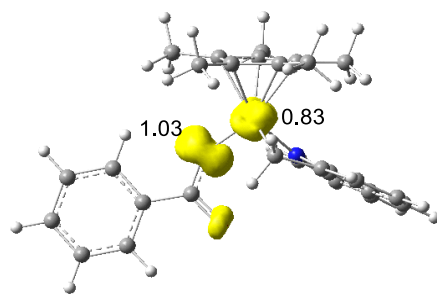


Fig. S6 Spin density plot for the 38 .

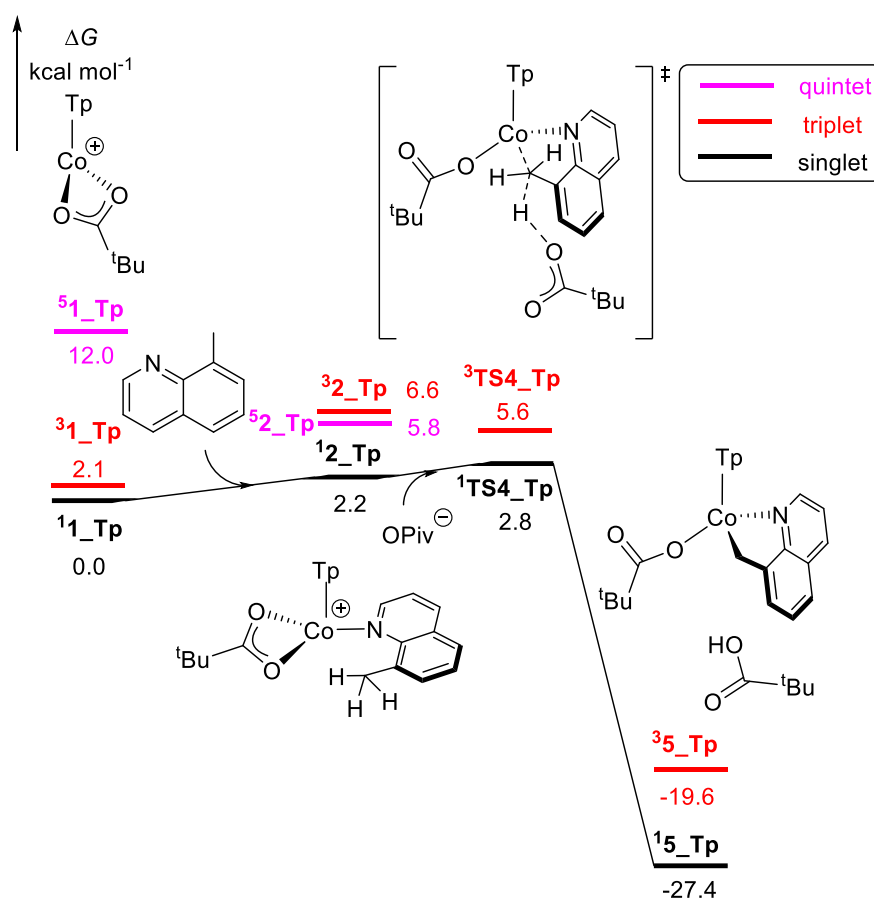


Fig. S7 Calculated free energy profiles for C(sp³)-H activation catalyzed by Tp ligated Co(III) complex via external base metalation/deprotonation (energies in kcal mol⁻¹, Tp = hydridotris(pyrazolyl)borate).

Table S1 Relative free energies of **1**¹, **3**¹, and **5**¹ calculated with different DFT functionals and DLPNO–CCSD(T) method (kcal mol⁻¹) on the basis of B3LYP-D3/BSI geometries.

	B3LYP–D3	B3P86	ωB97XD	PBE0	M06	CCSD(T) ^a
1 ¹	3.4	2.2	3.5	8	-1.5	3.5
3 ¹	0	0	0	0	0	0
5 ¹	11.6	13.3	36.1	10.2	10.5	18.1

^aThe DLPNO–CCSD(T) calculations were carried out using ORCA 4.0 software with def2–TZVP basis set.

Except for the M06 functional, all of the other methods predict the triplet ground state of **1**.

Table S2 Free energy differences (kcal mol⁻¹) of several potential Co(III) active species between singlet, triplet, and quintet states (the corresponding singlet states are taken as reference points).

	<i>G</i> (singlet)	<i>G</i> (triplet)	<i>G</i> (quintet)
[Cp*CoI ₂] ₂	0.0	-7.6	-2.5
Cp*Co(OPiv) ₂	0.0	-4.4	0.9
[Cp*Co(OPiv)] ⁺	0.0	-3.4	8.1
Cp*Co(OPiv)(SbF ₆)	0.0	0.4	9.1
[Cp*Co(SbF ₆)] ⁺	0.0	-11.6	-3.6

Table S3 Main electronic configurations (**Ψ**_{*i*}), natural orbitals (**ψ**_{*i*}), and the weight of contributions for the CASSCF(12,12) of ^{oss}**8**.

	Configuration state function	Weight
Ψ ₁	(ψ ₁) ² (ψ ₂) ² (ψ ₃) ² (ψ ₄) ² (ψ ₅) ² (ψ ₆) ² (ψ ₇) ⁰ (ψ ₈) ⁰ (ψ ₉) ⁰ (ψ ₁₀) ⁰ (ψ ₁₁) ⁰ (ψ ₁₂) ⁰	0.64
Ψ ₂	(ψ ₁) ² (ψ ₂) ² (ψ ₃) ² (ψ ₄) ² (ψ ₅) ² (ψ ₆) ⁰ (ψ ₇) ² (ψ ₈) ⁰ (ψ ₉) ⁰ (ψ ₁₀) ⁰ (ψ ₁₁) ⁰ (ψ ₁₂) ⁰	0.17
Ψ ₃	(ψ ₁) ² (ψ ₂) ² (ψ ₃) ² (ψ ₄) ² (ψ ₅) ⁰ (ψ ₆) ² (ψ ₇) ⁰ (ψ ₈) ² (ψ ₉) ⁰ (ψ ₁₀) ⁰ (ψ ₁₁) ⁰ (ψ ₁₂) ⁰	0.03
Ψ ₄	(ψ ₁) ² (ψ ₂) ² (ψ ₃) ² (ψ ₄) ⁰ (ψ ₅) ² (ψ ₆) ² (ψ ₇) ⁰ (ψ ₈) ⁰ (ψ ₉) ² (ψ ₁₀) ⁰ (ψ ₁₁) ⁰ (ψ ₁₂) ⁰	0.02

Cartesian coordinates and electronic energies (a.u., calculated at the level of B3LYP–D3/BSII(SMD,DCE)//B3LYP–D3/BSI) for all of the stationary points and the imaginary frequencies (cm⁻¹) of transition states

¹[Cp*CoI₂]₂, -4737.70347036

C	-2.23437500	2.32280400	0.70773100
C	-3.23514200	1.37769800	1.15742900
C	-3.91406900	0.88091600	0.00019900
C	-3.23541100	1.37737400	-1.15734700
C	-2.23457300	2.32263400	-0.70814600
C	2.23452400	-2.32265500	0.70810700
C	3.23535800	-1.37742600	1.15738100
C	3.91406500	-0.88092900	-0.00011700
C	3.23517900	-1.37766500	-1.15739500
C	2.23439200	-2.32278400	-0.70777100
C	1.38219000	-3.21702100	-1.55296500
H	1.76605200	-4.24340900	-1.49248400
H	0.34491000	-3.21814500	-1.20762100
H	1.38525200	-2.91171300	-2.59953200
C	1.38249000	-3.21675900	1.55361200
H	0.34518100	-3.21808300	1.20835800
H	1.76646100	-4.24312000	1.49335400
H	1.38561900	-2.91118900	2.60010200
C	3.59650300	-1.06257000	2.57623400
H	2.76145500	-1.26566200	3.24944400
H	4.45374800	-1.66293000	2.90510700
H	3.85735400	-0.00629700	2.67898100
C	5.16365500	-0.06120800	-0.00031600
H	5.22974000	0.57720400	0.88104900
H	6.02407100	-0.74419300	-0.00041700
H	5.22949300	0.57714700	-0.88174200
C	3.59612700	-1.06311200	-2.57636500
H	3.85687000	-0.00683900	-2.67939700
H	4.45339700	-1.66346600	-2.90518300
H	2.76102800	-1.26645000	-3.24943700
C	-3.59660500	1.06246000	-2.57617400
H	-4.45385900	1.66280600	-2.90504700
H	-2.76157700	1.26552200	-3.24941900
H	-3.85745800	0.00618200	-2.67886700
C	-5.16365500	0.06118600	0.00048600
H	-6.02407500	0.74416500	0.00065100
H	-5.22979800	-0.57722500	-0.88087600
H	-5.22942400	-0.57717200	0.88191500

C	-3.59603800	1.06320000	2.57642500
H	-4.45330900	1.66355400	2.90524200
H	-3.85676400	0.00692800	2.67951100
H	-2.76092300	1.26658100	3.24946300
C	-1.38213900	3.21707200	1.55286100
H	-1.76598500	4.24346300	1.49234000
H	-1.38518100	2.91181400	2.59944200
H	-0.34486700	3.21816300	1.20749400
C	-1.38259000	3.21672500	-1.55371600
H	-1.76659500	4.24307500	-1.49349400
H	-0.34527300	3.21810000	-1.20848900
H	-1.38573900	2.91110800	-2.60019300
I	-0.00000200	-0.00004400	-1.89447100
I	0.00000200	0.00005500	1.89448500
I	2.55132400	2.21541000	-0.00004600
I	-2.55130700	-2.21541300	0.00000600
Co	-1.84975000	0.32860800	-0.00000300
Co	1.84974900	-0.32860700	0.00001100

³[Cp*CoI₂]₂, -4737.70835508

C	2.27899100	2.40899800	-0.73997800
C	3.30201600	1.56291700	-1.18206300
C	3.95694300	1.02735900	-0.00044600
C	3.30213800	1.56365800	1.18102200
C	2.27911600	2.40948300	0.73858800
C	-2.29791500	-2.32666300	-0.70377600
C	-3.29332700	-1.37820200	-1.15881500
C	-3.96982300	-0.87261000	-0.00457900
C	-3.29919600	-1.37167200	1.15628700
C	-2.30236800	-2.32336600	0.71171400
C	-1.45912400	-3.22317900	1.56058300
H	-1.85088800	-4.24667400	1.50160300
H	-0.42140700	-3.23445900	1.21708900
H	-1.46022100	-2.91477400	2.60600600
C	-1.44843900	-3.22952800	-1.54322300
H	-0.41195900	-3.23472600	-1.19573700
H	-1.83666900	-4.25403300	-1.47902800
H	-1.44639700	-2.92796900	-2.59063100
C	-3.65531100	-1.07025100	-2.57884300
H	-2.82644500	-1.29074000	-3.25370800
H	-4.52382900	-1.66006800	-2.89723100
H	-3.90039100	-0.01100300	-2.68968600
C	-5.21100000	-0.04009900	-0.01050400
H	-5.26623700	0.59811100	-0.89281300

H	-6.07902400	-0.71334400	-0.01344600
H	-5.27350800	0.59990300	0.86998700
C	-3.66751600	-1.05510300	2.57277300
H	-3.91466800	0.00446700	2.67555600
H	-4.53615000	-1.64434100	2.89190700
H	-2.84074300	-1.26956700	3.25218000
C	3.69134300	1.24474900	2.59334900
H	4.60330200	1.77818700	2.88809700
H	2.89730500	1.52075600	3.29014300
H	3.87637300	0.17289600	2.71138400
C	5.25020400	0.28341100	-0.00036200
H	6.07466300	1.01062700	-0.00094300
H	5.35205100	-0.34777800	0.88349800
H	5.35160000	-0.34867200	-0.88364000
C	3.69120100	1.24329200	-2.59423500
H	4.60395100	1.77550200	-2.88874400
H	3.87490200	0.17118000	-2.71206000
H	2.89775200	1.52022500	-3.29132100
C	1.35993800	3.26458700	-1.54527500
H	1.61838600	4.32175900	-1.39927700
H	1.42133700	3.03852000	-2.61024000
H	0.31997600	3.13128100	-1.22963200
C	1.36019900	3.26557900	1.54351300
H	1.61875200	4.32264900	1.39697400
H	0.32019500	3.13221500	1.22804200
H	1.42169100	3.04005000	2.60859000
I	-0.08395800	-0.01589000	1.94353500
I	-0.08355000	-0.01725900	-1.94400100
I	-2.57645700	2.21842200	0.00020000
I	2.76880800	-2.29201800	0.00098500
Co	1.89271300	0.16043100	-0.00008000
Co	-1.89970700	-0.33387000	-0.00012000

⁵[Cp*CoI₂]₂, -4737.69694372

C	-2.25374700	2.48419400	0.72486200
C	-3.27521900	1.60576700	1.16781900
C	-3.95939100	1.10784600	0.00029500
C	-3.27567000	1.60564200	-1.16751600
C	-2.25403400	2.48411800	-0.72504100
C	2.20820200	-2.35707900	0.70692600
C	3.24104300	-1.44679000	1.15762100
C	3.93545600	-0.97148900	0.00079900
C	3.24212000	-1.44560100	-1.15723500
C	2.20902400	-2.35649500	-0.70844700

C	1.32751000	-3.22192900	-1.55424800
H	1.67808600	-4.26020900	-1.49625400
H	0.29119100	-3.19335900	-1.20722100
H	1.33763000	-2.91457900	-2.59994300
C	1.32555200	-3.22304200	1.55101300
H	0.28949200	-3.19336400	1.20328800
H	1.67546000	-4.26148700	1.49203500
H	1.33508400	-2.91694100	2.59707900
C	3.61783300	-1.14836600	2.57579400
H	2.78642600	-1.34454300	3.25497500
H	4.47024300	-1.76297700	2.89057000
H	3.89441400	-0.09660200	2.68395700
C	5.21018200	-0.19158400	0.00187800
H	5.29526800	0.44412300	0.88355900
H	6.04879600	-0.90117000	0.00239900
H	5.29659000	0.44441800	-0.87945400
C	3.62007500	-1.14560800	-2.57476400
H	3.89716500	-0.09382600	-2.68140900
H	4.47240500	-1.76021600	-2.88976200
H	2.78901600	-1.34054300	-3.25474000
C	-3.65533300	1.30593700	-2.58658200
H	-4.48432100	1.94203300	-2.92165600
H	-2.81200500	1.46970600	-3.26137900
H	-3.96788500	0.26369000	-2.69534800
C	-5.24346600	0.34462200	0.00055400
H	-6.08767500	1.04814900	0.00043500
H	-5.33314700	-0.29249100	-0.88108800
H	-5.33304500	-0.29208300	0.88249800
C	-3.65448000	1.30637200	2.58706100
H	-4.48329900	1.94262800	2.92224800
H	-3.96711300	0.26418300	2.69613900
H	-2.81093100	1.47018400	3.26157000
C	-1.33778800	3.32813100	1.54846400
H	-1.59977500	4.38791300	1.42864600
H	-1.39766600	3.08065400	2.60913000
H	-0.29642400	3.20770800	1.23184600
C	-1.33840900	3.32798500	-1.54908100
H	-1.60060700	4.38775000	-1.42955900
H	-0.29696600	3.20788400	-1.23261100
H	-1.39843300	3.08016400	-2.60966100
I	0.08545500	0.04456200	-1.95003800
I	0.08557000	0.04440700	1.95034100
I	2.66518900	2.16790700	-0.00020300
I	-2.81806400	-2.32990500	-0.00025300

Co	-1.84655000	0.11014900	0.00023700
Co	1.89148800	-0.35096600	0.00001500

NaOPiv, -508.969207358

C	1.10934100	0.01217900	-0.00000800
C	1.57325800	-0.74934100	1.25807900
H	1.14229900	-1.75317400	1.27597400
H	2.66625100	-0.83190400	1.27294100
H	1.26373600	-0.22567400	2.16985800
C	1.57322900	-0.74951200	-1.25799800
H	1.14226200	-1.75334300	-1.27575400
H	1.26369200	-0.22596500	-2.16984200
H	2.66622000	-0.83208200	-1.27287100
C	1.67730000	1.43671500	-0.00010900
H	1.34279000	1.99126500	-0.88086400
H	1.34281200	1.99138100	0.88058100
H	2.77332900	1.40782500	-0.00012300
C	-0.43676000	0.02837300	0.00002700
O	-1.04625000	1.14427300	0.00002500
O	-1.02843200	-1.10059600	0.00002400
Na	-2.90764900	0.00107000	-0.00002200

AgSbF₆, -986.893591865

Sb	-1.02195200	0.00005300	-0.00010300
F	0.24952400	-1.38739100	0.51390800
F	-1.98457300	-1.23086000	-1.01870200
F	-1.98406400	-0.26911400	1.57509100
F	0.24779100	1.14063700	0.94425700
F	0.24731800	0.24967100	-1.45977300
F	-1.98729500	1.49677400	-0.55425900
Ag	2.10683400	-0.00000300	0.00001200

NaI, -460.211256793

I	0.00000000	0.00000000	0.47280700
Na	0.00000000	0.00000000	-2.27806800

AgI, -444.916441225

I	0.00000000	0.00000000	1.23794400
Ag	0.00000000	0.00000000	-1.39597900

OPiv⁻, -346.705809073

C	0.53087000	0.01408800	0.00000500
C	0.99321100	-0.75049100	1.25107900
H	0.49817300	-1.72537400	1.27473800

H	2.08546700	-0.89517200	1.26965700
H	0.71203100	-0.20862500	2.16354700
C	0.99312800	-0.74985200	-1.25149100
H	0.49812800	-1.72474200	-1.27560000
H	0.71184800	-0.20753900	-2.16366400
H	2.08538800	-0.89447700	-1.27023800
C	1.10187100	1.43525100	0.00034300
H	0.74899500	1.98663100	-0.87632800
H	0.74907500	1.98618200	0.87732900
H	2.20412400	1.43210100	0.00029100
C	-1.06530200	0.03030000	0.00009300
O	-1.61109500	1.16073100	0.00000400
O	-1.59089200	-1.11382500	0.00000800

SbF₆⁻, -840.005686376

Sb	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	1.89494000
F	0.00000000	1.89494000	0.00000000
F	1.89494000	0.00000000	0.00000000
F	0.00000000	-1.89494000	0.00000000
F	-1.89494000	0.00000000	0.00000000
F	0.00000000	0.00000000	-1.89494000

NaSbF₆, -1002.23001606

Sb	-0.34726300	-0.00003500	-0.00001700
F	0.92492200	0.93369400	1.13862800
F	-1.31740200	-0.56223100	1.49233500
F	-1.31823800	1.57318600	-0.25805100
F	0.92359500	0.51952200	-1.37889400
F	0.92413400	-1.45378000	0.23813600
F	-1.32005200	-1.01009800	-1.23199300
Na	2.57798100	-0.00007500	-0.00005300

¹Cp*Co(OPiv)₂, -2466.36279553

C	0.02197800	-2.56739500	0.11819100
C	-0.77917400	-2.15261100	1.21634300
C	-2.05552500	-1.69974800	0.69265600
C	-0.71490100	-2.31844300	-1.09349700
C	-2.02361100	-1.84344700	-0.72079200
Co	-0.49726700	-0.54679800	-0.08348800
C	-0.21844900	-2.55057500	-2.48771700
H	0.81925000	-2.22009000	-2.58168600
H	-0.26503400	-3.61245900	-2.75853200
H	-0.81264000	-1.98941300	-3.21268000

C	-3.07617000	-1.42491000	-1.70096100
H	-2.71259000	-0.59385200	-2.31275400
H	-3.33038500	-2.25744100	-2.36519600
H	-3.98792800	-1.09667800	-1.19922200
C	-3.15849500	-1.12596500	1.53011700
H	-3.97110700	-0.73797100	0.91266500
H	-3.57442200	-1.88332100	2.20362300
H	-2.77676100	-0.30061100	2.13829900
C	-0.36000700	-2.14188600	2.65389600
H	-1.10289800	-1.63936300	3.27639200
H	-0.23384000	-3.16387800	3.02983000
H	0.58872600	-1.60713200	2.74668300
C	1.41309400	-3.11081800	0.19013000
H	1.38648600	-4.20716100	0.16342700
H	2.00623300	-2.76575300	-0.65984500
H	1.91268700	-2.78380500	1.10131200
C	3.49853700	0.66699600	-0.15836600
C	4.55957700	0.64820800	0.94963800
H	4.22000900	1.20850000	1.82443300
H	4.76389300	-0.37473200	1.27783100
H	5.49333400	1.09264800	0.58635400
C	3.98094900	-0.15131600	-1.37313300
H	4.17574700	-1.19274500	-1.09062600
H	3.22948700	-0.14542200	-2.16650700
H	4.91349300	0.26738600	-1.76873800
C	3.20376500	2.11666800	-0.59362900
H	2.43315300	2.13659900	-1.36813600
H	2.85365200	2.71322800	0.25666900
H	4.11121600	2.59050600	-0.98565600
C	2.18369400	0.04388800	0.36808400
O	1.25255900	-0.01389400	-0.54847500
O	2.07509000	-0.35123100	1.52959500
C	-1.42490000	3.18386700	0.01625500
C	-0.36198800	3.87049000	-0.87047300
H	-0.38397900	3.46575400	-1.88551400
H	-0.55783400	4.94710600	-0.91496900
H	0.64266800	3.71957000	-0.46504300
C	-2.82795500	3.39289000	-0.59070900
H	-2.88015600	2.97854300	-1.60064200
H	-3.59800500	2.90969000	0.02093200
H	-3.05648500	4.46266600	-0.63828300
C	-1.36395300	3.72917900	1.45019800
H	-2.10181100	3.23846800	2.09163400
H	-0.37815200	3.56257300	1.89142900

H	-1.56976200	4.80467200	1.44609000
C	-1.12330700	1.69467300	0.00625500
O	-0.76292400	1.05901800	1.04983900
O	-1.19835000	1.01598100	-1.07524900

³Cp*Co(OPiv)₂, -2466.36283833

C	1.11859400	-2.20670900	0.52530400
C	-0.04827000	-2.13299300	1.30966300
C	-1.15804300	-2.20157200	0.40088100
C	0.72557500	-2.40400600	-0.89841700
C	-0.65441500	-2.41141600	-0.96348400
Co	0.00277200	-0.25400700	0.02706000
C	1.71818400	-2.48116600	-2.01174400
H	2.23780200	-1.52019700	-2.10301800
H	2.46984800	-3.25548300	-1.81957100
H	1.23651600	-2.69841500	-2.96695400
C	-1.53916200	-2.49185500	-2.16807000
H	-0.96452600	-2.69536600	-3.07392600
H	-2.29041600	-3.28222300	-2.05717400
H	-2.06287000	-1.53957200	-2.30640200
C	-2.60042500	-2.16814900	0.77537600
H	-3.20364200	-1.75898400	-0.03891800
H	-2.96305500	-3.18423500	0.98223100
H	-2.75945600	-1.55624200	1.66466700
C	-0.15434600	-1.93487200	2.79273400
H	-0.83886600	-1.11126500	3.01679700
H	-0.52490600	-2.83694700	3.29406500
H	0.81546800	-1.68048800	3.22434500
C	2.53564100	-2.18374700	0.99330100
H	2.90980600	-3.20617900	1.13656700
H	3.17749700	-1.69957600	0.25252200
H	2.63411600	-1.63955800	1.93328700
C	3.37933200	1.88914300	-0.07446200
C	3.96614700	2.15520900	1.31858600
H	3.24539800	2.67585700	1.95359500
H	4.23038100	1.21881800	1.81920300
H	4.86971200	2.76892800	1.23389000
C	4.39197600	1.12622200	-0.95174400
H	4.68123600	0.17717500	-0.48524700
H	3.96689100	0.91037000	-1.93481200
H	5.30079100	1.72332900	-1.08380700
C	2.99618200	3.21859700	-0.76145100
H	2.55418600	3.03128800	-1.74344500
H	2.27094600	3.77456000	-0.15792100

H	3.88582700	3.84543000	-0.88792200
C	2.10141400	1.05351000	0.03283900
O	1.55054500	0.62197900	-1.04095600
O	1.56774300	0.78867100	1.14791700
C	-3.37221000	1.89115800	-0.08078400
C	-4.03415600	1.83774600	-1.46500700
H	-4.33861100	0.81677700	-1.71669000
H	-4.92544700	2.47458800	-1.47911900
H	-3.34541000	2.17774400	-2.24173100
C	-4.34027200	1.38022900	1.00340500
H	-4.66330000	0.35464600	0.79164300
H	-3.86118600	1.39044900	1.98504000
H	-5.23352800	2.01321200	1.03860500
C	-2.93591100	3.33646100	0.25018700
H	-2.44191200	3.37592300	1.22472600
H	-2.24004200	3.71651100	-0.50507700
H	-3.81046600	3.99604500	0.27162400
C	-2.10416300	1.03412300	-0.05742400
O	-1.53894100	0.77453700	1.05427900
O	-1.58480400	0.59553800	-1.13246800

⁵Cp*Co(OPiv)₂, -2466.35125451

C	1.14510000	-2.15856000	0.48166300
C	0.00041300	-1.99591000	1.31337300
C	-1.14393100	-2.15878700	0.48126400
C	0.69594200	-2.37351200	-0.89318000
C	-0.69426700	-2.37367900	-0.89343000
Co	-0.00018400	-0.05551900	0.04506000
C	1.62759900	-2.49376100	-2.05767700
H	2.18145900	-1.55772000	-2.19092500
H	2.35722900	-3.29722100	-1.90144400
H	1.08999700	-2.70194700	-2.98511900
C	-1.62552200	-2.49426600	-2.05821700
H	-1.08758600	-2.70252800	-2.98544900
H	-2.35505200	-3.29783400	-1.90207600
H	-2.17953000	-1.55836100	-2.19178500
C	-2.57177200	-2.14179700	0.91569800
H	-3.22070200	-1.78650800	0.11057300
H	-2.90712700	-3.15215500	1.18688100
H	-2.71347100	-1.49216600	1.78155800
C	0.00005000	-1.77679000	2.79817100
H	-0.87894000	-1.20372500	3.10365400
H	-0.00103300	-2.72486900	3.35056200
H	0.87983100	-1.20533800	3.10436400

C	2.57277800	-2.14110300	0.91656800
H	2.90815300	-3.15120000	1.18869400
H	3.22196400	-1.78636900	0.11140500
H	2.71410200	-1.49075000	1.78195500
C	3.52370200	1.77436000	-0.09655300
C	4.14664800	1.93727500	1.29725100
H	3.46931600	2.46775000	1.97038600
H	4.36544700	0.96345500	1.74620800
H	5.08355100	2.49984200	1.22378400
C	4.47548600	1.00244900	-1.03081500
H	4.72433200	0.01954400	-0.61551100
H	4.02038300	0.85410900	-2.01263500
H	5.41017700	1.55955000	-1.15496700
C	3.20454300	3.15838300	-0.70828400
H	2.74203500	3.04845000	-1.69290500
H	2.52066600	3.72180500	-0.06487200
H	4.12698100	3.73903000	-0.81656400
C	2.19711800	1.02236400	-0.00572500
O	1.64159600	0.58450000	-1.07133600
O	1.60766400	0.84157000	1.10618600
C	-3.52457000	1.77336300	-0.09649800
C	-4.47606200	1.00144800	-1.03102400
H	-4.72468800	0.01837200	-0.61600000
H	-5.41088700	1.55833900	-1.15511800
H	-4.02084700	0.85347000	-2.01284700
C	-4.14763900	1.93568700	1.29732800
H	-4.36614400	0.96166600	1.74600100
H	-3.47051700	2.46619800	1.97064200
H	-5.08472600	2.49796100	1.22396700
C	-3.20580600	3.15767500	-0.70781000
H	-2.52208000	3.72109700	-0.06423800
H	-2.74328500	3.04817700	-1.69247500
H	-4.12841500	3.73808400	-0.81589400
C	-2.19773300	1.02179200	-0.00581100
O	-1.60800600	0.84141500	1.10604300
O	-1.64226700	0.58389300	-1.07141700

¹1, -2119.58287379

C	-2.30007300	-0.74722800	-0.65305000
C	-1.85693700	-1.17507600	0.61843900
C	-2.30908100	0.71893400	-0.67024600
C	-1.52079100	0.01485200	1.38145300
C	-1.87190500	1.18195100	0.59094500
C	-1.61980800	-2.57397200	1.09049000

H	-2.27081200	-2.79533400	1.94297700
H	-1.81957500	-3.30680600	0.30858900
H	-0.58338900	-2.70055300	1.41721800
C	-2.66325100	-1.60141600	-1.82492200
H	-2.34240700	-2.63504700	-1.69221900
H	-3.75089700	-1.59555100	-1.96423800
H	-2.21830200	-1.22076500	-2.74905600
C	-2.68230000	1.54091500	-1.86186200
H	-2.23275300	1.14399900	-2.77689500
H	-3.76978000	1.51886000	-2.00086900
C	-1.65126900	2.59446000	1.02956200
H	-1.86588500	3.30643600	0.23247600
H	-2.29995100	2.82638800	1.88096200
H	-0.61462700	2.74265100	1.34654100
C	-0.96665700	0.03437200	2.76620500
H	-0.34966900	-0.84492300	2.96182400
H	-0.37108600	0.93170100	2.94538500
H	-1.79182800	0.03106300	3.49016700
C	1.88144400	0.01791300	-0.24128500
O	1.17068600	1.09308300	-0.23472300
O	1.17984800	-1.06648300	-0.21964800
C	3.38451700	0.01002600	-0.22295200
C	3.78431800	-0.36292600	1.23146900
H	4.87546000	-0.39339700	1.29778700
H	3.42231600	0.38203400	1.94720500
H	3.39363400	-1.34537300	1.50978600
C	3.89194700	-1.07145900	-1.20039200
H	3.61500500	-0.83323100	-2.23203800
H	4.98298300	-1.11801800	-1.14585400
H	3.48906600	-2.05553100	-0.95048200
C	3.92995900	1.39862400	-0.59239400
H	5.02203300	1.38043300	-0.54295100
H	3.63945700	1.68242300	-1.60787600
H	3.56649800	2.16767300	0.09349600
H	-2.37379600	2.58113200	-1.75355900
Co	-0.39765400	0.00211500	-0.25822800

³¹I, -2119.58352165

C	1.92628300	-0.69052900	1.16996700
C	2.09281700	-1.15573600	-0.21847200
C	1.93904300	0.70715600	1.15509500
C	2.26666300	-0.01823100	-1.06901800
C	2.11381000	1.13982600	-0.24282000
C	2.15353100	-2.59305200	-0.61436700

H	3.13513100	-3.00485900	-0.34552700
H	1.39917100	-3.18420200	-0.08814800
H	2.01753000	-2.72868600	-1.68823100
C	1.75039200	-1.60797700	2.33768000
H	0.95997400	-2.34142300	2.15026600
H	2.67535500	-2.16803000	2.51881400
H	1.50134400	-1.06322300	3.24906900
C	1.78042000	1.65201900	2.30328500
H	1.52014100	1.13134000	3.22555300
H	2.71615600	2.19735800	2.47372700
C	2.20103600	2.56722500	-0.66887300
H	1.45913300	3.18371500	-0.15415900
H	3.19081800	2.96581200	-0.41032400
H	2.06562600	2.68293900	-1.74515600
C	2.56429100	-0.03675600	-2.54039300
H	2.14430600	-0.92017500	-3.02619100
H	2.16343900	0.84526300	-3.04453100
H	3.64734300	-0.05021200	-2.70700700
C	-2.02022400	0.02811200	-0.13637900
O	-1.31728400	1.10876000	-0.16645000
O	-1.32729500	-1.06377900	-0.14693600
C	-3.52463900	0.01438000	-0.07595800
C	-4.03468700	-0.83783000	-1.26320400
H	-5.12557000	-0.89535400	-1.21475900
H	-3.76274600	-0.38533600	-2.22209700
H	-3.63071600	-1.85222600	-1.22581600
C	-3.91814800	-0.66176600	1.26207500
H	-3.55805500	-0.08479700	2.12000400
H	-5.00867300	-0.71294100	1.32435200
H	-3.51854400	-1.67687600	1.32507800
C	-4.07747200	1.44586200	-0.14791700
H	-5.16928100	1.41201600	-0.09975900
H	-3.71579000	2.05658600	0.68336700
H	-3.79081200	1.93806000	-1.08110900
H	1.00487300	2.39702000	2.09993500
Co	0.28428400	0.00865300	-0.20176900

⁵¹, -2119.56361928

C	2.19570400	-1.03133700	0.65684700
C	2.20102800	-1.01797700	-0.74316500
C	2.18305400	0.36691100	1.12179100
C	2.19124300	0.38922500	-1.18181600
C	2.13976000	1.22704300	-0.02239900
C	2.24748800	-2.18546900	-1.67807200

H	3.23098800	-2.24587400	-2.15977300
H	2.06991800	-3.12795600	-1.15875100
H	1.50437100	-2.09413100	-2.47655300
C	2.23574100	-2.21661800	1.56963700
H	2.06150900	-3.14888300	1.03108300
H	3.21594400	-2.28660700	2.05666500
H	1.48712800	-2.14056200	2.36455600
C	2.26234500	0.78755700	2.54968900
H	1.73538500	0.09377200	3.21025400
H	3.31374000	0.79489000	2.87019500
C	2.18600500	2.72867500	-0.00741700
H	1.68810900	3.13700500	0.87478000
H	3.22374100	3.08064600	0.00246900
H	1.69897300	3.15422600	-0.88750100
C	2.27958000	0.83619000	-2.60116500
H	1.75335200	0.15693900	-3.27729300
H	1.89050100	1.84697500	-2.73848700
H	3.33258000	0.84528500	-2.91625100
C	-2.16134300	0.03494700	-0.04921400
O	-1.49178700	1.13265300	-0.04054500
O	-1.45207600	-1.04342600	-0.05114800
C	-3.67111800	-0.01552200	-0.05672300
C	-4.10149300	-0.78630300	-1.32850000
H	-5.19187000	-0.86887400	-1.34222800
H	-3.79234900	-0.25813100	-2.23634500
H	-3.67589300	-1.79252100	-1.34383900
C	-4.11364200	-0.79828200	1.20352400
H	-3.81324500	-0.27873900	2.11924600
H	-5.20409700	-0.88092900	1.20599900
H	-3.68816300	-1.80462000	1.21342000
C	-4.25717700	1.40397500	-0.05281600
H	-5.34900100	1.34371600	-0.05833900
H	-3.94835400	1.96059900	0.83592000
H	-3.93987200	1.96896000	-0.93325100
H	1.86879200	1.79420600	2.70386100
Co	0.19158600	0.06296100	-0.03802300

¹Cp*Co(OPiv)(SbF₆), -2959.60992433

C	1.31264800	-2.44901400	-0.71144100
C	2.50820000	-1.73049200	-0.96203500
C	2.95780700	-1.16327600	0.29940800
C	1.02952800	-2.38047300	0.71172700
C	2.06286300	-1.62238900	1.32898900
Co	1.13405600	-0.44759400	-0.11175700

C	-0.10344500	-3.06776200	1.40596200
H	-1.02530600	-3.00057000	0.82901500
H	0.14560300	-4.12754400	1.54438300
H	-0.29422200	-2.62371000	2.38275000
C	2.07702700	-1.23120200	2.77332400
H	1.13081100	-0.75000700	3.03643900
H	2.19881800	-2.11862500	3.40352700
H	2.88628600	-0.53520600	2.99653400
C	4.15578500	-0.28024600	0.45924200
H	4.10172400	0.29700800	1.38419300
H	5.07871200	-0.87132900	0.47903900
H	4.21791200	0.42531500	-0.37252300
C	3.14710300	-1.43810500	-2.28319500
H	3.21109500	-0.35644900	-2.43701400
H	4.16319300	-1.84658700	-2.31352100
H	2.57978300	-1.86754200	-3.11004300
C	0.40114600	-3.09564500	-1.70605900
H	0.47202900	-4.18656200	-1.62540100
H	-0.63538700	-2.80907000	-1.51009800
H	0.64921800	-2.80916300	-2.72926200
C	1.14458000	3.36323200	-0.01588800
C	0.49570400	3.84558900	1.29009200
H	1.09272700	3.55851900	2.16067600
H	0.41029900	4.93682900	1.27393600
H	-0.49989100	3.41104100	1.40053700
C	2.57468000	3.92663000	-0.17192000
H	3.20697400	3.64679200	0.67815100
H	3.04249000	3.55930700	-1.08975300
H	2.53393800	5.01942700	-0.21685700
C	0.27791300	3.76307900	-1.23199000
H	0.72752400	3.41210200	-2.16431700
H	-0.72262500	3.33385100	-1.14262900
H	0.19251500	4.85386300	-1.27163700
C	1.24737200	1.85475500	-0.01052200
O	1.66128700	1.19841900	-1.03270500
O	0.90640300	1.13497700	0.98830800
Sb	-2.35711700	-0.03175100	-0.02885400
F	-1.89053000	1.78590100	0.19903100
F	-1.42501800	-0.47144000	1.56492900
F	-3.98700400	0.10643500	0.87367600
F	-3.06858600	0.34801800	-1.71971400
F	-0.60654300	-0.24094200	-0.97213000
F	-2.52740400	-1.89270500	-0.36758700

³Cp*Co(OPiv)(SbF₆), -2959.60190353

C	1.23307500	2.43320600	1.18996700
C	2.04993800	2.17668200	0.01471000
C	1.25056400	2.42395200	-1.18664700
C	-0.04682600	2.74737200	0.73102900
C	-0.03285800	2.74493100	-0.75980800
Co	0.57143800	0.59942000	0.00768600
C	-1.27287200	3.04212100	1.52721000
H	-1.11036500	2.88482000	2.59422100
H	-1.58276100	4.08342900	1.37289600
H	-2.09957000	2.40318400	1.20425300
C	-1.24569400	3.03092000	-1.58087600
H	-2.07379100	2.38523200	-1.27527100
H	-1.56740100	4.06982300	-1.43611300
H	-1.05950200	2.87297000	-2.64405100
C	1.76767700	2.25562300	-2.58242400
H	0.97883500	2.41148000	-3.32032800
H	2.57530500	2.96633300	-2.79208900
H	2.16080800	1.24282200	-2.71607800
C	3.49834400	1.82953600	0.02513700
H	3.75563600	1.22296800	-0.84538900
H	4.10405400	2.74511900	-0.00278000
H	3.75741800	1.27478000	0.92884000
C	1.71500100	2.27781700	2.60080400
H	2.50799000	2.99896000	2.82923200
H	0.90469600	2.42845700	3.31622000
H	2.11413700	1.26995600	2.75210200
Sb	-2.24546800	-0.90609600	-0.00054300
F	-0.97648100	-0.07932500	-1.25270900
F	-3.13681500	0.76776800	-0.02503700
F	-3.28205600	-1.56154000	-1.40797800
F	-1.11547700	-2.40956100	0.02623600
F	-0.99333600	-0.05386300	1.25326800
F	-3.30321300	-1.52878500	1.40610700
C	2.16611400	-1.22218500	0.03090600
O	1.77767400	-0.69285100	1.12108100
O	1.79607000	-0.67731700	-1.06369200
C	2.99053500	-2.50241600	0.00513200
C	2.05040300	-3.60466200	-0.53974300
H	2.57758800	-4.56456800	-0.55378500
H	1.15715300	-3.70176700	0.08406300
H	1.72453500	-3.36498600	-1.55502000
C	4.18460900	-2.30773600	-0.94934700
H	4.86345600	-1.53039200	-0.57955200

H	4.75373100	-3.23964400	-1.03001900
H	3.84133900	-2.01918500	-1.94570000
C	3.47375500	-2.86001000	1.41759800
H	4.04977100	-3.79084900	1.38832100
H	4.11362500	-2.07257800	1.82827800
H	2.62919900	-2.99161700	2.09795200

⁵Cp*Co(OPiv)(SbF₆), -2959.5869179

C	1.14121000	2.39767100	1.17290900
C	1.97989200	2.24681400	0.00254200
C	1.15402400	2.38223900	-1.17771300
C	-0.15711600	2.68999400	0.72568500
C	-0.14934500	2.68059000	-0.74756200
Co	0.50349300	0.40121000	0.00466600
C	-1.37700400	2.96174000	1.54247300
H	-1.20714600	2.76247800	2.60175700
H	-1.67818500	4.01219600	1.43708100
H	-2.21618900	2.34662100	1.20780000
C	-1.36052200	2.94194600	-1.58039800
H	-2.20345800	2.33179500	-1.24599200
H	-1.66205700	3.99388300	-1.49197400
H	-1.18005800	2.72852900	-2.63515600
C	1.65810300	2.23613400	-2.58194100
H	0.84099300	2.26830000	-3.30509400
H	2.36545000	3.03472400	-2.83492100
H	2.17179700	1.27688900	-2.69983700
C	3.44701800	1.98187000	0.01360700
H	3.75150800	1.42960500	-0.87820000
H	4.00965200	2.92482100	0.03536700
H	3.73116500	1.40299200	0.89571600
C	1.63156200	2.27028700	2.58371800
H	2.33823400	3.07108200	2.83173700
H	0.80784000	2.31452200	3.29867100
H	2.14253800	1.31206600	2.72059700
Sb	-2.35956600	-0.95608900	0.00130400
F	-1.09141000	-0.10459400	-1.25165400
F	-3.28222900	0.69305300	-0.01280600
F	-3.37286300	-1.63823200	-1.40788700
F	-1.16531300	-2.41159200	0.01656800
F	-1.09959700	-0.08917700	1.25285400
F	-3.38335900	-1.61849900	1.41236500
C	2.36842300	-1.13379000	0.02573900
O	1.89534400	-0.66826000	1.11604300
O	1.89643600	-0.68082800	-1.07382800

C	3.43237300	-2.22136000	0.01049500
C	2.74364600	-3.49821700	-0.52733000
H	3.46673900	-4.31983700	-0.56101600
H	1.91181500	-3.79674700	0.11851500
H	2.35190300	-3.33169900	-1.53391900
C	4.56158200	-1.79150300	-0.94779900
H	5.06451500	-0.88808900	-0.58500900
H	5.30999600	-2.58721600	-1.01976300
H	4.16743600	-1.58863700	-1.94638300
C	3.97924000	-2.45994100	1.42498000
H	4.73276600	-3.25391200	1.40187700
H	4.44552400	-1.55482900	1.82625300
H	3.18096100	-2.75442500	2.11027700

¹[Cp*Co(SbF₆)]⁺, -2612.78480565

C	2.43655300	-0.36365900	1.16905200
C	2.39906600	-1.21414900	0.00134800
C	2.43692100	-0.36614200	-1.16799900
C	2.40577500	0.99537500	0.72696400
C	2.40553300	0.99382000	-0.72879900
Co	0.78753400	-0.00071600	0.00008600
C	2.32610500	2.22337300	1.57343200
H	2.04894800	1.99351000	2.60250200
H	3.30115600	2.72461600	1.58534200
H	1.59536300	2.92959400	1.17139200
C	2.32630000	2.21956800	-1.57850700
H	1.60933400	2.93512800	-1.16857100
H	3.30650200	2.71009000	-1.60710000
H	2.03140700	1.98875500	-2.60249700
C	2.36082000	-0.86131600	-2.57368600
H	2.18310500	-0.05551000	-3.28538800
H	3.30643600	-1.35034400	-2.83521300
H	1.56434400	-1.60236000	-2.68458200
C	2.35429800	-2.70785000	0.00274000
H	1.84928000	-3.09341300	-0.88498400
H	3.37530600	-3.10849300	0.00854100
H	1.84018000	-3.09155300	0.88608400
C	2.36059700	-0.85564600	2.57580500
H	3.31143000	-1.33155500	2.84280500
H	2.16957700	-0.05009600	3.28438100
H	1.57333500	-1.60646800	2.68575800
Sb	-2.04019200	-0.00256600	-0.00001000
F	-0.61505800	-0.70008000	-1.22065100
F	-0.63422700	1.41335200	-0.00026000

F	-2.91099500	0.80503900	-1.41912500
F	-2.88548900	-1.64908500	0.00024100
F	-0.61527400	-0.69961900	1.22101500
F	-2.91130400	0.80573500	1.41851600

³[Cp*Co(SbF₆)]⁺, -2612.80196432

C	2.69209900	-1.15126500	0.01191300
C	3.06534300	0.00144000	-0.76070000
C	2.69100600	1.15193700	0.01454200
C	2.09275100	-0.69738700	1.29261700
C	2.09212200	0.69447000	1.29425000
Co	0.89258700	0.00027800	-0.59471100
C	1.51955900	-1.57358900	2.35812200
H	1.64236100	-2.63340600	2.13330400
H	2.00506300	-1.36635200	3.31829700
H	0.45122400	-1.36309400	2.48157300
C	1.51822600	1.56773000	2.36177600
H	0.44968800	1.35728200	2.48358800
H	2.00269000	1.35743600	3.32180100
H	1.64163700	2.62815800	2.14019400
C	2.91057300	2.57936800	-0.33784600
H	2.01949100	3.18137400	-0.13258600
H	3.71647200	2.98438200	0.29011800
H	3.19781800	2.71018900	-1.38152400
C	3.82366200	0.00327800	-2.05843500
H	3.59195200	0.88558700	-2.65873800
H	4.90261400	0.00333900	-1.86808900
H	3.59245300	-0.87764500	-2.66096600
C	2.91281700	-2.57763600	-0.34404000
H	3.71934800	-2.98350200	0.28256500
H	2.02238000	-3.18096700	-0.13988000
H	3.19974700	-2.70564000	-1.38815600
Sb	-2.16716900	0.00001700	-0.10524400
F	-0.60558000	1.25027100	-0.52712600
F	-1.34771700	-0.00237400	1.59940300
F	-3.26694200	1.44047700	0.27348500
F	-2.42126200	0.00221400	-1.95112400
F	-0.60590800	-1.24952200	-0.53021600
F	-3.26794000	-1.44057800	0.27001600

⁵[Cp*Co(SbF₆)]⁺, -2612.7858382

C	-2.64358800	1.17878900	0.07155300
C	-3.05963700	-0.00076200	-0.67291000
C	-2.64295700	-1.17922100	0.07284000

C	-2.07427500	0.73631800	1.29534000
C	-2.07379400	-0.73506300	1.29611700
Co	-0.89147600	-0.00012400	-0.74360800
C	-1.48953000	1.56233700	2.38238700
H	-1.60988900	2.63063700	2.20308600
H	-1.96004300	1.31391500	3.34150100
H	-0.42123800	1.33611500	2.48743200
C	-1.48832400	-1.55952800	2.38394000
H	-0.42020900	-1.33229500	2.48868800
H	-1.95897700	-1.31055200	3.34284300
H	-1.60780100	-2.62810400	2.20569400
C	-2.88457600	-2.60253100	-0.33289400
H	-2.11552400	-3.26670400	0.06650700
H	-3.85494600	-2.94443600	0.04644000
H	-2.89920400	-2.71928500	-1.41901000
C	-3.86810700	-0.00163800	-1.92944700
H	-3.68663900	-0.89119000	-2.53674700
H	-4.93529400	-0.00168700	-1.66738000
H	-3.68697800	0.88728900	-2.53776600
C	-2.88609300	2.60148300	-0.33580700
H	-3.85705700	2.94292700	0.04242400
H	-2.11792700	3.26672400	0.06351200
H	-2.89998900	2.71713000	-1.42205500
Sb	2.15177900	0.00002100	-0.09091400
F	0.61083200	-1.24945900	-0.56084500
F	1.28107100	0.00168000	1.58877600
F	3.24141200	-1.43813800	0.32367800
F	2.46117200	-0.00175800	-1.92901700
F	0.61111700	1.24904100	-0.56331700
F	3.24174200	1.43871000	0.32096100

8-Methylquionline, -441.436161643

C	-2.27039700	-0.35543200	0.00001400
C	-1.37827700	0.69893300	-0.00000200
C	0.02297500	0.40518700	-0.00003800
C	0.46334800	-0.95818200	-0.00000400
C	-0.49530500	-2.00498700	0.00001000
C	-1.83651300	-1.70403000	0.00001200
H	-3.33689400	-0.14597700	0.00002200
C	1.86116000	-1.19469100	-0.00000500
H	-0.15265400	-3.03641100	0.00001800
H	-2.57490800	-2.50049200	0.00002300
C	2.72899000	-0.12830900	-0.00001300
C	2.18994800	1.18184600	0.00003800

H	2.22763200	-2.21829100	-0.00001400
H	3.80472300	-0.27241000	-0.00004700
H	2.86270300	2.03894500	-0.00004000
N	0.89943400	1.45180600	-0.00000500
C	-1.83577600	2.13318200	0.00000000
H	-1.45019800	2.66606700	0.87471800
H	-1.45020800	2.66606800	-0.87472000
H	-2.92715900	2.19875400	0.00000700

Phenyl-1,4,2-dioxazol-5-one, -588.505106504

C	0.64137400	0.28017800	0.00000000
C	2.75521400	-0.31251300	0.00000600
O	3.75364300	-0.96145300	-0.00000900
O	1.46083800	-0.80987800	0.00000000
O	2.64694600	1.04376600	-0.00000500
N	1.27231200	1.40741800	0.00000100
C	-0.80498700	0.09080100	0.00000100
C	-1.34331300	-1.20414500	-0.00000200
C	-1.65409300	1.21024300	0.00000500
C	-2.72622600	-1.37549100	-0.00000200
H	-0.68072600	-2.06251400	-0.00000500
C	-3.03238800	1.02701900	0.00000600
H	-1.22561800	2.20680900	0.00000700
C	-3.57068800	-0.26400500	0.00000300
H	-3.14328900	-2.37752300	-0.00000400
H	-3.68960800	1.89081300	0.00000900
H	-4.64771600	-0.40150300	0.00000300

CO₂, -188.668744516

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16914100
O	0.00000000	0.00000000	-1.16914100

PivOH, -347.195642288

C	-0.94248800	0.18792200	-0.00005700
C	0.57315500	-0.01035700	0.00002600
O	-1.52295800	1.25160600	-0.00009500
O	-1.61299900	-0.99509200	-0.00006900
H	-2.55765600	-0.76725100	-0.00011200
C	1.25194800	1.36609500	-0.00000200
H	2.33964800	1.24335500	0.00006400
H	0.96559700	1.94516400	-0.88174200
H	0.96549700	1.94524900	0.88165000
C	0.96882200	-0.80602100	-1.26302000

H	2.05375600	-0.95266400	-1.27938700
H	0.48575900	-1.78590800	-1.28057300
H	0.68767200	-0.26618100	-2.17325300
C	0.96868400	-0.80590100	1.26319300
H	2.05361600	-0.95254500	1.27969300
H	0.68743500	-0.26597300	2.17334300
H	0.48561800	-1.78578500	1.28078600

Product, -841.367657364

C	-3.16350600	-1.91953100	-1.29430600
C	-3.66189800	-0.64501800	-1.42425800
C	-3.15651900	0.40218800	-0.60958000
C	-2.13038000	0.11766400	0.34723200
C	-1.63852100	-1.21846700	0.47684000
C	-2.15088000	-2.20070900	-0.34407200
H	-4.39837900	1.98620800	-1.41399100
H	-3.54116700	-2.72037700	-1.92264900
H	-4.43897600	-0.42031300	-2.14986600
C	-3.61826600	1.73923900	-0.69842300
H	-1.76276600	-3.21190700	-0.26356400
C	-2.05381500	2.32206000	1.02386200
C	-3.07252500	2.70221200	0.11759900
H	-1.60407300	3.07163400	1.67350100
H	-3.40163800	3.73520900	0.07536900
N	-1.59285700	1.09144600	1.14420500
C	-0.56204400	-1.52132200	1.50032600
H	-0.30042400	-2.57991500	1.47018000
H	-0.92551000	-1.27757400	2.50341500
C	1.64549100	-1.24208400	0.45298900
O	1.70068300	-2.41969300	0.10134400
N	0.65682900	-0.76190700	1.26421100
C	2.69796400	-0.24856200	0.04041400
C	2.45959000	1.13004700	-0.04813200
C	3.95770300	-0.74996100	-0.31039000
C	3.47412400	1.99384900	-0.46111100
H	1.47456300	1.53475200	0.16859900
C	4.97315600	0.11406600	-0.71251700
H	4.11236300	-1.82254000	-0.26316900
C	4.73430700	1.48895200	-0.78618700
H	3.27825800	3.05953500	-0.53605700
H	5.94997900	-0.28291300	-0.97300000
H	5.52443300	2.16311300	-1.10407100
H	0.57618300	0.22812000	1.44391400

12, -2561.06350769

C	0.77561600	2.22904300	-1.22732400
C	-0.53438600	2.25433400	-0.67368600
C	-0.40372100	2.29974800	0.77347000
C	1.71830000	2.18845900	-0.14237300
C	0.97827500	2.29946000	1.09411900
Co	0.51479100	0.54795200	0.03727000
C	3.20779500	2.11436000	-0.26984600
H	3.49635000	1.62202400	-1.20106900
H	3.64814100	3.11800400	-0.26840500
H	3.64180500	1.55430500	0.56149600
C	1.60092200	2.28357200	2.45316800
H	2.28052200	1.43161300	2.54954700
H	2.18464200	3.19750400	2.60738100
H	0.85307700	2.22266000	3.24520400
C	-1.55820700	2.38313500	1.72224100
H	-1.27608400	2.09085900	2.73473300
H	-1.93579200	3.41124900	1.76062800
H	-2.38130400	1.74020000	1.40107000
C	-1.83264900	2.37987100	-1.40942400
H	-2.62192500	1.79074100	-0.93951300
H	-2.15332500	3.42821800	-1.40658800
H	-1.75013200	2.05926500	-2.44845500
C	1.15268200	2.12619000	-2.67112500
H	1.80929300	2.95794600	-2.94615200
H	1.69774200	1.19424500	-2.85338700
H	0.28055600	2.15003000	-3.32546100
C	3.07593000	-2.32195900	-0.09692400
C	2.35726600	-3.51342700	0.58360900
H	1.45008300	-3.79199800	0.03747400
H	3.02506000	-4.37970400	0.59592200
H	2.08527600	-3.27171400	1.61469300
C	3.44352200	-2.67250000	-1.54697800
H	2.55810700	-2.94067100	-2.12873600
H	3.93488400	-1.83239700	-2.04658300
H	4.13166000	-3.52250100	-1.55334200
C	4.33057300	-1.93080700	0.71151600
H	4.84838600	-1.08243200	0.25171700
H	4.07153200	-1.66357900	1.73885300
H	5.02560300	-2.77483500	0.73715500
C	2.10441900	-1.16378500	-0.06975600
O	1.80060300	-0.56008100	1.02222300
O	1.49417500	-0.73198400	-1.10368200
C	-3.62103500	-1.07356900	-1.99773600

C	-2.35334800	-0.93614600	-1.45402500
C	-2.23611000	-0.89055600	-0.02774000
C	-3.41088900	-1.12270100	0.77044700
C	-4.68251700	-1.24823500	0.15387900
C	-4.78802700	-1.19828300	-1.21357600
H	-3.71570000	-1.11338100	-3.07901000
C	-3.27278800	-1.26150400	2.17215100
H	-5.55499900	-1.40492700	0.78083500
H	-5.75389400	-1.29546800	-1.69830800
C	-2.02745500	-1.17886800	2.74623700
C	-0.93782500	-0.84825600	1.92478700
H	-4.15680800	-1.45208300	2.77415800
H	-1.87169400	-1.31770700	3.80986500
H	0.04168500	-0.69876900	2.36218800
N	-1.02263900	-0.66229600	0.60501100
C	-1.16213200	-0.93576600	-2.37350000
H	-0.62093200	0.01035900	-2.36676200
H	-0.43752100	-1.69726400	-2.08060500
H	-1.47867700	-1.13278400	-3.39991000

³², -2561.0635766

C	0.75301000	2.35481800	-1.06806000
C	-0.55516200	2.41326300	-0.59398400
C	-0.50675700	2.28088300	0.87763300
C	1.63619000	2.17399300	0.10233500
C	0.84244400	2.18655500	1.29039900
Co	0.39244300	0.39556300	-0.06644000
C	3.12251900	2.09956400	0.03632600
H	3.44695400	1.54074300	-0.84405600
H	3.54265600	3.11134300	-0.03459000
H	3.53464500	1.62413000	0.92815500
C	1.37459300	2.03103800	2.68403000
H	1.99604000	1.13341000	2.75713200
H	1.98728100	2.89354400	2.96622500
H	0.56819300	1.94644100	3.41515100
C	-1.72310000	2.32421400	1.74019500
H	-1.52599900	1.95926800	2.74894000
H	-2.08270400	3.35800300	1.81946100
H	-2.53537600	1.73281000	1.30809200
C	-1.82139000	2.64226000	-1.36010200
H	-2.56569800	1.86734000	-1.15177800
H	-2.26490000	3.60432400	-1.07911800
H	-1.64441600	2.65902900	-2.43671100
C	1.25401500	2.43251700	-2.47577400

H	1.89494200	3.31092200	-2.60975100
H	1.84942100	1.54555000	-2.71560900
H	0.43517000	2.50065600	-3.19413900
C	3.43460200	-2.13358400	-0.17301500
C	2.89298500	-3.35124800	-0.95789800
H	2.51742500	-3.04986300	-1.93921100
H	3.69628900	-4.07994600	-1.10212100
H	2.08373300	-3.84600200	-0.41028100
C	4.55670100	-1.44844900	-0.98290300
H	4.19369900	-1.12398900	-1.96129100
H	4.95366900	-0.57710700	-0.45076100
H	5.38164200	-2.15088500	-1.13393200
C	3.95098100	-2.56781300	1.20618600
H	4.32123400	-1.71228400	1.77826900
H	3.16213300	-3.04650900	1.79202700
H	4.77216000	-3.28025900	1.08417800
C	2.28383000	-1.14960000	-0.02055400
O	1.79026400	-0.82781400	1.09746700
O	1.76616300	-0.61068900	-1.07562600
C	-3.66361200	-1.06653600	-2.10225700
C	-2.42710100	-0.89865500	-1.50115400
C	-2.36202500	-0.96367800	-0.07461400
C	-3.54216900	-1.29369500	0.67218100
C	-4.78267100	-1.44632900	0.00119100
C	-4.84311100	-1.31498500	-1.36496300
H	-3.72410700	-1.02946300	-3.18617700
C	-3.42764700	-1.48760700	2.07042500
H	-5.66845100	-1.68394300	0.58234000
H	-5.78597500	-1.43427400	-1.88844700
C	-2.20148000	-1.36815000	2.68250000
C	-1.09914200	-0.97633800	1.90440100
H	-4.31428900	-1.74706500	2.64211100
H	-2.07071100	-1.54207000	3.74431800
H	-0.12535200	-0.82715600	2.35611400
N	-1.17087700	-0.74690400	0.59233000
C	-1.19257100	-0.73023900	-2.35034000
H	-0.81097700	0.29700400	-2.34269900
H	-0.37999500	-1.38651900	-2.02778700
H	-1.41314900	-0.96423300	-3.39430500

⁵², -2561.04439083

C	0.59890500	2.29632400	-1.09459200
C	-0.75499400	2.40655600	-0.61482200
C	-0.73944500	2.35154000	0.83454400

C	1.43895600	2.26357500	0.05364500
C	0.58756300	2.26253500	1.25218800
Co	0.44658300	0.19723600	-0.24672100
C	2.93046100	2.29042800	0.07469900
H	3.35304200	1.96353000	-0.87735900
H	3.28467200	3.31197600	0.26577800
H	3.32079700	1.65097600	0.87006700
C	1.12824000	2.15590100	2.64073800
H	1.75344000	1.26112300	2.73766400
H	1.75973500	3.01937900	2.88073600
H	0.33262800	2.10813100	3.38663700
C	-1.97941500	2.36763800	1.67161200
H	-1.76123200	2.20281500	2.72803100
H	-2.49770600	3.32972100	1.58429400
H	-2.68482800	1.59396500	1.34761800
C	-1.99426100	2.56455500	-1.42879200
H	-2.72880600	1.78611100	-1.19011600
H	-2.47240200	3.52556500	-1.20159000
H	-1.79508800	2.53483500	-2.50110500
C	1.06473000	2.42028600	-2.51920600
H	1.35511400	3.45143100	-2.74985700
H	1.92783000	1.77623200	-2.70604300
H	0.28324900	2.13193000	-3.22625100
C	3.73340600	-1.93652300	-0.04980400
C	3.40720700	-3.30178200	-0.69688800
H	3.03046400	-3.17367700	-1.71443900
H	4.31417900	-3.91233600	-0.73457200
H	2.65830100	-3.84714000	-0.11280500
C	4.78116200	-1.18902300	-0.90796200
H	4.41922800	-1.04060200	-1.92825900
H	5.02297200	-0.21190200	-0.47607000
H	5.70372300	-1.77554700	-0.94685000
C	4.24582100	-2.12371800	1.38529800
H	4.46756800	-1.16231000	1.85670700
H	3.50865400	-2.64009400	2.00604000
H	5.16288100	-2.71979300	1.37242500
C	2.46400300	-1.10381200	-0.05826100
O	1.95021500	-0.62084500	1.00235100
O	1.87028900	-0.84765900	-1.17741300
C	-3.70244800	-1.29581600	-2.03721000
C	-2.47054300	-1.03398400	-1.46390700
C	-2.37568300	-1.04924500	-0.03918500
C	-3.52162000	-1.40195200	0.74620500
C	-4.76102500	-1.65835500	0.10399000

C	-4.85005000	-1.59193900	-1.26540500
H	-3.78717700	-1.29183600	-3.12007500
C	-3.37094300	-1.50337600	2.15031800
H	-5.62410200	-1.91560200	0.71033600
H	-5.79293700	-1.78788500	-1.76510300
C	-2.14469400	-1.26740600	2.73101900
C	-1.07755700	-0.87429600	1.90740200
H	-4.22997700	-1.77886100	2.75563400
H	-1.99059700	-1.35875500	3.79991800
H	-0.10442300	-0.64481900	2.32879800
N	-1.18424000	-0.74434000	0.58413500
C	-1.25673600	-0.80530800	-2.32567600
H	-0.82535300	0.19695300	-2.18602800
H	-0.47077100	-1.54314700	-2.13465800
H	-1.51141200	-0.86414200	-3.38617600

MECP3, -2561.05688814

C	-2.49939400	-1.53404600	-0.63277300
C	-2.64436100	-0.31172500	-1.31547700
C	-2.79827200	0.72480800	-0.30990700
C	-2.89860200	0.09834300	0.98602100
C	-2.63478600	-1.27284700	0.80196100
C	4.38003100	-1.42356100	-1.25706500
C	4.32621600	-1.41800400	0.11434600
C	3.07177900	-1.37474900	0.77232300
C	1.86078200	-1.30169300	0.00631500
C	1.93064700	-1.38658500	-1.41607400
C	3.18244900	-1.43233900	-2.00449600
H	3.90217000	-1.48060600	2.76392800
H	5.33402100	-1.45396900	-1.77199700
H	5.22978100	-1.45713800	0.71430700
C	2.98748300	-1.41244100	2.18288600
H	3.24210000	-1.49656100	-3.08669800
C	0.62220600	-1.20950700	1.99411200
C	1.75861300	-1.36740300	2.79793200
H	-0.34425200	-1.07256400	2.46175500
H	1.65290000	-1.40393900	3.87497500
N	0.65035500	-1.16997200	0.66165200
C	0.70359800	-1.47586500	-2.28067100
H	-0.04158900	-2.13523600	-1.83530700
H	0.25563700	-0.49541700	-2.44945400
H	0.96597200	-1.89050200	-3.25600700
C	0.35235200	1.88014700	0.01865400
C	1.35490300	3.01414600	-0.00249400

O	-0.18291700	1.45666400	1.09116500
O	0.06563500	1.23024100	-1.05231300
C	-2.98871700	2.17873900	-0.58620000
H	-2.69678800	2.78478000	0.27374300
H	-2.40009200	2.49852900	-1.44811800
H	-4.04414000	2.38397900	-0.80168900
C	-2.60494500	-0.06446200	-2.78895300
H	-3.60143000	0.20762700	-3.15276500
H	-1.92783900	0.75904500	-3.03046700
H	-2.27698700	-0.94788400	-3.33887800
C	-2.38153400	-2.90712200	-1.21135100
H	-3.33609000	-3.43538900	-1.09572400
H	-2.14302500	-2.88744400	-2.27512200
H	-1.62072400	-3.50282000	-0.69822600
C	-2.60683500	-2.34890000	1.83796100
H	-3.51208900	-2.96261900	1.75809300
H	-1.75267000	-3.01745700	1.70070700
H	-2.57128200	-1.94559200	2.85154100
C	-3.09823400	0.83336500	2.27143100
H	-4.08003400	1.31787500	2.28174400
H	-3.04881200	0.16515500	3.13301000
H	-2.33803000	1.60989300	2.39593500
Co	-0.94798000	-0.14006100	-0.02572200
C	1.04951700	4.00642400	1.12991600
H	1.80744300	4.79431000	1.14286200
H	0.07397400	4.48068100	0.98574700
H	1.04633700	3.50968900	2.10226200
C	1.33762100	3.71437700	-1.36995300
H	2.09441300	4.50331700	-1.38693100
H	1.55034300	3.01161800	-2.17789500
H	0.36522100	4.17654300	-1.56576500
C	2.73232900	2.34214800	0.23096800
H	3.51544700	3.10516000	0.21549200
H	2.76156600	1.83711200	1.20097800
H	2.95071400	1.60853600	-0.55038000
¹ TS2_3_CMD, -2561.04743727, i27.76			
C	-1.28869300	-2.27016300	-1.04506500
C	0.04717900	-2.70093000	-0.64298500
C	0.13124200	-2.59983500	0.76538800
C	-2.00814700	-1.90494600	0.11552100
C	-1.11482600	-2.03955300	1.24904500
C	-3.43751800	-1.47032900	0.17865700
H	-3.74192000	-0.96732200	-0.74000000
H	-4.08126900	-2.34789700	0.31786200

H	-3.61227800	-0.79303500	1.01637000
C	-1.50798800	-1.80889600	2.67520500
H	-2.00574700	-0.84275000	2.79577100
H	-2.21356000	-2.58477800	2.99653400
H	-0.65242800	-1.85022900	3.35230700
C	1.29704600	-3.01379600	1.60713000
H	1.38333700	-2.41949300	2.51880300
H	1.16823600	-4.05989000	1.91211000
H	2.24013400	-2.94445400	1.06099100
C	1.09471200	-3.30210300	-1.53369300
H	2.10136400	-2.96356600	-1.27327700
H	1.08252900	-4.39420200	-1.43404200
H	0.92037800	-3.07706200	-2.58727100
C	-1.82388100	-2.22313000	-2.44228700
H	-2.52068200	-3.05515400	-2.60077300
H	-2.36013200	-1.28742000	-2.61649500
H	-1.03305600	-2.30948900	-3.18946800
C	-2.70764500	2.73013300	0.01191200
C	-1.63398500	3.82056600	0.24066400
H	-1.05079700	3.99858700	-0.66919500
H	-2.11683700	4.76349900	0.51656100
H	-0.94768300	3.53934200	1.04442600
C	-3.65911200	3.15951600	-1.11641400
H	-3.11873900	3.32193200	-2.05155600
H	-4.42422100	2.40032600	-1.30347200
H	-4.16396200	4.09053200	-0.83975300
C	-3.49702400	2.50136800	1.31703200
H	-4.26613100	1.73148300	1.18863900
H	-2.83801300	2.20016200	2.13517200
H	-4.00523600	3.42557700	1.60974400
C	-1.97249200	1.44029100	-0.39859000
O	-1.27499100	0.86727700	0.55641900
O	-1.99926800	0.99044900	-1.55114700
C	3.36947200	1.09113100	-2.19710900
C	2.27937400	0.64047400	-1.47165900
C	2.35879100	0.66536600	-0.04927500
C	3.53000000	1.19955600	0.58541500
C	4.62519900	1.62563200	-0.20796400
C	4.54764100	1.56330400	-1.57868400
H	3.31006300	1.09324500	-3.28196600
C	3.54309500	1.31708700	1.99573900
H	5.50903500	2.01706100	0.28630600
H	5.37703100	1.89798900	-2.19288700
C	2.43679600	0.94611500	2.72358300

C	1.33372400	0.40567000	2.04078700
H	4.42369000	1.72323500	2.48510400
H	2.39553400	1.05580100	3.80112800
H	0.44418300	0.11480600	2.58548800
N	1.30168500	0.22654100	0.72348200
C	1.04731100	0.17082700	-2.19934200
H	1.10871900	-0.88354100	-2.47219200
H	0.08803500	0.37480800	-1.67784100
H	0.91102800	0.73035400	-3.13013300
Co	-0.30259100	-0.65948800	-0.01509700

13_CMD, -2561.04838316

C	2.51490100	-1.47550500	0.85338200
C	2.72887600	-0.05095600	1.07822700
C	2.73058800	0.59921100	-0.17767300
C	2.45170200	-0.39570900	-1.19278000
C	2.39604200	-1.68697300	-0.54001800
C	-4.22622800	-1.16556200	1.67286200
C	-4.29073400	-1.58123400	0.36451000
C	-3.10837700	-1.66065000	-0.41681100
C	-1.85405000	-1.30925100	0.17352100
C	-1.79991800	-0.91329400	1.53833400
C	-2.97872400	-0.83846900	2.25447900
H	-4.06792300	-2.33443000	-2.23721100
H	-5.12877300	-1.09218800	2.27037200
H	-5.23955700	-1.84457100	-0.09265600
C	-3.12445300	-2.06014300	-1.77426100
H	-2.94606800	-0.52691700	3.29437700
C	-0.76212900	-1.68644200	-1.85626200
C	-1.95090500	-2.08306700	-2.49230000
H	0.16010300	-1.63797500	-2.41697500
H	-1.92395700	-2.37409200	-3.53598300
N	-0.69793300	-1.32653800	-0.57902600
C	-0.47196900	-0.63437100	2.18139300
H	0.11962600	-1.54484600	2.29036500
H	0.09267800	0.19924000	1.68741800
H	-0.58776100	-0.19783000	3.17692300
C	-0.22212200	2.19062000	0.18715900
C	-1.12625500	3.27372500	-0.42304000
O	-0.03122200	1.16008800	-0.60544900
O	0.24659600	2.26723200	1.32721800
C	2.93888400	2.05586000	-0.43394700
H	2.36542500	2.38338700	-1.30277200
H	2.63119700	2.65451900	0.42327200

H	4.00037800	2.24479000	-0.63357100
C	2.89493000	0.62549600	2.40237000
H	3.94369900	0.90719000	2.54919200
H	2.28235200	1.52926700	2.44049000
H	2.60510800	-0.02508700	3.22945900
C	2.52684100	-2.55439900	1.89209200
H	3.52791300	-2.99695000	1.95736500
H	2.27629700	-2.17340400	2.88382500
H	1.82877400	-3.35846000	1.64373700
C	2.22006100	-3.02511700	-1.18826700
H	3.12044700	-3.62733100	-1.02462600
H	1.37592400	-3.57184700	-0.75895900
H	2.06886200	-2.94762700	-2.26548000
C	2.36399400	-0.09241900	-2.65565700
H	3.30792800	0.33652500	-3.00858500
H	2.16369700	-0.98274000	-3.25456600
H	1.57388900	0.64167400	-2.84035900
Co	0.88045300	-0.34103400	0.09051200
C	-0.55319600	3.70625900	-1.78760600
H	-1.19533700	4.47009600	-2.23715200
H	0.44757000	4.13842600	-1.67556800
H	-0.49067200	2.85860500	-2.47490800
C	-1.20755900	4.47453700	0.52928100
H	-1.86145000	5.24233500	0.10394000
H	-1.60376800	4.17863000	1.50357600
H	-0.22008500	4.91427500	0.69413600
C	-2.52479700	2.64390000	-0.61615000
H	-3.21400200	3.38593100	-1.03157700
H	-2.47840900	1.79070400	-1.29851900
H	-2.93621000	2.29955200	0.33922600

¹TS4_CMD, -2561.02798868, i1213.57

C	-1.96880700	-2.07245100	-0.80679800
C	-2.50235800	-0.77927800	-1.18315700
C	-2.73104500	-0.04095200	0.00585900
C	-2.33355000	-0.86102100	1.13313100
C	-1.92367600	-2.13041500	0.61857300
C	4.34490800	-0.30676300	-1.69528600
C	4.54768600	-0.75152900	-0.40794700
C	3.43548800	-1.05584400	0.41972200
C	2.12379200	-0.90714600	-0.12055200
C	1.92426600	-0.48344000	-1.45937000
C	3.03570700	-0.17224400	-2.21923100
H	4.53619900	-1.59235700	2.20813500

H	5.19439400	-0.05884200	-2.32348700
H	5.55004700	-0.85714300	-0.00469200
C	3.55030000	-1.46339000	1.77083400
H	2.90393400	0.17135200	-3.24114900
C	1.15361400	-1.46931100	1.92467400
C	2.41293200	-1.66886100	2.52113800
H	0.24640600	-1.57219300	2.50458100
H	2.46458200	-1.96176000	3.56349300
N	1.00642600	-1.12626300	0.65068700
C	0.51075100	-0.42317600	-1.94472100
H	0.13328900	-1.42823500	-2.13615100
H	-0.10995300	0.72460200	-1.52416200
H	0.44003300	0.08234000	-2.91509300
C	-0.16661500	2.17604400	-0.11104000
C	0.11140500	3.56628900	0.45033100
O	-0.26242200	1.18596500	0.68911300
O	-0.25974100	2.01728900	-1.36892400
C	-3.28305100	1.34571300	0.10527400
H	-2.89973900	1.85624100	0.99050600
H	-3.02884300	1.94299200	-0.77229800
H	-4.37562900	1.30749400	0.18413800
C	-2.76689000	-0.30273500	-2.57764700
H	-3.80739600	-0.50798800	-2.85386600
H	-2.59990500	0.77297000	-2.66652400
H	-2.12592700	-0.80615700	-3.30413100
C	-1.66160800	-3.21949600	-1.72105800
H	-2.50068400	-3.92487600	-1.73697500
H	-1.49517800	-2.89181300	-2.74926900
H	-0.77612300	-3.76935500	-1.38995700
C	-1.50698700	-3.34166800	1.39344000
H	-2.24044900	-4.13990000	1.23381100
H	-0.53647500	-3.71926000	1.05994000
H	-1.45601700	-3.15261200	2.46645600
C	-2.40942200	-0.42109200	2.56294800
H	-3.44658900	-0.21720800	2.84932000
H	-2.02259000	-1.17964100	3.24638600
H	-1.83299500	0.49798400	2.70634800
Co	-0.69370100	-0.52558300	-0.12248100
C	-0.08486300	3.59393900	1.97297300
H	0.13295300	4.59646500	2.35216300
H	-1.11591900	3.34709500	2.24583400
H	0.57656700	2.88280800	2.47377600
C	-0.82872100	4.57608900	-0.23826900
H	-0.60430300	5.58571800	0.11777900

H	-0.70535300	4.55215400	-1.32301700
H	-1.87750900	4.36368400	-0.00463600
C	1.58338700	3.88478600	0.09127100
H	1.83980100	4.88293200	0.45856000
H	2.26732100	3.16607500	0.55526500
H	1.73443200	3.86271100	-0.99098300

³TS4_CMD, -2561.01116768, i1401.66

C	-2.72338900	-1.21883100	-0.92375300
C	-2.86316500	0.24964100	-0.99604800
C	-2.77608800	0.74123200	0.29843100
C	-2.54740200	-0.40411000	1.20461000
C	-2.60680100	-1.60735900	0.44267300
C	4.20539200	-0.71130500	-1.70941400
C	4.35923100	-1.38128600	-0.51637700
C	3.21496400	-1.74591000	0.24107000
C	1.92239200	-1.40820400	-0.25753400
C	1.77086100	-0.75988700	-1.51883600
C	2.91604400	-0.40613700	-2.20932400
H	4.25259600	-2.69280700	1.89078300
H	5.07799500	-0.42174000	-2.28600900
H	5.34597400	-1.63079100	-0.13849200
C	3.28264300	-2.41430300	1.48835200
H	2.82487800	0.10466200	-3.16356800
C	0.89177000	-2.29115200	1.63762300
C	2.12494000	-2.69861300	2.18170400
H	-0.03486400	-2.46002000	2.17641100
H	2.14712400	-3.20830700	3.13819600
N	0.78759400	-1.67113600	0.46914900
C	0.38474300	-0.47887800	-2.00147600
H	-0.19124400	-1.40855100	-2.10867800
H	0.03995900	0.78069900	-1.53181500
H	0.37492800	-0.03294800	-3.00095100
C	0.42056000	2.03822500	0.01763600
C	1.16219900	3.22740600	0.62066600
O	0.08332700	1.06156000	0.76407200
O	0.20849400	2.02155800	-1.24012100
C	-2.84868500	2.16201300	0.75466600
H	-2.09857100	2.36096100	1.52388100
H	-2.68415400	2.85728600	-0.07083000
H	-3.83295600	2.37893400	1.18653600
C	-3.05855400	1.02001000	-2.26415400
H	-4.10376200	0.97059800	-2.59164200
H	-2.79128500	2.07037100	-2.13733800

H	-2.44406000	0.61614600	-3.07367200
C	-2.86227900	-2.15069300	-2.08369400
H	-3.92265300	-2.38874800	-2.23931600
H	-2.49118700	-1.70909000	-3.01130700
H	-2.33867800	-3.09396600	-1.90821400
C	-2.55505600	-3.02341600	0.94115400
H	-3.50256000	-3.53478900	0.74063800
H	-1.76121700	-3.59745600	0.45303000
H	-2.38601800	-3.06452000	2.01889800
C	-2.37164000	-0.25641200	2.67937500
H	-3.28198500	0.15410800	3.13238000
H	-2.15119400	-1.20771500	3.16639300
H	-1.55622500	0.44261200	2.89278400
Co	-0.82189000	-0.45616700	-0.16714700
C	1.04407300	3.23056200	2.15131800
H	1.60691500	4.07460300	2.56026700
H	0.00209200	3.33681100	2.47004000
H	1.43810200	2.30801400	2.58398200
C	0.60198100	4.53404300	0.02676600
H	1.17026400	5.38516600	0.41311000
H	0.67057200	4.53309300	-1.06296600
H	-0.44735700	4.67671000	0.30638900
C	2.64185400	3.04315300	0.19729200
H	3.23926800	3.86857000	0.59583500
H	3.05138700	2.10539700	0.58776700
H	2.73770400	3.03748600	-0.89154600

⁵TS4_CMD, -2560.99849041, *i*1338.72

C	1.45632600	-2.54160900	0.75019900
C	2.31554200	-1.51028200	1.34899400
C	2.93002900	-0.81446700	0.31620600
C	2.48434600	-1.38337100	-0.94465700
C	1.51149500	-2.41123400	-0.66685700
C	-4.47503900	1.03036000	1.75091900
C	-4.89311000	0.62222300	0.50436900
C	-3.98250400	-0.04248300	-0.35703000
C	-2.64727300	-0.27399600	0.09477000
C	-2.23474500	0.10254400	1.40817700
C	-3.15871600	0.76499200	2.19933300
H	-5.33430700	-0.32424100	-2.02351400
H	-5.16335100	1.54762900	2.41164900
H	-5.90773800	0.80494900	0.16461000
C	-4.32273700	-0.48029300	-1.65919100
H	-2.87030300	1.07462700	3.19974300

C	-2.07221900	-1.24793700	-1.95884100
C	-3.37660200	-1.09276700	-2.45675600
H	-1.29013000	-1.69093900	-2.56730600
H	-3.61326100	-1.43664900	-3.45699100
N	-1.71843400	-0.85596300	-0.73703200
C	-0.84240300	-0.22326500	1.84887800
H	-0.71444600	-1.31666600	1.91233300
H	0.08455800	0.81001400	1.44444700
H	-0.65627800	0.12198200	2.87066600
C	0.89456400	2.02221400	0.00757700
C	1.26860200	3.41039400	-0.49905700
O	0.79322400	1.05317500	-0.81403100
O	0.64611600	1.87930300	1.25377300
C	3.86625300	0.34748800	0.40940400
H	3.58876000	1.12350600	-0.31074800
H	3.86442400	0.79397900	1.40530600
H	4.89523800	0.04758800	0.17714100
C	2.46049700	-1.30041600	2.82184400
H	1.48454800	-1.23488700	3.31426000
H	2.99760500	-2.13683000	3.28552700
H	3.01069400	-0.38529200	3.04649400
C	0.74571900	-3.61401100	1.50807200
H	1.39811700	-4.49283000	1.60438100
H	0.48382200	-3.29712600	2.52051800
H	-0.16237200	-3.94399500	0.99587300
C	0.94051800	-3.38680600	-1.66258300
H	1.59224100	-4.26077000	-1.77696100
H	-0.04219800	-3.74973500	-1.34914500
H	0.82921800	-2.93318700	-2.65091300
C	2.92543200	-0.89870500	-2.28040100
H	4.01873200	-0.84587800	-2.33045000
H	2.57311300	-1.53464600	-3.09422300
H	2.54902200	0.11956300	-2.44419700
Co	0.19165700	-0.68355800	-0.06109600
C	1.85876500	3.33483700	-1.91507100
H	2.09123800	4.34319400	-2.26904000
H	2.78650800	2.75341100	-1.93123600
H	1.15819700	2.87489600	-2.61602100
C	2.27065800	4.05989700	0.47599300
H	2.49681700	5.07666100	0.14214100
H	1.86287100	4.10684200	1.48765000
H	3.21103400	3.50018700	0.50981900
C	-0.05099500	4.22314600	-0.51363700
H	0.15368700	5.24077300	-0.85913100

H	-0.78395100	3.77533900	-1.19304500
H	-0.48696200	4.27779200	0.48733700

¹⁵_CMD, -2561.045748

C	-2.90869800	-0.92185900	-0.42405600
C	-2.80038400	0.28651600	-1.19544800
C	-2.48996500	1.33874700	-0.28995400
C	-2.56442200	0.81407600	1.06606700
C	-2.85539600	-0.55768600	0.97921300
C	3.53627900	-1.75553600	-1.88057900
C	3.61205600	-2.35296600	-0.64062800
C	2.48573700	-2.33369700	0.22387000
C	1.29973400	-1.70128300	-0.23855700
C	1.20517700	-1.14422700	-1.53774300
C	2.33590900	-1.15222900	-2.33288400
H	3.35231000	-3.36368900	1.92574400
H	4.40434300	-1.75551400	-2.53233100
H	4.53055400	-2.82384900	-0.30408300
C	2.47102200	-2.85987400	1.53914800
H	2.30072200	-0.71230000	-3.32551000
C	0.23208400	-2.01195300	1.80285900
C	1.34511800	-2.70789600	2.31885800
H	-0.63615000	-1.83096100	2.42210100
H	1.30473700	-3.08942700	3.33292200
N	0.20157600	-1.53074200	0.56830000
C	-0.14612700	-0.62462000	-1.88859600
H	-0.78912600	-1.45106500	-2.20768400
H	0.24773400	1.57237200	-1.65188700
H	-0.12807000	0.09064100	-2.72121100
C	1.16392900	1.86123500	-0.05223700
C	2.37971000	2.48997000	0.59069100
O	0.41209200	1.08861100	0.55847700
O	0.98328400	2.13894000	-1.33270700
C	-2.28678900	2.78460600	-0.62355600
H	-1.54359400	3.24677900	0.03252900
H	-1.96709200	2.93017100	-1.65882000
H	-3.22440000	3.33938900	-0.49206800
C	-3.00150900	0.41104000	-2.67149100
H	-4.07038900	0.53576100	-2.88495200
H	-2.48236000	1.27959000	-3.08468700
H	-2.66302100	-0.47718500	-3.21004200
C	-3.24289900	-2.28308400	-0.94853300
H	-4.32516500	-2.46067600	-0.91035700
H	-2.92915100	-2.40319200	-1.98869800

H	-2.75767900	-3.06763800	-0.36055800
C	-3.11204800	-1.50491800	2.10753900
H	-4.19427500	-1.60804000	2.25841300
H	-2.72498100	-2.50598200	1.89869600
H	-2.68795900	-1.15241000	3.05163800
C	-2.33609300	1.62916300	2.29932700
H	-3.15156100	2.34724700	2.44825300
H	-2.27602400	1.00371900	3.19308900
H	-1.40333200	2.19796200	2.22568000
Co	-1.00524300	-0.13096600	-0.15583300
C	2.23061000	2.45933000	2.11869500
H	3.13005200	2.87993900	2.57773400
H	1.37255600	3.05541700	2.44713100
H	2.09788900	1.43862100	2.48642600
C	2.57844900	3.93061900	0.08573800
H	3.47491300	4.35172400	0.55069600
H	2.70513100	3.96470600	-0.99888300
H	1.72896900	4.56754500	0.35524100
C	3.57525800	1.60098200	0.15573400
H	4.49001700	1.99627500	0.60826800
H	3.44390300	0.56706200	0.49047000
H	3.69758400	1.60115100	-0.93087600

³⁵S_CMD, -2561.03621755

C	-3.06090700	-0.19150500	-0.97214200
C	-2.61278800	1.17831400	-0.71121400
C	-2.43654400	1.31950000	0.68348900
C	-2.69159700	0.04097300	1.28930100
C	-3.14204100	-0.87098400	0.28024800
C	3.64551500	-1.44256900	-1.89258400
C	3.74262300	-2.12342700	-0.69819000
C	2.59210100	-2.28617700	0.11846000
C	1.36085900	-1.74274100	-0.33669700
C	1.24922800	-1.09886800	-1.60176500
C	2.40358800	-0.93050800	-2.34536700
H	3.51408000	-3.35815600	1.76208900
H	4.52804100	-1.30542800	-2.50934600
H	4.69325200	-2.52533700	-0.36140800
C	2.59390100	-2.92025000	1.38571600
H	2.35545100	-0.42142500	-3.30351400
C	0.27178000	-2.34865700	1.63413700
C	1.43584300	-2.96604500	2.13367300
H	-0.63989400	-2.31915000	2.22085900
H	1.41074000	-3.44330800	3.10674300

N	0.23660900	-1.75442900	0.45033400
C	-0.11889300	-0.67491900	-2.00434900
H	-0.73169300	-1.53606900	-2.30794800
H	0.06236500	1.73618900	-1.46464700
H	-0.14926700	0.06279400	-2.81082100
C	1.17046000	1.80167400	0.04936900
C	2.41114300	2.44117700	0.63965000
O	0.50016900	0.94313500	0.62240400
O	0.84013700	2.24839800	-1.16440600
C	-1.99535600	2.54376800	1.42169000
H	-1.26492700	2.29729400	2.19792300
H	-1.54105700	3.27993900	0.75293500
H	-2.84812900	3.02973600	1.91260600
C	-2.53837300	2.26280100	-1.74319100
H	-3.52598200	2.71787000	-1.89250900
H	-1.85873400	3.06718400	-1.44654300
H	-2.21653100	1.87869100	-2.71605200
C	-3.52547500	-0.70328600	-2.30000400
H	-4.57651800	-0.43285000	-2.46422200
H	-2.94669200	-0.27890800	-3.12520700
H	-3.45596300	-1.79287500	-2.36268600
C	-3.60304800	-2.28228400	0.49479500
H	-4.67466400	-2.31192000	0.72808000
H	-3.44633600	-2.89788800	-0.39548600
H	-3.07712600	-2.76280500	1.32513500
C	-2.58001200	-0.23497800	2.75616800
H	-3.36947000	0.29077700	3.30784900
H	-2.68446100	-1.29951800	2.98075000
H	-1.62155200	0.11251200	3.15789500
Co	-1.06137100	-0.36648300	-0.27794000
C	2.74704700	1.75595500	1.97113300
H	3.64495400	2.21241200	2.39836300
H	1.93145100	1.86061400	2.69234000
H	2.93779500	0.68748200	1.82869800
C	2.11398100	3.94220100	0.85956800
H	2.99743800	4.42360300	1.29015300
H	1.87294500	4.44313500	-0.08192700
H	1.27977400	4.08351800	1.55577400
C	3.57647600	2.27190700	-0.35997600
H	4.47818800	2.72449900	0.06414800
H	3.78350900	1.21362100	-0.55050200
H	3.36026200	2.76111600	-1.31297800

55_CMD, -2561.00605325

C	-3.21147200	-0.92287800	-0.70263900
C	-3.10136300	0.48227100	-1.01637500
C	-2.77037500	1.16189400	0.15535000
C	-2.63998600	0.17449500	1.23633200
C	-2.88181900	-1.11204000	0.69621500
C	3.70539600	-1.09211400	-2.15670100
C	4.06771500	-1.67297700	-0.95994100
C	3.07132700	-1.95891200	0.00869800
C	1.71321000	-1.64413400	-0.29216300
C	1.32775500	-1.12217300	-1.56931500
C	2.34924100	-0.82357600	-2.45987700
H	4.36705600	-2.78633800	1.53546500
H	4.46607500	-0.85813100	-2.89499800
H	5.10488300	-1.90814200	-0.74222000
C	3.34519500	-2.51734100	1.28261900
H	2.09781300	-0.40298100	-3.42937100
C	1.02316500	-2.29306800	1.84740900
C	2.32488100	-2.70636800	2.19208400
H	0.20550800	-2.36104200	2.55925300
H	2.51027100	-3.13381700	3.17085100
N	0.73078600	-1.77979600	0.65922100
C	-0.12599300	-0.90830700	-1.83160200
H	-0.64227400	-1.87158800	-1.95997700
H	-0.08681400	1.30398300	-1.49147300
H	-0.30861800	-0.32863100	-2.74110900
C	0.79228900	1.98190800	0.03484000
C	1.88174100	2.92449800	0.50246300
O	0.25447400	1.14969200	0.78317900
O	0.49711800	2.05817200	-1.25348600
C	-2.59079700	2.63450100	0.34815800
H	-1.78487400	2.84449100	1.05659900
H	-2.36272100	3.14484800	-0.59039600
H	-3.50298300	3.08781800	0.75595500
C	-3.30749000	1.05509500	-2.38501800
H	-4.34858700	0.94246900	-2.70871400
H	-3.06698200	2.11970100	-2.42104300
H	-2.68584700	0.54248500	-3.12815300
C	-3.59182900	-1.99532500	-1.66314700
H	-4.68567900	-2.08093200	-1.72595000
H	-3.23157800	-1.77718500	-2.67253500
H	-3.20979900	-2.97271700	-1.35764500
C	-3.01063900	-2.41051200	1.44569200
H	-4.06315700	-2.65631400	1.62764400

H	-2.57093800	-3.24288900	0.88836800
H	-2.51321800	-2.36362300	2.41742700
C	-2.36530300	0.52978100	2.66421000
H	-3.21565500	1.07644300	3.08996000
H	-2.19832800	-0.35555700	3.28102300
H	-1.48731400	1.17828800	2.74627000
Co	-0.80915500	-0.52210100	0.07310400
C	1.84272200	3.04466200	2.03363600
H	2.65654400	3.69398000	2.36700500
H	0.89925900	3.48343900	2.37306700
H	1.95771800	2.07003600	2.51353400
C	1.72738200	4.30647700	-0.16218000
H	2.53982900	4.95729100	0.17232300
H	1.76765600	4.23648200	-1.25101300
H	0.78050800	4.77786800	0.11957600
C	3.20934300	2.25654100	0.04888700
H	4.04762000	2.88083500	0.37096800
H	3.32795600	1.26431300	0.49602200
H	3.24983700	2.15311100	-1.03841400

¹⁶, -2802.35676175

C	4.39536600	1.40527200	-2.10818500
C	3.93410100	2.56203000	-1.51705800
C	2.68095800	2.56310900	-0.84793800
C	1.93948800	1.34965700	-0.81636500
C	2.37884600	0.18367300	-1.49341000
C	3.61846600	0.21774200	-2.10610900
H	2.65753600	4.62948300	-0.18505200
H	5.36094200	1.40251900	-2.60416000
H	4.52275300	3.47385700	-1.54125200
C	2.12884200	3.68053800	-0.17534200
H	3.98816800	-0.66468900	-2.62022100
C	0.29462000	2.28672200	0.52986200
C	0.92884200	3.54583400	0.49039300
H	-0.62212200	2.15106000	1.08651000
H	0.47272800	4.38127700	1.00958300
N	0.78151500	1.21580000	-0.08606900
C	1.39710900	-0.93399100	-1.49024400
C	1.70112000	-0.81334400	1.86084600
C	1.82783400	-2.02066500	1.11383300
C	0.53418900	-2.63343500	1.06516300
C	0.36110500	-0.75766800	2.41892400
C	-0.34313900	-1.88158900	1.94157700
H	1.84462800	-1.91315400	-1.66249900

H	0.64990500	-0.76232500	-2.27131500
C	0.19311700	-3.93668900	0.40627600
H	0.42506500	-4.77925100	1.06838500
H	-0.86792300	-3.99000900	0.15577800
H	0.75469000	-4.07279100	-0.52050000
C	3.10213000	-2.55974800	0.54403300
H	3.70976200	-2.98287900	1.35207400
H	2.91890700	-3.35388300	-0.18151800
H	3.69348600	-1.77844200	0.05956500
C	2.80403400	0.15526400	2.16233600
H	3.29951000	-0.11037700	3.10342700
H	3.55972300	0.15530300	1.37417200
H	2.42412500	1.17483900	2.26455800
C	-0.09501700	0.26974600	3.41106500
H	0.39140600	0.09963400	4.37844400
H	0.16913400	1.28351900	3.09750700
H	-1.17324000	0.23403900	3.58063300
C	-1.75290600	-2.28647200	2.24978400
H	-1.75676600	-3.24242900	2.78448200
H	-2.26834800	-1.55708600	2.87718900
H	-2.33854600	-2.42942500	1.33634500
Co	0.39353200	-0.72925200	0.22163800
C	-2.40122400	-0.24590600	-1.02981800
C	-2.43000300	-1.93849300	-2.44974200
O	-2.74999500	-2.68058000	-3.31487800
O	-3.10548100	-0.78946500	-2.04808700
O	-1.33746200	-2.03592000	-1.63421900
N	-1.31715400	-0.91063300	-0.75988400
C	-2.93788500	0.92824700	-0.35993700
C	-3.66793000	1.87439400	-1.09711700
C	-2.78015000	1.07188900	1.02701900
C	-4.20749500	2.97948700	-0.44325800
H	-3.80585800	1.74179600	-2.16497600
C	-3.33544700	2.17258100	1.67280700
H	-2.23191400	0.31913500	1.57734200
C	-4.04265100	3.12939100	0.93717300
H	-4.76466200	3.71907900	-1.00857800
H	-3.22640000	2.28070200	2.74733300
H	-4.47700900	3.98640200	1.44227800

³⁶, -2802.3420191

C	4.60885100	0.82323700	-2.32568200
C	4.29418600	2.07850200	-1.85112600
C	3.06378000	2.29087800	-1.17417400

C	2.18236300	1.18418700	-1.01559300
C	2.47635900	-0.09039600	-1.57348500
C	3.70474400	-0.26007500	-2.18992400
H	3.30577100	4.39800100	-0.72065900
H	5.55745500	0.65831500	-2.82672300
H	4.98380900	2.90850300	-1.96968100
C	2.66552200	3.52750600	-0.60933000
H	3.96556800	-1.22920100	-2.60468300
C	0.69148400	2.45116500	0.24665900
C	1.47497700	3.61122600	0.08201500
H	-0.23052000	2.48435400	0.81551700
H	1.14078200	4.54430300	0.52142100
N	1.03151100	1.27528500	-0.26999700
C	1.41267200	-1.11852800	-1.45630300
C	1.71193000	-0.66960600	2.17587700
C	1.89406200	-1.83201100	1.39122000
C	0.59440700	-2.50464600	1.26728900
C	0.32430700	-0.59019200	2.52228100
C	-0.35543600	-1.74735700	2.00499100
H	1.77375700	-2.14350300	-1.52846800
H	0.60761200	-0.96123700	-2.18007700
C	0.36315300	-3.84144000	0.62886500
H	0.53900200	-4.64937000	1.34919300
H	-0.66145800	-3.93795300	0.26325000
H	1.03127400	-4.00586300	-0.21937900
C	3.20679000	-2.36455600	0.90650100
H	3.76771500	-2.79548400	1.74380900
H	3.07740100	-3.15085300	0.16102900
H	3.82438400	-1.57762500	0.46430400
C	2.75688800	0.34255900	2.53962500
H	3.07030300	0.23316700	3.58457100
H	3.64752900	0.23867300	1.91564800
H	2.38315800	1.36491000	2.41880800
C	-0.25594300	0.47885800	3.40114200
H	0.14727100	0.39073900	4.41662600
H	0.00794700	1.48211800	3.04697900
H	-1.34311100	0.41067600	3.47702500
C	-1.79465400	-2.11571700	2.22637900
H	-1.90570000	-2.73960100	3.12050500
H	-2.43003300	-1.23641100	2.36261300
H	-2.19263500	-2.68323700	1.38138200
Co	0.41612700	-0.63304400	0.24170200
C	-2.72823200	-0.25767600	-1.01172000
C	-2.78884400	-2.02213800	-2.33361500

O	-3.14035100	-2.83148400	-3.12284500
O	-3.49795300	-0.89740400	-1.92194000
O	-1.60996200	-2.00080000	-1.63393800
N	-1.58857700	-0.84597800	-0.81325700
C	-3.22222100	0.94441900	-0.36212600
C	-4.29226400	1.65803300	-0.92341800
C	-2.63530800	1.37234400	0.84020100
C	-4.75541400	2.80787600	-0.28649700
H	-4.74985600	1.31413300	-1.84469800
C	-3.10757900	2.51779900	1.47032900
H	-1.83296000	0.79143800	1.27877300
C	-4.16583000	3.23888800	0.90472100
H	-5.58025300	3.36493100	-0.71813700
H	-2.66533400	2.84100700	2.40762400
H	-4.53722900	4.13077000	1.39944600

⁵⁶, -2802.32564964

C	5.04129700	0.43749000	-1.97817600
C	4.68511000	1.71133100	-1.56240500
C	3.35712100	1.97457600	-1.12095600
C	2.39016300	0.92482400	-1.11554000
C	2.72793200	-0.36924000	-1.69326800
C	4.08872300	-0.58160300	-2.04634400
H	3.67452900	4.06533600	-0.66136600
H	6.06230400	0.23461800	-2.28466000
H	5.41206400	2.51712000	-1.54937100
C	2.96027100	3.24713000	-0.64856300
H	4.37179800	-1.55658300	-2.43112100
C	0.82251800	2.32739500	-0.10663600
C	1.67940300	3.43418000	-0.16925600
H	-0.16432500	2.41887800	0.33445000
H	1.34124300	4.39902000	0.19112500
N	1.16367400	1.10956700	-0.54436000
C	1.76609300	-1.34367900	-1.94855600
C	1.64163100	-0.53747500	2.13266200
C	1.54584300	-1.84433600	1.56231100
C	0.18625900	-2.28334000	1.68382600
C	0.33964500	-0.15577100	2.59617400
C	-0.55880000	-1.24533000	2.33673400
H	2.05233100	-2.31671500	-2.32949500
H	0.70402100	-1.14097000	-1.89745200
C	-0.35240800	-3.62953700	1.29220000
H	-0.27280900	-4.34233500	2.12202700
H	-1.40770600	-3.57429500	1.01110100

H	0.19233700	-4.05267200	0.44420500
C	2.68550100	-2.66347700	1.02932900
H	3.13031200	-3.27087100	1.82666100
H	2.35592400	-3.34700100	0.24259600
H	3.47650400	-2.03601700	0.61190500
C	2.88001000	0.30362300	2.23144700
H	3.34894300	0.20408500	3.21779800
H	3.62528700	0.01457100	1.48598500
H	2.65862600	1.36590300	2.08544500
C	0.02630000	1.12176800	3.32449300
H	0.37400400	1.07771900	4.36333200
H	0.51709100	1.98436100	2.86082500
H	-1.04822700	1.32332900	3.35686700
C	-2.00000400	-1.35523400	2.74879000
H	-2.11143900	-2.04793100	3.59078700
H	-2.41421000	-0.39488300	3.06482700
H	-2.62707100	-1.73750600	1.93586900
Co	0.15819300	-0.48196000	0.37528200
C	-2.71288900	-0.33281500	-1.05917900
C	-2.69238100	-2.19413700	-2.25016400
O	-2.99950800	-3.05784600	-2.99738000
O	-3.42984300	-1.05020200	-1.94993500
O	-1.54745100	-2.11080100	-1.49985100
N	-1.57890200	-0.89982000	-0.76490500
C	-3.23289800	0.92512900	-0.55364800
C	-4.27580400	1.56709800	-1.24177500
C	-2.69716400	1.49486100	0.61555300
C	-4.76144000	2.78392000	-0.76812800
H	-4.69382000	1.11702800	-2.13561800
C	-3.19058400	2.70843600	1.07953300
H	-1.92692100	0.97221600	1.17253500
C	-4.21994800	3.35605500	0.38584500
H	-5.56470400	3.28394900	-1.29880700
H	-2.78700400	3.14217900	1.98901100
H	-4.60628200	4.30189600	0.75227900

¹³, -2907.7827475

C	0.14040600	-0.50177700	1.92101000
C	-0.38814200	-1.75693100	1.50935000
C	-1.79899700	-1.76675500	1.82281000
C	-2.11133200	-0.54751800	2.52158700
C	-0.94008500	0.25671400	2.53037400
C	2.94925700	2.93555400	-1.06544700
C	2.03610900	3.82462100	-0.55214200

C	0.70244700	3.40330900	-0.31700000
C	0.32487400	2.03393100	-0.56732300
C	1.25886400	1.15962300	-1.20291900
C	2.54820500	1.62867700	-1.41831800
H	-0.00392700	5.35013800	0.29739100
H	3.97781100	3.23768000	-1.23771800
H	2.30474400	4.85511000	-0.33642500
C	-0.28213400	4.31282700	0.12948100
H	3.26124400	0.93778700	-1.86467000
C	-1.84740500	2.51490300	0.18368700
C	-1.57459000	3.88450000	0.32626700
H	-2.83077200	2.12919900	0.42444600
H	-2.36573700	4.55826400	0.63555400
N	-0.94410100	1.60951800	-0.19767100
C	0.89463600	-0.20706700	-1.70807200
H	0.64531700	-0.88609300	-0.89672400
H	0.02319800	-0.15503800	-2.36651000
H	1.75470500	-0.65414200	-2.21104600
C	4.04174800	-1.38304900	-0.78301100
C	5.45473300	-1.17961800	-0.13421400
O	3.93904100	-1.04805000	-1.99216500
O	3.12475900	-1.83525200	-0.03550700
C	-3.03348900	-0.68093000	-1.13737600
C	-3.98893100	-0.90653200	-2.29308700
O	-1.85614000	-1.15838500	-1.14647100
O	-3.33544300	0.03455200	-0.11643800
C	1.56585300	-0.05751600	1.87492500
H	1.64479500	1.01110600	1.66294500
H	2.00885300	-0.22757000	2.86553000
H	2.16189900	-0.61838600	1.14342400
C	-0.77798400	1.62003300	3.12736400
H	-0.32812100	1.54258400	4.12403500
H	-0.11797300	2.23833300	2.51513200
H	-1.73277300	2.14042900	3.22488900
C	-3.47568800	-0.16863800	3.00510900
H	-3.78928000	-0.84221300	3.81001200
H	-3.50098900	0.85308800	3.38793600
H	-4.20248700	-0.24970400	2.19149200
C	-2.75129400	-2.88340100	1.52658000
H	-2.67850200	-3.67206900	2.28446200
H	-3.78319300	-2.52503200	1.50709300
H	-2.52572100	-3.32986100	0.55541100
C	0.32906100	-2.85927400	0.80017700
H	0.45890100	-3.69991700	1.49416900

H	-0.27453500	-3.21804900	-0.03964100
H	1.31446300	-2.55712200	0.42579600
Co	-1.48323700	-0.20366500	0.55784200
C	5.46633000	-1.62765300	1.33234100
H	6.46671300	-1.50980100	1.77001200
H	4.75819600	-1.04072000	1.92600000
H	5.16540200	-2.67529100	1.41797900
C	6.47912700	-1.98919200	-0.94940800
H	6.27914800	-3.06423500	-0.86881800
H	6.41230300	-1.71218100	-2.00449700
H	7.50235000	-1.80927900	-0.59373100
C	5.80041600	0.31917000	-0.23012400
H	5.07406800	0.92523300	0.32690900
H	6.79651100	0.52497900	0.18288800
H	5.77949400	0.63944700	-1.27565200
C	-3.96520100	-2.40304800	-2.66392700
H	-4.33588700	-3.01959200	-1.83782000
H	-4.60837600	-2.57826800	-3.53194600
H	-2.95129900	-2.72852100	-2.90744800
C	-5.40740600	-0.45791200	-1.91216100
H	-6.08161400	-0.60870300	-2.76099400
H	-5.79083400	-1.03396200	-1.06435300
H	-5.42750800	0.59959000	-1.63670500
C	-3.45123200	-0.06264700	-3.47383700
H	-3.43909000	1.00313400	-3.22271700
H	-2.43525900	-0.36696800	-3.73860300
H	-4.09680600	-0.20040200	-4.34706000

³³, -2907.78449688

C	0.15666800	-0.58467000	2.04444500
C	-0.44630900	-1.77143300	1.59191300
C	-1.87353000	-1.63716700	1.83091300
C	-2.13182300	-0.37830400	2.50472300
C	-0.90654300	0.28157000	2.61504400
C	3.18558000	2.85349200	-1.30732900
C	2.37293000	3.81331400	-0.75122800
C	1.03913600	3.48487200	-0.39721200
C	0.57004000	2.14165000	-0.59074300
C	1.40324800	1.17778200	-1.23072700
C	2.69378700	1.55285900	-1.56721600
H	0.47603300	5.46476300	0.26417400
H	4.21071800	3.09133900	-1.57453100
H	2.72586900	4.82753100	-0.58633700
C	0.13682100	4.44177600	0.12276700

H	3.33406800	0.80650100	-2.03037100
C	-1.52761700	2.72996400	0.27828000
C	-1.15663700	4.07778900	0.42634100
H	-2.51904900	2.38705200	0.55177100
H	-1.88008000	4.79325300	0.80086400
N	-0.69855200	1.79262300	-0.17604200
C	0.88808400	-0.18925900	-1.58741000
H	0.71216700	-0.80312000	-0.69532800
H	-0.03208700	-0.13465500	-2.17712400
H	1.65674500	-0.75557300	-2.12041200
C	3.92711700	-1.55002400	-0.81220500
C	5.34753200	-1.38904000	-0.18159900
O	3.81989600	-1.30423500	-2.04029400
O	2.98251400	-1.91173200	-0.04585600
C	-3.23844500	-0.55632800	-1.13362900
C	-4.35160000	-0.90789800	-2.11831900
O	-2.14046300	-1.21566100	-1.17514100
O	-3.35643700	0.37572500	-0.28382800
C	1.61083200	-0.25704900	2.10767100
H	1.78262900	0.81167800	1.94580600
H	1.99777800	-0.50023200	3.10707000
H	2.19774900	-0.82877200	1.37569200
C	-0.62695900	1.60870700	3.24039800
H	-0.10638600	1.47346200	4.19663300
H	0.02562200	2.21517200	2.60571700
H	-1.54172800	2.17390300	3.42888500
C	-3.49202000	0.10210000	2.91234500
H	-3.95014000	-0.58019100	3.63716500
H	-3.44519800	1.09170100	3.37239600
H	-4.14965400	0.16605000	2.03975100
C	-2.89929200	-2.67448700	1.52274500
H	-2.89226000	-3.45464000	2.29531100
H	-3.90182000	-2.24233200	1.48655300
H	-2.68958400	-3.15085800	0.56278900
C	0.21415600	-2.98301800	1.00408500
H	0.34884800	-3.75194000	1.77557100
H	-0.40919200	-3.41305600	0.21435600
H	1.19371600	-2.74631300	0.57766600
Co	-1.27856500	-0.12488900	0.30053000
C	5.32136100	-1.63528700	1.33225000
H	6.33308100	-1.57283500	1.75321700
H	4.69516400	-0.89441400	1.84059100
H	4.90591600	-2.62104400	1.55672100
C	6.27657100	-2.40615700	-0.87170900

H	5.96072900	-3.43299100	-0.65411700
H	6.24407800	-2.26417400	-1.95499700
H	7.31193900	-2.29047800	-0.52638600
C	5.84429200	0.03841100	-0.47829100
H	5.19664900	0.78584400	-0.00309500
H	6.86335000	0.18666300	-0.09944600
H	5.83906100	0.21932700	-1.55652100
C	-4.63110200	-2.42170400	-2.01993600
H	-4.99238100	-2.69215500	-1.02146900
H	-5.40081900	-2.70657400	-2.74468100
H	-3.72568400	-2.99756100	-2.22512200
C	-5.62052300	-0.10324300	-1.80451700
H	-6.40727700	-0.35277300	-2.52408200
H	-5.99017400	-0.32597700	-0.79908200
H	-5.42817500	0.97137500	-1.85699100
C	-3.83009700	-0.56591800	-3.53235600
H	-3.61533700	0.50428300	-3.62366900
H	-2.91497900	-1.12134800	-3.75261600
H	-4.58681900	-0.82483200	-4.28038300

⁵³, -2907.76554381

C	0.31090400	-0.16595500	2.15168000
C	-0.43734300	-1.37031400	1.83019800
C	-1.79755000	-1.09025000	2.09670400
C	-1.91137300	0.31284300	2.52202500
C	-0.62793900	0.86146700	2.53810800
C	3.16710900	2.75285300	-1.61588100
C	2.32528000	3.76749000	-1.22303000
C	0.98662100	3.46824400	-0.85864900
C	0.54814000	2.10339900	-0.88263900
C	1.41096900	1.07388100	-1.35257900
C	2.70719700	1.41585000	-1.70026800
H	0.36101700	5.50156400	-0.47368900
H	4.19591700	2.97148100	-1.88540000
H	2.66144700	4.80008400	-1.19050500
C	0.05082200	4.45985300	-0.48468500
H	3.36945700	0.61863400	-2.03198600
C	-1.57817400	2.74179500	-0.12521500
C	-1.23878200	4.10494100	-0.14593200
H	-2.56276800	2.40677000	0.18371300
H	-1.98078400	4.84608700	0.12868900
N	-0.71988600	1.78007900	-0.45702500
C	0.91151800	-0.33476400	-1.51815400
H	0.68303200	-0.81565500	-0.54938100

H	0.04283600	-0.38574200	-2.18481000
H	1.71581500	-0.98114800	-1.89479300
C	3.85228300	-1.70455800	-0.65494500
C	5.30048500	-1.60016500	-0.07256600
O	3.73182800	-1.46656800	-1.88808000
O	2.91557200	-1.99019500	0.14720000
C	-3.30132700	-0.88423800	-1.02290600
C	-4.49771200	-1.43509100	-1.79043400
O	-2.16837700	-1.48399800	-1.11464400
O	-3.38333200	0.15196200	-0.29258200
C	1.78787000	-0.02273100	2.14306200
H	2.08879800	1.02229100	2.02564400
H	2.19337700	-0.37293700	3.10481200
H	2.26705400	-0.64647900	1.37154600
C	-0.22779400	2.26376100	2.87828900
H	0.40516900	2.28463000	3.77303500
H	0.35209300	2.71666200	2.06655400
H	-1.09400900	2.90185900	3.06506200
C	-3.21411200	0.97354200	2.83799900
H	-3.70119700	0.49106600	3.69437000
H	-3.08679300	2.03114700	3.07954000
H	-3.89736100	0.89027400	1.98545600
C	-2.93666500	-2.05846500	2.06942800
H	-3.11675600	-2.46356300	3.07384400
H	-3.85669100	-1.57091500	1.73730300
H	-2.72717900	-2.89633400	1.40207600
C	0.15398400	-2.71173800	1.49909300
H	0.34613100	-3.27606800	2.42096800
H	-0.53854900	-3.29840400	0.88884100
H	1.09955500	-2.61560600	0.95650100
Co	-1.25910700	-0.12987800	0.07642700
C	5.32095600	-1.91533100	1.42832100
H	6.34656300	-1.88448400	1.81866600
H	4.71850800	-1.19397700	1.98964800
H	4.89999200	-2.90568200	1.62076500
C	6.19761700	-2.58965100	-0.83870200
H	5.88424200	-3.62369300	-0.65357200
H	6.12385100	-2.40186900	-1.91278200
H	7.24622300	-2.49435300	-0.52826900
C	5.80256000	-0.16380200	-0.31734100
H	5.16423100	0.56802400	0.19440000
H	6.82669200	-0.03434800	0.05512700
H	5.78765300	0.06089600	-1.38749100
C	-4.69335300	-2.90906100	-1.37393100

H	-4.93071500	-2.98990500	-0.30765100
H	-5.52365100	-3.34552700	-1.93843700
H	-3.79002200	-3.49106400	-1.57061600
C	-5.75884200	-0.61566300	-1.48387100
H	-6.60906600	-1.02004100	-2.04261300
H	-6.00060700	-0.64715200	-0.41750100
H	-5.62628800	0.43272900	-1.76390200
C	-4.15391000	-1.36168900	-3.29516600
H	-4.00256700	-0.32483400	-3.61443400
H	-3.24436900	-1.92663100	-3.51307900
H	-4.97734500	-1.77996500	-3.88322000

¹TS4, -2907.7541085, i661.14

C	0.22008900	0.18272000	2.39220800
C	-0.21146400	-1.19377300	2.22102300
C	-1.63853100	-1.20108600	2.22255300
C	-2.09926900	0.15214200	2.29266400
C	-0.93463500	1.00230900	2.41003400
C	1.96702000	3.73915800	-1.37367900
C	0.74108100	4.36556200	-1.43988400
C	-0.44267900	3.62395200	-1.18850700
C	-0.31357500	2.24751400	-0.84341200
C	0.94366900	1.58335700	-0.86114300
C	2.07029400	2.35000200	-1.11123000
H	-1.88829000	5.20339200	-1.52764700
H	2.87310700	4.30706500	-1.56356200
H	0.66243700	5.42069600	-1.68600700
C	-1.75290700	4.16057500	-1.25269900
H	3.03559000	1.85528200	-1.15164700
C	-2.62431100	2.02179800	-0.56627900
C	-2.83727400	3.35484600	-0.98032500
H	-3.43439200	1.35034400	-0.30730800
H	-3.85273800	3.72918400	-1.04826300
N	-1.40670800	1.50500900	-0.46903600
C	0.96879300	0.09465200	-0.71906800
H	1.22379600	-0.36520600	0.23806500
H	0.29755500	-0.45797800	-1.37279600
H	2.10404900	-0.27735800	-1.09998500
C	4.00913400	-0.98574200	-0.31469800
C	5.54667900	-1.15981400	-0.41428200
O	3.45491800	-0.50589100	-1.37823200
O	3.41122800	-1.29587800	0.73399200
C	-2.85319800	-1.44904200	-0.97362400
C	-3.12205300	-2.50151300	-2.07282500

O	-1.59483100	-1.35615800	-0.65669000
O	-3.77171200	-0.79047800	-0.46907000
C	1.63146600	0.66436000	2.54705600
H	1.78174500	1.61418900	2.02573800
H	1.84096900	0.83276200	3.61079600
H	2.35906700	-0.04842500	2.15364200
C	-0.95091900	2.49488500	2.54390700
H	-1.05992000	2.78471700	3.59557500
H	-0.02512400	2.93609800	2.16892300
H	-1.78161300	2.93740600	1.98916000
C	-3.52860300	0.58829100	2.38595600
H	-3.91198200	0.41295200	3.39867400
H	-3.63389400	1.65517300	2.17602000
H	-4.14269800	0.03666200	1.67277600
C	-2.50597800	-2.41366100	2.10651100
H	-2.66630300	-2.85430000	3.09794700
H	-3.47359300	-2.16195300	1.67177600
H	-2.03563100	-3.16789900	1.47303500
C	0.67592500	-2.40109700	2.15359500
H	0.85001300	-2.80007500	3.16103500
H	0.20483100	-3.18970800	1.56140500
H	1.64341600	-2.17002400	1.70213200
Co	-0.91226800	-0.08096200	0.57656600
C	6.10515600	-1.70607100	0.90568700
H	7.19139900	-1.83791300	0.83525100
H	5.88886400	-1.02455600	1.73337900
H	5.64995500	-2.66910100	1.15173400
C	5.84666300	-2.13638100	-1.56897900
H	5.42149400	-3.12559500	-1.36501600
H	5.41560600	-1.76687900	-2.50276100
H	6.92885200	-2.25504200	-1.70047400
C	6.16807600	0.21546700	-0.72988400
H	5.95985000	0.93353000	0.07250600
H	7.25672600	0.13217600	-0.83046800
H	5.75912900	0.61432600	-1.66172200
C	-2.59873300	-3.86815900	-1.58566300
H	-3.12097200	-4.18692800	-0.67618700
H	-2.76603000	-4.63273000	-2.35242700
H	-1.52883900	-3.81861400	-1.36903100
C	-4.62718000	-2.58116700	-2.36051900
H	-4.82192700	-3.32592000	-3.14023100
H	-5.18380200	-2.86276100	-1.46240900
H	-5.01403300	-1.61510900	-2.69534500
C	-2.35625600	-2.07594600	-3.34274100

H	-2.69634800	-1.09578200	-3.69608400
H	-1.28263900	-2.01657500	-3.14732000
H	-2.52520800	-2.80020900	-4.14744500

³TS4, -2907.74872991, i1236.00

C	-0.05335200	0.40198900	2.32209900
C	-0.44387400	-0.98987300	2.28878400
C	-1.84963300	-1.02140400	2.22990000
C	-2.35234900	0.36210500	2.24559200
C	-1.25366300	1.22141600	2.31451500
C	2.43405900	3.69192800	-1.11334500
C	1.28328900	4.42496900	-1.30686600
C	0.02234900	3.77842100	-1.24288200
C	-0.01977800	2.37521500	-0.97476100
C	1.17948400	1.60560400	-0.85221200
C	2.38476800	2.29402800	-0.90161600
H	-1.21459500	5.51443600	-1.62988100
H	3.40147600	4.18408300	-1.15327200
H	1.32288000	5.49248700	-1.50429100
C	-1.21479800	4.45043100	-1.40736900
H	3.30705600	1.72801600	-0.82471000
C	-2.35081200	2.38787800	-0.93677600
C	-2.39794600	3.75588700	-1.27893300
H	-3.25052700	1.80517100	-0.76893700
H	-3.35825200	4.24359300	-1.40695100
N	-1.21113700	1.73192600	-0.77879300
C	1.11360300	0.12905700	-0.72072100
H	1.32355600	-0.31118300	0.25174700
H	0.38845500	-0.39626300	-1.34454600
H	2.27715900	-0.34836400	-1.10238100
C	4.01924500	-1.11160200	-0.15186200
C	5.50454100	-1.54050200	-0.25743500
O	3.51246000	-0.71229100	-1.28436400
O	3.41999000	-1.15306100	0.93140800
C	-2.51102700	-1.67132500	-1.04514900
C	-3.29833600	-2.67353100	-1.89241400
O	-1.30784300	-1.93490700	-0.72352600
O	-3.02785100	-0.57350000	-0.66444600
C	1.32428900	0.94170200	2.53120200
H	1.48894300	1.84344200	1.93299600
H	1.44615500	1.22804900	3.58528600
H	2.10202900	0.22055900	2.27428700
C	-1.24819600	2.71911300	2.36649800
H	-0.96840600	3.07949800	3.36409500

H	-0.52710100	3.13907600	1.65810600
H	-2.22879700	3.13478800	2.12456900
C	-3.80492700	0.71496700	2.18477000
H	-4.33432200	0.35473100	3.07539000
H	-3.95642600	1.79487900	2.11982200
H	-4.26834800	0.24787600	1.30969100
C	-2.72735100	-2.23163700	2.21300200
H	-3.10373800	-2.45779700	3.21909500
H	-3.59260500	-2.07159800	1.56382100
H	-2.18516300	-3.10617900	1.84905900
C	0.47913200	-2.17384800	2.32656400
H	0.60749400	-2.53972100	3.35305500
H	0.07255600	-2.99256800	1.72638800
H	1.46766800	-1.93352600	1.92775900
Co	-1.12977700	-0.09751700	0.29258100
C	6.01435800	-1.99300300	1.11670100
H	7.06488200	-2.29874500	1.04890200
H	5.93070100	-1.18631800	1.85009400
H	5.42768600	-2.83569700	1.49216800
C	5.60762200	-2.69374700	-1.27553100
H	5.03394700	-3.56485200	-0.93983700
H	5.21818200	-2.38396400	-2.24829100
H	6.65243000	-3.00362400	-1.39502000
C	6.31967600	-0.33177300	-0.76052100
H	6.25648300	0.50493100	-0.05468400
H	7.37687800	-0.60167500	-0.86617500
H	5.94548500	0.00762800	-1.72963300
C	-3.20153700	-4.06005300	-1.22456000
H	-3.67233800	-4.05441000	-0.23539200
H	-3.71432600	-4.80869400	-1.83797000
H	-2.15739600	-4.35769100	-1.10408200
C	-4.76495700	-2.23993400	-2.02269400
H	-5.31492700	-2.95945800	-2.63883600
H	-5.24836700	-2.18609700	-1.04247300
H	-4.84359300	-1.25272600	-2.48522100
C	-2.62443900	-2.71885700	-3.28185100
H	-2.67355700	-1.74134300	-3.77401200
H	-1.57376000	-3.00604800	-3.19107200
H	-3.13430600	-3.44687200	-3.92214700

⁵TS4, -2907.73665915, i1319.33

C	0.01806200	0.39761000	2.32671900
C	-0.42440000	-0.97042600	2.23060500
C	-1.84367300	-0.95672100	2.23357900

C	-2.29218600	0.42343200	2.28820200
C	-1.15259200	1.24705100	2.32693400
C	2.50486500	3.65254400	-1.12099200
C	1.36215900	4.40119700	-1.29868100
C	0.09504800	3.76738300	-1.23232800
C	0.03900000	2.36070100	-0.98024500
C	1.22813600	1.57332300	-0.87709900
C	2.43939300	2.25265900	-0.92694700
H	-1.11834900	5.52504700	-1.58419900
H	3.47803300	4.13314000	-1.16061400
H	1.41169100	5.47051500	-1.48316500
C	-1.13274100	4.45860200	-1.37408000
H	3.35598400	1.67600200	-0.86118000
C	-2.29867700	2.41464500	-0.90642300
C	-2.32737800	3.78388800	-1.23468900
H	-3.20399500	1.84499000	-0.72595100
H	-3.28068200	4.28957700	-1.34161100
N	-1.16431600	1.73794600	-0.77774800
C	1.15785200	0.09441300	-0.76262500
H	1.33528700	-0.36902400	0.20499400
H	0.45984300	-0.42376700	-1.42327700
H	2.36328000	-0.37933300	-1.11716200
C	4.06139600	-1.18726300	-0.16989800
C	5.54354900	-1.62207800	-0.27141900
O	3.57235700	-0.73561400	-1.29242300
O	3.44361800	-1.27092800	0.89962800
C	-2.68003600	-1.61598200	-1.01295800
C	-3.51350200	-2.61616800	-1.81330900
O	-1.45357200	-1.89198100	-0.76007900
O	-3.16143600	-0.51827400	-0.60266000
C	1.41888800	0.88495600	2.50867400
H	1.60513100	1.78599700	1.91472300
H	1.58428300	1.15625200	3.56094000
H	2.16332900	0.13851200	2.22532900
C	-1.10476200	2.74384400	2.38474900
H	-0.83935800	3.09468900	3.39000800
H	-0.35254500	3.14385500	1.69709800
H	-2.06591700	3.19098100	2.12051700
C	-3.73018200	0.84073400	2.26753000
H	-4.25013800	0.51377300	3.17649000
H	-3.83548300	1.92642000	2.20019300
H	-4.24458400	0.39205900	1.41133800
C	-2.74679200	-2.15032100	2.23170500
H	-3.02205000	-2.43727800	3.25494600

H	-3.67030100	-1.94041000	1.68545300
H	-2.26189800	-3.00867600	1.76213600
C	0.44567600	-2.19482100	2.23797400
H	0.53459400	-2.60505200	3.25221800
H	0.01499100	-2.97309600	1.60125100
H	1.45220700	-1.98514300	1.86858500
Co	-1.13041900	-0.10275300	0.18755100
C	6.03197200	-2.13136100	1.09060100
H	7.08097000	-2.44278600	1.02526100
H	5.94437800	-1.35287900	1.85348700
H	5.43372500	-2.98289800	1.42566600
C	5.65265100	-2.73601600	-1.33204400
H	5.06940500	-3.61559000	-1.03736400
H	5.27748700	-2.38623900	-2.29687200
H	6.69693400	-3.04810100	-1.45056300
C	6.37485000	-0.40170100	-0.71684800
H	6.30813500	0.40800900	0.01947500
H	7.43137400	-0.67583000	-0.81852100
H	6.01668900	-0.02268600	-1.67733000
C	-3.41223200	-3.99470900	-1.12831900
H	-3.84257500	-3.96677000	-0.12159900
H	-3.96229200	-4.74169400	-1.71040900
H	-2.36947800	-4.31002100	-1.04652600
C	-4.97666500	-2.15895300	-1.88998500
H	-5.56294500	-2.87865700	-2.47112500
H	-5.41750000	-2.08100800	-0.89174100
H	-5.05832700	-1.17816900	-2.36567000
C	-2.89647300	-2.69351100	-3.22783200
H	-2.94901700	-1.72296100	-3.73329500
H	-1.84839800	-2.99890200	-3.17587200
H	-3.44538200	-3.42148700	-3.83474000

¹⁵, -2907.79490776

C	0.49038700	-0.48662400	2.08481000
C	-0.20937200	-1.69622600	1.74390700
C	-1.60203700	-1.49189600	2.05581300
C	-1.77920600	-0.15823400	2.49102000
C	-0.47954800	0.47663200	2.48008700
C	2.15524900	3.52590600	-1.26208100
C	1.03644300	4.31342900	-1.08859000
C	-0.20295300	3.70814000	-0.74804900
C	-0.23026700	2.29669300	-0.58943700
C	0.90096200	1.47446400	-0.85129400
C	2.09196000	2.11197500	-1.15724400

H	-1.44500100	5.48516600	-0.64498800
H	3.10529100	3.99189200	-1.50922700
H	1.08909000	5.39300100	-1.19714500
C	-1.41792000	4.40510800	-0.52531100
H	2.97787900	1.51915500	-1.35892900
C	-2.47403800	2.30718500	0.03897400
C	-2.54855900	3.70486000	-0.16301200
H	-3.32400300	1.70768900	0.34261300
H	-3.49593900	4.20834300	-0.00321800
N	-1.34493600	1.63743600	-0.14084500
C	0.62728500	0.01140400	-0.77377100
H	1.50669000	-0.58641700	-0.53568900
H	0.16762600	-0.35265700	-1.69973800
H	2.90095900	-1.00127400	-2.18618400
C	4.17844000	-1.40419300	-0.85994700
C	5.55514700	-0.98359300	-0.34895700
O	3.80900700	-0.72357200	-1.97209000
O	3.46058100	-2.24023300	-0.34941600
C	-3.17588700	-0.99099600	-0.92227500
C	-3.79162000	-1.76709900	-2.11289700
O	-1.88655200	-1.10743100	-0.84969300
O	-3.89397000	-0.34327900	-0.14553400
C	1.97415500	-0.26503200	2.07123100
H	2.23627200	0.66691500	1.55927300
H	2.35328600	-0.19694200	3.09818300
H	2.49657600	-1.08154600	1.57198900
C	-0.18916800	1.89448200	2.87556100
H	-0.06978400	1.98590300	3.96205700
H	0.73002800	2.25398700	2.40595100
H	-0.99807200	2.56592900	2.57454800
C	-3.07417700	0.47329400	2.90611700
H	-3.34253200	0.19041300	3.93157700
H	-3.00999700	1.56455600	2.87723700
H	-3.87820600	0.16535000	2.23410300
C	-2.67608400	-2.52094500	1.88627800
H	-2.72545400	-3.17152000	2.76830900
H	-3.64929000	-2.05294900	1.73594300
H	-2.47149900	-3.15051800	1.01736200
C	0.39327000	-2.97898500	1.25294800
H	0.54990200	-3.68985500	2.07451000
H	-0.26893300	-3.45367500	0.52335600
H	1.35359800	-2.81001800	0.76271200
Co	-0.88457700	-0.16775800	0.49778500
C	5.86464700	-1.76476000	0.93588200

H	6.85965300	-1.49405500	1.30287400
H	5.13367900	-1.54129600	1.71789600
H	5.83838600	-2.84257800	0.75705800
C	6.60387100	-1.29631500	-1.43886600
H	6.63817700	-2.36877100	-1.65686300
H	6.38036800	-0.76273600	-2.36610500
H	7.59610200	-0.98998100	-1.09187400
C	5.53474000	0.53398100	-0.06130900
H	4.75099000	0.79108500	0.65897500
H	6.49746600	0.83840800	0.36188900
H	5.36404300	1.10827700	-0.97514000
C	-3.40737100	-3.25468400	-1.98423000
H	-3.81322400	-3.68524900	-1.06157700
H	-3.81106200	-3.82831400	-2.82675200
H	-2.32098900	-3.37165600	-1.96759100
C	-5.31811100	-1.61277600	-2.10725400
H	-5.75755200	-2.16046400	-2.94908500
H	-5.74629600	-1.99817600	-1.17785600
H	-5.60494900	-0.56078100	-2.18568300
C	-3.20253300	-1.19194400	-3.41687100
H	-3.45132000	-0.12970700	-3.52327600
H	-2.11398900	-1.28945200	-3.42253300
H	-3.60859200	-1.72145700	-4.28677500

³⁵, -2907.78266226

C	0.41477700	-0.29532800	1.97116200
C	-0.32499500	-1.54310100	1.88640300
C	-1.66791600	-1.25336000	2.18218200
C	-1.77902200	0.16801900	2.46826300
C	-0.49690400	0.74470700	2.37837400
C	2.57725600	3.37938600	-1.14196200
C	1.56176200	4.30405300	-1.01758300
C	0.22645200	3.85807500	-0.82462400
C	-0.01345400	2.45694500	-0.77482400
C	1.02704100	1.49939300	-0.98071700
C	2.31806600	1.98515500	-1.12814900
H	-0.75760800	5.78563300	-0.67260600
H	3.60071800	3.72031800	-1.27191900
H	1.76886400	5.37011200	-1.04589300
C	-0.89288300	4.70781500	-0.63199800
H	3.13590500	1.28845400	-1.27708600
C	-2.26491500	2.75580200	-0.28920700
C	-2.13475500	4.16083000	-0.38417700
H	-3.20682200	2.27127300	-0.05208100

H	-3.00642400	4.78946400	-0.23554700
N	-1.23727200	1.94349200	-0.46360900
C	0.61139300	0.08090500	-1.00912600
H	1.39707400	-0.64224800	-0.79996200
H	0.04905400	-0.19002000	-1.90695800
H	3.01685800	-1.12877000	-2.35247900
C	4.05198900	-1.65086400	-0.86812400
C	5.39577700	-1.39770000	-0.18764100
O	3.90750300	-0.93526900	-2.01180400
O	3.17889200	-2.39029300	-0.46209100
C	-2.96195900	-1.21424700	-1.01999200
C	-4.06126500	-1.95941400	-1.79276900
O	-1.77153400	-1.66236300	-1.07588100
O	-3.22947700	-0.17721100	-0.34213600
C	1.90577100	-0.15973300	1.93003200
H	2.21309200	0.77028000	1.44121500
H	2.31410900	-0.14387300	2.94956100
H	2.36727100	-0.99282000	1.39849900
C	-0.11593200	2.17495700	2.62745600
H	0.20595000	2.33443400	3.66477900
H	0.70954400	2.48444300	1.97956700
H	-0.95128500	2.85424800	2.43465400
C	-3.07218100	0.86066000	2.77351600
H	-3.47564200	0.54677000	3.74446400
H	-2.95121000	1.94685900	2.80107200
H	-3.81675000	0.61808400	2.00814800
C	-2.82277200	-2.20811400	2.19101700
H	-3.13144100	-2.45565200	3.21489800
H	-3.68517900	-1.77050600	1.67972800
H	-2.56972000	-3.14125300	1.68285900
C	0.25378400	-2.87955800	1.52352300
H	0.55487300	-3.44500100	2.41528100
H	-0.47679000	-3.47948600	0.97440600
H	1.13279400	-2.77540000	0.88353000
Co	-1.02995500	-0.10453500	0.23008300
C	5.45275400	-2.21128200	1.11314200
H	6.42261600	-2.06377700	1.59855300
H	4.66717500	-1.90122400	1.80737800
H	5.31823000	-3.27782000	0.91619400
C	6.52448000	-1.83368300	-1.14784400
H	6.45605400	-2.90208400	-1.37746000
H	6.48200200	-1.27556600	-2.08649300
H	7.49626800	-1.65060000	-0.67794100
C	5.52112500	0.11152200	0.11749000

H	4.69778400	0.45824500	0.75025400
H	6.45968400	0.29924100	0.64893700
H	5.52249000	0.70248800	-0.80189800
C	-4.06666100	-3.42921900	-1.32581700
H	-4.32313500	-3.50238700	-0.26339300
H	-4.80694100	-4.00481400	-1.89303400
H	-3.08194500	-3.88023500	-1.47002900
C	-5.43175100	-1.31485600	-1.54552600
H	-6.20784900	-1.85188500	-2.10271700
H	-5.68972900	-1.33764300	-0.48279000
H	-5.43571000	-0.26841400	-1.86219400
C	-3.70003700	-1.89516300	-3.29169800
H	-3.68436100	-0.85854100	-3.64689100
H	-2.71352500	-2.33204700	-3.46620700
H	-4.43984600	-2.44478900	-3.88477100

55, -2907.77131543

C	0.27722200	-0.49910800	1.85790700
C	-0.33707000	-1.74303300	1.49527500
C	-1.69646800	-1.69990700	1.94074000
C	-1.92053300	-0.43939700	2.57797300
C	-0.70475000	0.30231300	2.52792100
C	3.03667800	3.00701500	-1.09525600
C	2.13156800	3.95171800	-0.63488800
C	0.77107200	3.59039600	-0.41981100
C	0.33990900	2.25395000	-0.67726400
C	1.26697000	1.29564600	-1.27182100
C	2.62016000	1.71258200	-1.41034500
H	0.11646100	5.53692300	0.26408300
H	4.07890700	3.27904300	-1.23403200
H	2.44572300	4.96841200	-0.41823000
C	-0.18594000	4.51091300	0.07175800
H	3.33966200	1.00583600	-1.80881000
C	-1.80195000	2.74486800	0.09736800
C	-1.48002600	4.09677500	0.30326000
H	-2.78801100	2.34972400	0.31688600
H	-2.23886900	4.77964400	0.66947100
N	-0.91911100	1.85067600	-0.35157900
C	0.85869300	0.04035700	-1.71516500
H	1.59395900	-0.68510700	-2.04219300
H	-0.18174600	-0.25602700	-1.77871200
H	4.16281600	-1.07791400	-2.94144300
C	4.41215400	-1.53905200	-1.13410100
C	5.40143100	-1.40038000	0.01995800

O	4.84529400	-0.92229400	-2.26691300
O	3.33542200	-2.09800400	-1.09390900
C	-3.35087600	-0.65311500	-1.09277500
C	-4.52562500	-1.09927200	-1.96959400
O	-2.21169000	-1.20664700	-1.26648500
O	-3.49380800	0.23117500	-0.19689500
C	1.72633600	-0.13925100	1.70142500
H	1.86050900	0.92367900	1.47420600
H	2.29115300	-0.34380600	2.62189200
H	2.19187900	-0.70598500	0.89265300
C	-0.46061800	1.67912500	3.07607300
H	0.01427000	1.64828400	4.06582000
H	0.19932200	2.25885300	2.42126800
H	-1.39124500	2.24476600	3.17916300
C	-3.24125600	0.01120600	3.13458800
H	-3.54704400	-0.59995300	3.99291700
H	-3.20309900	1.05095100	3.47153900
H	-4.02737900	-0.06141300	2.37491500
C	-2.72899500	-2.77475200	1.75793100
H	-2.81844900	-3.41520500	2.64566600
H	-3.71641100	-2.34033700	1.56828500
H	-2.48481700	-3.41717800	0.90781300
C	0.32397400	-2.90763800	0.81117700
H	0.53781500	-3.72026300	1.51816000
H	-0.32081700	-3.31805400	0.02684800
H	1.26874200	-2.62435800	0.34052800
Co	-1.38726600	-0.13991400	0.33447200
C	4.94148000	-2.29148700	1.18310700
H	5.64603700	-2.19896200	2.01555600
H	3.94863100	-2.00772500	1.53568500
H	4.90011500	-3.34149500	0.88021200
C	6.81059300	-1.81824400	-0.45049900
H	6.82464500	-2.86350200	-0.77645400
H	7.15614900	-1.19555900	-1.27876200
H	7.51628800	-1.71527800	0.37998500
C	5.41163700	0.08655500	0.44848400
H	4.41601300	0.42027100	0.75416600
H	6.09089400	0.21426700	1.29741600
H	5.75556200	0.72808700	-0.36763300
C	-4.74814400	-2.60685500	-1.72323900
H	-5.01965100	-2.79801500	-0.67947500
H	-5.56034600	-2.97695500	-2.35886700
H	-3.83940600	-3.17078900	-1.94721700
C	-5.79354900	-0.30836800	-1.62070100

H	-6.62815300	-0.63895300	-2.24906900
H	-6.06796200	-0.45200600	-0.57219900
H	-5.64349200	0.76344400	-1.77798300
C	-4.13318300	-0.86840900	-3.44357300
H	-3.96615000	0.19607100	-3.64319400
H	-3.21571400	-1.41018400	-3.68606500
H	-4.93394900	-1.21501100	-4.10634800

MECP1, -2907.7814768

C	0.43920000	-0.33720000	2.02990000
C	-0.29490000	-1.57720000	1.89150000
C	-1.65510000	-1.29340000	2.15810000
C	-1.77140000	0.11120000	2.46860000
C	-0.47630000	0.68540000	2.43110000
C	2.49780000	3.23470000	-1.33300000
C	1.47580000	4.15000000	-1.20690000
C	0.16170000	3.69850000	-0.91550000
C	-0.04960000	2.30160000	-0.76100000
C	0.99340000	1.35010000	-0.95680000
C	2.26200000	1.84170000	-1.21790000
H	-0.84770000	5.61690000	-0.85490000
H	3.50500000	3.58060000	-1.54690000
H	1.66110000	5.21470000	-1.31570000
C	-0.96260000	4.54290000	-0.73530000
H	3.08000000	1.14810000	-1.37720000
C	-2.29240000	2.59760000	-0.22240000
C	-2.18460000	3.99380000	-0.41230000
H	-3.22340000	2.11340000	0.05140000
H	-3.06290000	4.61640000	-0.28040000
N	-1.25590000	1.78920000	-0.37470000
C	0.58970000	-0.07730000	-0.87740000
H	1.41580000	-0.74690000	-0.64340000
H	0.07710000	-0.40930000	-1.78470000
C	-3.22050000	-0.93120000	-0.88420000
C	-4.14080000	-1.72670000	-1.82870000
O	-1.96810000	-1.23290000	-0.95030000
O	-3.67900000	-0.06440000	-0.11530000
C	1.92870000	-0.19230000	1.99770000
H	2.23980000	0.70890000	1.46020000
H	2.31830000	-0.11320000	3.02070000
H	2.40470000	-1.05180000	1.52540000
C	-0.10840000	2.11270000	2.70230000
H	0.13620000	2.26880000	3.76060000
H	0.76490000	2.41540000	2.11710000

H	-0.92240000	2.79800000	2.45030000
C	-3.04410000	0.80920000	2.83290000
H	-3.31930000	0.59920000	3.87410000
H	-2.94570000	1.89410000	2.73430000
H	-3.86030000	0.48660000	2.18410000
C	-2.79020000	-2.26830000	2.14250000
H	-2.97370000	-2.67480000	3.14470000
H	-3.70760000	-1.78890000	1.79710000
H	-2.58210000	-3.10800000	1.47550000
C	0.29610000	-2.90950000	1.54450000
H	0.63920000	-3.43720000	2.44360000
H	-0.44190000	-3.54700000	1.05000000
H	1.15260000	-2.80930000	0.87440000
Co	-0.96320000	-0.15260000	0.39040000
C	-4.02210000	-3.22120000	-1.47280000
H	-4.36650000	-3.40900000	-0.45020000
H	-4.63570000	-3.82560000	-2.15000000
H	-2.98380000	-3.55290000	-1.55020000
C	-5.59160000	-1.25920000	-1.67170000
H	-6.24870000	-1.83270000	-2.33460000
H	-5.93420000	-1.39000000	-0.64200000
H	-5.69040000	-0.19780000	-1.91560000
C	-3.65990000	-1.50280000	-3.27450000
H	-3.71770000	-0.44310000	-3.54650000
H	-2.62310000	-1.82670000	-3.39000000
H	-4.28530000	-2.06600000	-3.97590000
H	2.99340000	-1.38150000	-2.21540000
C	4.11880000	-1.71780000	-0.74780000
C	5.47680000	-1.34940000	-0.15950000
O	3.88770000	-1.11570000	-1.93990000
O	3.30300000	-2.46020000	-0.24040000
C	5.60510000	-1.98670000	1.22960000
H	6.59100000	-1.75990000	1.64730000
H	4.84450000	-1.60190000	1.91410000
H	5.48780000	-3.07150000	1.17750000
C	6.57560000	-1.88790000	-1.10030000
H	6.51860000	-2.97730000	-1.18990000
H	6.49000000	-1.45400000	-2.09910000
H	7.55990000	-1.63260000	-0.69500000
C	5.58400000	0.18560000	-0.05560000
H	4.77500000	0.60080000	0.55250000
H	6.53430000	0.45200000	0.41800000
H	5.54820000	0.65510000	-1.04100000

ossTS7, -2802.34578334, i307.42

C	-4.01288100	1.94108700	2.08066800
C	-3.41155900	3.00342900	1.43890000
C	-2.20721400	2.80360100	0.71158300
C	-1.66569100	1.49100100	0.68000900
C	-2.24053700	0.41865000	1.40300900
C	-3.43021300	0.64667700	2.07096200
H	-1.88785300	4.82673000	-0.00668000
H	-4.94051100	2.09549300	2.62240000
H	-3.85499400	3.99381100	1.46834600
C	-1.51603200	3.80613900	-0.01356600
H	-3.90282000	-0.15862100	2.62534300
C	0.05624500	2.13297700	-0.75268100
C	-0.37978400	3.47394600	-0.72247300
H	0.92450200	1.83988800	-1.32860500
H	0.18029900	4.21840200	-1.27639100
N	-0.57553200	1.17255400	-0.08866400
C	-1.43089700	-0.82521300	1.41398600
C	-1.67512000	-0.79187500	-1.97413300
C	-1.99349200	-1.90433500	-1.13629200
C	-0.80785000	-2.71280300	-1.02391400
C	-0.32543300	-0.95687300	-2.46214900
C	0.19466300	-2.15258500	-1.89520800
H	-1.99152000	-1.74407300	1.56957200
H	-0.61417600	-0.78378600	2.13342800
C	-0.64413900	-3.97258300	-0.23540800
H	-0.72712900	-4.84395500	-0.89597600
H	0.33077700	-3.99776700	0.25426500
H	-1.40490700	-4.06358300	0.54121000
C	-3.35257200	-2.20950100	-0.59132000
H	-4.00398300	-2.53867100	-1.40876300
H	-3.32404700	-3.00906500	0.15004100
H	-3.81403400	-1.32954900	-0.13488300
C	-2.62332900	0.30262700	-2.35244900
H	-3.15802300	0.03454000	-3.27097700
H	-3.36597400	0.47097500	-1.57012300
H	-2.10241600	1.24493500	-2.53436200
C	0.36849000	-0.05663400	-3.43753700
H	0.28219000	-0.46019900	-4.45295700
H	-0.07327400	0.94161800	-3.44568100
H	1.43166700	0.04488100	-3.20899800
C	1.54947300	-2.74671400	-2.10347700
H	1.45677400	-3.72484500	-2.58778100
H	2.17679900	-2.11692100	-2.73648100

H	2.05302000	-2.89611800	-1.14423000
Co	-0.34724400	-0.78597100	-0.29921000
C	2.20537600	-0.34856700	1.10145100
C	1.92525400	-2.02365100	2.88892900
O	2.31032900	-2.25083000	3.98815100
O	2.65909500	-0.66289000	2.26044300
O	1.15263200	-2.44825500	2.01053700
N	1.24990100	-0.96828500	0.46390100
C	2.83331800	0.79783600	0.38475400
C	3.01368800	2.00751700	1.06689400
C	3.20168900	0.67569000	-0.96226700
C	3.53259700	3.10649200	0.38297300
H	2.74878000	2.07672400	2.11660400
C	3.73550900	1.77559900	-1.63404900
H	3.08886600	-0.28078600	-1.45990900
C	3.88745900	2.99426600	-0.96534200
H	3.67206200	4.04757100	0.90547000
H	4.04312300	1.68067600	-2.67089300
H	4.30154700	3.85056000	-1.48865400

¹TS7, -2802.33465934, i348.75

C	-4.01646600	1.93689800	2.07104100
C	-3.42579800	2.99791400	1.41728700
C	-2.21647500	2.80229400	0.69749700
C	-1.66032900	1.49531300	0.68539800
C	-2.22497600	0.42524900	1.41896900
C	-3.41809400	0.64943700	2.08134400
H	-1.91677300	4.81901400	-0.04696400
H	-4.94803700	2.08743700	2.60718500
H	-3.88090600	3.98331900	1.43204100
C	-1.53339700	3.80270100	-0.03807900
H	-3.88392700	-0.15378400	2.64449700
C	0.06055200	2.13709300	-0.74793000
C	-0.39042200	3.47358800	-0.73746600
H	0.93238900	1.84582000	-1.31900400
H	0.16318800	4.21673900	-1.29963000
N	-0.56271200	1.17823200	-0.07421900
C	-1.39657800	-0.80947800	1.44125600
C	-1.66046000	-0.76996600	-1.95356300
C	-1.97277800	-1.88736800	-1.12913400
C	-0.78357600	-2.69513100	-1.02304900
C	-0.30520400	-0.92498500	-2.43981100
C	0.21555400	-2.12664200	-1.88887400
H	-1.94977500	-1.73342000	1.59838100

H	-0.60593400	-0.74475400	2.18824700
C	-0.63473300	-3.97144200	-0.25749600
H	-0.86604500	-4.82781100	-0.90250400
H	0.38226300	-4.08418300	0.11962500
H	-1.30743200	-4.00450900	0.60116400
C	-3.32566600	-2.20246400	-0.57303800
H	-3.98036200	-2.54307500	-1.38305200
H	-3.28321500	-2.99766200	0.17251500
H	-3.79177800	-1.32494900	-0.11708400
C	-2.61148600	0.32362900	-2.32978000
H	-3.12375000	0.07131400	-3.26527300
H	-3.37208400	0.46878600	-1.56017900
H	-2.09651600	1.27498700	-2.47981600
C	0.38279900	-0.01934100	-3.41426900
H	0.30899700	-0.42914400	-4.42830700
H	-0.07334300	0.97223900	-3.43077300
H	1.44317200	0.09876500	-3.17984500
C	1.57254200	-2.71419800	-2.10718900
H	1.48237800	-3.70125700	-2.57284300
H	2.18445000	-2.09043800	-2.76116200
H	2.09321300	-2.84352500	-1.15386700
Co	-0.34101700	-0.77673200	-0.27780700
C	2.19137200	-0.35536900	1.13442800
C	1.87627400	-2.10919400	2.87999800
O	2.25110200	-2.35316500	3.97328000
O	2.64225000	-0.66142800	2.28491000
O	1.14462900	-2.47186500	1.95090700
N	1.22880400	-0.96757600	0.48827600
C	2.80701200	0.78090900	0.38592200
C	2.95457000	2.01104100	1.03914100
C	3.20345500	0.62539000	-0.94919500
C	3.47809600	3.09597300	0.33751200
H	2.66449500	2.10588400	2.08008900
C	3.73902900	1.71396800	-1.63858500
H	3.11028000	-0.34409700	-1.42435700
C	3.86380200	2.95116100	-0.99961300
H	3.59685400	4.05200500	0.83742700
H	4.06802300	1.59531900	-2.66629500
H	4.27944500	3.79792500	-1.53694100

³TS7, -2802.30950473, i645.02

C	1.58719900	4.10127500	-2.09400700
C	0.73259800	4.53623200	-1.10254300
C	0.10513400	3.59290900	-0.24498100

C	0.39181400	2.21643000	-0.45235000
C	1.20790300	1.76589000	-1.52080700
C	1.82633000	2.71906800	-2.31029200
H	-1.02344400	4.95480800	1.01261900
H	2.07688400	4.82546400	-2.73721500
H	0.54338200	5.59523900	-0.95677900
C	-0.76753100	3.91593500	0.82475900
H	2.47289700	2.40892600	-3.12578800
C	-0.89337900	1.57480500	1.37768800
C	-1.28077800	2.90972200	1.61826700
H	-1.24623100	0.76287100	2.00336600
H	-1.95781800	3.12639100	2.43674800
N	-0.07513700	1.24395900	0.38908500
C	1.25661300	0.29217700	-1.70524700
C	2.28478500	-0.03274200	1.78810000
C	3.00324500	-0.34931700	0.59224200
C	2.67364100	-1.70995900	0.22543100
C	1.50579100	-1.17763500	2.15547000
C	1.77912700	-2.22786500	1.22571700
H	2.14873200	-0.07694100	-2.20897000
H	0.36622600	-0.07506000	-2.22634100
C	3.26612100	-2.49525500	-0.90217500
H	4.09083600	-3.11685700	-0.53355600
H	2.51966700	-3.14810400	-1.35682600
H	3.66685500	-1.84509900	-1.68184700
C	4.01677700	0.53554400	-0.06084500
H	4.93447100	0.55634400	0.53855100
H	4.28227500	0.18244400	-1.05828200
H	3.65644800	1.56412000	-0.15030700
C	2.35216300	1.27726800	2.50592800
H	3.22606500	1.30332700	3.16802400
H	2.44726400	2.11039800	1.80443600
H	1.46742000	1.45137700	3.12122000
C	0.58208100	-1.29618100	3.32805300
H	1.06494000	-1.83881100	4.14899700
H	0.28381600	-0.31845000	3.71302100
H	-0.31944900	-1.85256300	3.05556700
C	1.22966200	-3.61528000	1.30292400
H	1.72050800	-4.16763800	2.11327500
H	0.15630600	-3.60045200	1.51074600
H	1.38109100	-4.15977200	0.37171200
Co	0.87323200	-0.55983600	0.09263200
C	-1.95231600	-1.38803300	-0.70488100
C	-0.73053500	-2.45972500	-2.32607300

O	-0.55956500	-2.82386500	-3.45260300
O	-1.96383700	-1.78925000	-1.97619700
O	0.03153200	-2.55374500	-1.27614600
N	-0.89332800	-1.51065900	0.02716800
C	-3.18547600	-0.78785300	-0.17649200
C	-4.09184300	-0.17972600	-1.06008300
C	-3.43754500	-0.79652900	1.20674800
C	-5.23610300	0.43208000	-0.55278200
H	-3.89557600	-0.19263800	-2.12644800
C	-4.58658900	-0.18819500	1.70110800
H	-2.74770400	-1.30472500	1.87282900
C	-5.48281900	0.43131800	0.82296700
H	-5.93951000	0.90251500	-1.23210200
H	-4.79475200	-0.20959100	2.76615300
H	-6.38105900	0.90168600	1.21084500

⁵TS7, -2802.27778876, *i*789.78

C	2.17699500	3.68356700	-2.29585200
C	1.47618400	4.33535200	-1.30331000
C	0.67875100	3.58837600	-0.39536900
C	0.62090200	2.17335400	-0.54640400
C	1.26953600	1.51207500	-1.63476600
C	2.07396300	2.28098100	-2.46477600
H	-0.03354600	5.23482000	0.82208700
H	2.80039800	4.25175300	-2.97890000
H	1.53608900	5.41384800	-1.19436100
C	-0.04167400	4.15725800	0.68390800
H	2.59842700	1.80346200	-3.28715300
C	-0.67553400	1.94433000	1.37393300
C	-0.73776500	3.34095200	1.55265800
H	-1.16293500	1.26982600	2.06943800
H	-1.30310500	3.75009100	2.38239800
N	-0.00832500	1.38031500	0.37541400
C	1.01264200	0.06755700	-1.80257000
C	2.52212800	-0.05435100	1.40311000
C	3.04332300	-0.81883100	0.31295300
C	2.50646100	-2.14791300	0.41168400
C	1.61991400	-0.90008900	2.15102000
C	1.60681000	-2.18221300	1.53569800
H	1.72704400	-0.46323600	-2.42975000
H	-0.00960700	-0.12407200	-2.15650400
C	2.77236600	-3.29929600	-0.49858900
H	3.10102400	-4.17260700	0.07575300
H	1.85661700	-3.58968200	-1.02743300

H	3.54001200	-3.06957300	-1.23868600
C	4.06871900	-0.34175200	-0.66447000
H	5.06743100	-0.35683900	-0.21164000
H	4.09965800	-0.96928800	-1.55715100
H	3.86838000	0.68565900	-0.98063400
C	2.90531000	1.35097500	1.73712800
H	3.78655200	1.35836700	2.39092800
H	3.15865200	1.91988700	0.83956600
H	2.10508100	1.87975200	2.25950400
C	0.88045800	-0.52150900	3.39668600
H	1.40861600	-0.88664200	4.28564200
H	0.78239100	0.56141400	3.49615900
H	-0.12091700	-0.96290000	3.41290900
C	0.84584000	-3.38775200	1.99210800
H	1.46574800	-4.00601600	2.65282600
H	-0.05244700	-3.10632900	2.54614600
H	0.53924000	-4.00133200	1.14280700
Co	0.65549200	-0.65566800	0.09164200
C	-2.23449200	-1.29562000	-0.54204000
C	-1.14746400	-2.70139100	-1.97938600
O	-1.00284000	-3.25561100	-3.02662600
O	-2.29688800	-1.87135300	-1.74767400
O	-0.39098500	-2.71371300	-0.90668600
N	-1.17174100	-1.45505500	0.18458600
C	-3.37643800	-0.49161100	-0.10651100
C	-4.28021900	0.00669300	-1.06016100
C	-3.54671600	-0.19806100	1.25912900
C	-5.34073900	0.80731700	-0.64326300
H	-4.14646600	-0.23512300	-2.10866100
C	-4.61272800	0.59741600	1.66305700
H	-2.86276200	-0.62291700	1.98684100
C	-5.50647400	1.10446500	0.71249000
H	-6.04207100	1.19392200	-1.37539300
H	-4.75978700	0.81145800	2.71684500
H	-6.34020300	1.72224800	1.03142200

oss8, -2613.69000163

C	3.33510500	1.27650500	2.00209700
C	3.24529800	2.29795800	1.08049200
C	2.06032700	2.45805300	0.31610000
C	0.98877100	1.55418100	0.55671400
C	1.06358100	0.54294800	1.53803800
C	2.24901200	0.39480000	2.23255500
H	2.67574300	4.12769800	-0.92332300

H	4.25235000	1.13825100	2.56510600
H	4.08130800	2.96877100	0.90932200
C	1.88483400	3.41310000	-0.71403300
H	2.35064700	-0.40060800	2.96431000
C	-0.26956800	2.44929900	-1.19285500
C	0.72312100	3.41183600	-1.46075700
H	-1.16817800	2.39004200	-1.79437200
H	0.56712100	4.12151000	-2.26510000
N	-0.14683000	1.55861700	-0.21397500
C	-0.17510900	-0.26693200	1.72985500
C	-3.20249000	0.88143200	-0.12104300
C	-3.06875800	0.16274300	1.11062400
C	-2.81404400	-1.20967500	0.78588500
C	-3.08327200	-0.04500500	-1.21326000
C	-2.85453800	-1.33457900	-0.66118700
H	-0.80908300	0.17047300	2.50222400
H	0.00430200	-1.32237800	1.93585400
C	-2.63527000	-2.36109700	1.72273800
H	-3.53789400	-2.98279500	1.72757600
H	-1.79369900	-2.98252400	1.40274200
H	-2.45095300	-2.02629600	2.74474500
C	-3.26663100	0.75898300	2.46940300
H	-2.94355100	0.08369300	3.26329400
H	-2.72605100	1.70414900	2.57882700
H	-4.32984100	0.96993600	2.63250500
C	-3.50803600	2.34420100	-0.20237100
H	-4.53512600	2.52224000	0.13723200
H	-2.84663400	2.92716500	0.44449600
H	-3.42963800	2.73136400	-1.21924500
C	-3.16184000	0.26254300	-2.67825600
H	-2.32854500	-0.19562400	-3.21929300
H	-4.08909400	-0.13467400	-3.10560700
H	-3.14718800	1.33682500	-2.87345900
C	-2.68940200	-2.61182600	-1.41718200
H	-3.65466400	-3.12914000	-1.48010100
H	-2.33439900	-2.42824100	-2.43256100
H	-1.97362100	-3.26978800	-0.92128500
Co	-1.21693100	-0.08800800	0.00309400
C	0.84893700	-2.06032200	-0.40040600
O	0.45500500	-3.07213900	0.20217100
N	-0.10603000	-1.20614000	-0.88163600
C	2.27723900	-1.73978900	-0.63960900
C	3.25331200	-2.54274200	-0.03345100
C	2.65653200	-0.62294300	-1.39994200

C	4.60055900	-2.22115800	-0.17703000
H	2.93525700	-3.40384000	0.54509600
C	4.00494000	-0.30423900	-1.53924200
H	1.89584700	-0.01440200	-1.88003800
C	4.97657800	-1.10142600	-0.92640000
H	5.35872700	-2.84120100	0.29111200
H	4.30083200	0.55815300	-2.12866000
H	6.02802200	-0.85384900	-1.03788700

¹⁸, -2613.6902545

C	-1.02173000	3.87616600	2.04189800
C	-1.17283400	4.25519700	0.72406800
C	-0.96131800	3.30950500	-0.31516300
C	-0.60478200	1.98964600	0.06296400
C	-0.37038000	1.62115600	1.40830700
C	-0.61118000	2.56270400	2.39194700
H	-1.35903400	4.56509600	-2.04118800
H	-1.19696200	4.59922200	2.83206800
H	-1.46369000	5.26914700	0.46773600
C	-1.09774800	3.56641900	-1.70316200
H	-0.44956500	2.31163200	3.43609200
C	-0.59785800	1.24600600	-2.14860700
C	-0.89014800	2.54768400	-2.61055700
H	-0.43341400	0.41855300	-2.82578600
H	-0.96455200	2.71941900	-3.67822700
N	-0.49269400	0.97770000	-0.85345100
C	0.20300800	0.25844500	1.57889400
C	-2.67277600	-0.78341900	0.06142600
C	-2.18626500	-1.26864800	1.29926400
C	-1.37227100	-2.44172600	1.02781900
C	-2.19725600	-1.66358700	-0.98249200
C	-1.45006200	-2.72193100	-0.36648700
H	-0.00310600	-0.21053300	2.53937300
H	1.27854800	0.25861000	1.39788200
C	-0.66997200	-3.27963100	2.04915700
H	-1.36654700	-3.99558100	2.50147000
H	0.14688200	-3.84437500	1.59597700
H	-0.25593500	-2.66807100	2.85445400
C	-2.55996000	-0.74417200	2.64941800
H	-3.59133500	-1.03501700	2.87899800
H	-1.92200400	-1.15103300	3.43570700
H	-2.50771500	0.34702800	2.68970700
C	-3.55638700	0.41059000	-0.12894800
H	-4.60795500	0.10320600	-0.15639600

H	-3.43697200	1.12686100	0.68629600
H	-3.33803300	0.92704900	-1.06642200
C	-2.52204400	-1.55446500	-2.43892400
H	-3.37715100	-2.19745300	-2.67954000
H	-2.79378300	-0.53422400	-2.71524100
H	-1.68150500	-1.87004700	-3.06130800
C	-0.78753900	-3.87228900	-1.05061000
H	-0.95549000	-3.85319600	-2.12819600
H	0.29243200	-3.84089400	-0.87630900
H	-1.17377700	-4.81831600	-0.65774800
Co	-0.50614200	-0.79208900	-0.00951200
C	1.97929500	-0.71273000	-1.23460800
O	1.80165200	-0.41213500	-2.42447100
N	0.96715400	-1.39678100	-0.61889400
C	3.21855100	-0.43285500	-0.47246800
C	4.13978000	0.47471400	-1.01441200
C	3.46878400	-1.03771500	0.77032700
C	5.29915500	0.78501100	-0.30851300
H	3.93028100	0.91776900	-1.98250300
C	4.63212800	-0.72497000	1.47066300
H	2.76562700	-1.76465900	1.16746800
C	5.54430900	0.18792900	0.93280000
H	6.01466100	1.48762400	-0.72398300
H	4.83481300	-1.19806200	2.42639500
H	6.45167400	0.42908800	1.47821700

³⁸, -2613.68833716

C	-4.04745600	-2.35364300	-1.70721600
C	-4.04879600	-2.78470300	-0.39696400
C	-3.04422400	-2.33021400	0.49957600
C	-2.07245400	-1.42936300	-0.00791100
C	-2.01669100	-1.05728200	-1.37303000
C	-3.02986000	-1.49724600	-2.20519100
H	-3.65613600	-3.38051200	2.29780600
H	-4.82471500	-2.69303100	-2.38445200
H	-4.81683600	-3.46120300	-0.03532200
C	-2.94260100	-2.68295800	1.86885600
H	-3.02544600	-1.22540100	-3.25654800
C	-1.05242400	-1.19947000	2.07514500
C	-1.93621900	-2.14116200	2.64335600
H	-0.27240100	-0.72282100	2.65791100
H	-1.82275300	-2.40780100	3.68789200
N	-1.14527200	-0.83846700	0.80392700
C	-0.79127300	-0.31166700	-1.76167800

C	-1.82690800	2.02949300	0.49966200
C	-1.46436200	2.29317000	-0.85212300
C	-0.05701100	2.60602800	-0.87190000
C	-0.67605400	2.26761400	1.33662000
C	0.40326300	2.65317100	0.49455900
H	-0.89578200	0.32320400	-2.63902100
H	0.05066800	-0.99565600	-1.87356600
C	0.74971700	2.95826900	-2.08289300
H	0.70240500	4.03645000	-2.27595900
H	1.79880400	2.68496200	-1.95358300
H	0.37964000	2.44371700	-2.97207700
C	-2.41431000	2.33817200	-2.00709900
H	-3.05400600	3.22349500	-1.91846100
H	-1.89212400	2.40461900	-2.96274700
H	-3.06709200	1.46095400	-2.03013500
C	-3.19052400	1.63449200	0.97432300
H	-3.76358400	2.52326200	1.26273900
H	-3.74796100	1.11461700	0.19263900
H	-3.13738000	0.97785800	1.84585100
C	-0.64372400	2.17772700	2.83089900
H	-0.87823600	3.15166400	3.27645500
H	-1.37958200	1.46376100	3.20738700
H	0.34299900	1.87928700	3.19436300
C	1.77776000	3.03026800	0.94713400
H	1.79046400	4.08117200	1.25882500
H	2.09888400	2.42596100	1.79871200
H	2.50984000	2.91293400	0.14685200
Co	-0.22916200	0.66479400	-0.06292300
C	2.07379900	-1.18252800	-0.22710500
O	1.41899400	-2.19718400	-0.51087300
N	1.36794600	-0.04208500	0.05054700
C	3.55307800	-1.14137100	-0.16232000
C	4.26956000	-2.28864100	-0.53424600
C	4.23686800	0.01018300	0.25516700
C	5.66086500	-2.27896000	-0.49199300
H	3.72101000	-3.16914100	-0.85177800
C	5.62877600	0.01508400	0.29714600
H	3.67659100	0.89020000	0.55400300
C	6.34053700	-1.12873500	-0.07750400
H	6.21759500	-3.16477800	-0.78094000
H	6.15999700	0.90399400	0.62291300
H	7.42585800	-1.12423400	-0.04480100

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C	-4.34397300	-1.77640600	-1.85462200
C	-4.51250900	-2.22923200	-0.56240200
C	-3.48529900	-2.03368200	0.39978900
C	-2.28959700	-1.38440100	-0.01150700
C	-2.07731700	-1.00989200	-1.37452400
C	-3.13476400	-1.16339800	-2.26246200
H	-4.47894400	-2.91250700	2.11677300
H	-5.13829800	-1.90969600	-2.58187100
H	-5.43423700	-2.71790700	-0.26170400
C	-3.58770200	-2.40003000	1.76611400
H	-3.01024300	-0.86523900	-3.29915300
C	-1.44696400	-1.37330500	2.15542600
C	-2.56286700	-2.09237400	2.63663700
H	-0.64738000	-1.06335000	2.82120300
H	-2.61054600	-2.36583000	3.68465300
N	-1.32872500	-1.01730900	0.88597700
C	-0.73147600	-0.55676800	-1.77347600
C	-1.72161200	2.05308900	0.36782200
C	-1.12901400	2.28218800	-0.93779800
C	0.25639500	2.65315600	-0.74510100
C	-0.70467700	2.21643100	1.33004000
C	0.52280700	2.58915400	0.63999200
H	-0.68716600	-0.00690700	-2.71137100
H	0.02485400	-1.33965500	-1.69707600
C	1.21839200	3.01248900	-1.83797600
H	1.12605700	4.07109900	-2.10788000
H	2.25305200	2.83495200	-1.53690900
H	1.03311600	2.42685400	-2.74258100
C	-1.89844000	2.39843400	-2.21429100
H	-2.40826000	3.36898400	-2.24880500
H	-1.24796200	2.33886000	-3.08928600
H	-2.66615600	1.62449100	-2.29613400
C	-3.16685100	1.74794300	0.61983900
H	-3.74153700	2.67466100	0.73300800
H	-3.60823800	1.18542400	-0.20591400
H	-3.30089400	1.16286500	1.53295100
C	-0.83835000	2.07651900	2.81474800
H	-0.97353000	3.05900300	3.28334800
H	-1.69978300	1.46237900	3.08619100
H	0.05612100	1.62908800	3.25788800
C	1.81631500	2.89274300	1.32837700
H	1.75463000	3.86025600	1.84082100
H	2.05358800	2.13906800	2.08471100

H	2.64774000	2.94446900	0.62341900
Co	-0.13991200	0.51523700	-0.09901900
C	2.21248600	-1.40850600	-0.16515300
O	1.61638000	-2.44132200	-0.50943600
N	1.42641500	-0.33331100	0.16266500
C	3.68362300	-1.26986300	-0.10712000
C	4.47859700	-2.34173900	-0.54082800
C	4.28411300	-0.09181200	0.36470100
C	5.86528300	-2.23171300	-0.50357900
H	3.99315900	-3.24323800	-0.89960800
C	5.67208500	0.01310000	0.40022300
H	3.66231300	0.72851100	0.70919900
C	6.46185800	-1.05579400	-0.03466000
H	6.48374300	-3.05858200	-0.83792400
H	6.14012600	0.92095900	0.76779700
H	7.54418900	-0.97348800	-0.00648100

oss^{TS9}, -2613.68878193, *i*244.46

C	-3.76960900	-2.76796100	-1.84148500
C	-4.04502600	-2.89947200	-0.49784200
C	-3.35776900	-2.09562800	0.44878500
C	-2.41534600	-1.14271300	-0.03406500
C	-2.15676800	-0.99664500	-1.41524900
C	-2.81698000	-1.82554800	-2.30282500
H	-4.22966000	-2.91980600	2.25483700
H	-4.28162900	-3.39619200	-2.56310000
H	-4.76818400	-3.62873700	-0.14621700
C	-3.51770600	-2.20562700	1.85126900
H	-2.61141100	-1.74928300	-3.36635600
C	-1.82721400	-0.51865000	2.13178000
C	-2.75183400	-1.42288900	2.68953600
H	-1.19098200	0.08451000	2.76679100
H	-2.83486400	-1.49683200	3.76779400
N	-1.67335600	-0.36688100	0.82214400
C	-1.19230200	0.06065100	-1.81950300
C	-0.69011200	2.51304600	1.08149800
C	-0.87636800	2.75577000	-0.30868200
C	0.38122000	2.50810400	-0.97586600
C	0.66102500	2.07639500	1.28732700
C	1.33342100	2.11573000	0.01409500
H	-1.67784400	1.00719800	-2.05436900
H	-0.50021100	-0.21763900	-2.61094100
C	0.68379700	2.66752900	-2.43269600
H	1.29799000	3.56160800	-2.58873000

H	1.23680300	1.80050500	-2.80394100
H	-0.22387900	2.77924700	-3.02776600
C	-2.14379600	3.27318200	-0.91764700
H	-2.12656500	3.22666800	-2.00783900
H	-3.01550600	2.71489800	-0.56330500
H	-2.29166900	4.32305000	-0.63960300
C	-1.74431300	2.73731000	2.12120600
H	-1.94813300	3.81099500	2.20221100
H	-2.68397400	2.24559400	1.85564600
H	-1.43699800	2.38864400	3.10805500
C	1.31720600	1.71593700	2.58503500
H	1.96477800	0.84241000	2.46835600
H	1.94128600	2.54597800	2.93637000
H	0.58864000	1.50132000	3.36952100
C	2.79705000	1.91233100	-0.21271900
H	3.30998100	2.87520300	-0.10018300
H	3.23008200	1.21438800	0.50510800
H	3.00027600	1.53986000	-1.21793100
Co	-0.26187300	0.71175300	-0.05276600
C	1.77319900	-0.82807600	-1.19576600
O	1.89471200	-0.49051700	-2.38065200
N	0.58415200	-0.72311000	-0.52378700
C	2.88804400	-1.41666300	-0.39205500
C	4.15380400	-1.49193900	-0.98858200
C	2.71205900	-1.82549500	0.94030900
C	5.23820200	-1.96784300	-0.25492900
H	4.26403200	-1.17282900	-2.01951500
C	3.80184200	-2.29480600	1.67120100
H	1.72432800	-1.78904800	1.39035200
C	5.06469900	-2.36493500	1.07456300
H	6.21829500	-2.03012300	-0.71744000
H	3.66778100	-2.61672100	2.69939800
H	5.91200900	-2.73468900	1.64402700

¹TS9, -2613.6845563, *i*211.26

C	-0.49517500	4.62296600	-0.94637600
C	-1.23768400	4.37258100	0.18742800
C	-1.21287300	3.08362700	0.77894200
C	-0.37223000	2.09200300	0.19636300
C	0.36760600	2.34651000	-0.97855800
C	0.28621800	3.60508300	-1.54570000
H	-2.65691700	3.43203100	2.35748500
H	-0.52476300	5.60485800	-1.40732900
H	-1.86244800	5.14446200	0.62592400

C	-2.00252800	2.70150400	1.89065100
H	0.81599300	3.81494100	-2.47002500
C	-1.09001600	0.48285100	1.72756400
C	-1.95661500	1.40164700	2.34954000
H	-1.03893800	-0.54756800	2.05526300
H	-2.57343100	1.06930600	3.17639500
N	-0.30365800	0.82141200	0.71293100
C	1.13353900	1.22072100	-1.59239800
C	2.20224000	-0.54775000	1.58757900
C	3.01366900	-0.11671900	0.50896900
C	2.93306800	-1.12178500	-0.53877700
C	1.57840600	-1.79232500	1.21164400
C	2.08191400	-2.16164400	-0.08864600
H	2.21597900	1.31546000	-1.55529300
H	0.81823000	1.02024600	-2.61424700
C	3.65760300	-1.11730400	-1.84878900
H	4.57047800	-1.71972200	-1.77448200
H	3.03783600	-1.54733300	-2.63930100
H	3.95355000	-0.11243700	-2.15576700
C	3.86740200	1.11501600	0.50361800
H	4.75802300	0.95935100	1.12291300
H	4.21316800	1.37049600	-0.49987800
H	3.33056200	1.97750600	0.90832200
C	2.03234400	0.18108500	2.88444900
H	2.84935800	-0.07874800	3.56711300
H	2.05264600	1.26375900	2.73893000
H	1.09470200	-0.07445100	3.38070200
C	0.66468100	-2.64012500	2.04526500
H	1.15916000	-3.58317300	2.30379900
H	0.39516500	-2.14889900	2.98195700
H	-0.25499500	-2.88765900	1.50509900
C	1.73684200	-3.39438100	-0.86299300
H	2.63313600	-4.00025400	-1.03206400
H	1.00915100	-4.01007700	-0.33165300
H	1.31851700	-3.12926500	-1.83851100
Co	0.98208900	-0.33391800	-0.17050300
C	-1.33283400	-0.35403200	-1.71027900
O	-1.63374500	0.64171000	-2.35903900
N	-0.04378800	-0.78950700	-1.46635600
C	-2.34716200	-1.24988900	-1.05328600
C	-3.58207500	-0.67211400	-0.72884800
C	-2.08119900	-2.58340300	-0.70432100
C	-4.53873000	-1.42046000	-0.04527700
H	-3.77114800	0.35448500	-1.02444000

C	-3.04486400	-3.32837900	-0.02453500
H	-1.13939000	-3.03797900	-0.99066300
C	-4.27023300	-2.74570500	0.31183600
H	-5.49713100	-0.97436400	0.20229500
H	-2.84841800	-4.36601800	0.22822300
H	-5.02030700	-3.32764000	0.83871700

³TS9, -2613.68072205, *i*278.28

C	-3.25352700	-3.51441600	-1.36737600
C	-3.82200700	-3.25838100	-0.13884800
C	-3.42338800	-2.11576900	0.60482600
C	-2.46248700	-1.23430600	0.03219000
C	-1.91621800	-1.48290700	-1.25163500
C	-2.28882300	-2.63672400	-1.91930500
H	-4.62554600	-2.47030700	2.37360100
H	-3.54074700	-4.40060900	-1.92373200
H	-4.55538900	-3.93583300	0.28744300
C	-3.88726900	-1.82251200	1.90969300
H	-1.85082400	-2.86051600	-2.88722800
C	-2.40599800	0.06833700	1.96264900
C	-3.37820500	-0.73432500	2.58754300
H	-1.96256700	0.90500200	2.48696300
H	-3.69673300	-0.49389000	3.59536000
N	-1.96921100	-0.15615600	0.72643800
C	-0.99053600	-0.47989900	-1.80910400
C	-0.83319100	2.78623800	0.53572500
C	-0.82060300	2.70217200	-0.90415700
C	0.47499500	2.30092700	-1.29364400
C	0.47458400	2.47821300	1.04354500
C	1.28983900	2.17196800	-0.07049900
H	-1.48028300	0.42347600	-2.17204500
H	-0.23168500	-0.83768300	-2.49607400
C	1.01266100	2.12440500	-2.67738700
H	1.73382300	2.91887200	-2.90196100
H	1.52579100	1.16352300	-2.78083100
H	0.21999300	2.17156900	-3.42604800
C	-1.99487500	3.01648000	-1.78261600
H	-1.81404900	2.72787000	-2.81988800
H	-2.90094700	2.50478300	-1.44135700
H	-2.20601600	4.09175000	-1.77561900
C	-2.00429600	3.28380200	1.32070800
H	-2.13954000	4.35320200	1.11710300
H	-2.93169000	2.78361000	1.02818100
H	-1.86561100	3.17412700	2.39756000

C	0.91127500	2.49138400	2.47859800
H	1.68276600	1.73898100	2.66130600
H	1.32807600	3.46696600	2.75455600
H	0.08042900	2.28807900	3.15928300
C	2.76039400	1.91504500	-0.05497500
H	3.28979800	2.87636800	-0.04390000
H	3.07038200	1.35149100	0.82711000
H	3.08605600	1.36869900	-0.94103400
Co	-0.33500300	0.69517700	-0.10932100
C	1.83172700	-1.05496100	-0.94119900
O	1.91769600	-1.03835900	-2.17416600
N	0.69637300	-0.72937700	-0.22765100
C	2.99097700	-1.43155600	-0.07146100
C	4.24496800	-1.58375600	-0.68311100
C	2.86761700	-1.58746700	1.31972300
C	5.36411300	-1.88120600	0.08946200
H	4.31764700	-1.46541400	-1.75884200
C	3.99214000	-1.88361500	2.08815800
H	1.89255200	-1.49175200	1.78515800
C	5.24013600	-2.02783400	1.47520300
H	6.33301700	-2.00073400	-0.38531200
H	3.89603700	-2.01152400	3.16204800
H	6.11462600	-2.26030200	2.07545900

⁵TS9, -2613.65892044, *i*194.27

C	3.16898500	3.73478100	-1.03279600
C	3.92054800	3.27379800	0.02641400
C	3.66577000	1.98819800	0.57746200
C	2.63931300	1.18984400	-0.00099300
C	1.91512000	1.64701700	-1.13928700
C	2.16043400	2.92766800	-1.61100600
H	5.14721500	2.03815600	2.15877000
H	3.35188400	4.72435900	-1.43820800
H	4.69935200	3.89031100	0.46481500
C	4.35203800	1.45998600	1.69673100
H	1.59040300	3.30242500	-2.45570500
C	2.93617800	-0.47796600	1.59603000
C	3.99655500	0.22312600	2.19757800
H	2.60609800	-1.43100800	1.98970500
H	4.50162200	-0.20623400	3.05524200
N	2.27178200	-0.01684400	0.53967000
C	0.96872300	0.72711300	-1.77750500
C	0.82293000	-2.89794000	-0.16105200
C	-0.00491000	-2.56027300	-1.31702600

C	-1.29193000	-2.22693400	-0.84304800
C	0.05314900	-2.68464700	1.01634300
C	-1.25179500	-2.27695900	0.61427900
H	1.42274700	-0.17990800	-2.20061500
H	0.22065600	1.14811100	-2.44047500
C	-2.48387300	-1.88618000	-1.67643700
H	-2.88091600	-2.78287800	-2.16772700
H	-3.28387600	-1.45028700	-1.07483400
H	-2.22838000	-1.16375400	-2.45825100
C	0.39057100	-2.74098200	-2.75398700
H	0.18700200	-3.76532800	-3.08868300
H	-0.16917600	-2.06574300	-3.40660100
H	1.45843700	-2.55954100	-2.90927200
C	2.21247300	-3.44484500	-0.26629900
H	2.19407500	-4.43824400	-0.73042500
H	2.84912000	-2.81246700	-0.89456200
H	2.69314400	-3.54346500	0.70827700
C	0.46043900	-2.94288300	2.44015000
H	-0.20545800	-3.67836000	2.90369800
H	1.47369800	-3.34540800	2.50787800
H	0.41216300	-2.03571500	3.05259500
C	-2.40655000	-1.99437100	1.51291300
H	-3.14837500	-2.80079800	1.44522200
H	-2.09500600	-1.91287200	2.55606900
H	-2.91273300	-1.06595300	1.23403200
Co	0.43552000	-0.62102000	-0.26533000
C	-1.84866500	1.20022700	-0.85862800
O	-1.88960100	1.38004400	-2.07953600
N	-0.78177100	0.64258700	-0.19302900
C	-3.00922800	1.51447300	0.03203300
C	-4.26637000	1.68833200	-0.56731500
C	-2.87541000	1.62391600	1.42643700
C	-5.37976500	1.96119900	0.22273700
H	-4.34501500	1.61163400	-1.64641600
C	-3.99291100	1.90436100	2.21102200
H	-1.89861400	1.50063800	1.88230900
C	-5.24465600	2.06831700	1.61122700
H	-6.35224100	2.09492600	-0.24075000
H	-3.88871400	1.99988700	3.28740100
H	-6.11438400	2.28424400	2.22438300

¹⁰, -2613.76612287

C	4.82220000	-1.79752000	0.10123800
C	4.89209000	-0.77534100	-0.81481500

C	3.72392100	-0.04903700	-1.15430100
C	2.46915100	-0.36260800	-0.52132700
C	2.40359400	-1.47077200	0.37737700
C	3.57904400	-2.14349300	0.66933400
H	4.70795400	1.20635100	-2.61397700
H	5.70972000	-2.36228900	0.36671700
H	5.82921800	-0.51713700	-1.29815200
C	3.76425800	0.97961500	-2.12618300
H	3.53198200	-2.99157100	1.34756200
C	1.44468000	1.36559800	-1.74627600
C	2.61959900	1.66921100	-2.45089200
H	0.53484900	1.92788200	-1.93042000
H	2.60833500	2.44696700	-3.20543500
N	1.36543700	0.42246800	-0.80987600
C	1.12204800	-1.99814700	1.00107000
C	-0.03741500	2.29338300	1.04514600
C	0.14149100	1.19839600	1.98510400
C	-1.13761900	0.54190300	2.14533400
C	-1.34441300	2.21571500	0.53389700
C	-2.03378500	1.12863800	1.22580300
H	1.13294400	-1.77329500	2.07818200
H	1.11190300	-3.09111200	0.92344900
C	-1.45462200	-0.59286800	3.06832900
H	-2.04792800	-0.22929200	3.91467500
H	-2.02822100	-1.37216000	2.56165900
H	-0.55180200	-1.05548200	3.46799400
C	1.38524400	0.97702700	2.78858200
H	1.52725500	1.80409700	3.49391700
H	1.33844500	0.05375300	3.36630700
H	2.27039700	0.93245600	2.14837100
C	1.01845900	3.30198200	0.71950300
H	1.05153100	4.05941900	1.51133700
H	2.00898800	2.84459300	0.66278500
H	0.82222000	3.81885900	-0.22157400
C	-1.98300000	3.11968600	-0.47575800
H	-2.57629500	3.89039500	0.03012600
H	-1.24086400	3.63135100	-1.09326700
H	-2.65558500	2.56460400	-1.13298900
C	-3.48339900	0.80156300	1.07070000
H	-4.07910300	1.52236100	1.64413700
H	-3.80439900	0.85744200	0.03003100
H	-3.71366300	-0.19661400	1.44313500
Co	-0.30876200	0.35499000	0.19680300
C	-1.08760000	-2.32658800	0.05602300

O	-1.19100300	-3.50448500	0.39783900
N	-0.06436900	-1.48747000	0.36992100
C	-2.11610100	-1.65380300	-0.81259900
C	-1.74716500	-0.58255400	-1.65068600
C	-3.44313600	-2.09346000	-0.80336600
C	-2.70852900	0.06897800	-2.43832200
H	-0.69083400	-0.38603100	-1.83884100
C	-4.39522400	-1.44661800	-1.58942100
H	-3.70157600	-2.94223500	-0.17847900
C	-4.03374400	-0.36001500	-2.40158600
H	-2.41077900	0.87046400	-3.10807000
H	-5.42639700	-1.78644500	-1.57643500
H	-4.78132900	0.12562400	-3.02091500

³¹⁰, -2613.77086429

C	-4.52082700	-2.23113200	-0.87263400
C	-4.71529200	-1.69024100	0.37441200
C	-3.72261300	-0.85512900	0.94892400
C	-2.52481600	-0.55680800	0.21465300
C	-2.33148800	-1.14387900	-1.07440700
C	-3.32593700	-1.96327400	-1.57712500
H	-4.78374100	-0.54580400	2.80670900
H	-5.26972100	-2.87921600	-1.31548300
H	-5.61606000	-1.89967800	0.94299000
C	-3.88025800	-0.31826900	2.24824000
H	-3.17387500	-2.42930100	-2.54634200
C	-1.75732200	0.74513700	2.02228300
C	-2.89329200	0.46950800	2.79644600
H	-0.96252800	1.36472500	2.41811500
H	-2.97390500	0.88085000	3.79579800
N	-1.57692100	0.27904200	0.78627100
C	-1.07184200	-0.92228000	-1.89803000
C	0.37072400	2.84212200	0.29005700
C	0.17061000	2.71933800	-1.13543900
C	1.19318400	1.88765800	-1.63166300
C	1.56557800	2.13404200	0.66658000
C	2.06923500	1.51727000	-0.50422900
H	-1.14641500	0.03456800	-2.44039300
H	-0.98350400	-1.71135800	-2.65011100
C	1.42654000	1.45309300	-3.04338900
H	2.31965100	1.94418600	-3.44643400
H	1.58838600	0.37292100	-3.09457700
H	0.58548400	1.70570100	-3.69136800
C	-0.95631300	3.35164500	-1.89739200

H	-0.77584200	4.42400900	-2.03511800
H	-1.07457500	2.90710300	-2.88745800
H	-1.90741500	3.24826900	-1.36608900
C	-0.47387300	3.70323100	1.17599300
H	-0.28951500	4.75736300	0.93590800
H	-1.54209800	3.52301800	1.02332000
H	-0.24215900	3.56707600	2.23382700
C	2.18139800	2.08106200	2.03392000
H	2.88626000	2.90855100	2.17396100
H	1.42889500	2.15911200	2.82375300
H	2.72538100	1.14626300	2.18258800
C	3.35271200	0.76809200	-0.65088900
H	4.14618300	1.46676500	-0.94528200
H	3.65278500	0.28216000	0.27809600
H	3.28238500	0.00123400	-1.42338700
Co	0.10020500	0.70288900	-0.18837900
C	0.90972600	-2.05438900	-1.03564500
O	0.76840700	-2.97417800	-1.83764500
N	0.13107100	-0.91409200	-1.07253000
C	1.95290000	-2.10388100	0.03750900
C	1.73076000	-1.59043900	1.32330400
C	3.17524900	-2.72350000	-0.25462300
C	2.73502100	-1.65671300	2.29187800
H	0.75787200	-1.18177100	1.58287000
C	4.18450200	-2.77073700	0.70487600
H	3.31662800	-3.15557100	-1.23995500
C	3.96922700	-2.23115600	1.97768700
H	2.54958400	-1.27879600	3.29316800
H	5.13643300	-3.23488000	0.46643800
H	4.75263900	-2.27895700	2.72787800

⁵10, -2613.74649119

C	-4.81774400	-1.87338500	-0.69573400
C	-4.93483900	-1.15700100	0.46918600
C	-3.84028100	-0.38941400	0.94443800
C	-2.61200600	-0.34038100	0.19899400
C	-2.50881400	-1.10236100	-1.01030700
C	-3.60291800	-1.84623900	-1.41535500
H	-4.85914100	0.28966100	2.72629800
H	-5.64477300	-2.47223100	-1.06232700
H	-5.85289100	-1.17399500	1.04855300
C	-3.93182700	0.32711600	2.16166100
H	-3.51980800	-2.43971100	-2.32126200
C	-1.68956800	1.06630200	1.83987300

C	-2.85472700	1.04867800	2.62190500
H	-0.81956900	1.62297100	2.16848800
H	-2.88551400	1.59573000	3.55704100
N	-1.56085000	0.42553500	0.68020900
C	-1.25932500	-1.13370100	-1.88179000
C	0.59348600	2.90120200	0.07463000
C	0.55399900	2.58313300	-1.33998000
C	1.63485200	1.68426000	-1.63801000
C	1.65931700	2.18839700	0.64782300
C	2.33194900	1.44054100	-0.42389000
H	-1.23918900	-0.24088100	-2.52553900
H	-1.29143700	-2.00659000	-2.54063700
C	1.99521500	1.15112100	-2.99430600
H	2.66233300	1.84334400	-3.52066600
H	2.50391600	0.18777700	-2.91936200
H	1.11000900	1.00723700	-3.61907800
C	-0.43834600	3.14051800	-2.30691500
H	-0.16758200	4.16992000	-2.57724800
H	-0.48012200	2.56154900	-3.23176900
H	-1.44253300	3.18122500	-1.87296500
C	-0.33310400	3.87891200	0.73016400
H	-0.18183200	4.88143900	0.31341200
H	-1.38435300	3.61934300	0.56473100
H	-0.16499800	3.94613400	1.80686600
C	2.14161800	2.22881100	2.06613400
H	3.05410600	2.83229100	2.14415800
H	1.40132500	2.66767000	2.73907800
H	2.38691900	1.22713100	2.43099900
C	3.59975500	0.66488500	-0.26294300
H	4.46204300	1.33946900	-0.34493600
H	3.65462300	0.17250000	0.70935500
H	3.70443900	-0.10177600	-1.03246800
Co	0.31541900	0.45892000	-0.27719000
C	0.64133200	-2.35935500	-0.93744400
O	0.46513600	-3.34548900	-1.64250900
N	-0.04493400	-1.16717100	-1.07927900
C	1.67032500	-2.31909200	0.15640500
C	1.39736000	-1.69062800	1.38493700
C	2.91190500	-2.93162500	-0.04523100
C	2.37162800	-1.65354700	2.38820800
H	0.39585600	-1.32095600	1.59563300
C	3.88725500	-2.87692700	0.95014900
H	3.09531500	-3.44570000	-0.98327900
C	3.62171700	-2.23445600	2.16538900

H	2.14381800	-1.20102700	3.34896100
H	4.85352300	-3.34345300	0.78520200
H	4.37932700	-2.20914100	2.94250900

¹¹, -2960.99063131

C	0.06469400	4.92059500	0.86167800
C	-1.11436900	4.60448100	1.49169400
C	-1.65353400	3.29832100	1.37420200
C	-0.98326700	2.31468100	0.56873400
C	0.25837400	2.65107500	-0.05072600
C	0.74576400	3.93644000	0.11309000
H	-3.34822900	3.66854500	2.66675200
H	0.48986900	5.91457500	0.95322400
H	-1.64136400	5.33642100	2.09607100
C	-2.83887500	2.92998100	2.05438000
H	1.69707600	4.19389300	-0.34475400
C	-2.63251700	0.74332100	1.12105800
C	-3.32009400	1.64634100	1.94767100
H	-2.98541800	-0.27482900	1.00632200
H	-4.21183500	1.32072300	2.47069200
N	-1.53488300	1.05654600	0.43731700
C	1.06968900	1.67525800	-0.87485500
C	-1.42238400	0.16806400	-2.66116500
C	-2.60667600	-0.32328100	-1.99391900
C	-2.36457400	-1.65248000	-1.59279900
C	-0.49025600	-0.92450700	-2.76354000
C	-1.03646400	-2.02805600	-2.05549100
H	2.11402700	1.99164400	-0.84511000
H	0.76454700	1.76229800	-1.92435200
C	-3.26604100	-2.56358900	-0.82103100
H	-3.56961200	-3.41256700	-1.44307400
H	-2.74390000	-2.96247700	0.05303500
H	-4.17328800	-2.05606900	-0.48599700
C	-3.85049500	0.48505000	-1.79883800
H	-4.41941900	0.50817900	-2.73572000
H	-4.50118400	0.06818500	-1.02825400
H	-3.61796400	1.51902000	-1.53185100
C	-1.34025000	1.50534900	-3.33713500
H	-2.09300900	1.57105900	-4.13108500
H	-1.53118900	2.32568900	-2.63808100
H	-0.36556300	1.66913600	-3.79949600
C	0.81819400	-0.88838200	-3.48663500
H	0.65078100	-1.07287400	-4.55409900
H	1.30555900	0.08511900	-3.39318700

H	1.50022300	-1.64575700	-3.10299800
C	-0.44110100	-3.38202600	-1.84374400
H	-1.00479900	-4.13026000	-2.41348100
H	0.60476200	-3.41566000	-2.14047200
H	-0.49037400	-3.64985100	-0.78550900
Co	-0.85844400	-0.39459200	-0.73311100
C	2.00649100	-0.59040300	-0.51910900
O	1.82639100	-1.80473300	-0.63146700
N	0.93190700	0.28571300	-0.44096700
C	3.40292600	-0.06609200	-0.34163200
C	3.72804500	0.88355600	0.63928900
C	4.42224600	-0.63064800	-1.11949600
C	5.05390800	1.27411000	0.82469300
H	2.94973100	1.29968700	1.27332600
C	5.74362800	-0.22257800	-0.94765300
H	4.16675300	-1.39422100	-1.84695900
C	6.06135200	0.72996200	0.02432000
H	5.30151400	1.99683800	1.59624600
H	6.52710700	-0.65470100	-1.56254300
H	7.09245500	1.03966500	0.16471200
C	-0.13778500	-1.48040700	1.88088900
C	-0.14978700	-2.53386400	2.97163400
O	-0.80559100	-1.61337300	0.83376100
O	0.62984200	-0.44354500	2.09948200
H	0.74099300	0.05177700	1.21704300
C	-1.20995900	-3.60229700	2.67068000
H	-1.20305500	-4.35564200	3.46295400
H	-2.21330300	-3.16744300	2.62395500
H	-1.01018700	-4.10399000	1.72031100
C	-0.43382600	-1.85098600	4.32712900
H	-0.40618700	-2.60214900	5.12145900
H	0.31125300	-1.08422100	4.54936800
H	-1.42572600	-1.38599300	4.33749700
C	1.26626700	-3.16479900	2.97756000
H	1.30360000	-3.95248600	3.73565600
H	1.50605100	-3.60619000	2.00550300
H	2.02702500	-2.41684500	3.21262500

³¹I, -2960.97277801

C	-2.08037500	-4.30584000	-1.83276200
C	-3.19960000	-3.51153400	-1.91149600
C	-3.09894200	-2.12476700	-1.63717500
C	-1.83639100	-1.55489800	-1.25569100
C	-0.66149900	-2.37352000	-1.29474800

C	-0.82435300	-3.72563400	-1.55112800
H	-5.17679600	-1.67926300	-2.04870100
H	-2.14639700	-5.37211000	-2.02280200
H	-4.16525000	-3.92735200	-2.18291500
C	-4.22283400	-1.26510700	-1.73434900
H	0.05665500	-4.36196000	-1.57273800
C	-2.85398200	0.52628000	-0.94909800
C	-4.09729700	0.07042200	-1.43213800
H	-2.73326100	1.54646700	-0.59948700
H	-4.93232700	0.75731400	-1.51190200
N	-1.77971500	-0.24255700	-0.84410200
C	0.77051500	-1.85199900	-1.28421100
C	-0.64208600	-1.44779200	2.34373500
C	-1.88189600	-0.82870300	2.21030200
C	-1.68419800	0.59214100	2.46523900
C	0.34795900	-0.42064300	2.76335100
C	-0.30986900	0.81610500	2.86005100
H	1.03308200	-1.72471700	-2.34542700
H	1.43202700	-2.64089800	-0.90396900
C	-2.73735700	1.64844600	2.42528700
H	-3.00858000	1.95124100	3.44452000
H	-2.36664500	2.53938400	1.90910600
H	-3.64398200	1.30219100	1.92590100
C	-3.18933800	-1.47897800	1.88102400
H	-3.78166500	-1.63558900	2.79033900
H	-3.79062200	-0.86889300	1.20356800
H	-3.04440800	-2.45277700	1.40915500
C	-0.31020400	-2.89520400	2.18195800
H	-0.23124500	-3.38189800	3.16251400
H	-1.06800800	-3.42398000	1.60180000
H	0.65340000	-3.02414800	1.68107200
C	1.75060100	-0.73825000	3.15871800
H	1.75377500	-1.23394300	4.13826000
H	2.22711600	-1.41836900	2.44795600
H	2.35787100	0.16375000	3.22323300
C	0.28308000	2.13381400	3.26089200
H	0.16626200	2.31294900	4.33581300
H	1.34629300	2.16628500	3.01540900
H	-0.20046300	2.95439600	2.72579700
Co	-0.26514700	0.29718000	0.69984900
C	2.15125900	-0.12064100	-0.10642100
O	2.03151400	0.87206700	0.66716900
N	0.97489500	-0.60507100	-0.56951600
C	3.49798000	-0.66881500	-0.41766000

C	3.82076200	-1.26944900	-1.64446200
C	4.49337400	-0.53624400	0.56519100
C	5.11133100	-1.74435800	-1.87492700
H	3.08453900	-1.33411500	-2.43672100
C	5.77510400	-1.03005500	0.33968000
H	4.24542200	-0.03751800	1.49510600
C	6.08587000	-1.63713000	-0.88053500
H	5.35710100	-2.19308500	-2.83235700
H	6.53499500	-0.93328500	1.10889900
H	7.08759500	-2.01556600	-1.05977200
C	-0.05998700	2.62236700	-1.05438700
C	-0.10116400	4.07813200	-1.48566300
O	-0.53001100	2.23955400	0.03378200
O	0.50479700	1.80639200	-1.91548600
H	0.58397800	0.88183600	-1.53583600
C	-0.85570200	4.91201400	-0.44036500
H	-0.87498000	5.95917100	-0.75431200
H	-1.88941100	4.57099200	-0.32812300
H	-0.37133800	4.85483800	0.53795200
C	-0.80263000	4.16604900	-2.85997100
H	-0.82410100	5.20944700	-3.18708200
H	-0.27554600	3.57691400	-3.61346900
H	-1.83729900	3.81076200	-2.80158400
C	1.36430700	4.56249800	-1.60680900
H	1.37042800	5.61308800	-1.91143200
H	1.88788600	4.48124100	-0.64905100
H	1.91158800	3.98039600	-2.35163800

⁵¹¹, -2960.95839783

C	-2.47326200	-3.61033100	-2.49976300
C	-3.54716200	-2.76381100	-2.36358900
C	-3.35393000	-1.46392700	-1.83237500
C	-2.04473400	-1.04127900	-1.42046900
C	-0.91915100	-1.88820600	-1.68500200
C	-1.17374100	-3.15605100	-2.18320100
H	-5.42250400	-0.85646800	-2.01613400
H	-2.60875400	-4.61556100	-2.88515800
H	-4.54685500	-3.07278000	-2.65348800
C	-4.43217600	-0.55437000	-1.68696200
H	-0.33378100	-3.81830300	-2.37583100
C	-2.93142700	0.98833400	-0.65685600
C	-4.22103900	0.68910500	-1.13704400
H	-2.73017100	1.92176500	-0.13909300
H	-5.02128600	1.41249500	-1.03022000

N	-1.89979500	0.16082500	-0.76337800
C	0.54314700	-1.44958200	-1.67078800
C	-0.57264200	-2.12318400	2.05310500
C	-1.78052900	-1.41831200	2.01355700
C	-1.54114200	-0.05482900	2.54047200
C	0.40674400	-1.28262100	2.65736400
C	-0.19631900	0.02617800	2.92650400
H	0.74981300	-1.10020900	-2.69449600
H	1.16924800	-2.33701100	-1.52234400
C	-2.61593600	0.95632200	2.81133000
H	-3.07454700	0.77076500	3.79085700
H	-2.21673500	1.97365100	2.82247600
H	-3.41579600	0.91023200	2.06823000
C	-3.11467700	-1.92826400	1.58500300
H	-3.70407300	-2.23498000	2.45967500
H	-3.69653300	-1.16297400	1.06502600
H	-3.02740100	-2.79636200	0.92822100
C	-0.32190600	-3.52321500	1.57595000
H	-0.33952300	-4.24270400	2.40331100
H	-1.06938300	-3.83910200	0.84453500
H	0.66078600	-3.60595900	1.09980400
C	1.79706400	-1.68442200	3.00266500
H	1.79287400	-2.36020400	3.86885600
H	2.26882500	-2.23178700	2.17968000
H	2.41895200	-0.82192700	3.24134300
C	0.48735700	1.14684600	3.65150900
H	0.61031500	0.90236300	4.71349300
H	1.47618300	1.33357700	3.22643100
H	-0.08849100	2.07248400	3.58667700
Co	-0.29991800	0.39737400	0.65527700
C	2.08132800	-0.23481800	-0.09962700
O	2.03958800	0.51126500	0.91901500
N	0.87989800	-0.41094400	-0.71045000
C	3.36859000	-0.82686000	-0.54322800
C	3.64031300	-1.13145000	-1.88693100
C	4.36545800	-1.03752000	0.42452300
C	4.87871900	-1.65831800	-2.25011000
H	2.90653500	-0.92457600	-2.65708000
C	5.59433800	-1.58056300	0.06118400
H	4.16165400	-0.76239200	1.45251800
C	5.85169300	-1.89517100	-1.27644900
H	5.08642700	-1.87813700	-3.29262400
H	6.35537200	-1.75004500	0.81646200
H	6.81251300	-2.31319400	-1.56085300

C	0.24571300	2.94530100	-0.64629900
C	0.29572700	4.45026600	-0.83786800
O	-0.26041600	2.41706100	0.36329400
O	0.78005300	2.24281400	-1.62141500
H	0.77571500	1.26338900	-1.40327900
C	-0.43314700	5.14925500	0.31861500
H	-0.38497600	6.23226200	0.17645700
H	-1.48671600	4.85725600	0.36053700
H	0.02407400	4.90679200	1.28124100
C	-0.37018200	4.79648600	-2.18936400
H	-0.32724600	5.87836900	-2.34321500
H	0.14015100	4.30721400	-3.02176500
H	-1.42368400	4.49669600	-2.20148900
C	1.78843900	4.86163700	-0.86341800
H	1.85782900	5.94471200	-0.99937400
H	2.28603600	4.60425400	0.07697800
H	2.31924900	4.37325200	-1.68381200

¹TS12, -2960.98606902, i1073.46

C	0.00115600	4.94738800	0.31324000
C	-1.18516600	4.68536300	0.95433400
C	-1.69969100	3.36439800	0.98341000
C	-0.99971000	2.30708800	0.30855700
C	0.25207100	2.58985300	-0.31554300
C	0.71673800	3.89372500	-0.29520400
H	-3.41809600	3.84653400	2.20621600
H	0.40774200	5.95302500	0.29372600
H	-1.73565300	5.47332000	1.45913300
C	-2.88640200	3.05281200	1.68935500
H	1.67660900	4.11239700	-0.75530700
C	-2.62503800	0.77725300	1.01783500
C	-3.33829900	1.75496200	1.73007500
H	-2.95336700	-0.25517300	1.01907900
H	-4.22767300	1.47242800	2.28136600
N	-1.52830200	1.03426900	0.31080200
C	1.10894700	1.54244700	-0.99095900
C	-1.37846700	-0.12237700	-2.69013500
C	-2.56158400	-0.54478600	-1.97994800
C	-2.32275400	-1.83396800	-1.45509500
C	-0.45360000	-1.22366800	-2.69465800
C	-1.00006200	-2.25699200	-1.88515900
H	2.14626400	1.88059800	-0.95422000
H	0.84656700	1.48599100	-2.05216100
C	-3.22222600	-2.66451400	-0.59567400

H	-3.52059300	-3.57468200	-1.12695200
H	-2.69723200	-2.96583800	0.31522200
H	-4.13226000	-2.12923800	-0.31594300
C	-3.80464700	0.27919300	-1.86285400
H	-4.37091100	0.21378700	-2.79939900
H	-4.45719300	-0.06392700	-1.05841200
H	-3.57242200	1.33360300	-1.69348400
C	-1.28047000	1.15105600	-3.47870300
H	-2.02279900	1.15502800	-4.28497200
H	-1.47167400	2.03000400	-2.85488300
H	-0.29891100	1.26761700	-3.94166200
C	0.83840700	-1.25553700	-3.44786700
H	0.62992800	-1.40810900	-4.51317900
H	1.38698800	-0.31409000	-3.35610000
H	1.48654700	-2.05678200	-3.09836700
C	-0.41278700	-3.58799600	-1.54322000
H	-1.02578800	-4.38855700	-1.97300500
H	0.60870500	-3.68757100	-1.90366300
H	-0.39527700	-3.71571100	-0.45753000
Co	-0.82645700	-0.51619100	-0.70662800
C	2.09281100	-0.69072300	-0.51387500
O	1.91199000	-1.88610300	-0.67938200
N	0.97819800	0.19833300	-0.39976100
C	3.46592500	-0.14504800	-0.29461900
C	3.72993500	0.85169900	0.65936800
C	4.52646000	-0.72862900	-1.00227400
C	5.04081900	1.26634700	0.88756100
H	2.91941300	1.27554500	1.24496800
C	5.83242100	-0.29446900	-0.78741700
H	4.31262100	-1.52223800	-1.71066900
C	6.09067900	0.70278800	0.15724100
H	5.24456900	2.02308900	1.63877700
H	6.64938300	-0.73928300	-1.34686800
H	7.11004600	1.03345500	0.33137800
C	-0.14252100	-1.18991000	1.99712100
C	-0.28334900	-2.00707200	3.27713900
O	-0.78322400	-1.54481000	0.95886800
O	0.62585200	-0.16748800	2.02657800
H	0.81777900	0.16901600	0.87473400
C	-1.28837100	-3.15240200	3.09371200
H	-1.36574000	-3.72577900	4.02193600
H	-2.28431100	-2.77293500	2.84508800
H	-0.97563000	-3.83205800	2.29645400
C	-0.75390600	-1.04982400	4.39466200

H	-0.83739800	-1.59952600	5.33678400
H	-0.04676900	-0.22854900	4.52984700
H	-1.73789400	-0.62532300	4.16424800
C	1.11736300	-2.56720600	3.61587200
H	1.06748900	-3.13808100	4.54791600
H	1.47617100	-3.23530900	2.82610400
H	1.84081300	-1.75804200	3.73930700

³TS12, -2960.9724695, i1120.84

C	0.16195900	4.54094300	2.03953100
C	1.50743500	4.35624300	1.83823800
C	2.00550100	3.07700000	1.47615100
C	1.10433900	1.96960800	1.33470200
C	-0.29344500	2.18572300	1.54799700
C	-0.72830700	3.45305900	1.88524600
H	4.07689200	3.69007200	1.33592600
H	-0.22647800	5.51733200	2.30960100
H	2.20697700	5.18003000	1.94448600
C	3.38324800	2.86022400	1.23382500
H	-1.79099700	3.62001000	2.03881800
C	2.87262600	0.57982000	0.74073800
C	3.82260000	1.61072500	0.86276800
H	3.18460900	-0.40679900	0.41822800
H	4.86779200	1.40793800	0.65805100
N	1.57489100	0.72797300	0.97311400
C	-1.29689800	1.06390000	1.42843000
C	0.13050700	-2.36415300	2.12329500
C	1.52847600	-2.37841300	1.85290300
C	1.69126000	-2.89868300	0.54317900
C	-0.58398000	-2.97359200	0.99228100
C	0.36746700	-3.28651300	0.01793300
H	-2.30689600	1.46804300	1.51386000
H	-1.16761700	0.36975600	2.26615000
C	2.95362600	-3.08851700	-0.22876200
H	3.06563800	-4.13833000	-0.52226100
H	2.91622000	-2.49705300	-1.15137700
H	3.83712300	-2.79906500	0.34302300
C	2.58755300	-1.92755700	2.81303300
H	2.62469000	-2.59330500	3.68263400
H	3.57912900	-1.92872600	2.35708000
H	2.39059200	-0.91573900	3.17995600
C	-0.49074000	-1.94725400	3.41376900
H	-0.41935400	-2.76857000	4.13975900
H	0.02737100	-1.08882900	3.85085900

H	-1.55008700	-1.70670400	3.30279700
C	-2.04986900	-3.27404400	0.98542700
H	-2.25953400	-4.13892600	1.62620200
H	-2.63719100	-2.43388500	1.36739900
H	-2.40323100	-3.49240400	-0.02173100
C	0.15421500	-3.89437200	-1.33191100
H	0.51031200	-4.93105600	-1.35519300
H	-0.90002400	-3.87969700	-1.60896200
H	0.70523600	-3.33112700	-2.09079200
Co	0.35120500	-1.07879100	0.18732800
C	-2.18385700	-0.29023700	-0.52713500
O	-1.89042500	-1.26442900	-1.22671700
N	-1.12298000	0.30919200	0.17093600
C	-3.56060600	0.26188400	-0.49028600
C	-3.79797800	1.64627900	-0.48749500
C	-4.64047800	-0.63141400	-0.54458600
C	-5.10550200	2.12682500	-0.52214200
H	-2.96268500	2.34074700	-0.49945800
C	-5.94602400	-0.14633300	-0.55424000
H	-4.44153600	-1.69728900	-0.58284700
C	-6.17906400	1.23192600	-0.54223100
H	-5.28816200	3.19667400	-0.54032500
H	-6.78102800	-0.83923000	-0.58304000
H	-7.19699800	1.60899400	-0.56000100
C	1.03741500	0.43103900	-2.11189100
C	1.86353100	0.77532400	-3.34922400
O	1.24405100	-0.68083600	-1.52074200
O	0.19098100	1.29535000	-1.71238400
H	-0.47333500	0.89735200	-0.74450800
C	2.83401800	-0.36134900	-3.69851500
H	3.41141900	-0.09148500	-4.58753400
H	3.53585200	-0.55042000	-2.88061900
H	2.29824400	-1.29139600	-3.90712200
C	2.64615900	2.06902900	-3.02444200
H	3.24363000	2.36276500	-3.89262800
H	1.96403000	2.88513100	-2.77568600
H	3.32712200	1.91832700	-2.17922400
C	0.88556100	1.03029700	-4.51710300
H	1.44840300	1.32060800	-5.40936400
H	0.31280700	0.12823500	-4.75621600
H	0.18380000	1.83005300	-4.27029300

⁵TS12, -2960.9595131, i1073.81

C	-0.77123100	4.56652500	2.02306500
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C	0.57619100	4.62076100	1.76894800
C	1.27581400	3.44778000	1.38246300
C	0.58172400	2.19585200	1.27431300
C	-0.82413300	2.16177200	1.54225200
C	-1.45800300	3.33791500	1.89922900
H	3.18918200	4.43207300	1.16179900
H	-1.31624400	5.45919300	2.31116400
H	1.12441200	5.55458000	1.84903500
C	2.65792800	3.48790600	1.08137500
H	-2.52643500	3.31656400	2.09457800
C	2.56213400	1.15584800	0.58725800
C	3.30563000	2.34381400	0.67689600
H	3.03201300	0.24469400	0.23765700
H	4.35870200	2.33936100	0.42024000
N	1.26834300	1.06162700	0.88821900
C	-1.64299300	0.89247900	1.47777900
C	1.80010100	-2.05560100	2.12367100
C	3.00238600	-2.09239200	1.32274000
C	2.68050800	-2.64463500	0.09349300
C	0.69784200	-2.59970400	1.35200300
C	1.25844300	-3.02142300	0.11366000
H	-2.69696800	1.13775600	1.62402200
H	-1.36221100	0.23356000	2.31402800
C	3.53555100	-2.80146100	-1.12005900
H	3.54127700	-3.83939800	-1.47229900
H	3.13637800	-2.18805800	-1.93779200
H	4.57001000	-2.50402700	-0.93770900
C	4.33081800	-1.58847500	1.80039500
H	4.73088600	-2.23062400	2.59413000
H	5.07053000	-1.56072200	0.99738500
H	4.25206400	-0.57981000	2.22312400
C	1.72673400	-1.52490600	3.51248300
H	0.71212200	-1.55130400	3.91406000
H	2.37388100	-2.10449600	4.18326100
H	2.08981000	-0.48980900	3.55229200
C	-0.61340900	-3.05455600	1.94879000
H	-0.46554000	-3.92672100	2.59594300
H	-1.07568700	-2.27120100	2.55857600
H	-1.32494100	-3.32100700	1.16780100
C	0.60561700	-3.78260700	-0.98819900
H	1.11167600	-4.74694100	-1.12332800
H	-0.45276400	-3.95507900	-0.80374900
H	0.69957500	-3.23307100	-1.93172000
Co	0.37506900	-0.74273700	0.19569100

C	-2.31080100	-0.84667200	-0.22233300
O	-1.78736900	-1.84179500	-0.73460100
N	-1.42413200	0.15586100	0.21688100
C	-3.77686800	-0.68111000	-0.12933100
C	-4.37833400	0.58479000	-0.23208700
C	-4.57723700	-1.82742900	-0.00582900
C	-5.76605000	0.69912100	-0.19837100
H	-3.76223600	1.46699600	-0.37991100
C	-5.96291400	-1.70571700	0.04879000
H	-4.09926900	-2.80020700	0.04308600
C	-6.55717500	-0.44353500	-0.04636000
H	-6.23179200	1.67452500	-0.29722400
H	-6.58101100	-2.59136100	0.15632600
H	-7.63838900	-0.35100000	-0.01168200
C	0.48260100	0.58337400	-2.28357200
C	1.13540800	1.07251600	-3.57549300
O	0.98847300	-0.41437200	-1.67276100
O	-0.52734900	1.24051700	-1.85594100
H	-1.03966900	0.78599500	-0.79737500
C	2.25595300	0.12061800	-4.01733000
H	2.70794000	0.48779100	-4.94350000
H	3.03959000	0.04942900	-3.25766500
H	1.87085500	-0.88660500	-4.20011100
C	1.71425500	2.47513700	-3.27141900
H	2.19494100	2.87689300	-4.16850600
H	0.92445800	3.16300500	-2.95992300
H	2.46779000	2.42841700	-2.47645900
C	0.05156600	1.17819900	-4.66846400
H	0.49327800	1.57419100	-5.58791600
H	-0.37632200	0.19606900	-4.89509400
H	-0.75661600	1.84191300	-4.35401300

MECP2, -2960.97605872

C	-0.19301100	5.03430800	0.48222500
C	-1.30580500	4.68946300	1.20931000
C	-1.72831100	3.33820800	1.26250700
C	-1.02094500	2.33252100	0.52323800
C	0.15881600	2.70483100	-0.19245300
C	0.54088900	4.03488800	-0.19045200
H	-3.37336400	3.69353600	2.61989700
H	0.14395500	6.06423500	0.44277500
H	-1.86563200	5.43537200	1.76408900
C	-2.83405800	2.94116300	2.05286500
H	1.44711500	4.31745500	-0.71807000

C	-2.47731400	0.69713400	1.32435300
C	-3.19568900	1.61667200	2.10802800
H	-2.74024300	-0.35515900	1.33342800
H	-4.01999400	1.27417600	2.72232600
N	-1.45967500	1.03174100	0.54490200
C	1.04441700	1.73850600	-0.94819100
C	-1.63778600	0.08877400	-2.55245900
C	-2.71527100	-0.42629400	-1.79207300
C	-2.39193200	-1.77672500	-1.46813900
C	-0.69640400	-0.99894700	-2.82398000
C	-1.16986000	-2.14438500	-2.16590200
H	2.06671200	2.12409600	-0.92430100
H	0.75215900	1.69747800	-2.00081800
C	-3.17764000	-2.72172000	-0.62335700
H	-3.49869400	-3.58456400	-1.21660400
H	-2.55987200	-3.09594800	0.19902000
H	-4.06861900	-2.25229800	-0.20320200
C	-3.95190900	0.32972400	-1.42427100
H	-4.65495400	0.33140700	-2.26638200
H	-4.46734900	-0.11392900	-0.57090300
H	-3.73293700	1.37224800	-1.17913900
C	-1.59671200	1.45986900	-3.15051300
H	-2.39967100	1.56794400	-3.88886400
H	-1.74652200	2.23907300	-2.39669600
H	-0.65626700	1.65485900	-3.66857800
C	0.47495000	-0.88978000	-3.74580400
H	0.12614300	-0.85362200	-4.78454100
H	1.05564500	0.02075200	-3.57057900
H	1.15139300	-1.73693200	-3.63823200
C	-0.54224500	-3.49877800	-2.09270900
H	-1.17514500	-4.24295100	-2.58860600
H	0.44009000	-3.50962200	-2.56314400
H	-0.41640400	-3.80769400	-1.05066300
Co	-0.73787200	-0.59774400	-0.67633400
C	2.14223300	-0.50245200	-0.73971000
O	1.90966100	-1.60377300	-1.19729300
N	1.00673100	0.36145800	-0.41144700
C	3.49988600	-0.01422900	-0.43052800
C	3.73792400	0.92810600	0.58466700
C	4.57905500	-0.57378300	-1.13302400
C	5.04279400	1.31065300	0.88115200
H	2.91537200	1.32693200	1.16870900
C	5.87892200	-0.17226100	-0.84540800
H	4.37845900	-1.31695600	-1.89707500

C	6.11086100	0.76995800	0.16084000
H	5.22893400	2.02423900	1.67713500
H	6.71126900	-0.59570500	-1.39710100
H	7.12641700	1.07661100	0.39021700
C	0.03211200	-1.40145100	1.94382000
C	-0.05448100	-2.40605100	3.09863700
O	-0.63357100	-1.70057600	0.86274500
O	0.73009100	-0.37881600	2.07854500
H	0.95428400	0.33157600	0.65080600
C	-1.10387100	-3.49395900	2.84592200
H	-1.13530600	-4.17942400	3.69825000
H	-2.10372200	-3.06605700	2.72418200
H	-0.87109300	-4.07572700	1.95080300
C	-0.39588000	-1.62169200	4.38046400
H	-0.40578600	-2.29960200	5.23892900
H	0.33931100	-0.83527600	4.56010700
H	-1.38571200	-1.15697700	4.30837200
C	1.34710900	-3.04107900	3.23357800
H	1.35780200	-3.73798500	4.07695700
H	1.61643300	-3.59814700	2.33034100
H	2.10444300	-2.27255200	3.40620600

TsN₃, -984.055669914

N	-2.15744800	-0.15369000	-1.08033500
N	-2.40438200	-1.34450900	-0.81604200
N	-2.66143600	-2.44112000	-0.66091600
C	0.24434200	0.36885300	0.18390400
C	1.03251000	1.13472400	-0.67729700
C	0.77896900	-0.68594200	0.92510300
C	2.38490500	0.82896800	-0.79193300
H	0.59036300	1.95352100	-1.23392700
C	2.13529300	-0.97357600	0.79352000
H	0.14565700	-1.25404000	1.59734100
C	2.95601000	-0.22519100	-0.06225700
H	3.00951200	1.41847200	-1.45705900
H	2.56401400	-1.79009700	1.36745300
S	-1.49677500	0.72806500	0.31394800
O	-2.01978200	0.10780400	1.53149800
O	-1.73419300	2.12173200	-0.03205200
C	4.43059000	-0.52342600	-0.17217900
H	4.81001100	-0.30225900	-1.17384900
H	5.00144500	0.08924300	0.53611200
H	4.64635200	-1.57140600	0.05306200

¹TS7', -3197.86954212, i618.78

C	4.22183500	-2.88105500	0.93975200
C	3.27935700	-3.70493100	0.36188900
C	2.01998400	-3.17645700	-0.02747800
C	1.77740400	-1.79607700	0.20881200
C	2.71965200	-0.96757200	0.86172900
C	3.94557300	-1.51289500	1.19482700
H	1.13584500	-4.97765700	-0.85396200
H	5.18928300	-3.28441000	1.22147900
H	3.49152700	-4.75465800	0.18432300
C	0.99554500	-3.91679700	-0.66746500
H	4.69467900	-0.89826600	1.68547200
C	-0.29876100	-1.89216900	-0.83426400
C	-0.16281900	-3.27787900	-1.05630200
H	-1.18185200	-1.36186900	-1.16098800
H	-0.96734900	-3.81259600	-1.54840600
N	0.63513800	-1.17496000	-0.22734400
C	2.22812400	0.40403900	1.17751700
C	1.43658500	0.79607000	-2.16645900
C	2.24942500	1.67878600	-1.40666400
C	1.38986900	2.68616400	-0.84264300
C	0.07273500	1.28701700	-2.13503900
C	0.06051600	2.46427200	-1.34532200
H	3.01689600	1.15739300	1.20938000
H	1.71501300	0.38418300	2.14410600
C	1.84596900	3.86628500	-0.04220800
H	2.40462100	4.56223800	-0.67855900
H	1.00571800	4.41855400	0.38171300
H	2.50992600	3.57077300	0.77580900
C	3.74166200	1.61543400	-1.29993900
H	4.19474600	1.91841400	-2.25052100
H	4.11911100	2.28599300	-0.52591100
H	4.08790500	0.60293600	-1.07455300
C	1.94177400	-0.38018200	-2.94347100
H	2.27455500	-0.05878900	-3.93706400
H	2.79227900	-0.84773100	-2.44207400
H	1.17205000	-1.14168400	-3.08088300
C	-1.09462500	0.72354900	-2.89033600
H	-1.30751800	1.33804100	-3.77271800
H	-0.89367100	-0.28887300	-3.24492100
H	-2.00075600	0.69888300	-2.27774500
C	-1.12728200	3.32568600	-1.05160500
H	-1.01548700	4.30166500	-1.53640900

H	-2.04955900	2.87075500	-1.41573600
H	-1.23775600	3.49757400	0.02224400
Co	0.77029700	0.78824200	-0.13285000
N	-0.51481500	1.17305200	1.11755900
N	0.04859500	2.17032700	2.31473900
N	0.36925500	3.19464800	2.61927600
C	-2.67785900	-0.35122500	0.98037900
C	-3.00589600	-1.68998000	0.75399200
C	-3.39000300	0.68821200	0.37214400
C	-4.04961700	-1.98594100	-0.11982900
H	-2.44255100	-2.47491500	1.24628600
C	-4.41869700	0.36888900	-0.50965200
H	-3.13840000	1.72060500	0.58358600
C	-4.76701400	-0.96813200	-0.76822000
H	-4.31635100	-3.02383400	-0.29745900
H	-4.97311700	1.16799100	-0.99358700
S	-1.38655600	0.01466500	2.15378500
O	-1.91128000	0.80684800	3.26930400
O	-0.60208400	-1.19595400	2.40789400
C	-5.91411100	-1.29785100	-1.68827800
H	-5.79702300	-2.28560200	-2.14178700
H	-6.85758300	-1.30389100	-1.12938300
H	-6.01454100	-0.55855100	-2.48773000

³TS7', -3197.86574562, i540.55

C	-2.78230100	4.08638000	1.04446300
C	-1.66828900	4.47321500	0.32996600
C	-0.73424600	3.49846100	-0.11257300
C	-0.98684000	2.14074500	0.21545800
C	-2.09056500	1.75379500	1.01278400
C	-2.99888400	2.72764000	1.38926600
H	0.65309700	4.80322700	-1.15306000
H	-3.50193100	4.83208300	1.36654100
H	-1.50163800	5.51698400	0.08258800
C	0.41642500	3.77547000	-0.89321900
H	-3.86210100	2.45798100	1.99036200
C	0.86351200	1.41058400	-0.99901500
C	1.21798000	2.73790200	-1.31886500
H	1.46133800	0.57501200	-1.33944200
H	2.11275000	2.91298900	-1.90446800
N	-0.20698200	1.12554700	-0.27231300
C	-2.10729600	0.33358500	1.43416700
C	-2.07629500	-0.36792000	-1.87560300
C	-2.99191300	-0.92071400	-0.92908200

C	-2.47911600	-2.20231500	-0.51548100
C	-1.01470900	-1.31772600	-2.07917500
C	-1.28278400	-2.46090900	-1.27501200
H	-3.09078200	-0.08405400	1.63699800
H	-1.42774800	0.15651400	2.26541400
C	-3.22084100	-3.14340700	0.38304200
H	-4.17939500	-3.40909000	-0.07786700
H	-2.66287500	-4.05786400	0.57264700
H	-3.43827900	-2.68105400	1.35025700
C	-4.33496100	-0.35476600	-0.59314600
H	-5.01493800	-0.50599600	-1.43976200
H	-4.77651400	-0.84577900	0.27566400
H	-4.28666400	0.72015600	-0.39837600
C	-2.26037700	0.92875700	-2.59732900
H	-2.83209000	0.76040800	-3.51770400
H	-2.81258400	1.64779300	-1.98929600
H	-1.30629900	1.37966300	-2.87672100
C	0.13148900	-1.19673600	-3.03591000
H	-0.04183400	-1.83007300	-3.91405200
H	0.26023400	-0.17294600	-3.39056000
H	1.06960600	-1.52620500	-2.57803100
C	-0.47575300	-3.71992200	-1.33723200
H	-0.52683300	-4.12398400	-2.35499700
H	0.57894700	-3.53216900	-1.11606300
H	-0.83740300	-4.48276600	-0.65006100
Co	-1.01731500	-0.66446500	0.00892500
N	0.27727600	-1.33306300	1.18794300
N	0.42077500	-2.84864700	1.66247500
N	-0.42352300	-3.62073500	1.68629200
C	2.78153300	-0.21372900	0.90967700
C	3.41462400	1.02818000	0.86157000
C	3.16565300	-1.25526200	0.06120800
C	4.43723700	1.22927500	-0.06535800
H	3.09104900	1.82544700	1.52153500
C	4.18110700	-1.03194800	-0.86531500
H	2.67427400	-2.22070700	0.12015300
C	4.83408200	0.21048300	-0.94342100
H	4.93431800	2.19442800	-0.10707600
H	4.48280100	-1.83581500	-1.53127600
S	1.45750600	-0.45136900	2.09173100
O	1.92069200	-1.29591800	3.18919300
O	0.86378300	0.86480300	2.36361200
C	5.95994500	0.42535300	-1.92348000
H	6.08069800	1.48240800	-2.17521300

H	6.90851100	0.08085900	-1.49478500
H	5.80060100	-0.13462100	-2.84954300

⁵TS7', -3197.84101497, i513.10

C	2.92985900	3.97840000	-1.16677300
C	1.81658000	4.44413200	-0.50022800
C	0.80846100	3.53724000	-0.07334000
C	0.96238600	2.15638700	-0.37360700
C	2.07093900	1.69403800	-1.14680000
C	3.06359900	2.60569500	-1.48375200
H	-0.48743700	4.96775400	0.91641700
H	3.70792900	4.66989500	-1.47298800
H	1.70693100	5.50039700	-0.27411300
C	-0.32758900	3.91873800	0.68398700
H	3.92621600	2.26950100	-2.05128300
C	-0.93555800	1.59848100	0.84882300
C	-1.20589900	2.95389000	1.12873900
H	-1.58373800	0.81579500	1.22451700
H	-2.08781600	3.20914200	1.70471300
N	0.11383100	1.21214700	0.13694900
C	2.06407400	0.29856300	-1.60386900
C	2.12739300	-0.15807200	1.83236700
C	2.99794900	-0.83535700	0.92587800
C	2.52099200	-2.21893800	0.78763300
C	1.08611400	-1.06334300	2.18477700
C	1.33408100	-2.33709800	1.53505300
H	3.02316300	-0.11842800	-1.90191900
H	1.27048800	0.09501800	-2.32694700
C	3.25189100	-3.27082000	0.01787700
H	4.26071600	-3.39686200	0.42872600
H	2.74055400	-4.23134400	0.05239600
H	3.36256600	-2.99453300	-1.03629600
C	4.33756500	-0.34861300	0.48011600
H	5.05813300	-0.45694200	1.30057100
H	4.71610200	-0.92168600	-0.36861000
H	4.31318400	0.70985200	0.20752700
C	2.33575700	1.22218400	2.37198200
H	2.91616800	1.17859000	3.30138100
H	2.88803800	1.84830900	1.66876700
H	1.38989000	1.72003500	2.59648100
C	-0.06085200	-0.80672400	3.10571400
H	0.08647900	-1.34391500	4.05120700
H	-0.16875300	0.25349200	3.33928200
H	-1.00157900	-1.16909400	2.67738400

C	0.47913600	-3.54899300	1.74554000
H	0.48710200	-3.83538400	2.80328100
H	-0.56136200	-3.35053900	1.46911600
H	0.82343300	-4.40024400	1.15910700
Co	0.98719000	-0.73726800	-0.16336000
N	-0.42358700	-1.54557600	-1.15259500
N	-0.42754100	-3.11628200	-1.51216800
N	0.51859600	-3.75759400	-1.40841900
C	-2.85121900	-0.33630600	-0.86568700
C	-3.47134800	0.90942100	-0.96374100
C	-3.16740000	-1.22218000	0.16724900
C	-4.41067400	1.27419400	0.00044200
H	-3.19977400	1.58678600	-1.76586000
C	-4.09940700	-0.83556800	1.12792200
H	-2.68251500	-2.19100600	0.22418000
C	-4.73639400	0.41560200	1.06059100
H	-4.89672800	2.24321400	-0.07109100
H	-4.34688600	-1.51735400	1.93708400
S	-1.62251000	-0.77645100	-2.09207700
O	-2.17848400	-1.73528200	-3.04227500
O	-1.01476200	0.47892800	-2.56544300
C	-5.77307300	0.80581700	2.08414600
H	-5.85507100	1.89167000	2.18285100
H	-6.75976800	0.42960000	1.78902300
H	-5.54693000	0.38506600	3.06819600

¹²Mn, -2329.25440412

C	0.96655600	2.37229300	-0.81335400
C	-0.43152500	2.46295100	-0.51182700
C	-0.60840600	2.18679200	0.87647300
C	1.65369800	2.04522500	0.40494300
C	0.67280600	1.91695800	1.44618000
C	3.13544800	1.92040800	0.58090100
H	3.62219700	1.63338600	-0.35284500
H	3.56201700	2.87669500	0.90419000
H	3.38050900	1.17339900	1.33957200
C	0.98556500	1.60628500	2.87841800
H	1.67378100	0.75914400	2.94924900
H	1.46449100	2.46707500	3.35791000
H	0.08658900	1.36882800	3.45044500
C	-1.92401500	2.21007500	1.59245300
H	-1.89332100	1.64143100	2.52312000
H	-2.19424500	3.24240300	1.84214300
H	-2.72593300	1.80054000	0.97287200

C	-1.53838700	2.83137100	-1.45617600
H	-2.41366500	2.18930500	-1.32222600
H	-1.85638500	3.86400200	-1.27411500
H	-1.22439200	2.76267100	-2.49930900
C	1.62411100	2.59930200	-2.14126100
H	2.10709800	3.58214200	-2.16920100
H	2.38604700	1.83848900	-2.32766000
H	0.90434100	2.55966500	-2.96171000
C	3.36124400	-2.09824500	-0.26466300
C	2.85609600	-3.26677200	-1.14698400
H	2.56627800	-2.91281900	-2.14018000
H	3.65557600	-4.00426000	-1.26349400
H	1.99796900	-3.76814900	-0.68715700
C	4.55385400	-1.40101000	-0.95291200
H	4.27071300	-1.01153100	-1.93384500
H	4.93262000	-0.57305600	-0.34519200
H	5.36780300	-2.11923300	-1.08655100
C	3.75378200	-2.60670400	1.13057600
H	4.09585100	-1.78762100	1.77010700
H	2.91219800	-3.09555400	1.62805900
H	4.56841300	-3.33067800	1.03953500
C	2.21871800	-1.11374200	-0.15777700
O	1.55699300	-0.90127700	0.90858200
O	1.81630500	-0.42517700	-1.16729200
C	-3.52258100	-0.86790300	-2.21815200
C	-2.33048000	-0.72154200	-1.53357800
C	-2.32849000	-0.90391300	-0.12065800
C	-3.52534100	-1.32583300	0.54029700
C	-4.72544900	-1.45652900	-0.20677900
C	-4.72598800	-1.21238700	-1.55936700
H	-3.53041900	-0.73795800	-3.29655500
C	-3.46129800	-1.62078300	1.92415400
H	-5.63217600	-1.76084700	0.30703700
H	-5.64070200	-1.31016800	-2.13456200
C	-2.26210400	-1.50856800	2.58865600
C	-1.14037700	-1.02965900	1.88817400
H	-4.35938100	-1.94761300	2.44037500
H	-2.16594000	-1.75415800	3.64003800
H	-0.19416500	-0.88927800	2.39371900
N	-1.16578400	-0.70041400	0.59792000
C	-1.03619200	-0.48708900	-2.26040900
H	-0.49829000	0.41111300	-1.90477000
H	-0.36232300	-1.34394200	-2.18390900
H	-1.19694700	-0.27781400	-3.32075900

Mn	0.40721700	0.43132200	-0.10056200
³² Mn, -2329.2789057			
C	0.78374700	2.30815100	-1.15030400
C	-0.54389600	2.34518800	-0.63738100
C	-0.46941400	2.32356400	0.80547400
C	1.68349000	2.21836200	-0.02700800
C	0.89488300	2.27289800	1.18263300
C	3.17977200	2.16607500	-0.09408100
H	3.51610900	1.73003700	-1.03724300
H	3.60582200	3.17310200	-0.01863800
H	3.58729200	1.56684000	0.72359000
C	1.46202200	2.20201400	2.56625600
H	2.15975200	1.36387200	2.65334100
H	2.01271100	3.12083600	2.79567400
H	0.68280800	2.08179500	3.32101400
C	-1.66264100	2.36113200	1.71023900
H	-1.42107200	2.02314000	2.71911300
H	-2.04598000	3.38538900	1.78196900
H	-2.47218500	1.73400500	1.32718400
C	-1.82007000	2.48756600	-1.41258500
H	-2.58966400	1.79618500	-1.06063400
H	-2.21094400	3.50455200	-1.29445500
H	-1.67320600	2.31157200	-2.47912200
C	1.21277600	2.30441300	-2.58627700
H	1.75233100	3.22786200	-2.82219300
H	1.88138000	1.46219300	-2.78735500
H	0.36166400	2.23100100	-3.26534200
C	3.23510800	-2.25695800	-0.12286500
C	2.53281800	-3.51301000	0.45066100
H	1.67668000	-3.80467600	-0.16657100
H	3.24013000	-4.34734400	0.46322300
H	2.18617000	-3.33801800	1.47272600
C	3.71046800	-2.51513700	-1.56063100
H	2.87828100	-2.79364500	-2.21184700
H	4.19023100	-1.62874300	-1.98574200
H	4.43883900	-3.33096100	-1.56223400
C	4.41617300	-1.85344300	0.78519400
H	4.92134200	-0.96023900	0.40294700
H	4.08015900	-1.65265300	1.80524500
H	5.14694500	-2.66662100	0.81343100
C	2.21238900	-1.14365000	-0.09945800
O	1.80817800	-0.61966100	1.00047400
O	1.65657300	-0.67784000	-1.15647200
C	-3.64518900	-1.09591600	-2.03802400

C	-2.38875500	-0.94707700	-1.47317400
C	-2.29029700	-0.94939600	-0.04724500
C	-3.46707800	-1.20010000	0.73674100
C	-4.72834900	-1.33620100	0.10162700
C	-4.81639100	-1.26607600	-1.26709100
H	-3.72878500	-1.10283500	-3.12095100
C	-3.33457000	-1.33691500	2.13967900
H	-5.60780600	-1.51230100	0.71346100
H	-5.77476600	-1.37238800	-1.76454200
C	-2.09360100	-1.24025400	2.72442600
C	-0.99391100	-0.92449000	1.90985400
H	-4.21990800	-1.53638300	2.73695500
H	-1.94842600	-1.37417600	3.79017000
H	-0.00969100	-0.79862100	2.34585800
N	-1.07637900	-0.74200000	0.58807100
C	-1.17562800	-0.86094500	-2.36089700
H	-0.70181300	0.12498900	-2.33521200
H	-0.40969600	-1.58266400	-2.06977500
H	-1.44979000	-1.05299800	-3.40043100
Mn	0.49594300	0.49172600	-0.03066800

⁵²Mn, -2329.3038595

C	0.69560100	2.48089100	-0.99350600
C	-0.55944200	2.49942200	-0.39026400
C	-0.37023500	2.27610700	1.06125600
C	1.68125200	2.22079800	0.06077200
C	1.00885700	2.17390200	1.32739500
C	3.15700500	2.14345800	-0.15152200
H	3.39556000	1.65378400	-1.09883600
H	3.58538900	3.15376000	-0.18262200
H	3.64546800	1.59669400	0.65734100
C	1.68508100	1.96194600	2.65034800
H	2.30106400	1.05768800	2.63115900
H	2.33479600	2.80940100	2.89343600
H	0.95990300	1.86088900	3.46046500
C	-1.49850600	2.27732300	2.04321500
H	-1.20322200	1.85771900	3.00655700
H	-1.84502600	3.30350700	2.21789300
H	-2.35437700	1.70843100	1.66766200
C	-1.89468100	2.77108200	-1.01378100
H	-2.61900300	1.98161400	-0.78748100
H	-2.30901900	3.70900300	-0.62629900
H	-1.82453900	2.86264000	-2.09905800
C	1.04862400	2.65598500	-2.43988200

H	1.65351500	3.55835400	-2.58294600
H	1.63589500	1.80733000	-2.80666500
H	0.15922400	2.74826700	-3.06619200
C	3.52150600	-2.15584900	-0.28590500
C	3.14261300	-3.48027700	0.41518500
H	2.28547200	-3.95521800	-0.07407900
H	3.98625400	-4.17497600	0.36388900
H	2.89443600	-3.30979400	1.46562000
C	3.85579100	-2.40313000	-1.76375000
H	3.01062700	-2.85151100	-2.29269500
H	4.11454200	-1.47149900	-2.27428100
H	4.70884000	-3.08412100	-1.83792000
C	4.72206100	-1.50745900	0.44070900
H	5.00966400	-0.56327900	-0.03431800
H	4.48654400	-1.31375600	1.49018100
H	5.58347400	-2.18023700	0.39518200
C	2.33810600	-1.20928000	-0.14499800
O	1.90361000	-0.87243000	1.00234000
O	1.74858400	-0.71611400	-1.18129300
C	-3.82943400	-0.88273000	-2.10314800
C	-2.57651200	-0.77241100	-1.52391800
C	-2.47417000	-0.96781600	-0.11240700
C	-3.63622100	-1.34439800	0.63975300
C	-4.89522000	-1.43429200	-0.00768200
C	-4.98947400	-1.19137400	-1.35670200
H	-3.92098400	-0.74618900	-3.17683000
C	-3.48376200	-1.64305200	2.01536300
H	-5.76825400	-1.71058100	0.57556600
H	-5.94672200	-1.26185000	-1.86257200
C	-2.24011400	-1.57892600	2.60305300
C	-1.15412500	-1.14995500	1.82321400
H	-4.35667600	-1.93711800	2.59144900
H	-2.08477800	-1.83045800	3.64573500
H	-0.16296200	-1.05767800	2.25844100
N	-1.26097500	-0.82600100	0.53143000
C	-1.36330800	-0.51451700	-2.38157200
H	-0.97246600	0.50298000	-2.25602100
H	-0.55125800	-1.21759700	-2.17152600
H	-1.61408500	-0.61176200	-3.44016500
Mn	0.40176900	0.32973000	-0.05623200

¹TS4_Mn, -2675.95392664, i880.31

C	-0.02799200	0.35863800	2.31030500
C	-0.44355000	-1.00963100	2.23969600

C	-1.87272200	-1.02726100	2.13625200
C	-2.33067800	0.33203500	2.09759900
C	-1.18724600	1.18106800	2.20727400
C	2.10205000	3.81839100	-1.11008400
C	0.90177300	4.47074500	-1.30333200
C	-0.31346200	3.74385700	-1.22544000
C	-0.24796500	2.35154300	-0.91986600
C	0.99203500	1.66630600	-0.80904700
C	2.15317900	2.42159100	-0.88817600
H	-1.68390200	5.36289700	-1.67769000
H	3.03221600	4.37671000	-1.16528500
H	0.86939600	5.53572900	-1.51498300
C	-1.59785600	4.31039900	-1.42077600
H	3.10916400	1.91207000	-0.82536600
C	-2.57086000	2.17145400	-0.89899700
C	-2.71848300	3.51958800	-1.28834400
H	-3.42870300	1.53325600	-0.72819300
H	-3.71464300	3.91809300	-1.44739700
N	-1.38412100	1.61340100	-0.69312800
C	0.96729800	0.18586000	-0.69561900
H	1.18959800	-0.29379900	0.25391700
H	0.30726800	-0.33622000	-1.38448900
H	2.13085900	-0.22805000	-1.06160600
C	3.93547400	-0.98485400	-0.17183000
C	5.45876000	-1.26286600	-0.24318500
O	3.43325700	-0.50327800	-1.26516300
O	3.30386700	-1.21362100	0.87484600
C	-2.23444700	-1.80042100	-0.97349100
C	-2.89346700	-2.84644400	-1.85778600
O	-1.04349400	-1.94071400	-0.54781100
O	-2.81559500	-0.71376100	-0.64442800
C	1.36973000	0.85742900	2.53187700
H	1.54993800	1.79007300	1.99083200
H	1.51778400	1.06027400	3.60012900
H	2.12374800	0.13658500	2.20898700
C	-1.19554900	2.67959100	2.26496100
H	-1.28733200	3.02236600	3.30249500
H	-0.27307600	3.09912000	1.85772400
H	-2.03006300	3.10250100	1.70068100
C	-3.76679100	0.75697400	2.02187100
H	-4.26632200	0.61170700	2.98713800
H	-3.86118400	1.81276200	1.75775900
H	-4.30390900	0.16894600	1.27221900
C	-2.74705300	-2.24467500	2.13389400

H	-3.05550500	-2.50340200	3.15381700
H	-3.65090100	-2.07859300	1.54235200
H	-2.22032500	-3.10471000	1.71547700
C	0.44946600	-2.21368700	2.29640400
H	0.55996900	-2.56217500	3.33089600
H	0.02506100	-3.02984800	1.70682900
H	1.44368700	-1.99925900	1.89689400
C	5.95570600	-1.83035400	1.09229700
H	7.03287100	-2.03003300	1.04527800
H	5.76451000	-1.12937200	1.90957100
H	5.43691700	-2.76132700	1.33653200
C	5.71685100	-2.26809100	-1.38302400
H	5.22331600	-3.22519300	-1.17952800
H	5.33006400	-1.88048200	-2.32867100
H	6.79137400	-2.45899300	-1.49072800
C	6.17326200	0.06680600	-0.55869900
H	5.99910500	0.80304500	0.23522400
H	7.25573500	-0.08769800	-0.64075800
H	5.80547200	0.48372700	-1.49976400
C	-2.50895300	-4.25064800	-1.35611700
H	-2.90457500	-4.43118200	-0.35113900
H	-2.92492300	-5.01076800	-2.02534400
H	-1.42365800	-4.36882700	-1.32130000
C	-4.41848800	-2.66126100	-1.85098700
H	-4.88439300	-3.39691900	-2.51453800
H	-4.82821600	-2.80149800	-0.84551200
H	-4.69603500	-1.66034300	-2.19042300
C	-2.33212200	-2.62612700	-3.28333000
H	-2.57948400	-1.62539900	-3.65260400
H	-1.24455400	-2.74131200	-3.29507700
H	-2.76649200	-3.36072600	-3.96949100
Mn	-1.13650800	-0.12569200	0.37006700

³TS4_Mn, -2675.96841211, i906.57

C	0.26200000	0.23809600	2.40653100
C	-0.22028400	-1.11514500	2.29183700
C	-1.65373100	-1.05768000	2.27658800
C	-2.05455100	0.32009900	2.30952700
C	-0.85704400	1.11134200	2.38873700
C	2.08500600	3.74820100	-1.30505900
C	0.87590800	4.40081000	-1.41376000
C	-0.33083000	3.67737800	-1.22750800
C	-0.24529500	2.29006400	-0.90803700
C	0.99994400	1.59940000	-0.88472600

C	2.14981200	2.35282000	-1.06569200
H	-1.72756600	5.29441000	-1.58550000
H	3.00974600	4.30126700	-1.44158000
H	0.82843400	5.46233400	-1.63929000
C	-1.62542100	4.24438900	-1.32354300
H	3.10786400	1.84272800	-1.06895000
C	-2.56886500	2.12315400	-0.68804200
C	-2.73889500	3.46452100	-1.08900600
H	-3.40322500	1.47709700	-0.43888100
H	-3.74139900	3.86928000	-1.17297300
N	-1.36664300	1.56905600	-0.57861700
C	1.00212400	0.11427100	-0.73881000
H	1.27957400	-0.35350200	0.20752700
H	0.33236900	-0.44259400	-1.39396100
H	2.16246800	-0.28604800	-1.14155900
C	3.97526100	-1.09504000	-0.34607700
C	5.50534900	-1.31808200	-0.43529500
O	3.45258300	-0.55125100	-1.39977500
O	3.34940200	-1.42168300	0.67846900
C	-2.93917300	-1.47738700	-0.95497900
C	-3.29228700	-2.59642600	-1.95153900
O	-1.65969300	-1.41207800	-0.67272300
O	-3.79374200	-0.72795700	-0.47334800
C	1.69442500	0.66570200	2.53532800
H	1.88871900	1.57906500	1.96500400
H	1.91741600	0.88058500	3.58796600
H	2.38733800	-0.09912000	2.17960100
C	-0.79820200	2.60922100	2.44967500
H	-0.86584200	2.95608800	3.48766600
H	0.13731900	2.98824800	2.03208500
H	-1.62073100	3.06601000	1.89366000
C	-3.46441400	0.82555600	2.37577500
H	-3.85714200	0.73728100	3.39628700
H	-3.52197900	1.87974400	2.09344900
H	-4.10957300	0.25919900	1.70178700
C	-2.57980500	-2.23580900	2.23946800
H	-2.77873100	-2.59243100	3.25729500
H	-3.53000900	-1.97312800	1.77223700
H	-2.14295100	-3.06101300	1.67334500
C	0.62067500	-2.35893500	2.30018900
H	0.83126200	-2.67222600	3.33077500
H	0.09883000	-3.18207900	1.80538200
H	1.57287600	-2.20506700	1.78715300
C	6.02469700	-1.94618200	0.86412600

H	7.10663500	-2.11219200	0.80182900
H	5.81927100	-1.29809900	1.72085400
H	5.53347300	-2.90364100	1.05699900
C	5.78984600	-2.24760700	-1.63206700
H	5.32810700	-3.23011300	-1.48272500
H	5.38718100	-1.81886300	-2.55308200
H	6.86934400	-2.39715700	-1.75316700
C	6.17751500	0.04892400	-0.67493000
H	5.98033900	0.73441700	0.15808700
H	7.26414600	-0.06731400	-0.76302800
H	5.79808700	0.50579300	-1.59251000
C	-2.84877300	-3.94457700	-1.34503200
H	-3.37498500	-4.14480600	-0.40486000
H	-3.07779900	-4.76134800	-2.03815300
H	-1.77419100	-3.94638500	-1.14620600
C	-4.80418400	-2.60236800	-2.21382800
H	-5.05873300	-3.39905500	-2.92122600
H	-5.36261100	-2.76643800	-1.28820300
H	-5.13400500	-1.64717300	-2.63113000
C	-2.52052100	-2.33894200	-3.26292100
H	-2.80469900	-1.37675200	-3.70371100
H	-1.44230300	-2.33070800	-3.08537500
H	-2.74837700	-3.12351500	-3.99279400
Mn	-0.94030300	-0.10884100	0.49830500

⁵TS4_Mn, -2675.99186817, i1291.74

C	0.08932200	0.25567500	2.32932000
C	-0.38925400	-1.08558600	2.33022000
C	-1.80762500	-1.01785700	2.28280500
C	-2.21946700	0.38991200	2.32802600
C	-1.06811200	1.16461500	2.34889900
C	2.51428700	3.69268200	-0.99518600
C	1.38269800	4.46680900	-1.13414700
C	0.10736100	3.84736100	-1.11886100
C	0.03098500	2.42845000	-0.96153700
C	1.21113500	1.61902000	-0.90098200
C	2.43105200	2.28375300	-0.89367900
H	-1.08789600	5.63736700	-1.36001400
H	3.49366700	4.16234500	-0.99526700
H	1.44876900	5.54508900	-1.24868200
C	-1.11410300	4.55974000	-1.21921800
H	3.34042800	1.69291300	-0.85747300
C	-2.30084900	2.49904900	-0.88780900
C	-2.31518700	3.88997100	-1.12627000

H	-3.21295400	1.92827900	-0.74302500
H	-3.26259400	4.41249100	-1.20259900
N	-1.17622500	1.80475800	-0.80393900
C	1.12304300	0.13233300	-0.88441200
H	1.33565400	-0.40894000	0.04102100
H	0.44974600	-0.34149500	-1.60149000
H	2.32624000	-0.32716100	-1.25450100
C	3.96134300	-1.25646000	-0.31066800
C	5.45700400	-1.65171900	-0.33582300
O	3.54608100	-0.69092500	-1.40750300
O	3.26323500	-1.47052600	0.69258200
C	-2.75255900	-1.54267700	-1.04978000
C	-3.61981200	-2.51017900	-1.85929700
O	-1.51593900	-1.84927000	-0.86599900
O	-3.21392100	-0.47207600	-0.56948400
C	1.50716100	0.70707400	2.48709900
H	1.70450300	1.60783600	1.89813800
H	1.69681500	0.96021600	3.53945100
H	2.22141000	-0.05883600	2.17925400
C	-0.95092800	2.65649600	2.41177000
H	-0.63237600	2.98403400	3.40934400
H	-0.20739700	3.02817700	1.70020900
H	-1.90062500	3.14611900	2.18550400
C	-3.64759700	0.84162300	2.32401600
H	-4.16450100	0.52113300	3.23699000
H	-3.72332200	1.93013100	2.26555700
H	-4.18134000	0.41502700	1.46940100
C	-2.76237600	-2.16846400	2.28051900
H	-3.12349000	-2.37463400	3.29679800
H	-3.63331900	-1.94519500	1.65864300
H	-2.29163700	-3.07727600	1.90045300
C	0.44973700	-2.33308900	2.34622300
H	0.64067700	-2.66518800	3.37451400
H	-0.05746200	-3.14977200	1.82459600
H	1.41432700	-2.17673600	1.85685200
C	5.84929300	-2.30398600	0.99595100
H	6.90779700	-2.58855900	0.98222700
H	5.68195000	-1.61856200	1.83145400
H	5.24857700	-3.19792700	1.18397400
C	5.68125800	-2.63478200	-1.50237600
H	5.10294100	-3.55396300	-1.35642100
H	5.37176000	-2.18443800	-2.44862600
H	6.74031900	-2.90985200	-1.57095100
C	6.28749800	-0.37351300	-0.57152500

H	6.13784200	0.34693400	0.24147700
H	7.35614900	-0.61420800	-0.61345300
H	5.99840700	0.10407100	-1.51112300
C	-3.54569300	-3.89873000	-1.19020100
H	-3.95561500	-3.86908700	-0.17462900
H	-4.12879400	-4.62377200	-1.76806300
H	-2.51104400	-4.24468000	-1.13227900
C	-5.07170300	-2.01571000	-1.91057400
H	-5.68354500	-2.71133900	-2.49487900
H	-5.49778900	-1.94052700	-0.90587900
H	-5.13395800	-1.02602800	-2.37072600
C	-3.02496800	-2.58811200	-3.28226700
H	-3.05792600	-1.61061400	-3.77595400
H	-1.98492300	-2.92159600	-3.24823700
H	-3.60155000	-3.29361700	-3.89026700
Mn	-0.99774600	-0.16325100	0.21192300

¹⁵Mn, -2675.98630866

C	0.06056600	0.09302600	2.25575600
C	-0.50295300	-1.21690200	2.13482900
C	-1.92377100	-1.08341800	2.14080700
C	-2.23565300	0.31795200	2.23425400
C	-1.00852900	1.03716100	2.30632600
C	2.32180200	3.49859100	-1.05961700
C	1.20295800	4.28683800	-1.23856600
C	-0.08957400	3.70751800	-1.13591200
C	-0.17195200	2.31796400	-0.84209300
C	0.97849400	1.48981800	-0.73958800
C	2.21882800	2.10527900	-0.82175100
H	-1.29778700	5.47272000	-1.51079000
H	3.30889600	3.94863900	-1.12435600
H	1.29433100	5.35006400	-1.44175000
C	-1.31222300	4.41266700	-1.27159200
H	3.12125400	1.50787900	-0.74111400
C	-2.49107700	2.37502300	-0.73578200
C	-2.50322800	3.74071300	-1.09398100
H	-3.40510200	1.82609900	-0.54517800
H	-3.45617400	4.24872000	-1.19969500
N	-1.36326700	1.68797300	-0.58871400
C	0.65632200	0.05672000	-0.54381000
H	1.44374100	-0.51962200	-0.05846300
H	0.36921000	-0.41372500	-1.49174800
H	2.67162300	-0.94107400	-1.37213800
C	4.18399800	-1.35242300	-0.30930300

C	5.70671600	-1.21496600	-0.29567600
O	3.64345300	-0.91049900	-1.46569700
O	3.51228100	-1.78119000	0.60934100
C	-2.55924500	-1.54913500	-1.02331100
C	-3.40989600	-2.43513700	-1.92870400
O	-1.35114200	-1.83865200	-0.76924600
O	-3.01601200	-0.47476100	-0.51013600
C	1.51186200	0.42573200	2.43705700
H	1.79290000	1.32557100	1.88317800
H	1.71786400	0.61311700	3.49845700
H	2.16337500	-0.38549300	2.10900000
C	-0.84923200	2.52303400	2.44509100
H	-0.84236100	2.82203300	3.50047400
H	0.08742800	2.86453300	1.99737100
H	-1.66307200	3.06260100	1.95330400
C	-3.61976900	0.89476900	2.27479100
H	-4.07419400	0.76230200	3.26442800
H	-3.61356300	1.96576000	2.05643300
H	-4.26263500	0.40419300	1.53840300
C	-2.92099800	-2.20299300	2.10668400
H	-3.20463300	-2.51280000	3.12008600
H	-3.83039900	-1.90124600	1.58074200
H	-2.51148600	-3.07654300	1.59375300
C	0.25977600	-2.50345900	2.01441100
H	0.36801100	-2.99585000	2.98906700
H	-0.25970200	-3.19059700	1.34137300
H	1.25947600	-2.34013200	1.60619600
C	6.24711400	-1.78679900	1.02201500
H	7.33694600	-1.68756800	1.05107300
H	5.82418300	-1.25992600	1.88129800
H	5.99044800	-2.84452800	1.12547300
C	6.29790200	-1.97733500	-1.50034200
H	6.05994000	-3.04481900	-1.44604200
H	5.91002700	-1.58656100	-2.44402200
H	7.38810700	-1.87421700	-1.50201500
C	6.04726800	0.28854900	-0.40880100
H	5.61045600	0.85468600	0.42129700
H	7.13326900	0.42457300	-0.37517900
H	5.67416600	0.70699800	-1.34710000
C	-3.20911100	-3.90607700	-1.51686500
H	-3.57495100	-4.08179600	-0.49971700
H	-3.76263000	-4.56470500	-2.19482600
H	-2.15097500	-4.17583700	-1.54900800
C	-4.89049100	-2.04105400	-1.82641200

H	-5.49130500	-2.66838600	-2.49365400
H	-5.26256700	-2.17155000	-0.80548000
H	-5.03900300	-0.99434400	-2.10340100
C	-2.89704500	-2.22233100	-3.37138900
H	-3.01528500	-1.17790200	-3.67950000
H	-1.83858600	-2.48635300	-3.44755700
H	-3.46450400	-2.84957000	-4.06762200
Mn	-1.19454700	-0.10665200	0.39538800

³⁵Mn, -2676.0028754

C	0.53844600	-0.51663600	2.02788500
C	-0.16817000	-1.72951400	1.73980100
C	-1.54599100	-1.50614300	2.07290300
C	-1.69963800	-0.15995800	2.51468500
C	-0.41116600	0.45923000	2.46607300
C	2.27611900	3.56312100	-1.07619500
C	1.17040400	4.37301700	-0.92129300
C	-0.10236300	3.78731600	-0.68733200
C	-0.18290100	2.36855100	-0.62180200
C	0.94267700	1.52836300	-0.87297500
C	2.16847900	2.14965000	-1.06188000
H	-1.28721800	5.59836200	-0.53437800
H	3.25168000	4.01351300	-1.23851300
H	1.25856000	5.45504200	-0.95898300
C	-1.30226300	4.51299900	-0.47879300
H	3.04915000	1.54271200	-1.24422600
C	-2.45135500	2.42864900	-0.07536100
C	-2.47102700	3.83402300	-0.20254600
H	-3.32934400	1.84893900	0.18784100
H	-3.40571300	4.36279100	-0.04902200
N	-1.33912200	1.72391000	-0.25823400
C	0.65472500	0.07083700	-0.87064300
H	1.52873000	-0.55704200	-0.70468700
H	0.12946100	-0.23898300	-1.78220000
H	2.98436900	-0.87056900	-2.31182700
C	4.17962100	-1.43323400	-0.96762200
C	5.54828300	-1.11751700	-0.36735400
O	3.89157800	-0.65065500	-2.03644300
O	3.40238700	-2.27109500	-0.55680700
C	-3.30040400	-0.97642000	-0.87976900
C	-4.01885600	-1.77011300	-1.99149400
O	-2.01168900	-1.15162000	-0.85347300
O	-3.92688200	-0.25356000	-0.09076000
C	2.02376600	-0.30825200	1.97083300

H	2.28188000	0.63826700	1.48451700
H	2.43971700	-0.28141700	2.98587500
H	2.51831100	-1.11229800	1.42503400
C	-0.08915700	1.87781000	2.84118300
H	0.14086700	1.96444400	3.91029000
H	0.77646800	2.24697000	2.28432300
H	-0.92646600	2.54777300	2.62743800
C	-2.98330600	0.48801700	2.94503800
H	-3.22760900	0.23094500	3.98328800
H	-2.91436800	1.57788200	2.88602600
H	-3.80766000	0.17309700	2.30197200
C	-2.64380800	-2.52052300	1.95218400
H	-2.72270400	-3.11582000	2.87042100
H	-3.60536100	-2.03812600	1.76868600
H	-2.45207000	-3.20663900	1.12407300
C	0.42765400	-3.02314300	1.26610500
H	0.66527300	-3.68819400	2.10678600
H	-0.27173800	-3.55284800	0.61313900
H	1.34530300	-2.85736900	0.69787200
C	5.77089300	-2.01702200	0.85659300
H	6.75891200	-1.82096800	1.28487100
H	5.01625400	-1.82982800	1.62539900
H	5.71063100	-3.07377600	0.58437100
C	6.63077100	-1.38111800	-1.43704500
H	6.63198900	-2.43145800	-1.74639500
H	6.47001100	-0.76093500	-2.32242100
H	7.61807200	-1.14916300	-1.02452300
C	5.57396300	0.37010800	0.04869100
H	4.77583700	0.59593900	0.76339300
H	6.53198500	0.59907300	0.52661600
H	5.45613100	1.02566900	-0.81764400
C	-3.72297600	-3.27062100	-1.79101200
H	-4.10780500	-3.62053000	-0.82651000
H	-4.20439300	-3.86111400	-2.57895500
H	-2.64677600	-3.45864100	-1.81910200
C	-5.53032600	-1.51416900	-1.92696000
H	-6.04284900	-2.07694400	-2.71546200
H	-5.93759200	-1.81901300	-0.95913000
H	-5.75333800	-0.45149400	-2.05475000
C	-3.45574000	-1.30925500	-3.35167600
H	-3.64150200	-0.24092800	-3.51111400
H	-2.37731200	-1.47977600	-3.40042200
H	-3.93641300	-1.86023500	-4.16825500
Mn	-0.92675100	-0.15870200	0.40449800

⁵⁵Mn, -2676.02532901

C	0.52006900	-0.38853500	1.95856000
C	-0.20174000	-1.63359100	1.93514900
C	-1.55560600	-1.33880500	2.20898100
C	-1.67490300	0.08319700	2.47077300
C	-0.40196200	0.66183000	2.33886400
C	2.48304400	3.53875900	-0.97152700
C	1.43196900	4.41460000	-0.80452300
C	0.11101900	3.90777600	-0.67996000
C	-0.08904300	2.49888700	-0.74704600
C	0.99579400	1.59656900	-0.99989200
C	2.27022600	2.14112500	-1.07256500
H	-0.92449100	5.79168100	-0.39859400
H	3.49681800	3.92220500	-1.04746600
H	1.59876200	5.48656900	-0.74732800
C	-1.03373600	4.71095500	-0.44351200
H	3.11640800	1.48378500	-1.24736700
C	-2.35562300	2.70624500	-0.26898200
C	-2.26398400	4.11741500	-0.25608500
H	-3.28532200	2.18120500	-0.07167900
H	-3.15336100	4.71051800	-0.07078800
N	-1.30737400	1.93385400	-0.49890200
C	0.67116500	0.15659500	-1.13286600
H	1.52008100	-0.51187300	-0.99660700
H	0.13527500	-0.07063300	-2.06243500
H	3.09125300	-0.88817600	-2.44782300
C	4.09050200	-1.56108500	-0.99782600
C	5.42685200	-1.39056600	-0.27818700
O	3.97844200	-0.74400100	-2.07558000
O	3.19799500	-2.31758800	-0.67215100
C	-3.19210300	-1.10332800	-0.95350700
C	-4.21197800	-1.91235500	-1.77038900
O	-1.94972300	-1.44934300	-1.08850400
O	-3.54022000	-0.17666300	-0.19441600
C	2.00874600	-0.23363200	1.86781800
H	2.28559100	0.69657500	1.36210600
H	2.45682400	-0.20861100	2.87032400
H	2.45849200	-1.06200200	1.31896900
C	-0.02299600	2.09697500	2.56374300
H	0.27940600	2.27271500	3.60430000
H	0.81533600	2.39342000	1.92721400
H	-0.85369600	2.77374600	2.34424900
C	-2.95607600	0.77984300	2.82018900

H	-3.26098900	0.55960400	3.85145100
H	-2.85552600	1.86533700	2.73264100
H	-3.76102500	0.46256200	2.15236800
C	-2.70171200	-2.30574900	2.25232200
H	-2.96436100	-2.56797800	3.28539100
H	-3.58879900	-1.87148600	1.78318200
H	-2.46259000	-3.23264900	1.72502600
C	0.39058600	-2.97867100	1.61724800
H	0.76559000	-3.47659600	2.52118300
H	-0.35243200	-3.64029400	1.16289400
H	1.22649200	-2.89501100	0.91678800
C	5.45782600	-2.32360600	0.94058400
H	6.42267800	-2.23378800	1.44953900
H	4.66689600	-2.07163800	1.65184700
H	5.31536000	-3.36532500	0.64212000
C	6.56482700	-1.74747400	-1.26000100
H	6.48787800	-2.78824200	-1.59140700
H	6.54305300	-1.10209700	-2.14161900
H	7.53134000	-1.62241000	-0.76112200
C	5.56289300	0.08241600	0.16807800
H	4.74073300	0.37362800	0.82927800
H	6.50149500	0.21209200	0.71653800
H	5.56987000	0.75702400	-0.69174300
C	-4.10236300	-3.38980600	-1.33780700
H	-4.34513400	-3.50663400	-0.27587000
H	-4.80214800	-4.00507500	-1.91453800
H	-3.08842000	-3.76388800	-1.49946300
C	-5.63134900	-1.38709300	-1.51779600
H	-6.35729400	-1.96821200	-2.09751700
H	-5.89299000	-1.45947000	-0.45859000
H	-5.71715900	-0.33568200	-1.80573900
C	-3.84713600	-1.78167400	-3.26340400
H	-3.90933400	-0.73825900	-3.59258000
H	-2.82984800	-2.13756200	-3.44353200
H	-4.54046100	-2.37026600	-3.87486100
Mn	-0.91519300	-0.24753200	0.15240700

²²Fe, -2441.9998331

C	0.81987600	2.28700500	-1.11338300
C	-0.52579300	2.32705800	-0.63924600
C	-0.49326000	2.28083900	0.79922700
C	1.68730000	2.18293100	0.03094300
C	0.86533900	2.21251200	1.21554200
C	3.18277600	2.11541500	0.00237800

H	3.53745300	1.67635400	-0.93260000
H	3.61600100	3.11828300	0.08927600
H	3.56251400	1.51142300	0.82947800
C	1.38770600	2.11175400	2.61449700
H	2.08893500	1.27679500	2.70160800
H	1.92175300	3.02907300	2.88519400
H	0.58543400	1.96522200	3.33978000
C	-1.70739600	2.31361600	1.67498900
H	-1.49897200	1.93418500	2.67634500
H	-2.06790900	3.34383500	1.77430200
H	-2.51995600	1.71922900	1.24954900
C	-1.77481100	2.49271100	-1.45146000
H	-2.56393500	1.81162500	-1.12469500
H	-2.15208200	3.51553500	-1.33926300
H	-1.59950700	2.31873700	-2.51386200
C	1.28770600	2.28831400	-2.53610000
H	1.86637700	3.19479400	-2.74272500
H	1.93142300	1.42463300	-2.72732600
H	0.45439900	2.25368800	-3.23957300
C	3.21970600	-2.22347500	-0.15380200
C	2.54643900	-3.50804700	0.38923000
H	1.69632100	-3.80321700	-0.23456500
H	3.27132400	-4.32724500	0.38273900
H	2.19547000	-3.36461500	1.41475000
C	3.69758300	-2.43525700	-1.59840100
H	2.86940400	-2.71195600	-2.25563600
H	4.16015500	-1.52932700	-2.00093900
H	4.44072700	-3.23728200	-1.62282500
C	4.39426000	-1.81758300	0.76145900
H	4.88031000	-0.90534000	0.39980300
H	4.05584300	-1.64763800	1.78644300
H	5.14203700	-2.61562100	0.77044300
C	2.17353900	-1.13257000	-0.10233600
O	1.75066300	-0.64789700	1.00487100
O	1.62072600	-0.63650100	-1.14487900
C	-3.62588500	-1.04032100	-2.05436600
C	-2.36945300	-0.91278100	-1.48408600
C	-2.27461600	-0.93358000	-0.05711800
C	-3.45501400	-1.19849000	0.71762700
C	-4.71563500	-1.31209500	0.07701200
C	-4.80084400	-1.21157300	-1.28989000
H	-3.70585500	-1.03328400	-3.13757800
C	-3.32775500	-1.37463300	2.11688800
H	-5.59705300	-1.49746700	0.68329400

H	-5.75896800	-1.30018200	-1.79133700
C	-2.08774600	-1.29993000	2.70445100
C	-0.98663500	-0.95691700	1.90157800
H	-4.21548200	-1.58624600	2.70626600
H	-1.94319900	-1.46471300	3.76599800
H	-0.00713000	-0.83048400	2.34627100
N	-1.06333800	-0.73762300	0.58700700
C	-1.15422900	-0.84486600	-2.37116900
H	-0.66471300	0.13227500	-2.35020500
H	-0.39973000	-1.57514200	-2.07332300
H	-1.43129600	-1.03949400	-3.40948500
Fe	0.48243100	0.50853400	-0.00851400

⁴²Fe, -2441.99981471

C	0.66684800	2.42447700	-1.04215000
C	-0.58390600	2.44826300	-0.41609600
C	-0.36694300	2.29319500	1.04211500
C	1.66670200	2.20516000	0.00663600
C	1.00981000	2.19749600	1.28882900
C	3.13886100	2.11789800	-0.21322500
H	3.37009900	1.67553900	-1.18437100
H	3.57920300	3.12336200	-0.18822700
H	3.61657200	1.52290500	0.56769200
C	1.70880900	2.01613600	2.60174200
H	2.30105700	1.09641900	2.59610200
H	2.38499500	2.85494600	2.79827600
H	1.00040200	1.96164900	3.43065500
C	-1.48198200	2.30117100	2.03534200
H	-1.16498400	1.92817400	3.01042800
H	-1.85502000	3.32406400	2.17064500
H	-2.32443400	1.69480200	1.69001400
C	-1.92887800	2.70055700	-1.02513900
H	-2.65299300	1.93062100	-0.74147900
H	-2.32422300	3.66277700	-0.67965000
H	-1.88084300	2.73301400	-2.11479700
C	0.99600400	2.58316400	-2.49639700
H	1.56183800	3.50633000	-2.66341200
H	1.60839800	1.74922200	-2.85337100
H	0.09522100	2.62899900	-3.11132600
C	3.40082500	-2.20409900	-0.24043100
C	2.94787000	-3.48297800	0.50030000
H	2.05689900	-3.91564500	0.03261600
H	3.74527400	-4.23102700	0.46052300
H	2.72266400	-3.26840600	1.54793400

C	3.70143700	-2.51208100	-1.71421400
H	2.82405900	-2.92215700	-2.22123100
H	4.01025800	-1.61240000	-2.25361500
H	4.51067900	-3.24557200	-1.77845000
C	4.64683000	-1.61217800	0.45602100
H	4.98588300	-0.70001400	-0.04716700
H	4.43522200	-1.37611600	1.50186900
H	5.46555400	-2.33687100	0.42067500
C	2.27800000	-1.18356500	-0.11109900
O	1.89418700	-0.76804400	1.02013100
O	1.68366000	-0.71310700	-1.16045000
C	-3.77890500	-0.97525800	-2.05740300
C	-2.52085900	-0.81651200	-1.50055400
C	-2.39254400	-0.95629000	-0.08476900
C	-3.53603700	-1.33137000	0.69583800
C	-4.80188000	-1.47247500	0.07103100
C	-4.92148000	-1.28136000	-1.28419200
H	-3.88748300	-0.88012300	-3.13397200
C	-3.36012400	-1.57802500	2.07908800
H	-5.65964700	-1.74693000	0.67740000
H	-5.88396000	-1.39119900	-1.77282500
C	-2.11052700	-1.46768100	2.64544300
C	-1.04371200	-1.04191300	1.83735100
H	-4.21919800	-1.87002600	2.67670300
H	-1.93541600	-1.67947900	3.69387900
H	-0.04966000	-0.91186000	2.25052900
N	-1.17326700	-0.76130600	0.53744000
C	-1.32652900	-0.56834000	-2.38518100
H	-0.93084300	0.44924700	-2.27823000
H	-0.50947400	-1.26587000	-2.17967000
H	-1.59800000	-0.67640200	-3.43761400
Fe	0.39022500	0.40561700	-0.14074600

⁶²Fe, -2441.99203713

C	0.78638200	2.41292900	-0.95418400
C	-0.56688800	2.43524300	-0.45100100
C	-0.51957600	2.23680600	0.96314200
C	1.65791700	2.22598100	0.15662700
C	0.85119600	2.10430400	1.34457300
C	3.15396900	2.17332400	0.11554900
H	3.51487600	1.80872000	-0.84928600
H	3.58057500	3.17160100	0.27219800
H	3.54799700	1.51964400	0.89729600
C	1.39566900	1.88445900	2.72193900

H	2.07995300	1.02988300	2.73626200
H	1.95779300	2.76294100	3.05920400
H	0.60233100	1.70114300	3.44961700
C	-1.71601800	2.22712400	1.86623400
H	-1.50850100	1.72653900	2.81443600
H	-2.03508600	3.25024200	2.09804900
H	-2.56586100	1.72037500	1.39882300
C	-1.81576400	2.71475900	-1.23241600
H	-2.61929400	2.01454700	-0.98254700
H	-2.18419200	3.72220400	-1.00470700
H	-1.64732500	2.66620800	-2.31003800
C	1.21911200	2.61036500	-2.37729900
H	1.56697300	3.63755500	-2.53776200
H	2.04091800	1.93711100	-2.63674300
H	0.40410900	2.42708300	-3.08150800
C	3.59003700	-2.06700400	-0.23556100
C	3.16100100	-3.43309400	0.35233500
H	2.36706900	-3.89068300	-0.24729100
H	4.01828400	-4.11255200	0.35042800
H	2.80594200	-3.32435100	1.38028800
C	4.07841700	-2.23046300	-1.68213800
H	3.30263000	-2.66464000	-2.31790100
H	4.36843500	-1.26882800	-2.11452900
H	4.94971500	-2.89147900	-1.70054000
C	4.69478700	-1.44399000	0.64707500
H	5.01820500	-0.47571700	0.25155200
H	4.34678100	-1.30396100	1.67339900
H	5.56421900	-2.10745900	0.66191200
C	2.37474300	-1.16031300	-0.17945400
O	1.85531200	-0.82650600	0.94397900
O	1.81564000	-0.69967900	-1.24144700
C	-3.78006400	-0.93188700	-2.12984300
C	-2.54123700	-0.81481100	-1.52428600
C	-2.47206900	-0.96890200	-0.10720100
C	-3.64977200	-1.31264500	0.63307700
C	-4.89488500	-1.41358000	-0.03984600
C	-4.95757100	-1.21090400	-1.39770100
H	-3.84802900	-0.82422100	-3.20851200
C	-3.52268300	-1.56559200	2.02050300
H	-5.78343800	-1.66392500	0.53152000
H	-5.90468700	-1.28874200	-1.92119000
C	-2.28890800	-1.48488700	2.62811100
C	-1.18645200	-1.08925700	1.85371400
H	-4.40663400	-1.83533100	2.59154300

H	-2.15488600	-1.69819000	3.68219700
H	-0.20368500	-0.97765800	2.30304100
N	-1.27012600	-0.81553900	0.55022500
C	-1.29792900	-0.59945800	-2.34772200
H	-0.84322800	0.38647900	-2.17344200
H	-0.53914900	-1.36478600	-2.15582000
H	-1.52574800	-0.62562700	-3.41564900
Fe	0.41291200	0.26781100	-0.10890300

²TS4_Fe, -2788.6864875, i740.90

C	0.22797800	0.18778300	2.40487700
C	-0.24996000	-1.16529200	2.23893000
C	-1.68138200	-1.12360100	2.22626000
C	-2.08690000	0.25075500	2.30739600
C	-0.89727500	1.05227000	2.41493600
C	2.10241000	3.72317200	-1.33881200
C	0.89286100	4.37798000	-1.43417000
C	-0.31260000	3.66330200	-1.21221300
C	-0.22409800	2.28278400	-0.86737800
C	1.01759300	1.58976300	-0.85673700
C	2.16750200	2.33261300	-1.07610000
H	-1.71192600	5.27683500	-1.58265700
H	3.02562900	4.27048500	-1.50543600
H	0.84444800	5.43506100	-1.67957600
C	-1.60796500	4.23152200	-1.30354800
H	3.12230300	1.81669600	-1.09381500
C	-2.54451500	2.11815400	-0.62908300
C	-2.71756100	3.45449900	-1.04922700
H	-3.37756200	1.47213100	-0.37536700
H	-3.72162800	3.85509500	-1.13464200
N	-1.34201700	1.56806200	-0.51375700
C	1.01215100	0.10559600	-0.70032100
H	1.30234900	-0.33698100	0.25182700
H	0.30688200	-0.44568800	-1.32077200
H	2.12770500	-0.30577100	-1.12430600
C	3.99077900	-1.08385800	-0.32990500
C	5.52576000	-1.28341300	-0.41707200
O	3.45683600	-0.58061200	-1.39459700
O	3.37692800	-1.39283500	0.70933000
C	-2.91007900	-1.43215100	-0.98086000
C	-3.26344500	-2.52402000	-2.01120200
O	-1.63581100	-1.34668600	-0.72635300
O	-3.77787100	-0.71775200	-0.46025200
C	1.65469200	0.62195700	2.56320200

H	1.84946800	1.54555600	2.00980900
H	1.85617400	0.82304600	3.62285000
H	2.36075000	-0.13073500	2.20732500
C	-0.85037800	2.54667300	2.52820100
H	-0.91723600	2.85697000	3.57761700
H	0.08128200	2.94503000	2.12043500
H	-1.67758400	3.01502800	1.98938300
C	-3.49946100	0.74464100	2.38095900
H	-3.89263800	0.61342800	3.39655000
H	-3.56347300	1.80826600	2.13952900
H	-4.13378200	0.19664800	1.68274000
C	-2.59557500	-2.30747400	2.15152000
H	-2.77760800	-2.70977100	3.15530400
H	-3.55189800	-2.03445800	1.70426000
H	-2.15586800	-3.10172000	1.54494300
C	0.59906500	-2.40066700	2.17368300
H	0.79512200	-2.77950500	3.18473300
H	0.08750100	-3.19009500	1.61745600
H	1.55878300	-2.20862300	1.68756300
C	6.05925300	-1.86932500	0.89622400
H	7.14383300	-2.01818400	0.83501600
H	5.84462700	-1.20349500	1.73693700
H	5.58521900	-2.82998200	1.11462400
C	5.82377000	-2.23748400	-1.59079800
H	5.38023100	-3.22405900	-1.41524800
H	5.41025600	-1.83937800	-2.52069500
H	6.90543000	-2.37078500	-1.71209100
C	6.17318400	0.08859800	-0.69278200
H	5.96565700	0.79137300	0.12323300
H	7.26159700	-0.01007200	-0.78097800
H	5.78335400	0.51514400	-1.62058500
C	-2.76851700	-3.88258200	-1.47314800
H	-3.26607600	-4.13667400	-0.53023800
H	-2.99096300	-4.67760200	-2.19339300
H	-1.68979200	-3.86108900	-1.29910900
C	-4.78143800	-2.56110800	-2.23253300
H	-5.03549900	-3.33616400	-2.96401000
H	-5.30898800	-2.77612600	-1.29918800
H	-5.14754800	-1.59933300	-2.60144600
C	-2.53720600	-2.19462000	-3.33212300
H	-2.85852500	-1.22329300	-3.72486600
H	-1.45507300	-2.16342900	-3.18335500
H	-2.76488900	-2.95482300	-4.08761800
Fe	-0.95686300	-0.08773600	0.54113300

⁴TS4_Fe, -2788.68686498, i1371.96

C	0.02742000	0.39289800	2.32132100
C	-0.37433700	-0.99528800	2.30240800
C	-1.78557100	-1.01328900	2.28873300
C	-2.27376700	0.37410600	2.34091800
C	-1.16738900	1.22096700	2.36742500
C	2.46575500	3.64373100	-1.16349600
C	1.31753000	4.39005100	-1.30969800
C	0.05324400	3.75208300	-1.22468500
C	0.00425900	2.34331400	-0.98707200
C	1.20009600	1.56078100	-0.90981900
C	2.40805800	2.24152600	-0.97866300
H	-1.17375900	5.50970800	-1.53357600
H	3.43656600	4.12762300	-1.21838200
H	1.36078100	5.46143800	-1.48427800
C	-1.18034200	4.44064500	-1.33645300
H	3.32773000	1.66790000	-0.93367700
C	-2.32670900	2.38210700	-0.87925900
C	-2.36828500	3.75810600	-1.18654000
H	-3.22639000	1.80379000	-0.69466500
H	-3.32560200	4.26078400	-1.27137100
N	-1.18986600	1.70912700	-0.77489700
C	1.13257300	0.07872200	-0.79954200
H	1.31249900	-0.38715200	0.16991600
H	0.44624700	-0.44142200	-1.46951600
H	2.33147400	-0.39394500	-1.15020800
C	4.04748600	-1.16579700	-0.20033900
C	5.53642600	-1.57832500	-0.30039000
O	3.54544500	-0.74898500	-1.33000700
O	3.43664500	-1.23336100	0.87433000
C	-2.70952000	-1.57158900	-1.05279200
C	-3.53617700	-2.53939700	-1.90322400
O	-1.45773300	-1.81481300	-0.89937000
O	-3.22402500	-0.55860600	-0.50289600
C	1.41739400	0.92062400	2.47544900
H	1.56286100	1.82873500	1.88219400
H	1.58942600	1.19152300	3.52665000
H	2.17664100	0.19598700	2.17615800
C	-1.14392200	2.71857400	2.40793600
H	-0.78588800	3.08331600	3.37857700
H	-0.47305300	3.12606200	1.64462200
H	-2.13575000	3.14265500	2.23706000
C	-3.72401500	0.74089500	2.34985400

H	-4.21033600	0.38851000	3.26803700
H	-3.86733000	1.82242100	2.29128900
H	-4.23647300	0.27806000	1.50137300
C	-2.67671500	-2.21508200	2.29986700
H	-3.03758400	-2.42666600	3.31483500
H	-3.54966000	-2.05086400	1.66261600
H	-2.15107300	-3.10117800	1.93825500
C	0.54133000	-2.18657700	2.34452100
H	0.71823900	-2.50556300	3.37956200
H	0.10109600	-3.03155100	1.80761300
H	1.51093200	-1.97347300	1.88829300
C	6.03850100	-2.05128100	1.06974700
H	7.09222500	-2.34634800	1.00563500
H	5.94134500	-1.25887000	1.81693100
H	5.45634200	-2.90590600	1.42470100
C	5.65968600	-2.71165300	-1.33861700
H	5.09182700	-3.59437700	-1.02411300
H	5.27610500	-2.38792600	-2.30917200
H	6.70852900	-3.00895300	-1.45414800
C	6.34462100	-0.35295900	-0.77391800
H	6.26576200	0.47076400	-0.05457200
H	7.40538300	-0.61095400	-0.87282600
H	5.97772700	-0.00057600	-1.74120300
C	-3.41779900	-3.94250800	-1.27054900
H	-3.83332400	-3.95362800	-0.25676500
H	-3.97253600	-4.67183600	-1.87063500
H	-2.37194800	-4.25384400	-1.21572100
C	-5.00428100	-2.09514300	-1.95117200
H	-5.58779800	-2.79448700	-2.55960900
H	-5.43849800	-2.06279500	-0.94785800
H	-5.09847700	-1.09552800	-2.38410500
C	-2.92942500	-2.55747200	-3.32235200
H	-2.99491200	-1.56887600	-3.79018800
H	-1.87782800	-2.85206100	-3.28833200
H	-3.47471900	-3.26705700	-3.95410500
Fe	-1.06912100	-0.17030200	0.28365100

⁶TS4_Fe, -2788.69175055, i1084.80

C	0.05231000	0.40459100	2.32131300
C	-0.45028300	-0.94380700	2.30893400
C	-1.87402800	-0.87554400	2.25678600
C	-2.25497900	0.50866400	2.21236900
C	-1.06601200	1.29399100	2.25332700
C	2.42460700	3.70828700	-1.05723800

C	1.28043100	4.45838300	-1.22563400
C	0.01630500	3.81720800	-1.20088100
C	-0.02964400	2.40472100	-0.99065600
C	1.15879300	1.61692100	-0.90495500
C	2.36728800	2.30087100	-0.91736300
H	-1.21369500	5.56722000	-1.53736700
H	3.39521100	4.19558800	-1.06679900
H	1.32864300	5.53326100	-1.37474900
C	-1.21801800	4.49604800	-1.35273800
H	3.28594500	1.72599200	-0.86321900
C	-2.36940700	2.42585100	-0.96009800
C	-2.40696300	3.80298600	-1.25940800
H	-3.27089900	1.84193700	-0.80723300
H	-3.36358300	4.29949000	-1.37876800
N	-1.22862400	1.76536600	-0.82126200
C	1.08457900	0.12688900	-0.86409900
H	1.25542600	-0.40424800	0.07557100
H	0.44889600	-0.36016100	-1.60631800
H	2.29345400	-0.30818400	-1.19223200
C	3.94988600	-1.21060000	-0.23859300
C	5.44693800	-1.60300800	-0.25408900
O	3.54050900	-0.64151100	-1.33481300
O	3.24578900	-1.43323600	0.75873500
C	-2.57130600	-1.71700300	-0.99218400
C	-3.38559900	-2.76246700	-1.74875600
O	-1.35501000	-1.97791400	-0.67992200
O	-3.05485600	-0.58625600	-0.67586900
C	1.48574200	0.81370900	2.48218700
H	1.70112100	1.73672400	1.93609900
H	1.70779900	1.00163100	3.54123100
H	2.17634700	0.04752400	2.12276700
C	-0.98545300	2.79148600	2.26867100
H	-1.01265000	3.17973500	3.29471100
H	-0.05758600	3.14544300	1.81168500
H	-1.81610800	3.24897700	1.72410800
C	-3.66662000	1.00635800	2.12836200
H	-4.19953500	0.85450300	3.07538800
H	-3.70347500	2.07464500	1.89949100
H	-4.21830500	0.47216500	1.34773300
C	-2.82452600	-2.03452600	2.28207500
H	-3.15226900	-2.25531300	3.30592500
H	-3.71721800	-1.82273500	1.68691100
H	-2.35808600	-2.93661400	1.88019900
C	0.37607500	-2.19521100	2.38380100

H	0.53537400	-2.49373900	3.42828800
H	-0.12621800	-3.02276900	1.87529700
H	1.35591600	-2.06379600	1.91824900
C	5.83425800	-2.25063400	1.08131400
H	6.89343900	-2.53340200	1.07427200
H	5.66090400	-1.56304200	1.91383000
H	5.23373200	-3.14472000	1.26906500
C	5.67813400	-2.58925700	-1.41656400
H	5.10120600	-3.50923100	-1.26969400
H	5.37047800	-2.14222000	-2.36507000
H	6.73804400	-2.86247600	-1.48115300
C	6.27725600	-0.32494100	-0.49026300
H	6.12379500	0.39756300	0.32021100
H	7.34651900	-0.56412600	-0.52800600
H	5.99041400	0.14975300	-1.43205200
C	-3.29667300	-4.10015500	-0.98558100
H	-3.75273000	-4.01837200	0.00654100
H	-3.82952800	-4.87979000	-1.53990800
H	-2.25551900	-4.40622100	-0.86050200
C	-4.84708500	-2.31286300	-1.88305500
H	-5.41867800	-3.06607000	-2.43533900
H	-5.31041400	-2.18074200	-0.90081300
H	-4.91963100	-1.36106100	-2.41556100
C	-2.73616900	-2.91577700	-3.14322400
H	-2.77764400	-1.97457500	-3.70219300
H	-1.68973700	-3.21760300	-3.05169300
H	-3.27221200	-3.67656400	-3.72034900
Fe	-1.06219400	-0.10760200	0.17933300

²⁵Fe, -2788.72390994

C	0.39339700	-0.31861000	2.20662700
C	-0.25553600	-1.56747000	1.92006900
C	-1.66584100	-1.37868500	2.10793800
C	-1.89271200	-0.01179100	2.45578200
C	-0.61661600	0.64228400	2.49880200
C	2.27704900	3.46195700	-1.20887200
C	1.15819800	4.26706900	-1.15525200
C	-0.11089900	3.68904500	-0.88445500
C	-0.16717200	2.28567400	-0.66845600
C	0.96911200	1.44213800	-0.81046900
C	2.18871300	2.05485300	-1.05017500
H	-1.33689700	5.47889700	-0.95531100
H	3.24891400	3.90802400	-1.40208800
H	1.23305900	5.34040600	-1.30468200

C	-1.33093300	4.40546600	-0.78445000
H	3.08043800	1.44683200	-1.16010100
C	-2.44887200	2.34565300	-0.20094200
C	-2.49312100	3.73195700	-0.47359700
H	-3.32557400	1.77157600	0.07789800
H	-3.44341200	4.25062000	-0.40607800
N	-1.31733600	1.65671600	-0.27035700
C	0.67100700	-0.00960900	-0.67660900
H	1.52479500	-0.60407100	-0.35197900
H	0.25288700	-0.41824800	-1.60480400
H	2.78467900	-1.05937900	-1.89007500
C	4.21584000	-1.43293100	-0.71531400
C	5.68544300	-1.09401900	-0.47147800
O	3.73923400	-0.86877300	-1.84960900
O	3.52026100	-2.11253600	0.01339000
C	-3.21268100	-1.04892900	-0.97148200
C	-3.81939000	-1.91906800	-2.09613600
O	-1.92242000	-1.13535900	-0.88154800
O	-3.93199100	-0.34734300	-0.24235800
C	1.87067000	-0.06037100	2.25324800
H	2.13626900	0.85276300	1.71051300
H	2.19646600	0.06674800	3.29300200
H	2.43960800	-0.88393400	1.82002000
C	-0.37216200	2.08904500	2.81425800
H	-0.27709900	2.24763400	3.89539700
H	0.54726400	2.44563800	2.34261400
H	-1.19162100	2.71934200	2.45839500
C	-3.22180600	0.61173500	2.76439400
H	-3.52483800	0.39761100	3.79692000
H	-3.18381700	1.69921100	2.65547800
H	-3.98849400	0.23408400	2.08553400
C	-2.71636600	-2.43879800	1.96382000
H	-2.84750400	-2.98570100	2.90570400
H	-3.67366100	-2.00148600	1.67677000
H	-2.43805200	-3.16118800	1.19291700
C	0.41803400	-2.85731600	1.55269000
H	0.63016000	-3.46176800	2.44386200
H	-0.22187500	-3.45141900	0.89461400
H	1.36137700	-2.68497400	1.03091500
C	6.13569300	-1.75676600	0.83776200
H	7.19100900	-1.53289700	1.02286200
H	5.54831100	-1.39251800	1.68499100
H	6.01120600	-2.84172500	0.79213300
C	6.52303900	-1.61547700	-1.65923700

H	6.44172200	-2.70351700	-1.75116400
H	6.19736500	-1.16488300	-2.60001600
H	7.57781100	-1.36770800	-1.50142000
C	5.81994600	0.44193800	-0.36966100
H	5.18729400	0.84270300	0.42975800
H	6.85828100	0.70502200	-0.14322900
H	5.53852500	0.92604100	-1.30824400
C	-3.43793200	-3.39031100	-1.83467300
H	-3.85002500	-3.73816400	-0.88061400
H	-3.83652900	-4.03439900	-2.62703400
H	-2.35170500	-3.50650400	-1.80101900
C	-5.34567800	-1.76330100	-2.11607900
H	-5.77876400	-2.38002000	-2.91205800
H	-5.78213500	-2.06802000	-1.16101300
H	-5.63023900	-0.72156600	-2.28652200
C	-3.21846500	-1.46030700	-3.44033100
H	-3.46513200	-0.41155000	-3.64174700
H	-2.13007900	-1.55853800	-3.42919500
H	-3.61852500	-2.06428500	-4.26309700
Fe	-0.97401800	-0.16027400	0.49602200

⁴⁵Fe, -2788.71949926

C	0.55497500	-0.15566700	1.98597400
C	-0.03758400	-1.47884200	2.00258000
C	-1.41846900	-1.31388400	2.24337100
C	-1.69037200	0.10371800	2.39103100
C	-0.46893500	0.80481800	2.27735900
C	2.16761200	3.48844200	-1.46418300
C	1.03384600	4.27001300	-1.40843300
C	-0.22725400	3.66051500	-1.16852600
C	-0.27584400	2.24840800	-0.99742300
C	0.89084500	1.43085000	-1.13179600
C	2.10093200	2.07774900	-1.33297600
H	-1.45965600	5.44458600	-1.17904900
H	3.13488200	3.95458300	-1.63043900
H	1.08993200	5.34833800	-1.52781600
C	-1.45118600	4.36585300	-1.04430300
H	3.00785300	1.48965400	-1.42898700
C	-2.55417800	2.28753500	-0.52275500
C	-2.61111100	3.68283600	-0.74358900
H	-3.42288100	1.70096500	-0.23887200
H	-3.55974700	4.20012500	-0.64632000
N	-1.42513000	1.60590600	-0.63408100
C	0.69435000	-0.03491100	-1.02065200

H	1.59387500	-0.60177200	-0.78855100
H	0.17790900	-0.45585400	-1.89182100
H	3.23771700	-1.00605400	-2.29429400
C	4.31608200	-1.29599800	-0.77661400
C	5.61426200	-0.83433900	-0.11773700
O	4.09540600	-0.68401800	-1.96716300
O	3.53534600	-2.10604700	-0.31928200
C	-3.23552900	-1.41669800	-0.88738600
C	-3.97719700	-2.44952300	-1.76164400
O	-1.93793700	-1.53152800	-0.90694900
O	-3.85211900	-0.57113600	-0.22333500
C	2.02175300	0.14106000	1.91004300
H	2.22022800	1.04403300	1.32399800
H	2.42837100	0.30679100	2.91642800
H	2.57160600	-0.68498300	1.45769600
C	-0.26100900	2.28780900	2.38235200
H	-0.03871300	2.59218900	3.41323200
H	0.57369200	2.61793600	1.75720100
H	-1.14705000	2.84273800	2.06071500
C	-3.04182700	0.68875300	2.67330200
H	-3.33511500	0.51646700	3.71690500
H	-3.04997600	1.76921800	2.50488900
H	-3.79691400	0.24068700	2.02360700
C	-2.46023100	-2.39067000	2.32828400
H	-2.69411800	-2.63430800	3.37265300
H	-3.38617300	-2.07164300	1.84293100
H	-2.12499300	-3.30846300	1.83912800
C	0.70995000	-2.76820600	1.81617100
H	1.13583900	-3.12373000	2.76398100
H	0.05028100	-3.55412100	1.43819900
H	1.53364200	-2.65815900	1.10606600
C	5.76103600	-1.54015000	1.23772600
H	6.70296500	-1.24219600	1.70884200
H	4.93986700	-1.27850800	1.91033200
H	5.75780000	-2.62647000	1.11799200
C	6.79398000	-1.19775600	-1.04653100
H	6.85664600	-2.28015600	-1.19943900
H	6.69120300	-0.71662500	-2.02237100
H	7.73316900	-0.86578900	-0.59227900
C	5.55374000	0.69704400	0.07742200
H	4.69303100	0.98518000	0.68932300
H	6.46119500	1.03564500	0.58770900
H	5.48416000	1.21587300	-0.88193700
C	-3.62653800	-3.85788100	-1.23730500

H	-3.95460000	-3.98266000	-0.19921700
H	-4.12535000	-4.62331400	-1.84282100
H	-2.54743200	-4.02602500	-1.27701400
C	-5.49175700	-2.21675800	-1.68421400
H	-6.01981300	-2.95350900	-2.30034600
H	-5.84815000	-2.30229700	-0.65418400
H	-5.75250300	-1.21535900	-2.03763600
C	-3.48608600	-2.30244100	-3.21602300
H	-3.71524500	-1.30507800	-3.60842100
H	-2.40538400	-2.45313400	-3.27474100
H	-3.98021200	-3.03912900	-3.85996000
Fe	-0.89326900	-0.33481700	0.23698900

⁶⁵Fe, -2788.716875

C	0.48220500	-0.07271900	2.01026900
C	-0.21129400	-1.32233600	1.99634500
C	-1.60688700	-1.05002300	2.16285500
C	-1.77548100	0.36548200	2.24920200
C	-0.48330200	0.96877400	2.15652900
C	2.41087800	3.46119800	-1.34966900
C	1.33006700	4.31817200	-1.32822000
C	0.02316600	3.78433900	-1.18377700
C	-0.12639400	2.37072200	-1.07386800
C	0.98618400	1.47400900	-1.19652500
C	2.24471500	2.05593800	-1.29435400
H	-1.08437400	5.64711200	-1.20049600
H	3.41514000	3.86625600	-1.44127300
H	1.46243300	5.39346900	-1.40594900
C	-1.15635900	4.56687500	-1.10164800
H	3.11706700	1.41473300	-1.36935700
C	-2.41946600	2.56039000	-0.69749700
C	-2.37580000	3.95962000	-0.88434700
H	-3.33804000	2.03595800	-0.45540800
H	-3.29101700	4.53831300	-0.81914700
N	-1.33463900	1.80774300	-0.77775200
C	0.68769700	0.02547300	-1.17238900
H	1.53045100	-0.61010200	-0.90511500
H	0.23676200	-0.31399000	-2.11639500
H	3.14067500	-1.04052400	-2.17890400
C	4.17870200	-1.50292800	-0.67460100
C	5.50320300	-1.18038300	0.01499400
O	4.03305900	-0.83663700	-1.84719600
O	3.32205400	-2.25178000	-0.25078300
C	-2.91522200	-1.63521600	-0.95007000

C	-3.97502100	-2.52869700	-1.59779600
O	-1.72463100	-2.08123900	-0.81477900
O	-3.18720000	-0.45723600	-0.56289200
C	1.96578800	0.12223400	1.92641600
H	2.22211600	0.97024800	1.28317800
H	2.39603700	0.32205500	2.91700800
H	2.45807100	-0.76264000	1.52075100
C	-0.17716100	2.43537700	2.23520400
H	-0.02929100	2.75852100	3.27419900
H	0.73363700	2.68357400	1.68312600
H	-0.98672900	3.04206400	1.81863800
C	-3.08906700	1.06934200	2.42526500
H	-3.46172000	0.97714200	3.45369200
H	-3.00438600	2.13676200	2.20358800
H	-3.84731700	0.64713300	1.75755600
C	-2.69905100	-2.07055800	2.28696400
H	-2.88512900	-2.32974300	3.33751100
H	-3.63719600	-1.69593700	1.86762300
H	-2.44066600	-2.99055000	1.75769400
C	0.39799500	-2.68503300	1.83336100
H	0.52648600	-3.18684600	2.80166500
H	-0.24200000	-3.31894000	1.21204900
H	1.37521800	-2.63529000	1.34735800
C	5.56989900	-1.94716600	1.34327400
H	6.52532800	-1.74652200	1.83834700
H	4.76148100	-1.64450800	2.01409900
H	5.47925900	-3.02416800	1.18061600
C	6.66153400	-1.60578800	-0.91381000
H	6.63526900	-2.68292500	-1.10903300
H	6.61323600	-1.08061200	-1.87099900
H	7.61893800	-1.37207700	-0.43671300
C	5.56815700	0.34206700	0.27017800
H	4.72744600	0.67656200	0.88613400
H	6.49510200	0.58423900	0.80021500
H	5.55150700	0.90128800	-0.66865100
C	-3.97685200	-3.89260600	-0.87857300
H	-4.27368600	-3.78365600	0.16972200
H	-4.68766300	-4.57056300	-1.36342300
H	-2.98270800	-4.34470800	-0.90674900
C	-5.35997700	-1.87271300	-1.51189800
H	-6.10905900	-2.51600600	-1.98634600
H	-5.65367100	-1.71099400	-0.47051100
H	-5.36642900	-0.90105100	-2.01234700
C	-3.56083700	-2.72186300	-3.07378000

H	-3.54246200	-1.76378900	-3.60484400
H	-2.56650700	-3.17124800	-3.13872800
H	-4.27716100	-3.37734400	-3.58105900
Fe	-1.04653800	-0.24496900	0.02047700

²²Ni, -2686.60877362

C	0.64983500	2.32210900	-1.17218800
C	-0.61678200	2.35275900	-0.59569100
C	-0.45315300	2.31608100	0.89457500
C	1.61371000	2.19803000	-0.08170600
C	0.90857500	2.29098500	1.18998900
C	3.09245700	2.13473000	-0.24450100
H	3.36366600	1.64688100	-1.18275100
H	3.50943400	3.15056100	-0.25828400
H	3.55417500	1.59277200	0.58314600
C	1.57838000	2.23243000	2.52753000
H	2.19085400	1.32857600	2.60420400
H	2.23434500	3.09787900	2.66893500
H	0.85199200	2.22656400	3.34211100
C	-1.60971900	2.37243000	1.83642500
H	-1.31291700	2.14424300	2.86104500
H	-2.05495000	3.37480800	1.82681400
H	-2.39278300	1.66862600	1.53862200
C	-1.94319500	2.51601000	-1.26118400
H	-2.65340800	1.75094700	-0.93498500
H	-2.37255000	3.49031100	-0.99811800
H	-1.86397200	2.46464100	-2.34772000
C	1.02803700	2.31369900	-2.62045900
H	1.70793100	3.14172400	-2.84647900
H	1.54181800	1.37964700	-2.87183900
H	0.15485400	2.40917900	-3.26781500
C	3.34894400	-2.18256700	-0.16548700
C	2.84964600	-3.42942500	0.60064700
H	1.95942100	-3.85449800	0.12496800
H	3.63039700	-4.19586000	0.60003700
H	2.60668100	-3.18111700	1.63696700
C	3.67672700	-2.54062100	-1.62226700
H	2.80262300	-2.94777700	-2.13687600
H	4.01590000	-1.66329800	-2.18030400
H	4.47254000	-3.29089300	-1.64592600
C	4.58837200	-1.59392400	0.54330700
H	4.95466500	-0.70149200	0.02402800
H	4.35895700	-1.32564400	1.57753200
H	5.39489400	-2.33296600	0.54598500

C	2.23882100	-1.14463500	-0.10660900
O	1.86308700	-0.65719400	1.01687500
O	1.63780400	-0.72624600	-1.15041800
C	-3.67778700	-1.07713200	-2.04475800
C	-2.41941500	-0.92366100	-1.48452200
C	-2.31357700	-0.96896900	-0.05854200
C	-3.47963600	-1.27898000	0.72274800
C	-4.74200400	-1.41707200	0.09067000
C	-4.84061200	-1.29609700	-1.27373600
H	-3.76796300	-1.05279400	-3.12695000
C	-3.33409800	-1.47528900	2.11716900
H	-5.61271700	-1.63858000	0.70026600
H	-5.79980600	-1.40442300	-1.76927800
C	-2.09149600	-1.37700500	2.69813300
C	-1.00775400	-0.99072200	1.89285200
H	-4.21046700	-1.72192000	2.71002200
H	-1.93447500	-1.55709600	3.75532900
H	-0.02426000	-0.84895600	2.32720600
N	-1.10614000	-0.75511600	0.58219500
C	-1.21661500	-0.79203800	-2.38099800
H	-0.81159000	0.22304700	-2.39029100
H	-0.40211900	-1.44573000	-2.06501600
H	-1.48405500	-1.04240500	-3.40982400
Ni	0.43438500	0.43220100	0.03535200

⁴²Ni, -2686.58858943

C	0.88867700	2.53130300	-0.79526500
C	-0.47821200	2.56239600	-0.24024900
C	-0.41616200	2.20531500	1.13767000
C	1.75935100	2.25489300	0.25883400
C	0.95255600	2.06983400	1.48108200
C	3.24879400	2.16328400	0.23527500
H	3.63895500	2.14929500	-0.78380700
H	3.69671200	3.01939900	0.75468500
H	3.58303700	1.25697600	0.74803900
C	1.53765700	1.74296200	2.80779500
H	2.08545700	0.79497900	2.74424500
H	2.26122800	2.51009800	3.10883400
H	0.77907300	1.66438400	3.58810700
C	-1.59873900	2.10170300	2.05516000
H	-1.37412800	1.49091200	2.93211600
H	-1.91646000	3.08927500	2.40899800
H	-2.45247000	1.64544800	1.54518800
C	-1.71580900	2.96482300	-0.97121300

H	-2.53071400	2.25136700	-0.80461900
H	-2.06732800	3.93720500	-0.60280100
H	-1.54934400	3.05667300	-2.04585100
C	1.24165800	2.87007100	-2.21201500
H	1.19372000	3.95330300	-2.37595200
H	2.25104600	2.53730200	-2.45949700
H	0.55688500	2.40206000	-2.92553200
C	3.36004600	-2.21352900	-0.37511600
C	2.88710400	-3.48109000	0.37568300
H	2.00719000	-3.92032800	-0.10619900
H	3.68490000	-4.22963900	0.36675200
H	2.63872300	-3.25116300	1.41519500
C	3.69812500	-2.54794700	-1.83526700
H	2.83418400	-2.96839900	-2.35605000
H	4.01873600	-1.65714200	-2.38260800
H	4.51034600	-3.28023000	-1.86506400
C	4.58515800	-1.60870600	0.34405000
H	4.94050700	-0.70883700	-0.16917300
H	4.34559500	-1.34955800	1.37855800
H	5.40299300	-2.33512700	0.34946700
C	2.22201200	-1.20922000	-0.30673200
O	1.84358900	-0.72526000	0.81841500
O	1.58813200	-0.82266700	-1.34662600
C	-3.86184200	-0.61388200	-2.04051100
C	-2.58547600	-0.57920600	-1.50791000
C	-2.41661600	-0.94368000	-0.13707000
C	-3.54402900	-1.40049400	0.61987300
C	-4.83117800	-1.41662100	0.02168000
C	-4.98686800	-1.01568000	-1.28310300
H	-4.00214600	-0.34326300	-3.08309000
C	-3.32967900	-1.83910200	1.94920600
H	-5.67899900	-1.75689500	0.60841300
H	-5.96723700	-1.02522600	-1.74783400
C	-2.06091300	-1.82136200	2.48215000
C	-1.00931200	-1.31251800	1.70006400
H	-4.17459000	-2.19599300	2.53140800
H	-1.85839600	-2.17004000	3.48829500
H	0.00006400	-1.24798700	2.09184000
N	-1.17291000	-0.87240300	0.45331400
C	-1.40216700	-0.23876600	-2.37412100
H	-0.87074900	0.66235300	-2.02760800
H	-0.67293200	-1.05212800	-2.41327400
H	-1.71488100	-0.00840100	-3.39506700
Ni	0.36760000	0.29360300	-0.20726200

²TS4_Ni, -3033.27296855, i1595.57

C	-0.15490300	0.41674900	2.29606900
C	-0.46924800	-0.98370600	2.29041800
C	-1.88334500	-1.10908900	2.31572800
C	-2.46067300	0.22325100	2.37390000
C	-1.40317700	1.15595700	2.34124400
C	2.44207000	3.69582600	-1.06634600
C	1.26746300	4.37748200	-1.28732300
C	0.03234000	3.67988200	-1.25912700
C	0.02153500	2.27167000	-0.99509300
C	1.25821600	1.55677200	-0.85485300
C	2.43404200	2.29772300	-0.86560000
H	-1.21934200	5.39313000	-1.68858400
H	3.39046400	4.22458700	-1.07739300
H	1.26499200	5.44589000	-1.48410900
C	-1.20905300	4.32785700	-1.47265700
H	3.37533400	1.76766000	-0.76808000
C	-2.31085100	2.24472400	-1.04957700
C	-2.37908800	3.60763200	-1.40145300
H	-3.20890700	1.65060200	-0.91330700
H	-3.34536100	4.06960700	-1.57180900
N	-1.16737500	1.60471300	-0.83400100
C	1.28643100	0.08227600	-0.74357600
H	1.39086400	-0.32451000	0.25810600
H	0.55235300	-0.45442900	-1.34083000
H	2.49064200	-0.33642800	-1.09045500
C	4.20488100	-1.02271000	-0.08127400
C	5.68339200	-1.47587900	-0.19525400
O	3.69752000	-0.67634600	-1.24413500
O	3.61433200	-0.99472400	0.99697100
C	-2.52428700	-1.58762800	-1.13160400
C	-3.22341100	-2.56524800	-2.07813700
O	-1.28715500	-1.72979400	-0.88496300
O	-3.16676400	-0.63687500	-0.57198900
C	1.19198500	1.04920700	2.47230000
H	1.30086300	1.94124300	1.84749200
H	1.31531800	1.37302000	3.51502000
H	2.01324700	0.37312700	2.22830200
C	-1.49377600	2.65244900	2.38293800
H	-1.22788400	3.04196500	3.37375000
H	-0.80808500	3.10979400	1.66207100
H	-2.50187700	3.00288300	2.14790600
C	-3.93360800	0.49739700	2.39596900

H	-4.38878500	0.13049200	3.32395200
H	-4.14740400	1.56645600	2.32073600
H	-4.42665900	-0.00807300	1.55898200
C	-2.67349200	-2.38217000	2.29525300
H	-3.05578300	-2.63751800	3.29205300
H	-3.53350900	-2.29105700	1.62411900
H	-2.06236300	-3.21804600	1.94695500
C	0.50501900	-2.12496000	2.22581900
H	0.52259200	-2.67922500	3.17218200
H	0.21781400	-2.82653800	1.43550700
H	1.52207200	-1.78961400	2.01166100
C	6.20154500	-1.86709300	1.19476200
H	7.24722400	-2.18793000	1.12742500
H	6.13683300	-1.02495900	1.88878900
H	5.61067000	-2.68425300	1.61672700
C	5.75605500	-2.67997800	-1.15564100
H	5.16772100	-3.52181900	-0.77455600
H	5.37077300	-2.41363300	-2.14275600
H	6.79432200	-3.01459200	-1.26121700
C	6.50718100	-0.30295400	-0.76511800
H	6.45939400	0.56877600	-0.10237700
H	7.55946900	-0.59318000	-0.86189900
H	6.13378700	-0.00788400	-1.74887900
C	-3.08361700	-3.97807400	-1.47122500
H	-3.58410500	-4.03920000	-0.49853500
H	-3.54198800	-4.71885700	-2.13530000
H	-2.03060200	-4.23407900	-1.33106800
C	-4.70451100	-2.19936100	-2.24600500
H	-5.19167400	-2.91120900	-2.92125400
H	-5.22594200	-2.21958100	-1.28506100
H	-4.81702900	-1.19442500	-2.66245300
C	-2.49422700	-2.50938700	-3.43685000
H	-2.57583400	-1.51316300	-3.88563700
H	-1.43412100	-2.74392000	-3.31462500
H	-2.93827000	-3.23067500	-4.13149800
Ni	-1.41458500	-0.06654300	0.42659800

⁴TS4_Ni, -3033.28456825, i1172.43

C	0.01139200	0.34782200	2.34838900
C	-0.38466800	-1.04280000	2.26596200
C	-1.80048700	-1.09005000	2.28058000
C	-2.29684000	0.26875300	2.36457400
C	-1.18057400	1.14483600	2.36639200
C	2.42434600	3.70130500	-1.05383300

C	1.25585800	4.40149000	-1.24982800
C	0.01241400	3.71956900	-1.21010100
C	-0.00316300	2.31152900	-0.95577700
C	1.21876100	1.57981500	-0.82765700
C	2.40470700	2.30091400	-0.85943900
H	-1.23969900	5.44161200	-1.60360400
H	3.37883000	4.21877400	-1.07553100
H	1.26497800	5.47245200	-1.43169400
C	-1.22986500	4.37501600	-1.39450400
H	3.34012700	1.75781200	-0.77805100
C	-2.33898400	2.29094900	-0.97720900
C	-2.40275600	3.66053100	-1.30464000
H	-3.23523100	1.69554800	-0.83798700
H	-3.36913100	4.13096200	-1.44899200
N	-1.19358100	1.64563000	-0.79438900
C	1.21808600	0.09706900	-0.71805900
H	1.33601200	-0.33138300	0.27339000
H	0.50844100	-0.43128700	-1.35231800
H	2.38839100	-0.32212500	-1.07526400
C	4.15059800	-1.10296200	-0.17049500
C	5.63831000	-1.51617400	-0.32095400
O	3.63622300	-0.64723500	-1.28491200
O	3.56008100	-1.20301900	0.90718800
C	-2.63183800	-1.55420300	-1.08828400
C	-3.42880600	-2.52149300	-1.96288100
O	-1.37973300	-1.72957200	-0.93923400
O	-3.19325000	-0.57843000	-0.49128900
C	1.39777200	0.88000100	2.53746800
H	1.55746700	1.79201300	1.95278100
H	1.55730700	1.14470000	3.59198800
H	2.16809700	0.16282200	2.24782200
C	-1.20769500	2.64398600	2.43118200
H	-1.07337000	3.00758600	3.45775600
H	-0.40678900	3.07931300	1.82558900
H	-2.15413100	3.04613200	2.05988000
C	-3.74700100	0.63928900	2.40729900
H	-4.20386900	0.32898000	3.35548300
H	-3.89163300	1.71814900	2.30903600
H	-4.29271100	0.14562600	1.59707500
C	-2.65957500	-2.31871700	2.25781600
H	-2.97301900	-2.61079900	3.26841300
H	-3.56263600	-2.14848900	1.66467900
H	-2.12473900	-3.16435000	1.81850800
C	0.53367000	-2.22878700	2.22030500

H	0.62163900	-2.69300800	3.21123400
H	0.14467200	-2.98856800	1.53525500
H	1.53784600	-1.96334700	1.88258700
C	6.16328200	-2.03360900	1.02436800
H	7.21440600	-2.32919700	0.92898500
H	6.08376300	-1.26491000	1.79770000
H	5.58537300	-2.89749600	1.36301100
C	5.73404300	-2.61753600	-1.39564700
H	5.16356100	-3.50473300	-1.09953500
H	5.33973500	-2.26179300	-2.35058000
H	6.77843500	-2.91942300	-1.53564100
C	6.44152200	-0.27888600	-0.77077300
H	6.37797900	0.52245300	-0.02542600
H	7.49921200	-0.53811300	-0.89475100
H	6.06134500	0.10465200	-1.72091100
C	-3.26130700	-3.93637400	-1.36780500
H	-3.67453000	-3.98834300	-0.35469500
H	-3.79040000	-4.66789500	-1.98791800
H	-2.20508500	-4.21242400	-1.32146600
C	-4.91156200	-2.12643900	-1.99724700
H	-5.47104600	-2.82971700	-2.62335400
H	-5.34480200	-2.13549900	-0.99320700
H	-5.04192700	-1.12021000	-2.40515100
C	-2.82361600	-2.48012500	-3.38219000
H	-2.92650300	-1.48305000	-3.82458200
H	-1.76158600	-2.73558600	-3.35612700
H	-3.34255600	-3.19341400	-4.03153800
Ni	-1.29392400	-0.08486100	0.32256400

²⁵Ni, -3033.33700448

C	0.50586700	-0.48829200	1.98664500
C	-0.18297600	-1.75653600	1.75634300
C	-1.53986700	-1.55640100	2.07279100
C	-1.71599700	-0.18038800	2.48695400
C	-0.44863300	0.45669800	2.48023100
C	2.36353800	3.43920600	-1.14348300
C	1.30328500	4.29469200	-0.93362900
C	0.01500600	3.76325400	-0.65536300
C	-0.13262900	2.35028600	-0.60581700
C	0.94937500	1.46462300	-0.89678500
C	2.19218700	2.03080400	-1.13105900
H	-1.07481800	5.62441500	-0.41876800
H	3.35167400	3.84553100	-1.34075800
H	1.43965800	5.37212500	-0.96188200

C	-1.14080600	4.53991900	-0.38334100
H	3.03857100	1.38841100	-1.34901600
C	-2.37010000	2.50187900	0.01405700
C	-2.32901500	3.91387100	-0.07243000
H	-3.26538200	1.94875900	0.28111600
H	-3.22897200	4.48444900	0.13118800
N	-1.30341300	1.75845600	-0.22641500
C	0.62324100	0.01469000	-0.92504900
H	1.47400300	-0.64430300	-0.75928800
H	0.06087200	-0.27681200	-1.81679900
H	3.07768500	-1.02429700	-2.43930200
C	4.18790500	-1.46420600	-0.98262500
C	5.52472400	-1.10753600	-0.33609800
O	3.95622200	-0.75800600	-2.11739100
O	3.38732000	-2.27309400	-0.55889100
C	-3.29810100	-0.89014000	-0.92325000
C	-4.08049000	-1.66852200	-2.01057200
O	-2.02243200	-1.09627500	-0.95001400
O	-3.89681600	-0.15838400	-0.11628700
C	1.98909000	-0.27744600	1.94790800
H	2.24487300	0.69043200	1.50430100
H	2.39953600	-0.29241300	2.96573200
H	2.48823900	-1.05781100	1.37268500
C	-0.14564500	1.87868100	2.85174700
H	0.12744500	1.97184400	3.91048800
H	0.68760300	2.27131200	2.26144600
H	-1.00533000	2.53089300	2.67478300
C	-3.02083300	0.42407700	2.90638500
H	-3.31446400	0.07005700	3.90297600
H	-2.95789500	1.51474200	2.95138000
H	-3.80569700	0.15922600	2.19511400
C	-2.65283600	-2.55178300	1.95134200
H	-2.90408500	-2.98440900	2.92828100
H	-3.55019400	-2.07325300	1.55205000
H	-2.38192900	-3.37058700	1.28132400
C	0.46732300	-3.03041900	1.30349700
H	0.85222600	-3.60758200	2.15462300
H	-0.24705000	-3.66343700	0.77057500
H	1.30546300	-2.83819800	0.63012900
C	5.68294200	-1.92137300	0.95607600
H	6.65122300	-1.69955800	1.41555900
H	4.89539300	-1.67877000	1.67453700
H	5.62857600	-2.99415700	0.75468900
C	6.65836100	-1.44522600	-1.32968300

H	6.67029700	-2.51428600	-1.56591700
H	6.54573000	-0.88681000	-2.26230000
H	7.62443600	-1.18689500	-0.88411100
C	5.53628600	0.40515000	-0.02246000
H	4.70430400	0.68121800	0.63345100
H	6.47009100	0.66440500	0.48667500
H	5.46667200	0.99981000	-0.93675400
C	-3.82411200	-3.17522600	-1.80421100
H	-4.18399600	-3.50268900	-0.82212300
H	-4.34957100	-3.76130300	-2.56745600
H	-2.75524800	-3.39432500	-1.86548000
C	-5.58085900	-1.36740500	-1.90122200
H	-6.13650800	-1.92010400	-2.66795900
H	-5.96505100	-1.65121500	-0.91771700
H	-5.77542200	-0.29918900	-2.02998000
C	-3.54953000	-1.23909000	-3.39266900
H	-3.71219300	-0.16782700	-3.55885000
H	-2.47761600	-1.43729700	-3.47010200
H	-4.06802600	-1.78554500	-4.18942400
Ni	-0.86556300	-0.20266900	0.36896600

⁴⁵Ni, -3033.3037136

C	0.75456200	-0.59153100	1.99517600
C	0.01750100	-1.80501100	1.80091400
C	-1.34779700	-1.53650300	2.08029900
C	-1.47637400	-0.13339800	2.40142200
C	-0.17648400	0.44496400	2.34221200
C	2.31121500	3.70169300	-0.79375200
C	1.18396300	4.48928100	-0.68191500
C	-0.09322800	3.87502000	-0.57597000
C	-0.16850200	2.45507800	-0.60582200
C	0.99391300	1.64106200	-0.82041000
C	2.22373200	2.29078000	-0.86653400
H	-1.29604100	5.66768700	-0.37407800
H	3.28976000	4.17009100	-0.85329700
H	1.25755200	5.57254400	-0.65188400
C	-1.30897400	4.58071600	-0.38753500
H	3.12645000	1.70476400	-1.00917200
C	-2.45838200	2.47376600	-0.16772100
C	-2.48640900	3.88626100	-0.20789100
H	-3.34017400	1.86986300	0.03000700
H	-3.42896100	4.40289900	-0.06160600
N	-1.33513600	1.79357700	-0.34913400
C	0.78080600	0.19963600	-0.92403900

H	1.64162600	-0.44376300	-0.78391300
H	0.15242000	-0.11241900	-1.76764700
H	3.08522700	-0.52305200	-2.37945200
C	4.22269200	-1.36532200	-1.13181900
C	5.61240400	-1.25218400	-0.50853000
O	4.00246400	-0.41391400	-2.07300500
O	3.37651000	-2.18577800	-0.83766300
C	-3.59113100	-0.92457600	-0.78075300
C	-4.35590500	-1.79701000	-1.80275600
O	-2.30871200	-1.12385000	-0.77580500
O	-4.19144000	-0.13226500	-0.04101200
C	2.23715000	-0.42089600	1.90642500
H	2.49897700	0.51488500	1.39999000
H	2.68764100	-0.38168000	2.90761500
H	2.70254900	-1.24349900	1.36105800
C	0.18814700	1.86636200	2.64912900
H	0.48185200	1.98346000	3.70046100
H	1.02658800	2.20509400	2.03388400
H	-0.64987400	2.54346800	2.46458900
C	-2.74626400	0.54636600	2.82245900
H	-3.02775900	0.25388400	3.84222700
H	-2.63433700	1.63391600	2.81197600
H	-3.56458800	0.28844000	2.14581600
C	-2.48378300	-2.51309500	2.04875000
H	-2.62143400	-2.99007800	3.02811900
H	-3.41757700	-2.01231900	1.78329100
H	-2.31051600	-3.30292100	1.31385200
C	0.60519500	-3.11926900	1.37590600
H	1.01313700	-3.67369900	2.23147000
H	-0.15101500	-3.75484600	0.90710600
H	1.41810700	-2.98069900	0.65673100
C	5.76876400	-2.34472300	0.55843100
H	6.76975400	-2.29145000	0.99791400
H	5.03284300	-2.22407600	1.35794200
H	5.62864300	-3.33909500	0.12693800
C	6.67007400	-1.42717200	-1.62047400
H	6.58881800	-2.41277500	-2.09047300
H	6.55820900	-0.66511900	-2.39568100
H	7.67263400	-1.34020600	-1.18925500
C	5.75126500	0.14755500	0.13109800
H	4.98595300	0.31053200	0.89674600
H	6.73221800	0.23494000	0.60928800
H	5.66205800	0.93637700	-0.62004100
C	-4.08663300	-3.27945800	-1.47242100

H	-4.44951400	-3.52978900	-0.46921100
H	-4.60278500	-3.92887800	-2.18892700
H	-3.01585300	-3.49459800	-1.51146800
C	-5.85953700	-1.50164800	-1.72723900
H	-6.40407800	-2.12014700	-2.45005600
H	-6.24810800	-1.70838400	-0.72647800
H	-6.06275700	-0.44948400	-1.94423200
C	-3.81801100	-1.47597500	-3.21199000
H	-3.98827000	-0.42350800	-3.46632800
H	-2.74426600	-1.67202400	-3.26866000
H	-4.32764800	-2.09028300	-3.96335900
Ni	-0.94985300	-0.19847300	0.24550400

¹I_Tp, -2432.01762965

Co	-0.10092500	0.00044900	-0.45474000
C	-3.88631400	0.00014500	-0.19164000
C	-4.46268600	1.27312700	-0.83727400
H	-4.26099300	1.29729500	-1.91239900
H	-5.54676900	1.28786900	-0.69625200
H	-4.04263600	2.17567600	-0.38737600
C	-4.46273200	-1.27185500	-0.83909600
H	-4.26127800	-1.29435900	-1.91430300
H	-4.04254300	-2.17508300	-0.39068600
H	-5.54678900	-1.28690000	-0.69789000
C	-4.17038800	-0.00091700	1.33680200
H	-3.75960800	-0.89508500	1.81628400
H	-3.75929100	0.89238700	1.81759400
H	-5.25274700	-0.00088400	1.49319100
C	-2.38691700	0.00025200	-0.31260100
O	-1.68049400	1.07840500	-0.33287800
O	-1.68040700	-1.07781600	-0.33521700
H	3.87295500	-0.00045500	0.91546400
N	1.69946900	-0.00098700	1.64693900
C	1.81393000	-0.00313700	2.98939500
C	0.54106300	-0.00403600	3.55145000
C	-0.34122900	-0.00252200	2.46741100
N	2.43236700	-1.24246200	-0.36413600
C	3.11079800	-2.36409200	-0.67384400
C	1.02609900	-2.56729100	-1.39659300
C	2.25345000	-3.23309000	-1.34459200
N	2.43236500	1.24325500	-0.36248300
C	3.11054800	2.36564100	-0.66996300
C	2.25315000	3.23559000	-1.33942300
C	1.02596200	2.56961400	-1.39278900

N	1.15840000	1.36349800	-0.81420100
N	1.15833100	-1.36225100	-0.81573200
N	0.37633700	-0.00058000	1.33548600
H	2.48540200	4.21415600	-1.72990900
H	2.48583000	-4.21094500	-1.73677900
H	0.28516600	-0.00548700	4.59957500
B	2.75771400	-0.00017500	0.49736600
H	2.79075100	-0.00366700	3.45009600
H	-1.41929500	-0.00251300	2.43816600
H	4.14928500	2.47086300	-0.39298400
H	0.07357000	2.87730100	-1.79948900
H	4.14961500	-2.46955200	-0.39725700
H	0.07371400	-2.87444800	-1.80370600

³¹Tp, -2432.01013251

Co	-0.18256900	0.00045800	-0.39054900
C	-3.97690600	0.00011900	-0.07137600
C	-4.58517600	1.27336300	-0.68835900
H	-4.44276500	1.29552300	-1.77285800
H	-5.65970100	1.28796700	-0.48744100
H	-4.14235400	2.17674700	-0.26237900
C	-4.58474800	-1.27423700	-0.68641200
H	-4.44246000	-1.29794900	-1.77089400
H	-4.14157200	-2.17682900	-0.25914400
H	-5.65925800	-1.28890900	-0.48539900
C	-4.17732600	0.00128300	1.47156000
H	-3.73874700	-0.89084800	1.92880600
H	-3.73898000	0.89422400	1.92743600
H	-5.25003700	0.00129500	1.68360100
C	-2.49136100	0.00032900	-0.27128100
O	-1.77670100	1.07538500	-0.32608500
O	-1.77650000	-1.07465900	-0.32647500
H	3.95715700	-0.00072200	0.56920700
N	1.92240800	-0.00014700	1.60397300
C	2.27203900	-0.00025600	2.90397800
C	1.11428700	-0.00018300	3.68064800
C	0.06664800	-0.00018900	2.75865600
N	2.37741200	-1.24037700	-0.51787500
C	3.03338400	-2.36259400	-0.86719600
C	0.91000900	-2.56806600	-1.46297400
C	2.13695100	-3.23423800	-1.48209500
N	2.37808800	1.23945100	-0.51817700
C	3.03473000	2.36135500	-0.86723100
C	2.13880800	3.23379900	-1.48174200

C	0.91142900	2.56844400	-1.46263200
N	1.07681400	1.36470500	-0.88633600
N	1.07616100	-1.36463700	-0.88625400
N	0.55974100	-0.00012100	1.50797700
H	2.34766100	4.21230100	-1.88549200
H	2.34524900	-4.21272300	-1.88617500
H	1.04752800	-0.00017800	4.75756200
B	2.79228600	-0.00047400	0.31472900
H	3.31337800	-0.00030200	3.19179800
H	-1.00182900	-0.00020500	2.92054500
H	4.08763400	2.46680800	-0.65039900
H	-0.06145100	2.87244100	-1.82041700
H	4.08616600	-2.46886300	-0.65018100
H	-0.06304900	-2.87127300	-1.82093100

⁵¹Tp, -2431.99348412

Co	0.18153000	0.00812800	0.23010600
C	4.08610500	0.01746000	0.09926400
C	4.48117500	-0.65405900	-1.23956800
H	4.11785300	-0.07721900	-2.09630200
H	5.57176800	-0.70355700	-1.30466400
H	4.08296900	-1.66969700	-1.30378100
C	4.64247800	1.44695300	0.17582300
H	4.28511400	2.05895000	-0.65640500
H	4.35118400	1.93889400	1.10784200
H	5.73467500	1.41279700	0.13316600
C	4.59402400	-0.83792500	1.28360600
H	4.32401200	-0.38607900	2.24360700
H	4.18455400	-1.85015100	1.24514400
H	5.68482400	-0.90116000	1.23668600
C	2.57632500	0.03323700	0.15618800
O	1.89385600	-1.05951700	0.16938200
O	1.88523100	1.11484800	0.17434700
H	-3.98975000	-0.02019400	-0.49268300
N	-2.48168200	-0.08269200	1.21353400
C	-3.29556700	-0.15341000	2.27899100
C	-2.52217400	-0.20178600	3.44275200
C	-1.20525800	-0.15554900	2.99872800
N	-2.15610600	1.28104400	-0.86584100
C	-2.66990100	2.36699600	-1.46858200
C	-0.48806300	2.65774700	-1.22390400
C	-1.63400100	3.27312600	-1.72042300
N	-2.11442800	-1.21407100	-0.99514400
C	-2.59501000	-2.25035200	-1.70313800

C	-1.53200100	-3.09515100	-2.04166800
C	-0.40519800	-2.49756400	-1.48405600
N	-0.76556300	-1.36039700	-0.85394300
N	-0.81217600	1.45365800	-0.70927900
N	-1.18433600	-0.08347900	1.64990200
H	-1.58247200	-4.01168800	-2.60890200
H	-1.71341700	4.23929400	-2.19429300
H	-2.87391100	-0.26218400	4.46098400
B	-2.81057300	-0.00910500	-0.31287700
H	-4.36803800	-0.16531600	2.14769900
H	-0.28024300	-0.17017100	3.55761100
H	-3.65125300	-2.32802000	-1.91771900
H	0.63199500	-2.79912300	-1.48394000
H	-3.72832500	2.43256200	-1.67631100
H	0.53974200	2.98871400	-1.19473500

¹²Tp, -2873.47534635

Co	0.54797000	-0.02177100	-0.05653900
C	2.01708000	3.49202200	-0.02795400
C	0.98692400	4.30589900	-0.85093500
H	-0.00708500	4.26292500	-0.39439500
H	1.30133700	5.35282700	-0.88518700
H	0.91812200	3.93245500	-1.87620300
C	2.11200300	4.03578500	1.40598200
H	1.13864500	4.02169000	1.90300200
H	2.80824200	3.44756900	2.01048300
H	2.47032000	5.06855400	1.37903800
C	3.39280200	3.52047400	-0.72684200
H	4.14197800	2.96421400	-0.15342900
H	3.33726200	3.09275800	-1.73064600
H	3.73674300	4.55543600	-0.80711900
C	1.51357900	2.07001200	-0.01170000
O	1.49494100	1.33434200	-1.06439000
O	1.03604200	1.50148100	1.03105300
C	-4.01140700	0.75282400	1.77191700
C	-2.80228100	1.14472300	1.21526700
C	-2.52486600	0.74204100	-0.12103200
C	-3.58977800	0.21340000	-0.92046100
C	-4.80132300	-0.18665600	-0.30174000
C	-4.98552000	0.03673800	1.04356100
H	-4.23689700	1.05461100	2.79112000
C	-3.43960300	0.23109000	-2.33037800
H	-5.58756500	-0.61958700	-0.91279200
H	-5.90896000	-0.26061200	1.52959500

C	-2.30600800	0.77926900	-2.88377800
C	-1.23178600	1.07446300	-2.02426800
H	-4.24861700	-0.13637500	-2.95563800
H	-2.18734900	0.90128400	-3.95412300
H	-0.26700600	1.35478100	-2.42763400
N	-1.27888900	0.95731000	-0.69973500
C	-1.93258500	2.15426700	1.92499400
H	-2.12945600	2.16006100	3.00084600
H	-0.86805000	2.01209500	1.75281000
H	-2.18123800	3.15471900	1.54867700
H	1.02080100	-4.23989000	0.42059300
N	2.19096700	-2.27668000	0.53380900
C	3.43231300	-2.68187300	0.86567700
C	4.25531200	-1.56582900	0.96071900
C	3.42547800	-0.47949900	0.66497900
N	-0.15147800	-2.48137900	1.26650500
C	-0.59887200	-3.01499500	2.42245000
C	-0.79234100	-0.81855400	2.51614300
C	-1.03269100	-1.98766900	3.24622800
N	0.44995400	-2.69772100	-1.15166400
C	0.54032500	-3.43718100	-2.27524100
C	0.53091900	-2.58259900	-3.36796400
C	0.45037300	-1.30043400	-2.81595900
N	0.37756100	-1.37921000	-1.47722700
N	-0.28767200	-1.12663100	1.31344500
N	2.18764100	-0.92297900	0.41016700
H	0.57909400	-2.84409900	-4.41355500
H	-1.45838900	-2.06663400	4.23435700
H	5.30501500	-1.54045900	1.20847500
B	0.86999300	-3.06432200	0.27939000
H	3.64068600	-3.73166300	1.00985600
H	3.65406800	0.57310100	0.62501900
H	0.61488400	-4.51277700	-2.21338900
H	0.45546800	-0.35068200	-3.32102300
H	-0.56344500	-4.08339900	2.57607200
H	-0.93649400	0.20467300	2.80639000

³²Tp, -2873.46225234

Co	-0.79716100	0.31675400	0.03832100
C	0.33687500	3.95125300	0.10460400
C	1.40931300	4.01378600	1.22327900
H	2.22969400	3.32088600	1.02063100
H	1.80424200	5.03216400	1.27505100
H	0.97558100	3.76156700	2.19459900

C	0.92246400	4.39503500	-1.24488100
H	1.80972500	3.81632100	-1.50775800
H	0.19285300	4.29051700	-2.05277600
H	1.20976300	5.44790400	-1.17818000
C	-0.88231700	4.82378400	0.48853700
H	-1.64801500	4.80349200	-0.29387700
H	-1.33124300	4.49053600	1.42721500
H	-0.55241000	5.85912100	0.61005800
C	-0.12469600	2.52609000	0.03372800
O	-0.73800900	1.94989600	1.02001200
O	0.03095500	1.74502400	-0.97433600
C	4.38667300	-0.88994200	-1.59415800
C	3.63417600	0.04152300	-0.90180700
C	2.99612700	-0.36992200	0.31168700
C	3.17484100	-1.70872800	0.79073400
C	3.94944700	-2.62756300	0.03620700
C	4.54012000	-2.22169700	-1.13755100
H	4.88023000	-0.59041400	-2.51459700
C	2.56243800	-2.05836300	2.02119900
H	4.07447600	-3.64193700	0.40412700
H	5.14032600	-2.91673100	-1.71645500
C	1.83270200	-1.11779700	2.71011500
C	1.68820200	0.16834500	2.13975900
H	2.68894400	-3.06494200	2.41082600
H	1.36339500	-1.34708400	3.66064000
H	1.10473600	0.93093500	2.65176300
N	2.22007300	0.53552100	0.98430300
C	3.46234600	1.44951700	-1.40530700
H	4.06099500	1.62151700	-2.30282700
H	2.41263000	1.65025300	-1.64101300
H	3.75908700	2.17703200	-0.64364500
H	-3.20674400	-3.16110600	-0.50715100
N	-3.26169000	-0.92092100	-0.93677100
C	-4.44442800	-0.78821700	-1.56833100
C	-4.61969900	0.54980200	-1.91283400
C	-3.46829300	1.19058000	-1.44804500
N	-1.17776700	-2.29104000	-1.07416600
C	-0.69384100	-3.19848900	-1.94318700
C	0.70314200	-1.48342400	-1.85264800
C	0.51200000	-2.72861800	-2.45554700
N	-2.25158800	-1.88974900	1.12764700
C	-2.77945800	-2.39553200	2.25759400
C	-2.36429000	-1.61512600	3.33425400
C	-1.57420400	-0.61158700	2.76995900

N	-1.50455800	-0.80094800	1.44161300
N	-0.31707200	-1.23918900	-1.01350000
N	-2.65529700	0.29932100	-0.85939300
H	-2.60358000	-1.75362600	4.37719600
H	1.16277900	-3.21805300	-3.16303900
H	-5.46044200	0.99050900	-2.42580600
B	-2.54703500	-2.17687200	-0.36597300
H	-5.07855100	-1.64759400	-1.73095800
H	-3.18194600	2.23100200	-1.50379400
H	-3.41817300	-3.26565100	2.21858800
H	-1.06397200	0.22098000	3.22821300
H	-1.24269900	-4.10708000	-2.14282200
H	1.51073800	-0.77709700	-1.95669300

⁵²Tp, -2873.46393555

Co	-0.56723600	0.11275500	0.02588900
C	2.35767800	2.85202700	0.06272100
C	3.62995400	1.97881000	0.21873200
H	3.72510800	1.26470700	-0.60432400
H	4.51215400	2.62589800	0.21912800
H	3.61320300	1.42284800	1.16094900
C	2.40288200	3.61249000	-1.27497700
H	2.48552300	2.92295200	-2.11853700
H	1.50390800	4.22138700	-1.41424400
H	3.26879600	4.28076300	-1.28716700
C	2.22994800	3.82270600	1.24805700
H	1.32733000	4.43533400	1.16245000
H	2.18675300	3.28451500	2.19808600
H	3.09477600	4.49221200	1.26821500
C	1.19467500	1.88002600	0.05549000
O	0.55816700	1.56876800	1.11407000
O	0.84189500	1.27004300	-1.00949200
C	3.61933900	-1.57868500	-2.03830400
C	2.36644100	-1.42160600	-1.46703500
C	2.28941300	-1.37726700	-0.03968100
C	3.47784600	-1.59233800	0.73986000
C	4.73154100	-1.73906400	0.09544100
C	4.80080200	-1.71147300	-1.27652800
H	3.69154900	-1.61870300	-3.12163400
C	3.36301100	-1.66943700	2.14912600
H	5.62066300	-1.88558800	0.70110200
H	5.75421000	-1.82367100	-1.78241900
C	2.13207700	-1.54651700	2.75066300
C	1.02266500	-1.27489400	1.93292500

H	4.25772500	-1.83942300	2.74158900
H	2.00448400	-1.62529500	3.82398400
H	0.04461100	-1.11453300	2.37853100
N	1.09153900	-1.16048000	0.60985700
C	1.15814000	-1.34699100	-2.36780200
H	1.33132800	-1.92928400	-3.27633400
H	0.25904700	-1.74244300	-1.89390200
H	0.95239100	-0.31605300	-2.66191300
H	-4.86257000	-0.52049100	-0.20667400
N	-3.15478200	0.46772700	-1.33290600
C	-3.80058900	1.01982300	-2.37434800
C	-2.87013400	1.68190000	-3.17739000
C	-1.64595000	1.48592000	-2.54160100
N	-2.93260400	-1.71783200	-0.15818300
C	-3.40347400	-2.97711000	-0.20898900
C	-1.20235800	-3.03228600	-0.04992800
C	-2.32428200	-3.85584200	-0.14571900
N	-3.27807400	0.35984700	1.16421700
C	-4.03232500	0.82884600	2.17410100
C	-3.19594000	1.42933300	3.11510500
C	-1.91098900	1.28999800	2.59178900
N	-1.96748800	0.63654500	1.41420000
N	-1.57493800	-1.73647200	-0.05908500
N	-1.82489400	0.74821900	-1.42604800
H	-3.48474800	1.90415100	4.03997400
H	-2.35279600	-4.93427000	-0.16611700
H	-3.06247100	2.22782900	-4.08799100
B	-3.67923200	-0.36775700	-0.14171100
H	-4.87054600	0.91006400	-2.47648400
H	-0.65527700	1.82752900	-2.79763100
H	-5.10595000	0.70973000	2.15639400
H	-0.95817000	1.62811100	2.96799600
H	-4.46515600	-3.16279000	-0.28273700
H	-0.15838200	-3.29465800	0.01804300

¹TS4_Tp, -3220.19990033, i463.61

C	1.64668700	4.59401500	-0.02245200
C	2.25702000	4.24593800	-1.20863400
C	2.09527300	2.93608300	-1.72279400
C	1.31462200	1.99675100	-0.98145400
C	0.63647400	2.37841200	0.20739200
C	0.82979800	3.67306100	0.66861000
H	3.25756100	3.19880800	-3.53043100
H	1.77096800	5.59562900	0.37802200

H	2.86263700	4.95901100	-1.75993600
C	2.66865400	2.50042900	-2.94201400
H	0.31746800	3.98479800	1.57375500
C	1.74505600	0.32185500	-2.55188700
C	2.47057500	1.20816400	-3.36959100
H	1.61692100	-0.71637100	-2.82664200
H	2.88614300	0.84633800	-4.30308200
N	1.21231000	0.69338800	-1.40021800
C	-0.27980900	1.45373200	0.91246900
H	-0.82370600	0.64224100	0.39297200
H	0.02891700	1.18353500	1.91737800
H	-1.41519200	1.95413800	1.01564200
C	-3.44157900	1.24642900	0.86882800
C	-4.96513600	1.43557500	0.63709600
O	-2.77684600	2.34631100	0.99467200
O	-2.95418300	0.10069000	0.90768700
C	3.08592100	-0.12419600	0.88261700
C	3.85958900	0.20963200	2.18123700
O	1.82653400	-0.38043200	1.11579700
O	3.64299900	-0.13112800	-0.21683600
C	-5.64107900	0.07297100	0.43872400
H	-6.71966500	0.19829600	0.28269600
H	-5.21762100	-0.44548200	-0.42633600
H	-5.48299100	-0.56894500	1.30941900
C	-5.55264800	2.15474800	1.86693200
H	-5.43668300	1.54331400	2.76916400
H	-5.03832400	3.10502100	2.03183100
H	-6.62290100	2.35042000	1.72713600
C	-5.15904700	2.31483200	-0.61366100
H	-4.74953700	1.82080500	-1.50254700
H	-6.22438600	2.50386400	-0.79375100
H	-4.64495000	3.27099600	-0.48948800
C	3.75566600	-0.99247100	3.14114900
H	4.20754200	-1.88733100	2.69883400
H	4.28239500	-0.77643700	4.07756100
H	2.71142300	-1.21899500	3.37017000
C	5.32878000	0.49531300	1.84241500
H	5.88721500	0.72661200	2.75641800
H	5.79308200	-0.36706500	1.35693100
H	5.41384000	1.34183400	1.15588600
C	3.21232600	1.45222800	2.82632700
H	3.22638600	2.30633900	2.14082100
H	2.17180000	1.25349900	3.09508500
H	3.75697700	1.73477600	3.73423200

Co	0.41117300	-0.54906500	-0.12654200
H	-1.94076600	-4.02476100	-0.89523100
N	-1.82846900	-1.81349900	-1.43345100
C	-2.90926300	-1.62343100	-2.21285200
C	-2.92875300	-0.29439000	-2.62019600
C	-1.80050600	0.27878700	-2.02296000
N	0.18936300	-3.22562100	-1.10924000
C	0.85339800	-4.31643800	-1.54045600
C	2.30107600	-2.67233200	-1.21059200
C	2.20528500	-4.00730400	-1.62772000
N	-1.25528900	-2.68190200	0.81757000
C	-1.81356300	-3.24527400	1.90738100
C	-1.36560500	-2.56349900	3.03111000
C	-0.51511700	-1.56791100	2.53237800
N	-0.46591200	-1.65378000	1.20199700
N	1.07763700	-2.21433300	-0.91152400
N	-1.14731700	-0.65218800	-1.31692800
H	-1.62269000	-2.75266600	4.06164100
H	3.00912000	-4.65437200	-1.94343600
H	-3.66255700	0.19362200	-3.24205100
B	-1.29296000	-3.04225800	-0.67777500
H	-3.58148700	-2.44186000	-2.42206700
H	-1.44903000	1.29941200	-2.03367800
H	-2.48027000	-4.08809300	1.80361200
H	0.06263600	-0.81414900	3.04196000
H	0.31641400	-5.22965400	-1.75041700
H	3.14759100	-2.00929800	-1.09897900

³TS4_Tp, -3220.1919531, *i*259.59

C	3.77556700	3.92039700	-0.53452300
C	4.06245400	3.09282500	-1.59467400
C	3.24694600	1.96382200	-1.86654100
C	2.13161300	1.64567800	-1.02077000
C	1.84310000	2.52493600	0.08665500
C	2.66182200	3.64020000	0.27425500
H	4.36251200	1.38632500	-3.62735100
H	4.39276600	4.78812100	-0.32473200
H	4.90623100	3.29339100	-2.24884700
C	3.51177300	1.15135500	-2.99355800
H	2.42797500	4.30906600	1.09709000
C	1.62269900	-0.17070000	-2.39269600
C	2.68295900	0.09546800	-3.27315700
H	0.98005500	-1.02420700	-2.56293300
H	2.83580500	-0.54778400	-4.13222200

N	1.35832500	0.54146100	-1.30064300
C	0.71801300	2.33913500	1.01807700
H	0.62995000	1.33786200	1.43437200
H	0.70650000	3.07525800	1.82182300
H	-0.30874000	2.50388800	0.45857200
C	-2.42646100	2.34763800	1.04187000
C	-3.96177000	2.31020000	0.69487200
O	-1.70202900	2.69832800	0.01564600
O	-2.03055900	2.03803900	2.15609800
C	2.52207800	-0.90389500	1.19850800
C	3.26126800	-0.89687200	2.55799000
O	1.25995800	-0.59803500	1.30816200
O	3.11341300	-1.17695800	0.14926900
C	-4.31830100	0.81281600	0.61922700
H	-5.39385000	0.70562400	0.43497100
H	-3.78259400	0.32118600	-0.19533000
H	-4.06661800	0.30307200	1.55165800
C	-4.69717200	2.98264200	1.86569000
H	-4.42634100	2.50991500	2.81154900
H	-4.45180200	4.04810900	1.92994600
H	-5.77918100	2.89340900	1.71566800
C	-4.29595200	3.00926900	-0.62987400
H	-3.80234200	2.51771100	-1.47090200
H	-5.37851700	2.97313400	-0.79669500
H	-3.98765600	4.05883200	-0.61576600
C	2.59919800	-1.94655500	3.47329100
H	2.68681200	-2.95019300	3.04248400
H	3.08347300	-1.95664500	4.45685700
H	1.53668100	-1.72753900	3.60507000
C	4.74298400	-1.23342200	2.34559800
H	5.27139600	-1.24419800	3.30594200
H	4.85555400	-2.21185400	1.87158000
H	5.22071400	-0.49848300	1.69152000
C	3.12063400	0.50378900	3.18805600
H	3.53912500	1.27494600	2.53073000
H	2.07010900	0.74486200	3.36851400
H	3.65610700	0.54774500	4.14350200
Co	0.01745300	-0.44811300	-0.12956400
H	-3.17030900	-3.18893000	-1.12678200
N	-2.28362100	-1.18151600	-1.71240900
C	-3.10597700	-0.82831600	-2.72116700
C	-2.73156300	0.43116200	-3.17457600
C	-1.64207000	0.78817800	-2.36670400
N	-0.89856600	-3.18308700	-1.10974100

C	-0.62796400	-4.47891600	-1.38848200
C	1.25735600	-3.37858700	-1.03265100
C	0.74836000	-4.65007300	-1.35641000
N	-2.28687700	-2.03835000	0.62337200
C	-3.06786500	-2.44226200	1.64809600
C	-2.62467500	-1.82017800	2.80835800
C	-1.53468200	-1.03512600	2.39896800
N	-1.34472400	-1.17702800	1.08564300
N	0.25818400	-2.50238300	-0.88853600
N	-1.38093700	-0.18944900	-1.49065400
H	-3.03307700	-1.91376100	3.80282500
H	1.30163700	-5.55965700	-1.53620100
H	-3.18594300	1.00958300	-3.96418600
B	-2.24273700	-2.47582100	-0.85796900
H	-3.89559400	-1.49336300	-3.03757100
H	-1.05757100	1.69408100	-2.34640200
H	-3.87568200	-3.13810700	1.47631900
H	-0.89212700	-0.37537600	2.95934600
H	-1.42918500	-5.17693400	-1.58397400
H	2.27117800	-3.03709500	-0.87735400

¹⁵Tp, -3220.2510703

C	-3.16899100	2.43063500	0.76227800
C	-3.17939600	2.40263100	-0.61727000
C	-2.22081800	1.62130900	-1.31407600
C	-1.27207800	0.89940600	-0.54472900
C	-1.30610200	0.86635000	0.87084100
C	-2.24504900	1.65385600	1.50835900
H	-2.84695700	2.03291500	-3.34908000
H	-3.88889500	3.04697800	1.29314800
H	-3.90319700	2.98360900	-1.18169000
C	-2.13129400	1.50762400	-2.72232100
H	-2.29095100	1.66619000	2.59345600
C	-0.19106600	0.10861300	-2.44191900
C	-1.13860500	0.73266700	-3.27996000
H	0.64746200	-0.44545300	-2.84467700
H	-1.04574800	0.62139900	-4.35446600
N	-0.25017700	0.20381500	-1.12637200
C	-0.31436500	-0.06149400	1.50169800
H	-0.74915200	-1.05065400	1.70749000
H	0.08520700	0.33993600	2.43510800
H	-2.81300000	-1.32699000	1.76347600
C	-4.17044500	-1.11164100	0.47704000
C	-5.66710900	-0.84353300	0.32762000

O	-3.77638400	-1.19188900	1.76557400
O	-3.40255200	-1.28668900	-0.45011400
C	1.57001100	2.51585000	-0.23020000
C	1.84586200	3.83752600	0.53217000
O	1.58613100	1.48223200	0.55869100
O	1.35600300	2.51613900	-1.44648500
C	-5.93839600	-0.36669500	-1.10734700
H	-7.01257200	-0.21177700	-1.25033400
H	-5.42057200	0.57664000	-1.30446800
H	-5.58600800	-1.09880300	-1.83733300
C	-6.38664800	-2.18766400	0.59235800
H	-6.06447600	-2.95332300	-0.12078000
H	-6.18501900	-2.54870100	1.60503200
H	-7.46776500	-2.05308800	0.48288500
C	-6.14057700	0.21222900	1.34447000
H	-5.62095100	1.16161600	1.18909800
H	-7.21487600	0.38376000	1.21969200
H	-5.95775900	-0.11263300	2.37105100
C	3.22579000	3.73742600	1.21153200
H	4.01913700	3.60552000	0.46720200
H	3.44165100	4.65194800	1.77659000
H	3.26087400	2.88524600	1.89469300
C	1.82201200	5.01639700	-0.44956200
H	2.01848800	5.95572600	0.08049600
H	2.57725400	4.88944300	-1.22976300
H	0.85089400	5.08971900	-0.94636800
C	0.74878600	4.01542500	1.60132500
H	-0.24434400	4.06235000	1.14119500
H	0.75303800	3.17583100	2.30110000
H	0.90860500	4.94343400	2.16303700
Co	1.11325400	-0.32787400	0.16698100
H	3.84981500	-3.65085300	0.02617200
N	1.63417900	-3.15872100	-0.13383200
C	1.09683000	-4.36924800	-0.39142300
C	-0.27372400	-4.21381800	-0.55123100
C	-0.50348900	-2.84039900	-0.37512500
N	3.41810600	-1.71244900	-1.09196900
C	4.44056900	-1.66451900	-1.97369300
C	3.20879200	0.16435900	-2.16382900
C	4.34294600	-0.47936900	-2.68895700
N	3.19293100	-1.93243500	1.36969700
C	4.06510800	-2.02254500	2.39676500
C	3.84114500	-0.95527500	3.25633200
C	2.79334300	-0.23339700	2.66325900

N	2.41224500	-0.83701700	1.53568000
N	2.65790700	-0.59104600	-1.20660000
N	0.65576900	-2.22012300	-0.12225600
H	4.36106500	-0.72911100	4.17458000
H	4.99765100	-0.12820600	-3.47212900
H	-1.00312900	-4.97982600	-0.76568100
B	3.10099400	-2.71405800	0.03883600
H	1.72749600	-5.24434000	-0.44350300
H	-1.42523700	-2.27777300	-0.42463600
H	4.77834400	-2.83245600	2.43581200
H	2.31422200	0.68660800	2.95852300
H	5.15715200	-2.47137800	-2.02374800
H	2.75887100	1.12062500	-2.39202800

³⁵Tp, -3220.22818968

C	3.20654600	2.41683600	-0.97275900
C	3.34148900	2.35090900	0.39833400
C	2.45716000	1.54008400	1.15872100
C	1.45753000	0.80873600	0.46639700
C	1.36130600	0.82893100	-0.95182900
C	2.21923800	1.65728600	-1.65064800
H	3.23175100	1.96024300	3.14053600
H	3.87026000	3.05315400	-1.55049300
H	4.10377900	2.93091600	0.91090800
C	2.47704700	1.42434800	2.57087900
H	2.15033300	1.71533500	-2.73285900
C	0.53480400	0.01126000	2.43472400
C	1.53249300	0.64769100	3.20509800
H	-0.27124600	-0.54843300	2.89881400
H	1.51949000	0.54526000	4.28464100
N	0.49959400	0.09452700	1.11904200
C	0.35049000	-0.07067900	-1.55967300
H	0.64918900	-1.12157000	-1.60728300
H	-0.07415900	0.28174000	-2.49876200
H	2.89563200	-1.34868900	-2.09204600
C	4.07706200	-1.35086300	-0.63269200
C	5.54206100	-1.14266000	-0.25394400
O	3.84915200	-1.21617400	-1.95775800
O	3.19384800	-1.65117300	0.14695000
C	-1.30574600	2.66321700	0.23331700
C	-1.51505000	4.04301700	-0.44061300
O	-1.47521400	1.66572900	-0.58003000
O	-0.99691500	2.58064900	1.42876200
C	5.62256100	-0.87836200	1.25756100

H	6.66912300	-0.77277100	1.56044100
H	5.08957600	0.04042400	1.51885700
H	5.17083100	-1.69604300	1.82347800
C	6.28074500	-2.45543700	-0.60896000
H	5.86102900	-3.30411100	-0.05939800
H	6.21398800	-2.66703700	-1.68013700
H	7.33843600	-2.36469500	-0.34088000
C	6.15428400	0.03171400	-1.04052200
H	5.62196100	0.96251400	-0.82708400
H	7.20229800	0.15830900	-0.74942800
H	6.11281100	-0.14509600	-2.11757100
C	-2.93624400	4.09005900	-1.03500800
H	-3.69231500	3.98393600	-0.24893900
H	-3.10838500	5.04698000	-1.54214200
H	-3.08044600	3.27893500	-1.75300200
C	-1.33137200	5.16219200	0.59243500
H	-1.47826500	6.14200000	0.12276000
H	-2.04655500	5.05622900	1.41261600
H	-0.32961000	5.12774700	1.02900600
C	-0.47452400	4.18708300	-1.56946400
H	0.54519800	4.13687600	-1.17211500
H	-0.58995900	3.38391400	-2.30206900
H	-0.59435800	5.14975000	-2.08070200
Co	-1.16043900	-0.24744000	-0.17387100
H	-4.22968600	-3.36431700	0.17199200
N	-1.97200800	-3.13973500	0.16925700
C	-1.59250500	-4.41777100	0.37702400
C	-0.20530600	-4.45636000	0.44961300
C	0.19702900	-3.12301600	0.27435400
N	-3.51953500	-1.46800400	1.19928700
C	-4.43774400	-1.35425000	2.18384300
C	-3.02652400	0.34669400	2.29061800
C	-4.15941000	-0.20566200	2.91225100
N	-3.50520900	-1.78151000	-1.28386200
C	-4.43581500	-1.88633500	-2.25679600
C	-4.17046400	-0.92400900	-3.22295900
C	-3.03312100	-0.25272700	-2.74620900
N	-2.64077800	-0.77990300	-1.58336200
N	-2.65094300	-0.42548800	1.26460200
N	-0.87645300	-2.34018200	0.10512400
H	-4.72156300	-0.73434900	-4.13146200
H	-4.69950100	0.17915200	3.76400700
H	0.42093200	-5.32095300	0.60961100
B	-3.38383800	-2.51805100	0.07196600

H	-2.33209400	-5.20066900	0.46021700
H	1.18735900	-2.68842000	0.26732200
H	-5.21522000	-2.63115000	-2.19015600
H	-2.49399200	0.58851800	-3.15707500
H	-5.21702500	-2.09459000	2.29092800
H	-2.46633100	1.25033500	2.48958300