

Supporting Information

**Palladium-Catalyzed Regio- and Chemoselective
Double-Alkoxy carbonylation of 1,3-Diynes: A
Computational Study**

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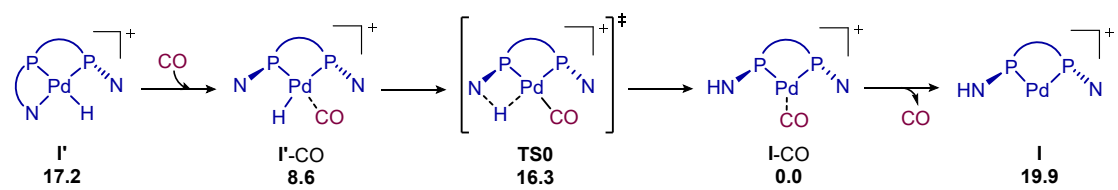
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Table of Contents:

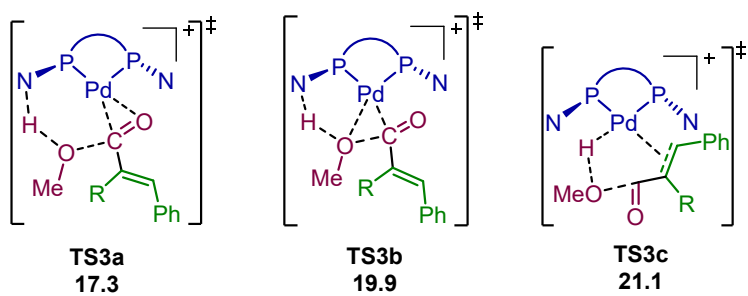
1. Interconversion between I and I'	S2
2. Other possibilities for methanolysis of IM4	S3
3. Other possible pathways for the methoxycarbonylation of (E)-3a	S4
4. 2,1-hydropalladation of (E)-3a	S5
5. The N-H proton shuttle transfer of (E,E)-2a	S6
6. The alternative 2,1-insertion of (E,E)-2a	S7
7. Frontier molecular orbitals of TS4 and TS8	S8
8. Non-covalent interactions of TS1 and TS7	S9
9. Table of calculated energies and energy corrections	S10
10. Cartesian coordinates	S12

1. Interconversion between I and I'



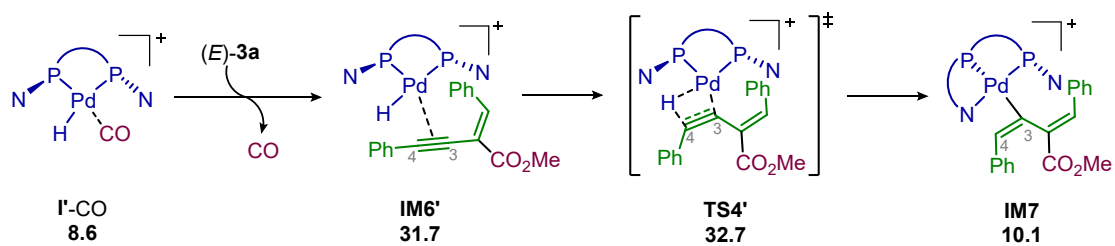
Scheme S1. Interconversion between I and I'. Energies are given in kcal/mol.

2. Other possibilities for methanolysis of IM4

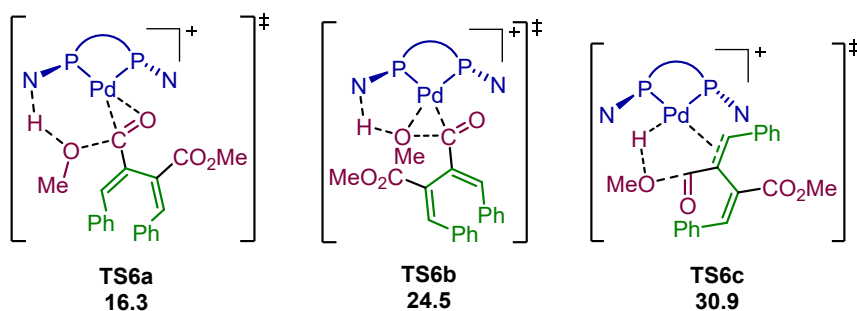


Scheme S2. Other possibilities for methanolysis of **IM4**. Energies are given in kcal/mol.

3. Other possible pathways for the methoxycarbonylation of (*E*)-3a

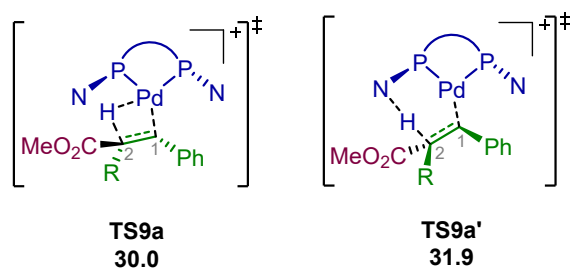


Scheme S3. 4,3-insertion of (*E*)-3a. Energies are given in kcal/mol.



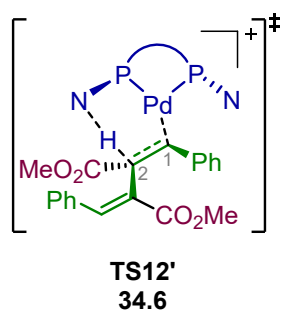
Scheme S4. Other possibilities for methanolysis of **IM9**. Energies are given in kcal/mol.

4. 2,1-hydropalladation of (*E*)-**3a**



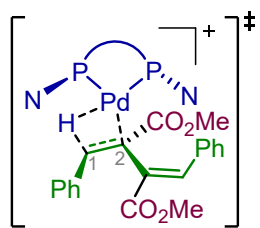
Scheme S5. 2,1-hydropalladation of (*E*)-**3a**. Energies are given in kcal/mol.

5. The N-H proton shuttle transfer of (*E,E*)-2a



Scheme S6. The N-H proton shuttle transfer of (*E,E*)-2a. Energies are given in kcal/mol.

6. The alternative 2,1-insertion of (*E,E*)-2a



Scheme S7. 2,1-insertion of (*E,E*)-2a. Energies are given in kcal/mol.

7. Frontier molecular orbitals of TS4 and TS8

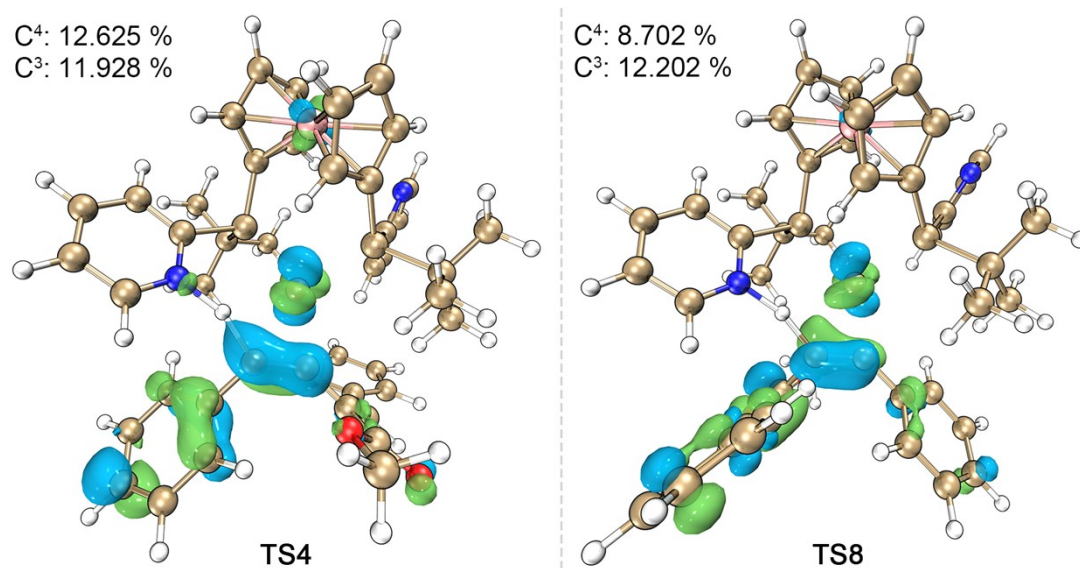


Figure S1. Frontier molecular orbitals of TS4 and TS8.

8. Non-covalent interactions of TS1 and TS7

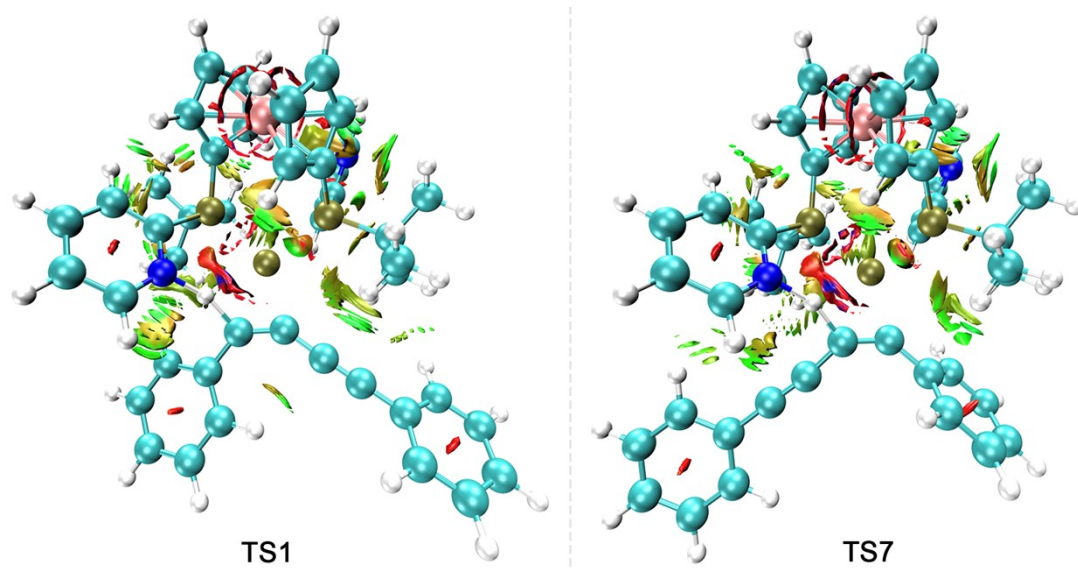


Figure S2. Non-covalent interactions of TS1 and TS7.

9. Table of calculated energies and energy corrections

Stationary point	Single-point energy- M06-SMD Def2-TZVPP (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
1a	-615.3659547	0.159911
CO	-113.291689	-0.014102
MeOH	-115.7100919	0.028751
I'	-3271.363748	0.505113
I	-3271.361303	0.506964
I'-CO	-3384.687720	0.509584
I-CO	-3384.702839	0.511049
I'-MeOH	-3387.086171	0.557160
I-MeOH	-3387.079013	0.556198
I'-1a	-3886.740456	0.691125
I-1a	-3886.767060	0.694175
IM1'	-3886.739846	0.690768
IM1	-3886.763648	0.695807
TS1'	-3886.736328	0.689655
TS1	-3886.741512	0.689299
IM2	-3886.783892	0.694081
IM3	-4000.095624	0.702044
TS2	-4000.089320	0.700653
IM4	-4000.100791	0.700455
IM4-CO	-4113.424132	0.705107
TS3	-4115.822783	0.757176
IM5	-4115.868975	0.758096
(E)-3a	-844.458528	0.219741
IM6	-4115.859112	0.759366
TS4	-4115.836001	0.753111
IM7	-4115.867829	0.759172
IM8	-4229.173378	0.765244
TS5	-4229.169038	0.764671
IM9	-4229.195749	0.764546
IM9-CO	-4342.516268	0.768833

TS6	-4344.909410	0.818409
IM10	-4344.948245	0.821304
<i>(E,E)</i> - 2a	-1073.549122	0.281977
TS7	-3886.735735	0.687482
IM11	-3886.777500	0.694167
IM12	-4115.861057	0.757655
TS8	-4115.826822	0.751466
IM13	-4115.866528	0.755678
IM14	-4115.871034	0.760409
TS9	-4115.833555	0.751670
IM15	-4115.856347	0.755180
IM16	-4229.155245	0.760177
TS10	-4229.135397	0.755527
IM17	-4229.166917	0.765853
IM17-CO	-4342.482405	0.767953
TS11	-4344.870688	0.817721
IM18	-4344.896690	0.817735
6a	-1073.515000	0.279170
IM19	-4344.912626	0.813289
TS12	-4344.912611	0.813631
IM20	-4344.933656	0.818215

10. Cartesian coordinates

1a

C	-4.06645600	2.61719100	-0.00000100
C	-2.67494500	2.61178700	0.00055100
C	-1.96054900	3.82661700	0.00028200
C	-2.67524400	5.04127400	-0.00057600
C	-4.06675000	5.03553900	-0.00113100
C	-4.76643000	3.82627700	-0.00084500
H	-4.60728600	1.67519900	0.00023100
H	-2.12490000	1.67641200	0.00121900
H	-2.12542100	5.97678100	-0.00079400
H	-4.60781500	5.97739600	-0.00179700
H	-5.85256700	3.82614800	-0.00128500
C	-0.53965700	3.82675600	0.00087400
C	0.68091600	3.82683100	0.00135100
C	2.03992400	3.82670700	0.00193700
C	3.26049400	3.82664100	0.00267700
C	4.68140300	3.82663200	0.00360500
C	5.39672900	3.82502600	-1.21068200
C	5.39516700	3.82824900	1.21880100
C	6.78823300	3.82503800	-1.20422200
H	4.84738700	3.82379200	-2.14646900
C	6.78668500	3.82823100	1.21412200
H	4.84463500	3.82949600	2.15388800
C	7.48728500	3.82663300	0.00540200
H	7.32979100	3.82380100	-2.14579500
H	7.32702800	3.82947900	2.15639300
H	8.57342100	3.82664200	0.00609500

CO

C	-2.59715300	0.94320500	0.03385200
O	-1.45941700	0.94320500	0.03385200

MeOH

C	0.04472400	0.66412500	0.00000000
H	-0.44079900	1.08744500	0.89321800
H	-0.44079900	1.08744500	-0.89321800
H	1.09085000	0.98208000	0.00000000
O	0.05023800	-0.75344100	0.00000000
H	-0.87064000	-1.05286800	0.00000000

I'

C	7.15322000	5.82169100	2.42830700
C	7.45524700	7.15088600	1.97708500

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H	8.19328500	5.30827900	-0.72895500
C	7.42178800	4.92367200	1.33227200
H	7.30428700	3.84909100	1.36223300
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C	10.46804200	6.48347600	3.32988800
H	10.18608100	7.10009500	4.16964800
C	10.92856700	6.95674800	2.06876400
H	11.06650900	7.99464800	1.79779800
C	11.10686300	5.83554700	1.20778200
H	11.40693800	5.87194400	0.16931300
C	10.76885300	4.65838500	1.93371700
H	10.76825500	3.64914600	1.54702700
C	6.88766300	6.40397800	5.33021200
C	6.71994000	5.98334300	6.65708300
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H	4.70080700	7.28085500	2.65539600
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C	9.80229900	-0.45029300	3.42717700

H	9.69215900	-1.50788400	3.21405700
C	8.70552100	0.28227000	3.88300500
H	7.72766900	-0.16499700	4.02261100
C	10.72070200	4.16758900	6.11758300
C	10.48981700	5.58758500	6.66235800
H	10.94636300	5.66380500	7.65611200
H	9.42640400	5.81864300	6.76360500
H	10.95771000	6.34536900	6.02955200
C	12.21559800	3.93872300	5.85716100
H	12.59621700	4.60436000	5.07532100
H	12.42494400	2.90379400	5.57094500
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Fe	9.13396200	5.93407400	1.86896000
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N	8.80608800	1.58806300	4.15978000
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C	5.92234300	6.25746900	5.30575200

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C	11.19395900	2.56388600	5.54813500
C	10.82421200	2.93367800	6.99433900
H	11.46651600	2.37956000	7.68907800
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H	11.59225900	0.48881200	6.02185900
H	11.25162200	0.75707100	4.30626200
H	9.92679500	0.77647800	5.48930200
Fe	9.46877100	6.72574600	3.56932200

N	6.86139000	7.10758100	5.80906800
N	11.58478400	3.46752600	2.16777900
P	6.38834400	5.21197000	3.86785300
P	9.97744500	3.47834100	4.42752600
Pd	7.65182500	3.51286700	4.62264200
H	7.73735400	7.19283300	5.27667700

I'-CO

C	7.56204300	6.35457600	2.70173900
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C	8.72727700	8.15257900	1.83273800
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H	8.53051800	4.84314000	1.34381900
C	10.33168300	5.24685000	4.25314900
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H	8.97973800	6.08579400	5.84532300
C	10.43369800	7.47425700	4.87669000
H	10.20619400	8.41944300	5.35062800
C	11.39749400	7.25994600	3.84902300
H	12.03251900	8.01514900	3.40576900
C	11.34727200	5.89298700	3.46434500
H	11.94668400	5.41856700	2.70384600
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C	6.48749100	5.21772500	6.51120800
H	6.65909400	4.15059900	6.41128300
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H	6.43334800	5.20541900	8.67019000
C	6.16511300	7.18460200	7.84546000
H	6.06885100	7.68916200	8.80099500
C	6.08293700	7.91138100	6.65459100
H	5.91907900	8.98608200	6.67151900
C	4.81374600	5.37426500	2.96287700
C	4.82772600	4.57308800	1.64980900
H	3.84952400	4.65785400	1.16299200
H	5.02405100	3.50826900	1.81319800
H	5.57934800	4.95836500	0.95226000
C	3.80338500	4.78445700	3.95837400
H	2.81239300	4.75587700	3.49172100
H	3.72914200	5.39410700	4.86379900
H	4.05167300	3.76158600	4.25730100

C	4.45446500	6.84090100	2.66704900
H	5.11220700	7.26951600	1.90620400
H	4.51568600	7.46308700	3.56325100
H	3.42701700	6.88162800	2.28666300
C	10.62973100	2.88049000	2.64143600
C	9.89185500	2.34154600	1.58357300
H	8.80891800	2.29259200	1.63818000
C	10.57979800	1.85880300	0.46853000
H	10.03737200	1.43600500	-0.37158700
C	11.97061200	1.92341600	0.45922500
H	12.54658000	1.55544000	-0.38325500
C	12.61947800	2.47274200	1.56865000
H	13.70424300	2.53646100	1.60324900
C	10.57600000	2.67041300	5.63780700
C	9.63152400	2.89281400	6.83274300
H	10.07559900	2.44653000	7.72988100
H	8.65690100	2.42005600	6.66682200
H	9.47313400	3.95736200	7.03750700
C	11.95539100	3.28707200	5.92964000
H	11.87544400	4.34144400	6.20773300
H	12.61810100	3.20507500	5.06557200
H	12.40764000	2.74876100	6.77069900
C	10.72181000	1.16991900	5.34693700
H	11.09338200	0.66997100	6.24849200
H	11.43623900	0.98509200	4.54050500
H	9.76677200	0.70324700	5.08224800
Fe	9.49330800	6.73199700	3.16322500
N	6.19382300	7.35453200	5.44358000
N	11.97004000	2.94664000	2.63689700
P	6.54566600	5.26255700	3.70669300
P	9.79354100	3.53009000	4.14847600
Pd	7.49710000	3.04351900	3.95624100
H	8.19196900	1.62907000	4.12609800
C	5.87378000	1.96622900	3.85564700
O	5.00978300	1.22392500	3.81119800
I-CO			
C	7.84479200	6.62645500	3.17777400
C	8.12768200	8.00432500	3.48542500
H	7.68128100	8.59248200	4.27362900
C	9.16406400	8.45123700	2.61540200
H	9.61941800	9.43228900	2.63020400
C	9.53626900	7.36603600	1.77130900
H	10.32659900	7.37387700	1.03338700

C	8.73901600	6.24044500	2.11661300
H	8.82638300	5.25298400	1.69006400
C	10.58064100	5.18659800	4.68839800
C	10.05651900	6.10568800	5.66635600
H	9.24737000	5.88542500	6.35065300
C	10.75773500	7.33732000	5.54767500
H	10.56686900	8.23662200	6.11783300
C	11.71889400	7.19416300	4.50347800
H	12.37923300	7.97044500	4.13975600
C	11.61993200	5.87517400	3.97825400
H	12.16871300	5.46157900	3.14731700
C	5.78344400	6.48865200	5.16813300
C	5.24818100	7.76562700	5.01238000
H	5.41621100	8.30458100	4.08949500
C	4.49210500	8.33339500	6.04044100
H	4.06873700	9.32510800	5.91452700
C	4.27109000	7.62657100	7.22686000
H	3.68780500	8.04721700	8.03735400
C	4.81808200	6.36068100	7.35359600
H	4.70611500	5.73437500	8.23097600
C	5.39275600	5.04302200	2.67857400
C	5.99078000	3.96198300	1.75985800
H	5.23912300	3.66566200	1.01878100
H	6.27903400	3.07325600	2.32938000
H	6.86866800	4.32164600	1.21627700
C	4.17822200	4.46024100	3.42063600
H	3.44639900	4.10053700	2.68858100
H	3.67604000	5.21098000	4.04123600
H	4.46182900	3.61480500	4.05707000
C	4.99086400	6.27284000	1.85657400
H	5.85182400	6.73132200	1.36158200
H	4.49592100	7.03308400	2.46942700
H	4.27618800	5.97179900	1.08140400
C	10.07544600	3.06986100	2.72816500
C	9.14446600	2.17826800	2.17851300
H	8.34532000	1.78348900	2.79832100
C	9.26266500	1.81859700	0.83637900
H	8.55741900	1.12607500	0.38629200
C	10.29877700	2.37044300	0.08574500
H	10.42793300	2.12749200	-0.96380000
C	11.18181400	3.24760100	0.71972600
H	12.00815400	3.69261800	0.16993800
C	11.07860300	2.38959300	5.41082400
C	11.02917200	2.78488000	6.89582400

H	11.67298400	2.11103100	7.47332800
H	10.01258200	2.70792100	7.29707400
H	11.38822000	3.80726300	7.05384200
C	12.50860300	2.52955200	4.87072500
H	12.88602200	3.54923200	4.99331600
H	12.57282900	2.26920800	3.81047500
H	13.17327600	1.85644500	5.42590700
C	10.57286000	0.94918400	5.23551500
H	11.21024900	0.26620100	5.80900500
H	10.60478500	0.63191600	4.18783800
H	9.54563600	0.83807800	5.60041300
Fe	9.79935500	6.83908200	3.76819700
N	5.54274900	5.85386800	6.34017300
N	11.08480300	3.59010800	2.00970800
P	6.74000600	5.42592800	3.96737700
P	9.87560600	3.52787400	4.50367800
Pd	7.57500200	3.60947400	5.21256400
H	5.96364700	4.89186600	6.39020000
C	6.92301700	2.49726400	6.63268600
O	6.59561000	1.77300000	7.46982900

I'-MeOH

C	7.90148200	6.61245200	3.18536000
C	8.22406700	7.99398000	3.43585300
H	7.82297800	8.61296700	4.22319100
C	9.23985900	8.39003200	2.51909900
H	9.71590600	9.36083200	2.48847000
C	9.56143400	7.27089400	1.69907600
H	10.32591900	7.23750100	0.93501900
C	8.74837400	6.17763800	2.10482400
H	8.79340000	5.17758300	1.70289300
C	10.60581800	5.16416600	4.64020600
C	10.09052600	6.09258300	5.61421600
H	9.26671900	5.89610300	6.28762500
C	10.81640400	7.30850200	5.49158800
H	10.63232600	8.21443200	6.05309100
C	11.78466300	7.14464700	4.45694100
H	12.46167400	7.90758600	4.09626200
C	11.66681100	5.82861300	3.93168200
H	12.21930200	5.40174900	3.11027100
C	5.91096800	6.52075900	5.30444300
C	5.48631100	7.83194300	5.06525800
H	5.69084100	8.30779000	4.11580600
C	4.78576600	8.51521000	6.06007600

H	4.45097000	9.53400100	5.89043300
C	4.51855400	7.87052600	7.26509800
H	3.97940300	8.36523000	8.06552500
C	4.94793900	6.55341900	7.41584500
H	4.74236500	5.99914800	8.32756600
C	5.42174800	5.04615200	2.82170100
C	5.95900000	3.93340700	1.90561100
H	5.18602600	3.66450600	1.17601200
H	6.20885900	3.03587600	2.47980700
H	6.84590600	4.24543400	1.34722200
C	4.21191000	4.51045600	3.60731600
H	3.45168100	4.16741500	2.89591800
H	3.75473500	5.28580800	4.22991800
H	4.48046500	3.66690400	4.25001000
C	5.01430700	6.26560400	1.98389400
H	5.86006100	6.68642000	1.43197600
H	4.57251500	7.05469000	2.59968300
H	4.25360200	5.96086700	1.25528200
C	10.04901900	3.05418300	2.65734300
C	9.08476200	2.20480400	2.10468600
H	8.27398200	1.83090600	2.72056600
C	9.18959400	1.86338700	0.75591700
H	8.45653100	1.20771900	0.29580600
C	10.24757200	2.38331300	0.01374200
H	10.36549000	2.15141600	-1.03952900
C	11.16901600	3.21240200	0.65896800
H	12.01526200	3.62787700	0.11718100
C	11.14592800	2.36598900	5.31109000
C	11.06576500	2.65189600	6.81913600
H	11.79544500	2.02254700	7.34134900
H	10.07317800	2.42512500	7.22034600
H	11.30324600	3.69657400	7.04616600
C	12.57136900	2.65157100	4.80311100
H	12.89610000	3.66373200	5.05828600
H	12.65806400	2.52541800	3.72078900
H	13.26020600	1.94762600	5.28373300
C	10.77189800	0.90602800	5.01739400
H	11.45528100	0.24665300	5.56405100
H	10.86134400	0.67003500	3.95216800
H	9.75213400	0.67332400	5.34066900
Fe	9.86476800	6.80115400	3.70745400
N	5.62407800	5.89480800	6.46590000
N	11.08158000	3.54203000	1.95240900
P	6.79922900	5.46956300	4.06322200

P	9.92583500	3.51039500	4.43735500
Pd	7.77309200	3.47387000	5.13752800
H	8.32227400	2.17324300	5.81153200
C	5.81454500	2.34571600	7.34889700
H	6.01536200	1.33348200	6.99833100
H	4.80595800	2.39227600	7.77223800
H	6.55548900	2.62181300	8.10625100
O	5.89119100	3.21319200	6.20460000
H	5.72371000	4.16482500	6.47213200

I-MeOH

C	7.46201500	6.41147000	2.88257700
C	7.65049600	7.83842100	2.96027400
H	7.10877100	8.52807200	3.59374100
C	8.65707200	8.21153200	2.02439400
H	9.04517700	9.21114200	1.88078100
C	9.08500900	7.03669000	1.34344600
H	9.86429100	6.98463400	0.59521900
C	8.36143500	5.93211000	1.87047600
H	8.48133700	4.89167000	1.60130200
C	10.47350800	5.27881900	4.29958200
C	9.94856900	6.18087700	5.28578800
H	9.27005600	5.89043600	6.07451500
C	10.48612300	7.48338000	5.06041400
H	10.27792600	8.37520100	5.63756600
C	11.34159400	7.40746300	3.92586400
H	11.86998300	8.23295000	3.46801600
C	11.33646100	6.05935600	3.45854300
H	11.84661800	5.71195700	2.57350300
C	6.04268600	6.08643400	5.34080200
C	5.02230800	5.71150600	6.23504300
H	4.31379100	4.95495600	5.92811800
C	4.94521400	6.27166800	7.49809500
H	4.14519700	5.97788800	8.16998000
C	5.91273600	7.20534500	7.92516200
H	5.88332100	7.64141700	8.91603600
C	6.91346200	7.54628300	7.04923000
H	7.71133900	8.24195000	7.27997300
C	4.73404700	5.41829700	2.77166700
C	5.09861200	5.00837400	1.33178800
H	4.18711100	4.98917100	0.72337200
H	5.54412300	4.00739900	1.30353500
H	5.79681700	5.71050000	0.86868600
C	3.69477100	4.42148700	3.31112700

H	2.87177500	4.33304500	2.59225500
H	3.25114300	4.75013800	4.25528700
H	4.12980000	3.42659500	3.45594600
C	4.18334900	6.84951200	2.79262200
H	4.90878900	7.56605300	2.39472900
H	3.90492800	7.16329400	3.80481000
H	3.28287700	6.91036000	2.16895300
C	10.71659400	2.84881800	2.72044600
C	12.04141100	3.09808700	2.34153200
H	12.66876600	3.74408300	2.94139800
C	12.55499500	2.49086400	1.19515900
H	13.58075100	2.67555300	0.89011300
C	11.73599400	1.63906200	0.45841600
H	12.09269000	1.14392200	-0.43832700
C	10.43559300	1.42395700	0.91221400
H	9.76466600	0.75331000	0.38127400
C	10.80370000	2.67196000	5.65096900
C	10.15118600	3.15358500	6.95893500
H	10.53089400	2.55619100	7.79637900
H	9.06097400	3.04418100	6.92625600
H	10.39116500	4.20105100	7.16804900
C	12.31120900	2.94628800	5.69135000
H	12.52888900	4.01958400	5.72517000
H	12.82585800	2.51213900	4.82971600
H	12.74395000	2.49050900	6.59052400
C	10.53136700	1.16787800	5.46962100
H	10.95293100	0.61617300	6.31825300
H	10.99244800	0.77800700	4.55629700
H	9.45745300	0.95533200	5.42460800
Fe	9.42967800	6.81579900	3.37851100
N	6.93531100	7.00703200	5.80405400
N	9.93427700	2.01097300	2.00622500
P	6.36469600	5.23368000	3.75127200
P	9.88614400	3.54164000	4.23199100
Pd	7.54307300	3.39299900	4.08837700
H	7.71618600	7.23968700	5.18176700
C	6.44570600	0.94476700	2.06095900
H	5.48187600	0.84984500	2.56578700
H	6.37067900	1.73737900	1.30367300
H	6.67685500	-0.00693500	1.56464800
O	7.41671200	1.25508800	3.05581200
H	8.28853500	1.43133900	2.62121100

I'-1a

C	7.45873300	6.30251000	3.02542000
C	7.27882600	7.66848200	3.43137300
H	6.53939000	8.02197300	4.13572900
C	8.28049500	8.45670400	2.79772400
H	8.43506400	9.51760100	2.94180200
C	9.07868800	7.59580300	1.98854000
H	9.94696500	7.88702400	1.41306200
C	8.58007800	6.27020200	2.12389300
H	9.00092400	5.38791400	1.66636700
C	10.07459900	5.46204400	4.96232500
C	9.19562700	6.16359200	5.86105100
H	8.32012800	5.73750200	6.33102600
C	9.62274200	7.51774300	5.91950900
H	9.13544000	8.31032200	6.47127400
C	10.76290600	7.66487000	5.07348000
H	11.28986600	8.58841600	4.87351000
C	11.05164200	6.40386800	4.48311100
H	11.81798300	6.17912600	3.75836400
C	5.46048400	5.58905500	4.91036900
C	4.27958100	6.31551600	4.73478100
H	3.87908900	6.49689700	3.74660900
C	3.62389800	6.81865700	5.85991300
H	2.70321900	7.38360400	5.74872300
C	4.17146500	6.58881800	7.11844000
H	3.69465400	6.96028400	8.01929100
C	5.35857500	5.85863800	7.19860100
H	5.81739600	5.64646800	8.16006000
C	5.41804200	4.48076400	2.05831100
C	6.28642600	3.60887000	1.12989200
H	5.70741400	3.35232800	0.23405400
H	6.59151900	2.68036300	1.61530100
H	7.18601200	4.13679500	0.79856500
C	4.17881600	3.68208800	2.49566200
H	3.60979500	3.38505600	1.60657100
H	3.51371700	4.26970200	3.13430700
H	4.45296500	2.77290700	3.03555900
C	5.00657900	5.74474200	1.28527700
H	5.88019800	6.29751500	0.93120400
H	4.39471700	6.43217900	1.87409900
H	4.41527600	5.44901900	0.41024800
C	10.39329800	3.47027000	2.81428300
C	9.70372500	2.55786300	2.00912000
H	8.85559500	2.01570100	2.40856100
C	10.12512500	2.37257900	0.69151000

H	9.60852300	1.67088900	0.04460800
C	11.21421400	3.10914900	0.23116300
H	11.57510300	3.00650400	-0.78702000
C	11.84717200	3.98807900	1.11457500
H	12.70724500	4.57171700	0.79488700
C	11.13964800	2.80349500	5.59635200
C	10.70849200	2.89537400	7.06885500
H	11.45868800	2.39752600	7.69407300
H	9.74477200	2.40452100	7.23871100
H	10.63188600	3.93582200	7.40228400
C	12.52161800	3.45877400	5.41901000
H	12.53024300	4.48647600	5.79134800
H	12.83984600	3.47098500	4.37364000
H	13.25698200	2.88556900	5.99529100
C	11.19344800	1.33821100	5.13939100
H	11.90133100	0.79192000	5.77298900
H	11.53403000	1.25005000	4.10257300
H	10.21795300	0.84803500	5.22623700
Fe	9.13712200	6.95779100	3.96977500
N	5.98649100	5.36387500	6.12918200
N	11.45525500	4.16815500	2.38069900
P	6.50445200	4.86029900	3.56787700
P	9.85743000	3.72326000	4.56242800
Pd	7.68078400	3.02714300	4.71956600
H	8.42170700	1.92628700	5.54207500
C	7.07915400	0.10976500	2.27297000
C	6.58743000	0.62193300	3.26664800
C	5.65224200	1.85782200	5.34846600
C	6.10376400	1.27813100	4.35476200
C	7.73637700	-0.35326800	1.10531300
C	8.93023000	-1.09551900	1.21250400
C	7.24424300	-0.00558900	-0.16969000
C	9.61962100	-1.47057600	0.06402100
H	9.30378200	-1.36157700	2.19578200
C	7.94308700	-0.38768200	-1.31080100
H	6.32432800	0.56418400	-0.24758000
C	9.13095000	-1.11674000	-1.19713900
H	10.53926400	-2.04058300	0.15109200
H	7.56079600	-0.11939700	-2.29082200
H	9.67173100	-1.41340200	-2.09055100
C	4.94754600	2.35278000	6.48443800
C	3.63086000	2.82907900	6.34362900
C	5.56503100	2.36162700	7.74945300
C	2.94308900	3.29669400	7.45900000

H	3.16275600	2.82431500	5.36540500
C	4.86259900	2.82081500	8.85829000
H	6.58617400	2.00761300	7.84212100
C	3.55291600	3.28867200	8.71616700
H	1.92689000	3.66200200	7.34874300
H	5.33557100	2.81375800	9.83553000
H	3.00804900	3.64584900	9.58475700

I-1a

C	5.98480600	7.43824800	4.54841400
C	5.96674400	8.83269500	4.89128500
H	5.80913300	9.21374600	5.88754200
C	6.27627700	9.58239600	3.72214300
H	6.38730400	10.65763500	3.67245900
C	6.47762700	8.67101500	2.64328900
H	6.75933400	8.93420100	1.63240800
C	6.29567400	7.35250300	3.14569300
H	6.40143400	6.42736000	2.59504900
C	9.34134400	6.92164100	4.44364600
C	9.09474200	7.64221000	5.66501400
H	8.75361400	7.21394400	6.59516100
C	9.30697800	9.02649800	5.41812000
H	9.15943600	9.82274000	6.13477600
C	9.67592300	9.18435300	4.05145200
H	9.86136500	10.12228400	3.54553700
C	9.69906500	7.89544100	3.44470100
H	9.89498300	7.70179800	2.40047000
C	6.28875400	6.37147200	7.25742300
C	6.79190600	5.33154900	8.05009000
H	6.84384800	4.32640500	7.64479400
C	7.22545000	5.61670700	9.34428000
H	7.61790500	4.82901800	9.98083300
C	7.15105400	6.93154200	9.79989100
H	7.48284100	7.20434300	10.79630200
C	6.62929900	7.90129700	8.94102400
H	6.54647200	8.93720500	9.26238900
C	3.83703800	5.87109300	5.72600900
C	3.28582200	5.46692000	4.34950900
H	2.19510500	5.36949900	4.40764100
H	3.69218000	4.50671300	4.02326200
H	3.51436500	6.22170600	3.58894900
C	3.50374500	4.80041100	6.77554800
H	2.41898700	4.64445600	6.80364300
H	3.82245100	5.10807900	7.77695800

H	3.96758200	3.84046100	6.54267100
C	3.24882400	7.22409300	6.15105600
H	3.41141600	7.99261000	5.39029400
H	3.67882900	7.57901800	7.09180600
H	2.16643800	7.11380900	6.29136600
C	9.61863400	4.81939300	2.54941300
C	10.78295100	5.24051700	1.91004100
H	11.45310500	5.91712100	2.42278500
C	11.08092400	4.77743000	0.62630700
H	11.99750600	5.09399500	0.13842500
C	10.21093800	3.89858600	-0.02437400
H	10.42906600	3.50242300	-1.00851500
C	9.05166000	3.51481600	0.62639200
H	8.32456200	2.82833000	0.21521200
C	10.44961300	4.32262700	5.30079400
C	9.91989700	4.22274400	6.74280500
H	10.68249400	3.74937000	7.37282700
H	9.01167000	3.61429300	6.78516800
H	9.69636600	5.20393600	7.17165300
C	11.75275000	5.13012900	5.27833600
H	11.60545500	6.15453100	5.63093100
H	12.19876000	5.16783800	4.27989700
H	12.48477300	4.64730900	5.93677000
C	10.67894700	2.90667000	4.74962500
H	11.36972600	2.37109100	5.41154500
H	11.12938500	2.92672500	3.75160400
H	9.75043600	2.33205900	4.69500700
Fe	7.81756000	8.25373600	4.18262900
N	6.20094600	7.63689500	7.70116200
N	8.80336400	3.98728500	1.86113100
P	5.71938600	5.95001800	5.55153100
P	9.04771000	5.13936200	4.29879500
Pd	6.94497800	4.13327300	4.62058800
C	8.57786700	0.87894000	2.32841200
C	7.76695900	1.38822600	3.08947000
C	5.83154000	2.36495000	4.49742700
C	6.93346800	2.15700000	3.87122800
C	9.52596500	0.44625000	1.36295700
C	10.90910500	0.54886500	1.62054800
C	9.09930800	0.00363200	0.09252100
C	11.83339900	0.23044100	0.63012700
H	11.24031400	0.87355700	2.60114100
C	10.03250200	-0.30635100	-0.89323100
H	8.03581100	-0.09456100	-0.10288400

C	11.40047500	-0.19096700	-0.63056700
H	12.89586600	0.30594800	0.84232400
H	9.69239200	-0.64865600	-1.86606400
H	12.12496800	-0.44055000	-1.39968300
C	4.57361800	1.84296300	4.98032800
C	3.42998300	1.85069900	4.16392900
C	4.47674700	1.34271100	6.29121800
C	2.21494300	1.37785400	4.65476800
H	3.50256800	2.23120900	3.14982300
C	3.26106100	0.86169100	6.77057100
H	5.35960500	1.34036100	6.92347500
C	2.12483000	0.88491400	5.95804900
H	1.33672900	1.39161700	4.01604200
H	3.19894300	0.47218600	7.78239500
H	1.17621700	0.51773600	6.33740800
H	7.96924800	3.66240700	2.38344700

IMI'

C	7.27756800	6.54570400	3.23283900
C	7.17642500	7.91048700	3.66640100
H	6.56228700	8.26270000	4.48119500
C	8.04786000	8.69656900	2.86283400
H	8.22926000	9.75674700	2.97864100
C	8.68313600	7.83710500	1.91910500
H	9.43188700	8.12891600	1.19502200
C	8.21210900	6.51244000	2.13926900
H	8.53271700	5.62845300	1.60724200
C	10.18717300	5.67796600	4.63812200
C	9.49412400	6.37277000	5.69055200
H	8.73528300	5.95264000	6.33201800
C	9.93371300	7.72492600	5.69059300
H	9.56155700	8.50928400	6.33573400
C	10.90188700	7.87743300	4.65521700
H	11.39398500	8.79999700	4.37757500
C	11.06885700	6.62397600	4.00634000
H	11.71382300	6.40481700	3.17015300
C	5.74542100	5.73767700	5.50014500
C	6.28984000	5.27052300	6.70147100
H	7.04947100	4.49563000	6.68799300
C	5.82476400	5.80038700	7.90510900
H	6.22687700	5.45439900	8.85175800
C	4.81766600	6.76065900	7.86762600
H	4.41041800	7.18636500	8.77807600
C	4.31812600	7.14823600	6.62235700

H	3.52060800	7.88412800	6.55009100
C	4.95599000	4.92284200	2.69426200
C	5.49530100	4.13164700	1.48866500
H	4.70152200	4.03038400	0.73860200
H	5.82244000	3.12668100	1.76885800
H	6.33385700	4.64811900	1.00875400
C	3.80537900	4.15457300	3.36024800
H	2.98627600	4.05104400	2.63842100
H	3.42050600	4.69410700	4.22963200
H	4.10297500	3.15275200	3.67242600
C	4.44931900	6.29712600	2.22372200
H	5.21695100	6.84432900	1.67027100
H	4.12423000	6.90860700	3.06744200
H	3.59619900	6.14316300	1.55125500
C	10.46131200	3.75296200	2.46778600
C	9.61105100	3.13120500	1.54703100
H	8.63644300	2.77455600	1.85883200
C	10.04636700	2.97642600	0.23051800
H	9.40860700	2.49080700	-0.50197900
C	11.30901000	3.44997300	-0.11727500
H	11.69098900	3.35283200	-1.12812800
C	12.08680300	4.05707800	0.87263100
H	13.07936400	4.43693400	0.64279800
C	11.22449700	3.02671500	5.26342200
C	10.66279700	2.91696200	6.69128200
H	11.40918100	2.43766900	7.33532300
H	9.74904000	2.31431400	6.72231900
H	10.44587500	3.90418900	7.11480400
C	12.54519100	3.81855400	5.28285300
H	12.42568200	4.78790300	5.77367300
H	12.92795200	3.98737200	4.27397600
H	13.28831900	3.24353000	5.84733700
C	11.46609700	1.63130700	4.67115200
H	12.16256100	1.08590300	5.31796100
H	11.90952100	1.68750900	3.67239100
H	10.54367800	1.04355100	4.61304700
Fe	9.09794400	7.18771200	3.85369000
N	4.77040600	6.66026900	5.46181100
N	11.68071600	4.20726000	2.13795800
P	6.41283200	5.10228500	3.89811900
P	9.93627200	3.94330100	4.22728000
Pd	7.78469100	3.11790500	4.34878600
H	8.69216900	1.88680600	4.68620200
C	4.42917000	2.66007900	6.82920600

C	5.09420900	2.20197800	5.91271400
C	5.81251800	1.76257200	4.85269300
C	6.42245900	1.32714500	3.86292300
C	3.66161100	3.29828400	7.83248700
C	2.57271000	4.11157100	7.45910500
C	4.01490700	3.18605000	9.19185300
C	1.86135000	4.80639200	8.43069000
H	2.30765800	4.19415500	6.41056800
C	3.29688900	3.88807800	10.15449100
H	4.85003600	2.55312200	9.47391200
C	2.22317300	4.69985500	9.77687200
H	1.02332500	5.43232300	8.14005700
H	3.56981400	3.79915900	11.20145000
H	1.66360900	5.24276900	10.53254400
C	6.71032000	0.59684800	2.66256300
C	8.01201000	0.17913700	2.33129700
C	5.64496200	0.30628100	1.78591000
C	8.24083900	-0.51578500	1.14783900
H	8.82913200	0.40676400	3.00496300
C	5.88661700	-0.38350600	0.60206100
H	4.64121800	0.62712300	2.04425300
C	7.18279600	-0.79397000	0.27842700
H	9.24750900	-0.84114500	0.90380100
H	5.06143000	-0.60372300	-0.06795100
H	7.36621300	-1.33294300	-0.64593500

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C	7.10878700	6.77170100	3.50141700
C	7.27566300	8.19749100	3.46927700
H	7.27548000	8.83204900	4.34070600
C	7.53452600	8.58441800	2.12491700
H	7.75604500	9.58889800	1.78896400
C	7.51730700	7.41491300	1.30827400
H	7.71377300	7.37865700	0.24503200
C	7.25280200	6.29844900	2.14838900
H	7.19988300	5.25995300	1.84968900
C	10.35195500	5.82910400	3.36116600
C	10.33553400	6.93160100	4.28695600
H	10.05537100	6.88516700	5.32713700
C	10.67075900	8.11795200	3.57778300
H	10.69936500	9.11375300	3.99841500
C	10.88429000	7.77655600	2.21188800
H	11.11012600	8.46582400	1.40950700
C	10.68563700	6.37306000	2.06859700

H	10.72571500	5.82976000	1.13616400
C	7.51515100	6.35719500	6.38560300
C	7.75573700	5.49908800	7.46739600
H	7.53001600	4.44126900	7.37743700
C	8.28817700	6.02579500	8.64281300
H	8.47872600	5.38360900	9.49771800
C	8.57815100	7.38807800	8.69497000
H	9.00093100	7.84270100	9.58485600
C	8.30478600	8.16548700	7.56828100
H	8.51006500	9.23371100	7.57031600
C	4.91474900	5.84884300	5.16702400
C	4.18835800	5.32893700	3.91576000
H	3.10527100	5.39182000	4.07518800
H	4.43304900	4.28581300	3.70658900
H	4.43419900	5.93323500	3.03634600
C	4.53303000	5.02536000	6.40716100
H	3.44214100	5.01953300	6.51294100
H	4.95500500	5.45909400	7.31949700
H	4.86167800	3.98697200	6.32473300
C	4.55966500	7.32546000	5.39638300
H	4.77539000	7.93529900	4.51470900
H	5.09794500	7.75152900	6.24794700
H	3.48519000	7.40390100	5.60257000
C	10.40964000	3.21597300	2.27126100
C	11.57143000	3.36089200	1.51489600
H	12.27597200	4.14156600	1.76706700
C	11.81122600	2.50108700	0.44071200
H	12.71819700	2.61185700	-0.14556600
C	10.89419100	1.49425300	0.12468100
H	11.06490600	0.80978300	-0.69765000
C	9.74737200	1.37614100	0.89196300
H	8.98063500	0.62451400	0.74528200
C	11.21311900	3.56551000	5.04803400
C	10.80070500	4.14319300	6.41338000
H	11.48783700	3.76745800	7.18095700
H	9.78631600	3.83755900	6.68119800
H	10.84794300	5.23451100	6.43565400
C	12.62417100	4.03938700	4.68080900
H	12.66553800	5.12170500	4.52761800
H	13.00372200	3.54140700	3.78360400
H	13.31047700	3.78909500	5.49848100
C	11.15756600	2.03311000	5.12710200
H	11.85799000	1.68416100	5.89466600
H	11.44202200	1.55755500	4.18195900

H	10.15522600	1.69219100	5.40223900
Fe	8.96510000	7.22050400	2.79239500
N	7.77889400	7.67304500	6.43973400
N	9.55180100	2.23826200	1.90581500
P	6.77033600	5.62476900	4.86202400
P	9.87754300	4.13506100	3.81101600
Pd	7.66906000	3.48646300	4.30664100
C	3.65887600	1.94264500	5.02749600
C	4.83636800	1.95435300	4.70313100
C	6.15919600	2.04691400	4.34210700
C	7.21705300	1.47089400	3.87378200
C	2.29420000	1.97143100	5.41851300
C	1.27774100	1.63611200	4.50207600
C	1.93981400	2.35356700	6.72870800
C	-0.05785300	1.69071300	4.88863800
H	1.54988700	1.33829500	3.49467600
C	0.60156400	2.39999600	7.10587000
H	2.72243900	2.60453400	7.43689700
C	-0.40010700	2.07161800	6.18855000
H	-0.83480800	1.43296700	4.17520100
H	0.33807300	2.69214500	8.11801200
H	-1.44351300	2.11010600	6.48643400
C	7.63213800	0.23957100	3.22404800
C	8.82916300	-0.42292500	3.55201800
C	6.85090600	-0.26959100	2.16450800
C	9.23423900	-1.55324400	2.84410300
H	9.43220100	-0.04741700	4.37023400
C	7.26588700	-1.39398000	1.45251500
H	5.92297000	0.23313600	1.90953900
C	8.46279700	-2.03757200	1.78433900
H	10.15435200	-2.05931600	3.12191200
H	6.65030400	-1.77324700	0.64184100
H	8.78256800	-2.91545700	1.23137400
H	8.70277800	2.15629400	2.50637900
TS1'			
C	7.50677600	6.91014800	3.71405000
C	7.51965900	8.10960000	4.50408500
H	6.96981700	8.26334900	5.42036600
C	8.40867600	9.03569900	3.89171000
H	8.66526600	10.01342600	4.27677000
C	8.94167000	8.43193700	2.71574700
H	9.67604400	8.86814300	2.05223100
C	8.39115500	7.12499300	2.59971100

H	8.62855000	6.40718500	1.82900500
C	10.40538200	5.52986700	4.61988200
C	9.80604200	5.92551800	5.86870500
H	9.04978000	5.37367500	6.40721100
C	10.33979600	7.19158100	6.23438800
H	10.05195500	7.77224500	7.10031300
C	11.27301500	7.58559500	5.23071500
H	11.81486000	8.52150700	5.20140200
C	11.32640600	6.56798100	4.23929500
H	11.90873100	6.56941300	3.33160300
C	5.76396000	5.81267100	5.65486300
C	6.23855400	5.23944600	6.83861700
H	7.02540700	4.49334100	6.80554000
C	5.65580700	5.62028000	8.04709300
H	5.99984200	5.19161500	8.98326400
C	4.61102800	6.54046700	8.02729600
H	4.11245200	6.84734300	8.94001300
C	4.19030500	7.03978200	6.79348000
H	3.36540100	7.74524200	6.73276500
C	5.24556100	5.41324300	2.69227900
C	5.87965800	4.76403200	1.44874300
H	5.15220200	4.77671400	0.62837300
H	6.15675500	3.72161900	1.64104600
H	6.76934300	5.30255800	1.10903100
C	4.02824000	4.58577800	3.12685000
H	3.29121900	4.59618500	2.31492600
H	3.55895700	5.00975100	4.01681000
H	4.28632000	3.54380100	3.32763400
C	4.80874800	6.85266600	2.36996900
H	5.63620900	7.45005000	1.97828300
H	4.40776800	7.34814600	3.25587900
H	4.02663800	6.81591100	1.60159400
C	10.27866000	4.27488400	1.96419400
C	9.38490600	3.73202300	1.03339800
H	8.51156200	3.18605900	1.37299500
C	9.63348800	3.92392300	-0.32617700
H	8.95622100	3.51870900	-1.07205000
C	10.76142800	4.64815800	-0.70447300
H	10.99349000	4.82713700	-1.74906200
C	11.60010300	5.14356500	0.29740900
H	12.49386700	5.70810300	0.04279400
C	11.28636000	2.77416400	4.31933100
C	10.96148200	2.39314400	5.77360000
H	11.72245100	1.69603200	6.14306000

H	9.98562000	1.90156000	5.85421700
H	10.96521000	3.26834100	6.43182800
C	12.67923200	3.42359000	4.24337300
H	12.76530100	4.27436600	4.92401700
H	12.91247500	3.77054800	3.23341900
H	13.43048700	2.68048500	4.53524000
C	11.24524900	1.52874000	3.42399600
H	12.00562300	0.81777300	3.76656800
H	11.46118800	1.76985900	2.37805700
H	10.27863700	1.01922300	3.47272600
Fe	9.39283700	7.25672100	4.37431400
N	4.75508800	6.69675500	5.63048100
N	11.37331700	4.96306900	1.60302700
P	6.57120100	5.39614100	4.05080000
P	9.96772500	4.00978100	3.76013300
Pd	7.75977600	3.31179700	4.12602900
H	8.42869300	1.87046200	4.03109200
C	4.10356800	2.92413400	6.30048700
C	4.99173200	2.48592500	5.58554300
C	6.04104300	2.08716300	4.81514400
C	6.80956000	1.29890200	4.18209600
C	3.11367700	3.48640300	7.14386700
C	2.08492000	4.28294400	6.60350100
C	3.18967200	3.30550500	8.53958100
C	1.16623200	4.89834200	7.44739600
H	2.02084400	4.41302700	5.52914100
C	2.26325000	3.92289200	9.37337200
H	3.97959000	2.68616000	8.95176900
C	1.25433600	4.72412700	8.83131600
H	0.37637600	5.51216500	7.02538900
H	2.32525400	3.77796200	10.44760500
H	0.53264600	5.20402500	9.48531100
C	7.04405300	-0.00921500	3.61965800
C	7.93901200	-0.21817900	2.55787900
C	6.31493200	-1.09684600	4.13876600
C	8.10886300	-1.49383000	2.02729000
H	8.48387300	0.62530500	2.14648100
C	6.49621900	-2.36877800	3.60633700
H	5.62106700	-0.93207400	4.95683500
C	7.39253200	-2.57137900	2.55244100
H	8.79959700	-1.64748900	1.20403600
H	5.93830900	-3.20550900	4.01498400
H	7.52985000	-3.56659100	2.14132800

TS1

C	7.20899400	6.91878700	3.54754900
C	7.38204000	8.34430700	3.58935000
H	7.35817200	8.93803500	4.48906700
C	7.67494900	8.79162400	2.27125900
H	7.90743700	9.80981100	1.98832100
C	7.67599300	7.66158800	1.40065700
H	7.90155600	7.67403300	0.34278100
C	7.38674900	6.50717700	2.17847500
H	7.33891000	5.48475800	1.82757100
C	10.46103000	5.97106800	3.43371500
C	10.42710600	7.02349600	4.41640500
H	10.13274300	6.91710500	5.44863900
C	10.77555200	8.24505500	3.77781000
H	10.79694500	9.21780200	4.24973000
C	11.01556900	7.97427700	2.40031200
H	11.25561200	8.70453800	1.63938800
C	10.82055600	6.58084500	2.17943100
H	10.87584000	6.08751600	1.22114800
C	7.59248400	6.35401900	6.41126200
C	7.91391700	5.42331200	7.40682000
H	7.73762700	4.36659100	7.23291900
C	8.46196600	5.88115700	8.60452300
H	8.71857700	5.18306700	9.39583800
C	8.67991300	7.24856400	8.76073800
H	9.11082400	7.65153500	9.67132600
C	8.32325000	8.10102300	7.71337700
H	8.47003900	9.17520500	7.79963300
C	4.98006400	5.93195600	5.15460200
C	4.25758000	5.48870700	3.87199400
H	3.17431500	5.54732800	4.03143200
H	4.49875200	4.45936400	3.60084600
H	4.50828300	6.14290300	3.03058900
C	4.59411000	5.04010700	6.34513100
H	3.50512700	5.06287100	6.46819700
H	5.04228900	5.40093700	7.27663900
H	4.89032900	3.99996100	6.19091800
C	4.63100400	7.39604100	5.46525800
H	4.86404800	8.05453500	4.62392900
H	5.15700900	7.76887700	6.34839100
H	3.55356700	7.46713500	5.65733300
C	10.27046400	3.36330500	2.20995500
C	11.36785200	3.53239600	1.36176400
H	12.13809300	4.25189000	1.60559200

C	11.45971700	2.76535600	0.19837100
H	12.30881600	2.88950600	-0.46665400
C	10.45979000	1.83983600	-0.09983600
H	10.49988700	1.23051400	-0.99565600
C	9.40165700	1.70402000	0.79243000
H	8.59846200	0.98907600	0.64985600
C	11.34692000	3.59340800	4.94410800
C	11.06103800	4.12824100	6.35748400
H	11.80408800	3.71863200	7.05195000
H	10.06917700	3.82602200	6.70323800
H	11.12763300	5.21810300	6.40937700
C	12.74731600	4.02493600	4.49178900
H	12.83370900	5.11296400	4.41462700
H	13.01937300	3.58181000	3.52943300
H	13.48522600	3.68010200	5.22593800
C	11.22915700	2.06193800	4.95462600
H	11.92596000	1.64827400	5.69266900
H	11.48571700	1.62936300	3.98180400
H	10.21947400	1.73704400	5.22652300
Fe	9.08427100	7.39195800	2.91283100
N	7.78528800	7.67394300	6.56475700
N	9.33134700	2.45193200	1.89925000
P	6.83208500	5.72836000	4.85215600
P	9.97591100	4.26789400	3.81634900
Pd	7.72515100	3.66009300	4.27061300
C	3.74427600	1.95558300	4.71762500
C	4.92928400	2.07306300	4.43600200
C	6.24970700	2.26155300	4.11142500
C	7.29144400	1.62318800	3.60594800
C	2.36840000	1.82696900	5.03382900
C	1.48904700	1.18986400	4.13389200
C	1.86185800	2.33854500	6.24689100
C	0.13723100	1.07715400	4.44021100
H	1.88046900	0.79467700	3.20212700
C	0.50929600	2.21481300	6.54570300
H	2.54003600	2.82006600	6.94304000
C	-0.35542300	1.58749700	5.64443200
H	-0.53454700	0.58827000	3.74133300
H	0.12666800	2.60703400	7.48307100
H	-1.41099000	1.49458400	5.88111400
C	7.52088200	0.19717200	3.34606200
C	8.81554600	-0.34988200	3.31165700
C	6.42262300	-0.65201300	3.10553600
C	9.00796100	-1.70537800	3.05138300

H	9.66984400	0.28575500	3.51205200
C	6.62100300	-2.00308400	2.83831300
H	5.41915200	-0.24015700	3.13127700
C	7.91302800	-2.53605800	2.80782600
H	10.01442800	-2.11389200	3.04247200
H	5.76419200	-2.64470000	2.65455400
H	8.06343000	-3.59111700	2.60058600
H	8.34834100	2.25915000	2.82238600

IM2

C	6.85384100	6.59371400	2.80988000
C	6.93234200	8.02754200	2.82680900
H	6.68996900	8.64594600	3.67602100
C	7.45191800	8.45190100	1.57186700
H	7.67436700	9.47447200	1.29679000
C	7.69665200	7.29729000	0.77011700
H	8.12688900	7.28684000	-0.22218400
C	7.33324700	6.15030100	1.52530500
H	7.40184500	5.12211700	1.20486100
C	10.11515200	6.12073500	3.71394800
C	9.91653000	7.45006900	4.23078200
H	9.46809000	7.70401600	5.17897400
C	10.35122800	8.37502400	3.24021800
H	10.30225200	9.45251000	3.32032300
C	10.79009800	7.63917400	2.10150700
H	11.13717800	8.05905500	1.16713700
C	10.64137000	6.25199500	2.38384000
H	10.85568400	5.43913000	1.70576000
C	6.37989100	6.13587000	5.70534400
C	6.24354600	5.27223400	6.80136300
H	6.07198600	4.21273500	6.64061800
C	6.34729500	5.79950700	8.08725400
H	6.23545000	5.15830500	8.95641500
C	6.61278300	7.16069400	8.23336100
H	6.71109400	7.61456300	9.21383700
C	6.75517900	7.93587900	7.08159200
H	6.96839200	8.99982900	7.15262400
C	4.30075900	5.49582100	3.72099800
C	4.01931500	5.05332700	2.27532100
H	2.94107100	5.12857800	2.09152300
H	4.32064200	4.01891300	2.10187700
H	4.52766600	5.69334300	1.54826800
C	3.60680000	4.54740200	4.71089700
H	2.52895500	4.55604600	4.51225700

H	3.75226600	4.86103200	5.74935000
H	3.95769300	3.51934100	4.59589200
C	3.80385100	6.93616300	3.93397100
H	4.25288600	7.63074800	3.21880400
H	4.00974300	7.30084800	4.94449300
H	2.71803200	6.95639700	3.78374800
C	10.23843700	3.20903600	3.48648800
C	11.47601900	2.97062200	2.89882900
H	12.28555800	3.68182400	3.01505800
C	11.63921500	1.79993900	2.15003900
H	12.59225100	1.58445300	1.67688500
C	10.57071000	0.91481400	2.01313400
H	10.66922700	0.00239700	1.43555800
C	9.35215900	1.22523300	2.61714100
H	8.47402900	0.59679500	2.52007400
C	10.46837900	4.42448600	6.16780100
C	10.02492400	5.57892200	7.08203000
H	10.40325300	5.39318600	8.09409500
H	8.93706300	5.66363100	7.14306900
H	10.43586200	6.53500100	6.74926200
C	11.99266900	4.45531300	5.99054800
H	12.32027600	5.36390100	5.47391200
H	12.35628300	3.58481300	5.43669600
H	12.47264500	4.44066900	6.97643900
C	10.00876400	3.08155300	6.76100100
H	10.47619000	2.94015100	7.74229000
H	10.29521200	2.23403900	6.12986200
H	8.92189200	3.05353400	6.89379500
Fe	8.80204800	7.19314400	2.52832000
N	6.63170200	7.44531700	5.84082600
N	9.20237000	2.34484900	3.33237300
P	6.16539000	5.43376900	4.01296300
P	9.58321700	4.59569300	4.51387600
Pd	7.49303300	3.58481800	3.86400100
C	7.10825700	2.77015800	0.42590800
C	6.57450700	2.52905800	1.50122800
C	6.18200100	2.41153600	2.83904800
C	5.29987400	1.57003000	3.42733200
C	7.86639200	3.13529700	-0.71774700
C	7.34593600	3.05600300	-2.02306500
C	9.18184300	3.61638800	-0.53166000
C	8.12060200	3.45278700	-3.10981500
H	6.33620300	2.68663100	-2.16955700
C	9.94806600	4.00842100	-1.62435700

H	9.58071100	3.67526100	0.47636200
C	9.41971700	3.92957600	-2.91646900
H	7.71003300	3.38938800	-4.11291600
H	10.95991600	4.37385700	-1.47193000
H	10.01858800	4.23570100	-3.76870300
C	4.45885500	0.53414300	2.82441800
C	3.64839300	-0.23655900	3.68047600
C	4.40940200	0.26934400	1.44168400
C	2.82158200	-1.23798800	3.18012000
H	3.67502000	-0.04214300	4.75016700
C	3.58089000	-0.73157500	0.94433500
H	5.01967300	0.84948100	0.75979400
C	2.78495600	-1.49017600	1.80757100
H	2.20616800	-1.82050800	3.85932600
H	3.55394600	-0.92229400	-0.12471300
H	2.14110500	-2.27014900	1.41244400
H	5.18932900	1.65264500	4.50730700

IM3

C	7.45306100	6.64543700	3.41998000
C	7.11266300	7.89639800	4.04449000
H	6.47889600	8.01468000	4.91097600
C	7.80430500	8.93540800	3.36258100
H	7.79100100	9.98356100	3.62962300
C	8.56593800	8.34833000	2.31057000
H	9.23396400	8.87141900	1.63973600
C	8.35218500	6.94261800	2.33634800
H	8.81152200	6.22117400	1.67841800
C	10.47322400	6.14193200	4.74667200
C	9.68136000	6.56988800	5.87034800
H	8.99733200	5.94016500	6.42123500
C	9.88103700	7.96687500	6.03825900
H	9.38608000	8.59251400	6.76881700
C	10.79576300	8.41113000	5.03714100
H	11.11439900	9.43264100	4.87744100
C	11.17133300	7.29441500	4.24212200
H	11.81631600	7.29396500	3.37795700
C	6.04271100	5.35503300	5.50534200
C	4.79706200	5.95113100	5.71104200
H	4.16618800	6.22889500	4.87671000
C	4.37654400	6.18977900	7.02128200
H	3.40645500	6.63717300	7.21146800
C	5.21464400	5.83613900	8.07307600
H	4.91835800	5.98469500	9.10510400

C	6.44418900	5.24824400	7.76952400
H	7.12691200	4.94870400	8.56075400
C	5.45990800	4.76046300	2.52844500
C	6.18190100	4.10964200	1.33293900
H	5.47136300	3.98705400	0.50717900
H	6.57050800	3.12255000	1.59347900
H	7.00826400	4.72983400	0.96948700
C	4.31682700	3.84812700	3.00532500
H	3.56811300	3.79446300	2.20638100
H	3.82115900	4.23233700	3.89997200
H	4.65207400	2.83495600	3.21229900
C	4.87882500	6.11482700	2.07703900
H	5.63639800	6.75880600	1.62617500
H	4.41209500	6.67219300	2.89358800
H	4.10549900	5.92285100	1.32447700
C	10.70634200	4.53790100	2.30367600
C	9.98184700	3.68559400	1.46088900
H	9.26292900	2.98786800	1.87879200
C	10.18918400	3.76467300	0.08333500
H	9.63788400	3.11980000	-0.59446700
C	11.11151200	4.68853900	-0.40252600
H	11.30295500	4.79021600	-1.46554700
C	11.79769400	5.48689700	0.51627700
H	12.53321600	6.21306500	0.17854400
C	12.00091900	3.65360600	4.80697900
C	11.78452200	3.42426400	6.31259000
H	12.69576400	2.99830400	6.74797900
H	10.96397000	2.73180100	6.52070300
H	11.57579900	4.36543100	6.83212700
C	13.20668700	4.58801500	4.60346700
H	13.10304600	5.50896600	5.18294200
H	13.34179100	4.85779600	3.55326500
H	14.11145000	4.07292500	4.94745600
C	12.25291200	2.32976200	4.06850000
H	13.10036300	1.81344700	4.53326100
H	12.50204700	2.50110700	3.01680300
H	11.39726700	1.64986700	4.10669900
Fe	9.12785000	7.52212500	4.14270200
N	6.85396000	5.00878900	6.52074200
N	11.60718000	5.41748900	1.83814800
P	6.80176700	5.01426200	3.85861700
P	10.42903400	4.45534000	4.12714100
Pd	8.34635900	3.24002500	4.41417000
H	7.46867000	1.12639100	2.60476500

C	5.06069000	2.30659000	6.37019200
C	5.79604400	2.06371000	5.42567800
C	6.69167100	1.92951800	4.36775900
C	6.63658000	1.08669500	3.30710600
C	4.16682500	2.65162300	7.41658700
C	2.88411500	3.14701300	7.10895700
C	4.56515500	2.56514800	8.76453600
C	2.03282900	3.56533700	8.12676100
H	2.57592200	3.20564500	6.06994400
C	3.70490600	2.98240800	9.77617600
H	5.55016900	2.17597700	9.00113100
C	2.44143400	3.48987800	9.46147600
H	1.04586400	3.94609700	7.88099400
H	4.01853000	2.90916200	10.81327100
H	1.77290100	3.81351100	10.25345700
C	5.59268100	0.14057600	2.91358900
C	5.77259900	-0.56094700	1.70461800
C	4.41534000	-0.09208500	3.65198200
C	4.81515600	-1.45897900	1.24464800
H	6.67826600	-0.39452000	1.12575600
C	3.46001600	-0.99161400	3.18883700
H	4.25528700	0.42821800	4.58746400
C	3.65225500	-1.67709300	1.98631600
H	4.97526400	-1.98959100	0.31086200
H	2.55938700	-1.16154400	3.77153300
H	2.90244800	-2.37782100	1.63178500
C	9.07383200	1.59086500	5.13527500
O	9.40324300	0.61385400	5.62569000

TS2

C	7.39579000	6.70599600	3.35071900
C	7.09054500	7.97451500	3.95401000
H	6.46016200	8.12493900	4.81833500
C	7.81963300	8.98142600	3.26162500
H	7.83645800	10.03372200	3.51174800
C	8.56998800	8.35509200	2.22376000
H	9.25649700	8.84760000	1.54849800
C	8.31345000	6.95705200	2.27123400
H	8.75842500	6.20898800	1.63265200
C	10.42603500	6.14690800	4.70235100
C	9.62569300	6.59221900	5.81294300
H	8.93698600	5.97273500	6.36974500
C	9.83753900	7.98851300	5.97271000
H	9.34174600	8.62404200	6.69411800

C	10.76750800	8.41591300	4.97859200
H	11.09866000	9.43280400	4.81484500
C	11.13965500	7.28923900	4.19594000
H	11.79439000	7.27553400	3.33927500
C	6.02929100	5.41429100	5.49379300
C	4.80897100	6.06273800	5.69913900
H	4.21630200	6.40867600	4.86149600
C	4.36649900	6.26385400	7.00804000
H	3.41659900	6.75430300	7.19586600
C	5.15931500	5.82229900	8.06241100
H	4.84512600	5.94065400	9.09307300
C	6.36621600	5.18840300	7.76207200
H	7.01300200	4.82090600	8.55449800
C	5.44761200	4.68437300	2.57987900
C	6.16680000	3.96669400	1.42017800
H	5.44692200	3.76010700	0.61952600
H	6.59170100	3.01306200	1.74601100
H	6.96949300	4.57992200	0.99629200
C	4.39599200	3.74373200	3.18890500
H	3.69983000	3.43018000	2.40212200
H	3.81536400	4.23149500	3.97671700
H	4.84584300	2.84523700	3.61005100
C	4.77806900	5.95856400	2.03859700
H	5.49493700	6.61098600	1.53345700
H	4.28866000	6.54490200	2.82124600
H	4.00854100	5.67166200	1.31199500
C	10.68327600	4.51247300	2.28548600
C	9.96793700	3.65070300	1.44523400
H	9.24973000	2.95572400	1.86760800
C	10.18665300	3.71789700	0.06896900
H	9.64345100	3.06512700	-0.60789500
C	11.11060000	4.63981400	-0.41769300
H	11.31101900	4.73200500	-1.47993700
C	11.78636600	5.44892900	0.49927500
H	12.52267700	6.17411400	0.16111200
C	11.94336800	3.64021200	4.82188600
C	11.71093400	3.46891300	6.33303800
H	12.60809600	3.03158000	6.78622900
H	10.87020000	2.80552700	6.55072000
H	11.52886300	4.43294400	6.81989000
C	13.17120900	4.53665200	4.58643300
H	13.08347300	5.48593400	5.12183800
H	13.32315900	4.75507900	3.52650100
H	14.06088100	4.01826200	4.96308300

C	12.14966400	2.28044500	4.13682300
H	12.99490400	1.76601200	4.60768200
H	12.38142400	2.39846400	3.07335500
H	11.27578600	1.63037700	4.23093100
Fe	9.09808700	7.54434700	4.07220900
N	6.79486900	4.98189200	6.51329600
N	11.58467100	5.39119100	1.82001200
P	6.79851700	5.07523200	3.85163900
P	10.39732400	4.44854600	4.10814000
Pd	8.36732100	3.31571500	4.43770400
H	7.74130700	0.88543400	2.86441300
C	5.24911100	2.10124900	6.57043400
C	6.01819800	1.79470100	5.67437200
C	6.95913900	1.58955000	4.66438400
C	6.85278400	0.89665300	3.49450200
C	4.31057400	2.52187600	7.54766000
C	3.05430200	3.01556300	7.14393000
C	4.63729200	2.50273100	8.91738300
C	2.15500400	3.49363200	8.09147400
H	2.80446500	3.02511200	6.08787000
C	3.72861600	2.97921100	9.85772000
H	5.60259900	2.11515900	9.22647400
C	2.48973400	3.48033600	9.44861600
H	1.18839500	3.87298700	7.77353000
H	3.98469900	2.95673800	10.91268900
H	1.78316500	3.84969400	10.18568500
C	5.72039300	0.17663800	2.93693900
C	5.86102300	-0.35173300	1.63654800
C	4.49229900	-0.00084200	3.60818400
C	4.81078500	-1.02122500	1.01928500
H	6.80696000	-0.22943000	1.11450300
C	3.44729700	-0.67671000	2.98882400
H	4.36750300	0.38394500	4.61227100
C	3.59880000	-1.18483900	1.69479400
H	4.93590400	-1.41977700	0.01728100
H	2.50876800	-0.81240300	3.51765700
H	2.77734300	-1.71053700	1.21762600
C	8.79779400	1.61974600	5.21454300
O	9.29975100	0.77249300	5.83258300
IM4			
C	7.39494900	6.95281800	3.22188200
C	7.28222400	8.26687500	3.79112200
H	6.72698100	8.52639300	4.68049100

C	8.08978000	9.15265900	3.02320600
H	8.24581400	10.20308100	3.22908700
C	8.70425700	8.40391400	1.97713200
H	9.40717600	8.78669400	1.24980400
C	8.28799200	7.04976500	2.09615200
H	8.61542800	6.22800900	1.47643400
C	10.46556000	6.11562400	4.50780100
C	9.78644800	6.73838800	5.61405000
H	9.10137900	6.23826400	6.28522000
C	10.14562900	8.11352000	5.63683800
H	9.76661900	8.85563000	6.32655500
C	11.04402600	8.35491400	4.55530700
H	11.46052200	9.31448900	4.27917400
C	11.24735400	7.13198400	3.85818400
H	11.83493100	6.97834400	2.96691400
C	6.01576500	5.70170100	5.49255600
C	5.06063800	6.64654100	5.86685400
H	4.70840300	7.38601600	5.15747500
C	4.55440700	6.60568900	7.16933200
H	3.79814500	7.31850800	7.48376800
C	5.02345800	5.63645300	8.05318600
H	4.63862700	5.55808700	9.06390000
C	5.99983200	4.74376300	7.60801200
H	6.40374300	3.97477700	8.25741600
C	5.31181100	4.88773600	2.73684400
C	5.91608100	4.28449300	1.45679400
H	5.10787300	3.99774000	0.77356700
H	6.49866300	3.38624100	1.68118400
H	6.56000000	4.99673000	0.93071500
C	4.50895900	3.80677800	3.47989000
H	3.73998400	3.40228000	2.81119200
H	4.01000300	4.20839400	4.36738700
H	5.14262700	2.97221900	3.79395900
C	4.42384200	6.08870900	2.38874100
H	4.99244000	6.88205400	1.89372100
H	3.94432900	6.50949500	3.27762500
H	3.62612700	5.76844100	1.70759200
C	10.33929300	4.24522400	2.27557100
C	9.45427400	3.39120500	1.60810800
H	8.74013500	2.80506700	2.17423300
C	9.48741600	3.33970500	0.21451100
H	8.80437200	2.69261300	-0.32806300
C	10.40261000	4.14142100	-0.46309900
H	10.46202300	4.14119300	-1.54641900

C	11.25427800	4.95548500	0.28905600
H	11.98777400	5.59145000	-0.20100100
C	11.85606800	3.52645600	4.73478500
C	11.87639100	3.68367400	6.26590300
H	12.77778600	3.19846200	6.65875700
H	11.01013300	3.21769200	6.74063800
H	11.91504700	4.73880100	6.55643000
C	13.10808100	4.18065700	4.12823000
H	13.18497900	5.23487900	4.40791200
H	13.12462100	4.11486600	3.03808100
H	13.99365000	3.66482100	4.51830100
C	11.79007200	2.04371300	4.33632300
H	12.67659000	1.52715500	4.72103300
H	11.77775800	1.91794200	3.24780500
H	10.91099100	1.54692500	4.75665200
Fe	9.23654000	7.60993100	3.83014700
N	6.47671400	4.77244300	6.36104500
N	11.23040100	5.01057700	1.62481600
P	6.76385500	5.38273200	3.83842000
P	10.28536200	4.35889100	4.12019200
Pd	8.20341800	3.65814300	4.82213200
H	8.40861100	1.04366700	3.64380000
C	5.20780500	1.66312200	6.91790600
C	6.14702800	1.41786900	6.18222500
C	7.30440000	1.36106600	5.37862900
C	7.41434100	0.94382000	4.07434700
C	4.10119000	2.05935600	7.71499300
C	2.92715100	2.53281600	7.09579500
C	4.19272500	2.06356900	9.12061300
C	1.87418700	3.00925600	7.87010100
H	2.86207200	2.52886100	6.01238200
C	3.13290700	2.54208900	9.88565900
H	5.09521600	1.69156800	9.59515900
C	1.97477000	3.01813900	9.26427800
H	0.97196000	3.37288200	7.38760100
H	3.20699200	2.53881900	10.96886700
H	1.14994400	3.38850000	9.86536900
C	6.42025000	0.39311200	3.17391500
C	6.81528300	0.16600700	1.83781800
C	5.08462800	0.12240200	3.53738400
C	5.90670300	-0.29366000	0.89159000
H	7.84781700	0.35399100	1.55259600
C	4.18148500	-0.34303600	2.58813800
H	4.76430200	0.27322300	4.56035700

C	4.58409400	-0.54714700	1.26469000
H	6.22735300	-0.46330100	-0.13169100
H	3.15743000	-0.55353200	2.88117700
H	3.87247600	-0.91122100	0.52996700
C	8.54192200	2.06747600	5.96043400
O	9.16820700	1.81029700	6.94254700

IM4-CO

C	7.57086100	6.85297900	3.21832000
C	7.57619800	8.23795400	3.60111900
H	6.96385900	8.68164900	4.37176100
C	8.55350000	8.90980700	2.81741200
H	8.82268400	9.95391700	2.90338000
C	9.15195800	7.95887700	1.94037900
H	9.95933600	8.15217700	1.24701600
C	8.55499000	6.69134800	2.18326800
H	8.82905600	5.76597700	1.70271100
C	10.28768300	5.81464400	4.90755600
C	9.72849300	6.74760400	5.85308300
H	8.95346100	6.52208600	6.57222800
C	10.36371300	8.00435100	5.66189900
H	10.13067200	8.91778800	6.19229700
C	11.31819100	7.86408900	4.61134900
H	11.92807800	8.65721600	4.19956200
C	11.28047700	6.52157300	4.14387200
H	11.83596800	6.10412900	3.31946600
C	5.50847800	6.55891200	5.11020800
C	5.85079900	6.61889200	6.46720700
H	6.69117500	6.05059100	6.85355800
C	5.09013700	7.42295500	7.31765900
H	5.33651300	7.49042300	8.37301200
C	4.01179000	8.12714500	6.78787900
H	3.38902900	8.76009700	7.41125700
C	3.74332600	7.99909000	5.42277300
H	2.90918000	8.52873100	4.96880900
C	5.41118000	4.99344400	2.53069000
C	6.20047800	3.95248400	1.71812700
H	5.58311400	3.61405400	0.87699000
H	6.45801300	3.07672000	2.31861600
H	7.12430000	4.36328100	1.30087500
C	4.15877500	4.32703900	3.12100800
H	3.52768400	3.97031000	2.29839700
H	3.56896300	5.02540200	3.71851600
H	4.40892600	3.45697300	3.73569400

C	5.01155400	6.17162900	1.62632000
H	5.88552400	6.63436800	1.15924900
H	4.47131300	6.93298500	2.18990400
H	4.36273100	5.79421200	0.82621100
C	9.85934900	3.48981800	3.11176900
C	9.08029400	2.38058200	2.76958400
H	8.42906300	1.92636400	3.50493700
C	9.15863000	1.87600000	1.47226900
H	8.56145600	1.01597800	1.18562900
C	10.00610100	2.50709500	0.56438700
H	10.09809100	2.15912700	-0.45925800
C	10.75091400	3.60657800	1.00074200
H	11.42923100	4.12000500	0.32340500
C	11.26205500	3.16563000	5.65110300
C	11.35998000	3.55533100	7.13476300
H	12.28932100	3.14121700	7.54305900
H	10.53318400	3.16614000	7.72757400
H	11.39476700	4.64152300	7.26625000
C	12.56557800	3.58066000	4.94382800
H	12.81261500	4.62791800	5.13227800
H	12.52539000	3.42334600	3.86316800
H	13.38103900	2.96738300	5.34517200
C	11.06299300	1.65065700	5.49139600
H	11.86814800	1.13185800	6.02460300
H	11.11049500	1.34651600	4.44146200
H	10.11478600	1.30704100	5.90514200
Fe	9.41983700	7.35887100	3.91392200
N	4.47457300	7.24223200	4.59796500
N	10.69155700	4.09099000	2.24745200
P	6.54120300	5.55529400	3.94082700
P	9.79604700	4.08476900	4.85534700
Pd	7.49124500	3.87577200	5.49703400
H	8.78900100	1.74353500	9.33744000
C	7.28835600	0.35138800	5.18909900
C	7.65488600	0.80222700	6.25965900
C	8.06842100	1.51044100	7.41431800
C	8.52278300	0.99126500	8.59771500
C	6.91846700	-0.13760400	3.90468500
C	7.66420400	-1.15752000	3.28281600
C	5.83923300	0.44639500	3.21240200
C	7.33571300	-1.57676600	1.99607400
H	8.49835600	-1.60436600	3.81394900
C	5.52281500	0.02568900	1.92428300
H	5.25841000	1.22475200	3.69559700

C	6.26926400	-0.98522100	1.31223400
H	7.91301100	-2.36639300	1.52487800
H	4.69011700	0.48306700	1.39875600
H	6.01700200	-1.31563600	0.30932700
C	8.71162700	-0.37791500	9.01675200
C	9.22347200	-0.59121800	10.31629300
C	8.41723000	-1.50265700	8.21457300
C	9.43456400	-1.87673200	10.79910500
H	9.45088800	0.26792000	10.94156200
C	8.62989800	-2.78551100	8.70224700
H	8.01957800	-1.36337700	7.21760300
C	9.13779200	-2.97786500	9.99188500
H	9.82714700	-2.02298800	11.80037200
H	8.39734000	-3.64336200	8.07875200
H	9.29984400	-3.98422500	10.36605600
C	8.03639600	2.99597800	7.29384400
O	8.22664200	3.77796800	8.19668000
C	5.69530500	3.30054000	6.04501900
O	4.65970000	2.95204900	6.37318800

TS3

C	7.89289200	5.64165800	0.89908300
C	7.53328400	7.03185000	0.78395700
H	7.06393300	7.65089600	1.53352200
C	7.92614800	7.49003900	-0.50522600
H	7.82941600	8.50473700	-0.86815600
C	8.51602900	6.39909000	-1.20682400
H	8.95103100	6.44083000	-2.19619100
C	8.49787400	5.26319700	-0.35524700
H	8.92495100	4.29090600	-0.56354200
C	11.25139900	5.91394500	1.35441400
C	10.67284700	6.84745000	2.28156100
H	10.28960500	6.60259000	3.25999600
C	10.65665000	8.13436000	1.67201600
H	10.24894500	9.03791500	2.10531800
C	11.21658000	8.01063700	0.36705700
H	11.30468500	8.80270200	-0.36455400
C	11.58922500	6.64947100	0.17119500
H	12.00585700	6.22474900	-0.73116800
C	8.03523400	5.11849800	3.83622300
C	7.74494300	6.44924700	4.14864500
H	7.26715200	7.07840300	3.41287900
C	8.09394600	6.97234000	5.39294500
H	7.87873200	8.00951100	5.63104100

C	8.72858400	6.14632000	6.31660600
H	9.03530900	6.50889500	7.29123900
C	8.95771500	4.82185700	5.95877400
H	9.44277400	4.13907200	6.64863600
C	5.89713400	3.94509400	2.18240700
C	5.59509800	3.30409000	0.81609700
H	4.54303400	2.99634500	0.78575500
H	6.21120500	2.41849500	0.64017800
H	5.76067900	4.01099300	-0.00305800
C	5.62183700	2.94470600	3.31446100
H	4.55560900	2.69020200	3.32132600
H	5.86819500	3.36152300	4.29764600
H	6.18393600	2.01995000	3.17755500
C	5.03275300	5.19830400	2.38101300
H	5.20259800	5.93820200	1.59412700
H	5.21068800	5.66985200	3.35359800
H	3.97416800	4.91406900	2.34565500
C	12.00241800	3.49715300	0.02637000
C	13.30292000	3.58640900	-0.47776600
H	14.08085700	4.09304400	0.07743300
C	13.59303400	3.00058700	-1.71108600
H	14.60221400	3.03537100	-2.10934700
C	12.57306500	2.36861600	-2.41421800
H	12.75855200	1.88090800	-3.36420100
C	11.29779400	2.35386400	-1.84912400
H	10.46885400	1.87440400	-2.36433500
C	12.88090400	4.06762900	2.88499000
C	12.25966200	4.24324000	4.28549100
H	13.05880500	4.24371600	5.03661800
H	11.57496300	3.42860100	4.52631200
H	11.72002000	5.19189700	4.37494000
C	13.90932000	5.19079900	2.67167500
H	13.46035600	6.17904600	2.80403600
H	14.37037600	5.16703400	1.68132100
H	14.71361600	5.08266300	3.40941000
C	13.55034700	2.68685200	2.79183600
H	14.26205400	2.57369700	3.61829500
H	14.10056500	2.56548000	1.85534300
H	12.82719200	1.87197000	2.86238900
Fe	9.56574500	6.75217400	0.56067000
N	8.61980500	4.31452800	4.76203800
N	11.01349600	2.89331600	-0.66036300
P	7.74461500	4.35322700	2.16504100
P	11.42611700	4.13366500	1.66669700

Pd	9.46761800	2.82145600	2.07172100
C	10.33004000	1.08184600	4.03176000
O	11.31146300	0.93595600	4.69181000
C	9.92253800	0.77119700	2.69197800
C	8.52553100	0.91359400	2.32158300
H	7.84397400	0.90401200	3.16245000
O	9.09692300	1.75152000	4.83718300
H	8.93319500	2.82181900	4.65547200
C	9.11192400	1.43099800	6.25235300
H	8.27978800	1.97412400	6.70058500
H	8.95471200	0.35697000	6.34954100
H	10.06771100	1.71309100	6.69656800
C	7.93934000	0.37564000	1.08068800
C	8.55007700	0.52564200	-0.17847800
C	6.68697700	-0.25842700	1.14773800
C	7.92366500	0.04810000	-1.32623900
H	9.49574600	1.04615000	-0.24967400
C	6.06434100	-0.73931200	-0.00269100
H	6.20117600	-0.37610000	2.11321500
C	6.68116100	-0.58754200	-1.24558800
H	8.40395800	0.17556000	-2.29289100
H	5.09924800	-1.23149700	0.07140900
H	6.19755800	-0.95898100	-2.14396700
C	10.91571700	0.21881500	1.83355000
C	11.70709500	-0.13621000	0.98357200
C	12.57906700	-0.44387700	-0.09507300
C	13.95848900	-0.17704900	-0.01292500
C	12.04808400	-0.96692600	-1.29120700
C	14.78309100	-0.42037900	-1.10771100
H	14.36740300	0.21926800	0.91063800
C	12.88190300	-1.20666300	-2.37951000
H	10.98428100	-1.17551700	-1.34803600
C	14.24959900	-0.93232900	-2.29356300
H	15.84723600	-0.21553800	-1.03456000
H	12.46568200	-1.61544100	-3.29578300
H	14.89820800	-1.12672000	-3.14253400

IM5

C	7.95751000	5.70222500	0.76323500
C	7.64413600	7.10625800	0.70760200
H	7.14881800	7.69350800	1.46634200
C	8.13761600	7.62050100	-0.52458700
H	8.09408500	8.65533100	-0.83730100
C	8.74683900	6.55110600	-1.24379900

H	9.25135300	6.63445000	-2.19688600
C	8.64199900	5.37065200	-0.46119600
H	9.06556500	4.40056400	-0.68638100
C	11.28873700	5.86773800	1.48488500
C	10.66745400	6.78219000	2.40458800
H	10.22433300	6.51506700	3.35281600
C	10.71943000	8.09143600	1.84498800
H	10.30296800	8.98870000	2.28313600
C	11.36489000	8.00101500	0.57751700
H	11.51689200	8.81602400	-0.11736300
C	11.72063000	6.63920400	0.35726800
H	12.18694300	6.23733200	-0.53112700
C	7.81768600	5.23075200	3.64662300
C	7.29728900	6.44383100	4.09231800
H	6.70766900	7.05011200	3.42006900
C	7.54117200	6.87309700	5.39853500
H	7.13898100	7.82242000	5.73837000
C	8.29959000	6.08478800	6.26970100
H	8.50363600	6.39859200	7.28652600
C	8.79473400	4.87816000	5.80448100
H	9.39542000	4.19645000	6.39306800
C	5.88021000	3.94700400	1.84849400
C	5.75229000	3.22808600	0.49139000
H	4.72147500	2.87581800	0.36900700
H	6.41362700	2.36146500	0.42449100
H	5.97610100	3.90437800	-0.34028800
C	5.53703100	2.98759100	2.99704800
H	4.50010500	2.64905100	2.88973600
H	5.62305300	3.47472000	3.97625800
H	6.17934400	2.10560400	2.98728700
C	4.95314700	5.16845900	1.88079500
H	5.20532000	5.89319400	1.10133700
H	4.96724300	5.67236400	2.85333700
H	3.92181900	4.83948400	1.70622100
C	11.97118100	3.47430900	0.08846200
C	13.26851000	3.54385600	-0.42535600
H	14.06703800	4.00373100	0.14184600
C	13.52835200	2.99876300	-1.68421700
H	14.53406100	3.01811900	-2.09194200
C	12.48323800	2.42390200	-2.39861600
H	12.64511900	1.96577600	-3.36730100
C	11.21416600	2.42129900	-1.81858100
H	10.36751700	1.98135100	-2.34037600
C	12.90389400	3.97129400	2.95445200

C	12.28243500	4.10359300	4.36005900
H	13.07400300	4.04665800	5.11662900
H	11.57040800	3.29770900	4.55396400
H	11.77273200	5.06659000	4.48578000
C	13.92831700	5.10265100	2.76758800
H	13.48103700	6.08770600	2.92771500
H	14.38276700	5.10365700	1.77337800
H	14.73761900	4.97524300	3.49670800
C	13.58259100	2.59801100	2.82595000
H	14.32958100	2.49392400	3.62218100
H	14.09778000	2.48893100	1.86850500
H	12.87719500	1.77255800	2.92796400
Fe	9.67672200	6.78050900	0.60973100
N	8.53899700	4.50535000	4.53905000
N	10.95710500	2.92539600	-0.60855400
P	7.71534800	4.39205000	1.97975800
P	11.43309900	4.07306900	1.75468400
Pd	9.43779200	2.83261400	2.19188600
C	10.49777400	0.89199500	4.19838700
O	11.60033800	0.55527500	4.57438000
C	9.99559100	0.80057500	2.80293300
C	8.58470000	0.86204000	2.55975800
H	7.97235400	0.86154900	3.45581100
O	9.57534700	1.42504000	5.07538400
H	8.95877400	3.62340200	4.14413200
C	9.97354500	1.36252300	6.45405900
H	9.10975800	1.71031700	7.02368700
H	10.22486200	0.33887900	6.73929000
H	10.84636600	1.99733000	6.63598200
C	7.90080300	0.35736000	1.35312300
C	8.40548800	0.54542700	0.05102100
C	6.65885400	-0.28256300	1.50042400
C	7.68746800	0.10055300	-1.05560300
H	9.33972400	1.07488200	-0.08650600
C	5.94296200	-0.72882100	0.39001600
H	6.25539200	-0.43444500	2.49850600
C	6.45450600	-0.53905600	-0.89418900
H	8.08761200	0.26059600	-2.05352100
H	4.98710900	-1.22535700	0.52893100
H	5.89863700	-0.88352000	-1.76099500
C	10.91812900	0.29511300	1.84126100
C	11.66406400	-0.05338700	0.94872400
C	12.48667300	-0.36851400	-0.16543800
C	13.87710700	-0.15276600	-0.12481900

C	11.90206400	-0.85622600	-1.35167500
C	14.65793400	-0.40559700	-1.24913100
H	14.32795000	0.21215800	0.79209900
C	12.69181000	-1.10700100	-2.47009100
H	10.83093200	-1.03118900	-1.37586400
C	14.06986700	-0.87877400	-2.42546200
H	15.73057400	-0.23938900	-1.20685600
H	12.23297400	-1.48836500	-3.37793600
H	14.68407200	-1.08125200	-3.29790000

(E)-3a

C	-4.28487900	2.05532100	-0.79435500
C	-2.90551600	2.20911400	-0.89362300
C	-2.16080500	2.67168900	0.20960000
C	-2.83307900	2.97221500	1.41092600
C	-4.21271900	2.81504500	1.50051000
C	-4.94300100	2.35760700	0.40053800
H	-4.84914500	1.69732400	-1.65073900
H	-2.38828500	1.96987000	-1.81758400
H	-2.25788500	3.32754900	2.25969300
H	-4.72126600	3.05016000	2.43112800
H	-6.01977300	2.23607400	0.47447100
C	-0.75238600	2.83446300	0.11501600
C	0.45267400	2.97357900	0.02342000
C	1.85782500	3.12755100	-0.03211800
C	2.63563900	3.06673900	-1.15090300
H	3.69821700	3.18426500	-0.95239100
C	2.28586100	2.86551300	-2.54628500
C	3.34835700	2.72484800	-3.46403300
C	0.96686100	2.81212300	-3.04383100
C	3.10923500	2.52428300	-4.81915400
H	4.36967200	2.77092600	-3.09525500
C	0.73172200	2.61725400	-4.40072300
H	0.13524700	2.93463400	-2.36330600
C	1.79682900	2.46857700	-5.29349600
H	3.94380100	2.41453100	-5.50556300
H	-0.29066500	2.58354800	-4.76688600
H	1.60482900	2.31481000	-6.35156200
C	2.59050700	3.36334900	1.25536600
O	3.79488500	3.49973900	1.35377500
O	1.75226700	3.40839900	2.30991200
C	2.38529300	3.62952500	3.57712900
H	2.91275100	4.58724900	3.58094600
H	1.57784500	3.63184500	4.30967600

H	3.10056400	2.83148600	3.79348000
IM6			
C	7.18462800	6.85454200	3.51733900
C	7.39086500	8.27534700	3.55212300
H	7.39351800	8.86997900	4.45135600
C	7.67607900	8.71662700	2.22980600
H	7.92854900	9.72909000	1.94313600
C	7.63982600	7.58625900	1.36039300
H	7.85028000	7.59276100	0.29921300
C	7.33409700	6.44025000	2.14600400
H	7.25677100	5.41776400	1.79975500
C	10.39833700	5.83472300	3.37302600
C	10.39053200	6.88773800	4.35515800
H	10.08241600	6.79812500	5.38478700
C	10.77206300	8.09922700	3.71498000
H	10.81772400	9.07104000	4.18705900
C	11.00669400	7.82280500	2.33781400
H	11.26980100	8.54585600	1.57766000
C	10.77526700	6.43435200	2.11776000
H	10.82455400	5.93759700	1.15994700
C	7.44938200	6.30540300	6.40080800
C	7.58794200	5.39685800	7.45920100
H	7.31254600	4.35698300	7.32644100
C	8.08622400	5.85505100	8.67693900
H	8.19415600	5.16900300	9.51081600
C	8.44441300	7.19697100	8.79415500
H	8.84436600	7.59759500	9.71999000
C	8.27068000	8.02704100	7.68540800
H	8.53143100	9.08187600	7.73747200
C	4.89187400	5.95935800	5.02403600
C	4.20808200	5.38586900	3.77242800
H	3.11989500	5.47013300	3.88028900
H	4.45657900	4.33356600	3.61535500
H	4.49878800	5.93996200	2.87333900
C	4.42426000	5.22227200	6.28651500
H	3.32953400	5.25273200	6.34004600
H	4.81811500	5.69016000	7.19380500
H	4.72958100	4.17684300	6.27871000
C	4.57315800	7.45575500	5.15790700
H	4.80996300	8.00674500	4.24418500
H	5.11955200	7.91534300	5.98719600
H	3.50025900	7.57476200	5.35339200
C	10.39030600	3.28456600	2.14582700

C	11.58756500	3.41239400	1.44422100
H	12.32030800	4.13800900	1.77124500
C	11.82627200	2.60699500	0.32838800
H	12.76090900	2.70326100	-0.21552700
C	10.87139500	1.67301900	-0.08445700
H	11.03931700	1.03179100	-0.94148400
C	9.68965200	1.56997500	0.63046100
H	8.89248700	0.87062300	0.40780600
C	11.05723300	3.44824300	4.98353300
C	10.60327900	3.98534200	6.35303000
H	11.23387700	3.54257200	7.13378000
H	9.56441700	3.72064100	6.56292200
H	10.70427100	5.07039200	6.42792000
C	12.50836300	3.85872500	4.70964000
H	12.61438000	4.94376200	4.62035300
H	12.90394600	3.39148700	3.80251800
H	13.14030800	3.52633000	5.54185000
C	10.91365900	1.91958800	4.98367800
H	11.54424500	1.49449700	5.77331400
H	11.22936900	1.47293200	4.03419500
H	9.87739000	1.62714900	5.17631000
Fe	9.06132700	7.28848100	2.85214000
N	7.77812800	7.60314500	6.51448400
N	9.49789900	2.37789500	1.68873300
P	6.75521500	5.66220700	4.81660900
P	9.82642600	4.14474600	3.70600100
Pd	7.61535900	3.52629300	4.17264300
C	6.17875500	2.02177300	4.35760200
C	7.12502300	1.51512400	3.66336700
C	7.50656000	0.35740800	2.87390100
C	8.67362900	-0.38460800	3.13091600
C	6.71087900	0.00322100	1.76413000
C	9.03658900	-1.44628800	2.30354000
H	9.28885500	-0.12704500	3.98538100
C	7.08422600	-1.05457900	0.93537600
H	5.80122000	0.56554600	1.57960300
C	8.25175000	-1.77983200	1.19640500
H	9.93336800	-2.01760300	2.52563900
H	6.45714300	-1.32018900	0.08895600
H	8.53726700	-2.60602200	0.55249300
H	8.62746600	2.30206800	2.25634600
C	4.92665300	1.84678100	5.04002400
C	3.66465300	1.82125100	4.23616500
O	2.54597200	1.76495200	4.70308100

O	3.90906400	1.89767500	2.90687800
C	2.73233700	1.94141800	2.08067400
H	2.12342900	2.81218400	2.33547200
H	3.09833100	2.01380100	1.05660600
H	2.13624700	1.03631400	2.21768200
C	4.78287300	1.77413100	6.38918500
H	3.75652600	1.70076200	6.74065300
C	5.80912100	1.89263900	7.41870200
C	5.41743600	2.39117500	8.67742900
C	7.16705300	1.56652900	7.22555400
C	6.34908400	2.59762100	9.69097700
H	4.37129200	2.63054900	8.84699500
C	8.09482200	1.75908300	8.24697400
H	7.48423000	1.13832400	6.28554100
C	7.69427700	2.28272100	9.47894000
H	6.02463700	2.99019300	10.64998500
H	9.13376200	1.48685500	8.08443900
H	8.42011600	2.42292200	10.27489300

TS4

C	7.22815400	6.94999800	3.54343600
C	7.41663900	8.37058100	3.64396100
H	7.39816500	8.92693200	4.56747800
C	7.71108400	8.87030200	2.34488400
H	7.95434800	9.89691300	2.10459800
C	7.70062200	7.77745600	1.42807000
H	7.92675400	7.83118000	0.37160100
C	7.40062700	6.59427300	2.15808500
H	7.34104400	5.58768200	1.76498700
C	10.46232200	5.98975800	3.43082500
C	10.44408200	7.03543600	4.42183300
H	10.14092600	6.93306400	5.45219900
C	10.81220900	8.25523400	3.78995400
H	10.84921100	9.22457100	4.26793700
C	11.04691100	7.99031200	2.41043200
H	11.29933800	8.72174500	1.65468100
C	10.83005300	6.60175700	2.18037500
H	10.87986200	6.11089600	1.22016400
C	7.45821600	6.26222800	6.41082000
C	7.61903500	5.28954200	7.40571000
H	7.37371500	4.25348400	7.20116200
C	8.10071300	5.68299400	8.65280100
H	8.22713400	4.94888800	9.44191900
C	8.41880900	7.02442600	8.85691200

H	8.80448000	7.37580000	9.80838300
C	8.22428500	7.92045200	7.80355700
H	8.45434800	8.97648500	7.92499500
C	4.90970300	5.97684800	4.98146900
C	4.24990100	5.48766500	3.68223300
H	3.15973500	5.54528800	3.78504300
H	4.51758900	4.45459600	3.44942900
H	4.53943900	6.11234200	2.83067300
C	4.43280700	5.15050000	6.18397400
H	3.33809700	5.18149000	6.23287300
H	4.82282600	5.54832200	7.12573400
H	4.73468200	4.10746700	6.09955600
C	4.58164800	7.46057100	5.21020900
H	4.83902500	8.07269400	4.34212600
H	5.10261600	7.86576200	6.08285200
H	3.50335300	7.56038200	5.38407800
C	10.30212200	3.39690100	2.17760500
C	11.45670500	3.55185100	1.40728700
H	12.21671000	4.26268400	1.70493400
C	11.61540300	2.78493200	0.25091800
H	12.50940900	2.89571600	-0.35499200
C	10.62208000	1.87743200	-0.11676000
H	10.71312500	1.26830500	-1.00899700
C	9.50089400	1.75976300	0.69856000
H	8.69581300	1.06220900	0.49505900
C	11.17584200	3.58000800	4.99035300
C	10.78442600	4.09405800	6.38698700
H	11.47267800	3.66954500	7.12804500
H	9.76913600	3.79152200	6.65373200
H	10.85155700	5.18202200	6.46467600
C	12.61498800	3.99043300	4.65656700
H	12.72733200	5.07767200	4.61194000
H	12.95097800	3.56520800	3.70619500
H	13.28858000	3.61364200	5.43551000
C	11.02984000	2.05104200	4.96808100
H	11.66766100	1.61328900	5.74484300
H	11.33994700	1.62513700	4.00815300
H	9.99743200	1.74628000	5.16715000
Fe	9.10718300	7.43377000	2.92499000
N	7.74712800	7.55895200	6.60588500
N	9.36690400	2.50623500	1.80086200
P	6.77392800	5.71966000	4.78949400
P	9.91544600	4.29651600	3.76450900
Pd	7.66569900	3.67202200	4.14157700

C	6.24936800	2.21167100	4.05887800
C	7.22452700	1.65490800	3.39220200
C	7.46511500	0.25950600	2.99034300
C	8.72902700	-0.33738500	3.12557900
C	6.41009900	-0.49493000	2.44557700
C	8.92988600	-1.66333500	2.74414200
H	9.54843800	0.23535900	3.54409500
C	6.61931100	-1.81658500	2.05854200
H	5.43946000	-0.02773700	2.31956800
C	7.87769100	-2.40629000	2.20611700
H	9.90914700	-2.11662700	2.86881300
H	5.79661200	-2.38921000	1.64032300
H	8.03564500	-3.43739900	1.90522900
H	8.32047300	2.33342200	2.66848100
C	4.99224800	1.90559800	4.69252000
C	3.73685000	1.89875500	3.87843800
O	2.61720400	1.77854000	4.32991500
O	3.99539500	2.06545000	2.56153900
C	2.83160600	2.12755900	1.71651000
H	2.20118900	2.97189700	2.00554500
H	3.21494200	2.25907900	0.70522800
H	2.25270600	1.20486800	1.79754700
C	4.84577800	1.69426400	6.02723700
H	3.82232000	1.54263200	6.36316000
C	5.86849200	1.75529500	7.06706000
C	5.47858200	2.21200100	8.34163900
C	7.22006900	1.40993900	6.86603500
C	6.41086600	2.36897600	9.36396200
H	4.43536900	2.45945000	8.51740100
C	8.14806200	1.55321700	7.89557600
H	7.53093800	0.99140400	5.91903600
C	7.75191800	2.04316300	9.14292000
H	6.08945400	2.73067100	10.33601300
H	9.18176500	1.26499000	7.72826400
H	8.47772000	2.14403900	9.94478400

IM7

C	6.93509700	5.95301800	2.55273900
C	7.01864800	7.31752200	2.11367500
H	6.90147700	8.17552900	2.75652700
C	7.35108300	7.31534600	0.73006800
H	7.53402000	8.19337300	0.12483400
C	7.47441600	5.96125700	0.29772100
H	7.75630400	5.63378100	-0.69389800

C	7.22156100	5.11725700	1.41452200
H	7.24641700	4.03628000	1.42782900
C	10.24028100	5.67336200	3.16390800
C	10.14994600	7.11053100	3.18398400
H	9.83275600	7.71821800	4.01705700
C	10.47591200	7.58870900	1.88285200
H	10.46690400	8.62484100	1.57264200
C	10.74190900	6.46647700	1.04623000
H	10.97823100	6.50054800	-0.00871900
C	10.59421400	5.28525300	1.82679800
H	10.70102600	4.27028400	1.47146200
C	6.80094200	6.40551800	5.49692600
C	6.76814100	5.89734500	6.80379000
H	6.57752200	4.84288500	6.97658000
C	7.00022400	6.77015700	7.86476500
H	6.97210400	6.40968800	8.88870400
C	7.28381000	8.10668200	7.58438100
H	7.47693400	8.82124600	8.37758200
C	7.32467200	8.51078700	6.24891200
H	7.55540500	9.54101800	5.98867900
C	4.48097200	5.44223800	3.99795300
C	4.01684400	4.61047800	2.79188100
H	2.92185400	4.64270700	2.74111800
H	4.31685600	3.56472800	2.86213900
H	4.40536300	5.02454100	1.85661100
C	3.83968800	4.95663900	5.30753300
H	2.75036000	4.94522200	5.18899100
H	4.07381100	5.63030300	6.13805200
H	4.15599400	3.95196400	5.58432400
C	4.10697400	6.91841000	3.77487000
H	4.49380000	7.29960300	2.82703500
H	4.46421300	7.56557600	4.58058800
H	3.01340200	6.99298300	3.74415200
C	10.38500100	2.89361800	3.96320700
C	11.61757800	2.46752100	3.47659300
H	12.42643800	3.17490200	3.33872200
C	11.77853800	1.11540900	3.16099200
H	12.73032500	0.75144000	2.78639500
C	10.70430300	0.24181300	3.32644300
H	10.79541200	-0.81252600	3.08892900
C	9.48854800	0.74568400	3.78677700
H	8.60567400	0.12388500	3.88600400
C	10.82571300	4.99373000	6.00819800
C	10.46167900	6.41445100	6.46981400

H	10.91349500	6.58923600	7.45337900
H	9.38449400	6.55411100	6.57084400
H	10.85562700	7.17321000	5.79039900
C	12.32740800	4.92511300	5.69819700
H	12.59565500	5.55189100	4.84079400
H	12.65705300	3.90074600	5.50564900
H	12.88891900	5.29116700	6.56619600
C	10.44354000	3.98098100	7.09536600
H	11.01065700	4.19361500	8.00933900
H	10.66905000	2.95428000	6.79512600
H	9.37847100	4.02783900	7.33885500
Fe	8.81843200	6.34438100	1.83578200
N	7.07914900	7.68754800	5.21997400
N	9.34180800	2.03800000	4.09791900
P	6.35878500	5.26157000	4.12151000
P	9.77837100	4.55121300	4.50166200
Pd	7.62753000	3.37461200	4.43039700
C	6.20622400	1.92583400	4.14792700
C	6.38341100	1.18329500	3.03308900
C	5.78873800	-0.11892000	2.69565600
C	5.68528100	-0.48620900	1.34288400
C	5.33920700	-1.02893200	3.67021100
C	5.11203900	-1.70006200	0.97140900
H	6.04339000	0.20038200	0.57907100
C	4.76887900	-2.24383000	3.29869800
H	5.44176700	-0.78530300	4.72255300
C	4.64637300	-2.58237500	1.94866600
H	5.02985400	-1.95916200	-0.08020000
H	4.42616600	-2.93241200	4.06558700
H	4.20213600	-3.53062000	1.66158000
H	7.06615900	1.56337100	2.27219200
C	5.18234600	1.70861500	5.17746400
C	3.73367000	1.49964200	4.78881700
O	2.83841400	1.31742400	5.59074700
O	3.53127200	1.53273200	3.46296900
C	2.20146300	1.20772900	3.02930100
H	1.47613500	1.90006100	3.46253800
H	2.22472600	1.29214400	1.94348700
H	1.95385100	0.18705300	3.33037800
C	5.37466400	1.74341000	6.52204700
H	4.47132700	1.70998300	7.12692300
C	6.63416800	1.75291100	7.26006100
C	6.70232300	2.38205400	8.51734900
C	7.75508700	1.03040300	6.81219100

C	7.85929900	2.30813900	9.29044200
H	5.82909600	2.91015800	8.89239500
C	8.90114400	0.93567300	7.59577800
H	7.68805400	0.49560900	5.87344900
C	8.95923900	1.57590900	8.83628300
H	7.89339700	2.79516200	10.26055700
H	9.74586100	0.34871700	7.24562800
H	9.85090600	1.49522300	9.45058400

IM8

C	7.24930000	6.25654100	3.20422000
C	6.99399800	7.66873700	3.33287200
H	6.63905500	8.15158100	4.22863300
C	7.36761200	8.29567200	2.11305400
H	7.34053300	9.35953400	1.91806000
C	7.85139200	7.29260400	1.22153400
H	8.25006000	7.46132600	0.23021100
C	7.77610700	6.03618800	1.88154300
H	8.06863800	5.07917000	1.47950400
C	10.57025200	6.27113500	3.69230100
C	10.05213900	7.14238700	4.71238000
H	9.63655200	6.83348600	5.65852000
C	10.14107500	8.47888600	4.23644200
H	9.78695700	9.35783000	4.75781300
C	10.71390500	8.45031700	2.93104100
H	10.87531400	9.30580500	2.28908800
C	10.98915000	7.09723000	2.59350800
H	11.41099600	6.74343200	1.66549200
C	7.36606900	5.64639600	6.07167800
C	8.00029400	4.85152100	7.03142800
H	8.29940300	3.83871800	6.78603700
C	8.25346700	5.39080200	8.29307800
H	8.75029700	4.79783900	9.05518400
C	7.86392100	6.70270000	8.55079700
H	8.04514100	7.16736300	9.51424600
C	7.22145400	7.41473900	7.53428300
H	6.89106900	8.43772500	7.69820900
C	5.09288100	4.73937800	4.48541500
C	4.62398000	3.87334600	3.30889000
H	3.52856800	3.89279600	3.26886200
H	4.93349600	2.83569300	3.42809500
H	5.00035500	4.25060700	2.35267500
C	4.68393200	4.10487000	5.82448500
H	3.60010300	3.94052500	5.81521600

H	4.91149000	4.76354700	6.66750500
H	5.15790000	3.13934200	5.99426200
C	4.42718900	6.12354000	4.38062200
H	4.56941100	6.57347100	3.39558600
H	4.79874600	6.81523900	5.14012700
H	3.35009700	5.99068200	4.53828900
C	11.30843200	4.03040200	2.11364300
C	10.51511900	3.37508300	1.16724000
H	9.48689900	3.11232200	1.38798000
C	11.07482600	3.08025100	-0.07855000
H	10.48395800	2.57554600	-0.83727900
C	12.39560400	3.44079100	-0.32786600
H	12.87088500	3.22674200	-1.27946600
C	13.10718600	4.09246200	0.68387100
H	14.14143100	4.39184600	0.53121000
C	11.99917800	4.10687800	5.03105800
C	11.34434900	4.06925700	6.42184400
H	12.11870200	3.90010300	7.17952400
H	10.61160800	3.25858600	6.49943400
H	10.84188300	5.01020800	6.66557000
C	13.07210000	5.20929800	4.98819500
H	12.66433500	6.18320800	5.27099800
H	13.51166400	5.29031500	3.99262500
H	13.86352500	4.95404000	5.70360400
C	12.64977900	2.74777900	4.73198600
H	13.40544100	2.54548800	5.50004100
H	13.14858000	2.74273200	3.76067600
H	11.93387800	1.92343900	4.76469100
Fe	8.97492600	7.29412600	2.97885800
N	6.97101200	6.90469800	6.32400500
N	12.58136900	4.38800900	1.87611400
P	6.99603100	4.93352700	4.40907100
P	10.62111500	4.47137700	3.77147300
Pd	8.58842100	3.12424100	4.04872500
C	7.07945800	1.65712100	4.21358500
C	6.62553600	1.38044100	5.45243800
C	5.52149500	0.51310400	5.88931000
C	5.57621900	-0.01447500	7.19087600
C	4.40861800	0.20515300	5.08855900
C	4.57690500	-0.86108600	7.66417900
H	6.42206800	0.23310900	7.82814700
C	3.40434600	-0.62994100	5.56560400
H	4.33223000	0.62175600	4.09125300
C	3.48831400	-1.17543300	6.85002700

H	4.64442600	-1.26951800	8.66808000
H	2.55011800	-0.85672700	4.93445300
H	2.70458200	-1.83191100	7.21560100
H	7.13790800	1.86563100	6.28254700
C	6.71105600	1.01102300	2.94656100
C	6.64093800	1.90804400	1.75722700
O	7.33458700	2.90969300	1.60489100
O	5.74437400	1.52343900	0.84004200
C	5.68494400	2.31544900	-0.36152000
H	6.64571200	2.29011000	-0.88174000
H	4.90595400	1.85718600	-0.96905900
H	5.42926700	3.34945600	-0.11999300
C	6.54363500	-0.32076600	2.68109400
H	6.22630500	-0.53068200	1.66313300
C	6.68242400	-1.52788700	3.48018200
C	6.07277300	-2.69195100	2.96587500
C	7.39234800	-1.63244100	4.69272200
C	6.13026300	-3.89980700	3.65173400
H	5.53874100	-2.63331800	2.02109100
C	7.47039000	-2.84602600	5.36447600
H	7.88605700	-0.76388600	5.10401200
C	6.83060400	-3.98028400	4.85678000
H	5.63842700	-4.77782900	3.24469900
H	8.02469400	-2.90748200	6.29610400
H	6.88354400	-4.92199200	5.39474400
C	9.58292000	1.46971000	3.95339100
O	10.07125400	0.44244500	3.84402500

TS5

C	7.19553400	6.30578800	3.17902700
C	6.94001000	7.71747100	3.28303900
H	6.56328500	8.21065800	4.16458600
C	7.35057700	8.32770100	2.06628100
H	7.33217200	9.38890400	1.85622400
C	7.85243800	7.31180600	1.19873700
H	8.27559600	7.46747400	0.21544900
C	7.75652600	6.06443200	1.87326300
H	8.06253000	5.10025300	1.49502000
C	10.53566600	6.30426400	3.71207000
C	10.00018500	7.16686500	4.73004400
H	9.58115500	6.85030200	5.67184100
C	10.08345300	8.50681600	4.26344200
H	9.71815200	9.37961200	4.78735500
C	10.67077800	8.49032300	2.96440900

H	10.83409300	9.35067600	2.32946200
C	10.95782000	7.14099300	2.62155900
H	11.39279100	6.79683400	1.69615700
C	7.30784400	5.74696000	6.05540900
C	7.93610700	4.97801300	7.04081300
H	8.26261900	3.96955100	6.81301300
C	8.14706800	5.53716900	8.30131300
H	8.63776700	4.96459900	9.08282200
C	7.72373200	6.84379900	8.53258300
H	7.87190500	7.32431200	9.49394000
C	7.09159800	7.52925000	7.49189100
H	6.73618700	8.54700100	7.63519000
C	5.13696300	4.64759100	4.47898800
C	4.75585400	3.76604200	3.28247900
H	3.66497000	3.66368100	3.24164900
H	5.18243000	2.76731700	3.38182700
H	5.08936300	4.19926000	2.33389100
C	4.82821600	3.91434200	5.79405400
H	3.78560000	3.57574600	5.78148400
H	4.95699100	4.56894000	6.66063100
H	5.45590300	3.03118300	5.92870900
C	4.34700200	5.96459900	4.42152500
H	4.46473400	6.46488600	3.45654400
H	4.65339100	6.65858000	5.20836200
H	3.28205400	5.73936800	4.55835700
C	11.35128700	4.08803900	2.14077100
C	10.61004500	3.41548800	1.16591600
H	9.58722900	3.11258100	1.35468400
C	11.21782300	3.15200300	-0.06420100
H	10.66864700	2.63339300	-0.84456200
C	12.53244900	3.55930900	-0.27006100
H	13.04359900	3.37004000	-1.20825900
C	13.19014900	4.22500900	0.76831200
H	14.21785900	4.56063500	0.65082400
C	11.94783200	4.11657400	5.07480300
C	11.25988500	4.06554700	6.44852500
H	12.01573700	3.88065200	7.22105900
H	10.52101200	3.25821000	6.49628600
H	10.75853200	5.00707600	6.69270400
C	13.03135600	5.20893800	5.07620200
H	12.62479900	6.18028800	5.37120700
H	13.49164500	5.30752100	4.09189500
H	13.80521800	4.93188100	5.80259400
C	12.57727200	2.74949500	4.76319900

H	13.28456800	2.49894900	5.56262300
H	13.12814100	2.76566100	3.82036100
H	11.83416200	1.94952100	4.71956100
Fe	8.93724500	7.32817600	2.98024900
N	6.88061400	6.99962200	6.28212000
N	12.61743700	4.49149700	1.94553300
P	7.00372500	4.99262900	4.39913000
P	10.61304300	4.50203800	3.78409300
Pd	8.62981500	3.21944200	4.00856000
C	7.36710800	1.34978200	4.05636900
C	7.00099900	1.08454600	5.33331500
C	5.83371700	0.39311300	5.87768900
C	5.91028000	-0.05805500	7.20858600
C	4.63752400	0.18499600	5.16595500
C	4.84463700	-0.72933400	7.79997400
H	6.82356400	0.11135500	7.77373500
C	3.56795300	-0.47044300	5.76319700
H	4.54655500	0.54590900	4.14916700
C	3.66944300	-0.93927200	7.07666600
H	4.92739800	-1.08248200	8.82321600
H	2.65026400	-0.62109200	5.20271700
H	2.83308000	-1.45832500	7.53482900
H	7.68660300	1.43217600	6.10624400
C	6.81431900	0.84472300	2.79170000
C	6.75683800	1.80934700	1.65708300
O	7.46328600	2.80802300	1.56428600
O	5.85380800	1.49234800	0.72108800
C	5.80169200	2.35897600	-0.42835800
H	6.75815100	2.34617400	-0.95664700
H	5.00952500	1.95453800	-1.05662900
H	5.56906200	3.38073500	-0.12076700
C	6.45264400	-0.44325300	2.51838300
H	6.01004600	-0.59635300	1.53790700
C	6.49830900	-1.64361300	3.34218500
C	5.50049800	-2.61212200	3.12030800
C	7.47420100	-1.89482200	4.32413900
C	5.43786100	-3.76419900	3.89836500
H	4.75889100	-2.44100000	2.34440500
C	7.42563700	-3.05885500	5.08102300
H	8.28266100	-1.19056200	4.47335500
C	6.39947500	-3.98865000	4.88452800
H	4.64904400	-4.49031600	3.72794900
H	8.19137900	-3.24620900	5.82771900
H	6.36087200	-4.89105900	5.48709300

C	9.36370400	1.46563400	3.86681300
O	10.00776100	0.51494500	3.69543000

IM9

C	7.10991700	6.38214700	3.33762000
C	6.96149800	7.80852400	3.42744000
H	6.63853200	8.33794600	4.30977900
C	7.39149600	8.37203600	2.19434200
H	7.44724300	9.42909100	1.97011000
C	7.79521200	7.31141500	1.32883600
H	8.20445500	7.42310400	0.33379900
C	7.62051300	6.08377300	2.02298200
H	7.84612500	5.09459000	1.65216700
C	10.48290500	6.13947900	3.76996600
C	10.00270700	7.00718900	4.81110700
H	9.57712900	6.69264300	5.75104600
C	10.14867400	8.35135100	4.37098300
H	9.83618600	9.23053400	4.91801300
C	10.71511800	8.33228700	3.06279800
H	10.91336100	9.19632100	2.44286900
C	10.92699700	6.97721900	2.68888300
H	11.33147900	6.63117600	1.74979100
C	7.18318300	5.87704100	6.22237500
C	7.81310200	5.12307500	7.21920200
H	8.14759800	4.11521400	7.00039400
C	8.01499500	5.69722500	8.47419900
H	8.50594600	5.13756000	9.26492900
C	7.58216800	7.00402900	8.68765900
H	7.72274000	7.49679700	9.64398100
C	6.95277800	7.67457700	7.63583700
H	6.59282600	8.69254300	7.76608400
C	5.05265800	4.70035200	4.61534700
C	4.76162200	3.79037700	3.41245600
H	3.68740400	3.57288000	3.36993600
H	5.29699100	2.84186400	3.49938800
H	5.05137800	4.26172000	2.46769100
C	4.73844100	3.96107400	5.92573600
H	3.70965900	3.58400900	5.89271000
H	4.82608600	4.62391100	6.79149200
H	5.39417400	3.10047400	6.08156900
C	4.21984700	5.98660900	4.52135100
H	4.37397700	6.49718200	3.56635700
H	4.46677800	6.68624700	5.32464600
H	3.15568600	5.73174800	4.60218900

C	11.24821300	3.95661500	2.15520500
C	10.43834900	3.53857100	1.09660300
H	9.38179000	3.35578600	1.24550900
C	11.03028700	3.34588300	-0.15228300
H	10.43007000	3.02334500	-0.99802500
C	12.39871700	3.56271300	-0.29274700
H	12.89974000	3.41807600	-1.24427000
C	13.12368400	3.97053900	0.82945700
H	14.19495700	4.14628800	0.76652900
C	11.80273100	3.88803600	5.12423900
C	11.08996100	3.89962100	6.48698000
H	11.81939000	3.66434100	7.27121200
H	10.29374400	3.14780500	6.52654900
H	10.65624100	4.87663200	6.72051300
C	12.95038000	4.91389200	5.13195400
H	12.59666200	5.91434900	5.39651700
H	13.44063300	4.96038100	4.15876300
H	13.68601700	4.60561100	5.88500200
C	12.34839300	2.47823700	4.84787500
H	13.04893400	2.21328900	5.64889200
H	12.88534400	2.43267500	3.89844500
H	11.55481700	1.72779800	4.83148900
Fe	8.92111200	7.26635900	3.08638900
N	6.74936700	7.13089700	6.43055100
N	12.56538400	4.17341400	2.02689900
P	6.90554900	5.09169000	4.57962500
P	10.51630900	4.33221100	3.80830400
Pd	8.46846700	3.27319700	4.05244600
C	7.74003300	0.95607000	3.70599200
C	7.30564300	0.96914100	5.00536300
C	6.03125700	0.59250500	5.60345400
C	6.00038800	0.47047600	7.00698800
C	4.83393500	0.39596500	4.88770800
C	4.82192000	0.15530300	7.67524200
H	6.91597700	0.62752300	7.57166800
C	3.65510300	0.09328000	5.55846500
H	4.82296500	0.49844800	3.81180400
C	3.64332800	-0.03247600	6.95081600
H	4.82058300	0.06105100	8.75655800
H	2.73857800	-0.04676000	4.99347900
H	2.71919700	-0.27310900	7.46733600
H	8.06757200	1.23249900	5.74101600
C	6.99030800	0.52320800	2.49941100
C	6.78232600	1.56323200	1.46313600

O	7.29209000	2.67850200	1.51515300
O	5.97720300	1.18366200	0.46554100
C	5.75028600	2.15871300	-0.57084700
H	6.69528100	2.43232700	-1.04572900
H	5.08765300	1.67048900	-1.28378400
H	5.27994900	3.05145000	-0.15246800
C	6.55474800	-0.74583300	2.30525900
H	5.95908600	-0.92315100	1.41329500
C	6.73831300	-1.88595000	3.19713000
C	5.68380800	-2.80647500	3.33155800
C	7.92491700	-2.09509100	3.92388400
C	5.78638200	-3.87516600	4.21784100
H	4.77489000	-2.66454800	2.75306100
C	8.03202900	-3.17703600	4.79079900
H	8.77204600	-1.43469100	3.77146400
C	6.95935400	-4.05990300	4.95212700
H	4.95867300	-4.56898400	4.32696200
H	8.95768800	-3.34198400	5.33384700
H	7.04655500	-4.90076300	5.63348000
C	9.13288500	1.48598700	3.46959300
O	10.07619800	0.95338400	2.96229800

IM9-CO

C	8.17940100	7.28199100	4.22517100
C	8.54107700	8.15980500	5.30796400
H	8.03732600	8.23506000	6.25987400
C	9.72209000	8.85937900	4.93266700
H	10.26234800	9.56143500	5.55342400
C	10.09963700	8.43229000	3.62596700
H	10.97807400	8.74835600	3.08031700
C	9.15550400	7.46634400	3.18531300
H	9.19041600	6.92817200	2.25191700
C	10.49268500	4.83671100	4.65431800
C	9.86254000	5.01821800	5.93691500
H	8.91710900	4.58538300	6.23707800
C	10.65969300	5.91629300	6.69841000
H	10.42510200	6.28617200	7.68749400
C	11.78772900	6.28945400	5.90852800
H	12.55679600	6.99489000	6.19400700
C	11.69468500	5.62973300	4.65235600
H	12.36055000	5.73783600	3.81143500
C	6.22403500	6.08959700	5.91893500
C	5.60210200	7.22126100	6.45845300
H	5.49927300	8.12688400	5.87465500

C	5.13178800	7.17021400	7.77116700
H	4.64159800	8.03332000	8.21119300
C	5.30477400	5.99821300	8.50430300
H	4.95437500	5.91508500	9.52766100
C	5.94546600	4.92204000	7.88862700
H	6.10378700	3.98845900	8.42297900
C	5.60041900	6.59563700	2.98182500
C	6.13899700	6.23462600	1.58343100
H	5.40064200	6.52478400	0.82654800
H	6.31604000	5.15834300	1.48586900
H	7.07158200	6.75913600	1.35401400
C	4.28305500	5.84210400	3.22771500
H	3.51686200	6.23057100	2.54663500
H	3.91561400	5.97172800	4.25093500
H	4.38082700	4.77195800	3.02338100
C	5.36920100	8.11256700	3.06082000
H	6.30572700	8.67310800	2.98981500
H	4.85562800	8.40548600	3.98036900
H	4.72835200	8.41943800	2.22569100
C	10.12227000	4.58561400	1.74810500
C	9.20226300	4.41648100	0.70723100
H	8.33290200	3.78283800	0.84067000
C	9.44622200	5.06296500	-0.50592000
H	8.75126200	4.95351000	-1.33312100
C	10.59106100	5.84563900	-0.63435600
H	10.81648700	6.37092800	-1.55662200
C	11.46140500	5.93212000	0.45548400
H	12.37560000	6.51752400	0.39012100
C	10.97482600	2.26521000	3.35369000
C	10.75759200	1.47700000	4.65413300
H	11.51743400	0.68940900	4.72315700
H	9.78238600	0.99309200	4.67848300
H	10.86634000	2.11771200	5.53636600
C	12.43605500	2.74659200	3.29243200
H	12.72961300	3.27045200	4.20484300
H	12.62227600	3.40433100	2.44009400
H	13.08068300	1.86562800	3.18986300
C	10.68619700	1.39522700	2.12116900
H	11.37595000	0.54367800	2.12470200
H	10.84663200	1.94934200	1.19120800
H	9.67589400	0.99102100	2.11287400
Fe	10.02290900	6.79450500	4.91811400
N	6.39407400	4.96012800	6.62917300
N	11.24067400	5.31785600	1.62245700

P	6.91580100	5.99259200	4.20813300
P	9.80533500	3.76613800	3.37209300
Pd	7.42541400	3.61297200	3.74849000
C	7.28188400	0.47316700	3.49121200
C	7.39492800	0.46414000	4.84493400
C	7.32251800	-0.64193600	5.78214100
C	7.84185900	-0.43059600	7.07544100
C	6.76718400	-1.90172400	5.47665300
C	7.84507100	-1.45082300	8.02053900
H	8.26012300	0.54200500	7.32357900
C	6.75951400	-2.91519700	6.42818100
H	6.32614000	-2.07920600	4.50353500
C	7.30561700	-2.69806800	7.69717300
H	8.26220900	-1.27561800	9.00742900
H	6.32480500	-3.87873900	6.18108100
H	7.30220800	-3.49620700	8.43331400
H	7.60611800	1.42846600	5.30541400
C	7.15541200	-0.71828400	2.61818500
C	8.22372300	-1.76427800	2.65090000
O	8.16272300	-2.83026000	2.07341600
O	9.27958200	-1.38753400	3.40437300
C	10.31686600	-2.37142700	3.53905200
H	10.71580900	-2.64462900	2.55950600
H	11.08355800	-1.90144800	4.15466800
H	9.92410700	-3.26562500	4.02933100
C	6.17816700	-0.87940300	1.69718100
H	6.28264200	-1.73417200	1.03208700
C	5.02076900	-0.00943500	1.48926100
C	4.56531500	0.22144900	0.18066400
C	4.35023600	0.61208900	2.55729000
C	3.51039700	1.09903700	-0.05921400
H	5.06119700	-0.27351600	-0.64955200
C	3.28412600	1.47549500	2.31819400
H	4.64854300	0.39042500	3.57561100
C	2.87078000	1.73406100	1.00820400
H	3.17953900	1.27946000	-1.07754100
H	2.76415800	1.93343500	3.15467200
H	2.03814800	2.40604700	0.82209200
C	7.39388900	1.77609200	2.79742200
O	7.33727800	1.93982400	1.59924100
C	5.70128600	3.10257400	4.53701400
O	4.74183800	2.79741500	5.07608100

TS6

C	6.92861400	6.63298900	4.48309200
C	6.64877700	7.88074400	5.14383300
H	6.46140900	8.01557900	6.19881400
C	6.73579500	8.92515500	4.17943400
H	6.62479900	9.98201100	4.38202700
C	7.05594400	8.34177600	2.91930200
H	7.23575100	8.87578300	1.99626400
C	7.17423200	6.93617800	3.09793000
H	7.44802000	6.22324300	2.33540700
C	10.26233100	6.82400800	4.21427600
C	9.97297500	7.18387500	5.57881600
H	9.76660500	6.48653500	6.37698800
C	9.92489300	8.60336100	5.67238600
H	9.68337300	9.17488800	6.55871600
C	10.18646400	9.13588700	4.37579800
H	10.17409500	10.18376000	4.10657500
C	10.40296900	8.05152100	3.48062000
H	10.56524800	8.10884400	2.41633400
C	6.77533700	5.27631800	6.96702400
C	5.61926300	5.87180900	7.48352000
H	4.84145700	6.19610100	6.80591600
C	5.46878200	6.04787100	8.85732400
H	4.56941600	6.50752000	9.25531500
C	6.48519000	5.61737000	9.70725900
H	6.41092200	5.71838800	10.78416200
C	7.61275100	5.04346400	9.13445200
H	8.42852800	4.67754400	9.75028300
C	5.33229900	4.21741600	4.53725000
C	5.70461900	3.46015100	3.24689000
H	4.79665600	3.03349400	2.80384500
H	6.40072000	2.64423700	3.45347800
H	6.16116900	4.12255800	2.50404900
C	4.76448200	3.23110000	5.56712700
H	3.92420600	2.68986200	5.11660700
H	4.38764000	3.73988500	6.45952400
H	5.50087700	2.48934000	5.87527400
C	4.28217100	5.28651100	4.19470400
H	4.62987300	5.97330600	3.41979400
H	3.97931700	5.88501300	5.05875100
H	3.38225300	4.78264700	3.82219300
C	9.73761100	5.09247600	1.93121100
C	9.00687900	3.98066000	1.49315500
H	8.87083600	3.13020100	2.14872200
C	8.47230300	3.99513100	0.20390800

H	7.89917600	3.14759300	-0.16098100
C	8.68164400	5.11341100	-0.59948800
H	8.27872200	5.17235300	-1.60537100
C	9.43544900	6.16860700	-0.07922800
H	9.63153400	7.05593300	-0.67737800
Fe	8.52623300	7.86724800	4.32163300
N	7.76242400	4.88571000	7.80722500
N	9.95578700	6.16532900	1.15210800
P	6.99406400	4.94503800	5.14426400
P	10.37407900	5.09557600	3.66993800
Pd	8.91729400	3.65226200	4.94944800
C	11.01281400	4.73314300	8.27386800
H	11.41916300	5.36442800	7.48337600
H	10.46573500	5.33104700	9.00207200
H	11.81074400	4.17238500	8.75440800
O	10.06241000	3.78334200	7.72344900
H	9.06378600	4.24641100	7.53327700
C	8.36078400	2.07146500	6.31752000
C	7.40949100	0.98808400	5.98073000
C	6.62244200	0.45590900	7.01407800
C	7.27419900	0.45321500	4.69064300
C	5.72469500	-0.58119600	6.76972200
H	6.73924000	0.84306900	8.02299000
C	6.37491100	-0.58176200	4.44510400
H	7.87296000	0.85884000	3.88310500
C	5.59610500	-1.10316200	5.48177800
H	5.13237900	-0.98502900	7.58537400
H	6.27769800	-0.98112600	3.43942000
H	4.89492100	-1.90885500	5.28587000
H	8.09532800	2.54413600	7.25743300
C	10.32410600	0.71393100	5.38359700
C	10.58222600	0.75117200	3.92390900
O	9.98837000	1.48587800	3.14607300
O	11.49060700	-0.14955100	3.52345900
C	11.68201400	-0.26440200	2.10146400
H	10.74267600	-0.53285300	1.61138000
H	12.04897600	0.67897700	1.69238300
H	12.42314000	-1.05233700	1.97393700
C	10.35606600	-0.48746000	6.00369500
H	10.65117700	-1.34228100	5.40035100
C	9.88863200	-0.79822700	7.35797200
C	9.11351400	-1.95768700	7.53050900
C	10.14294000	0.01677100	8.47347900
C	8.55636200	-2.26340900	8.76891900

H	8.91875600	-2.59769100	6.67473300
C	9.60055600	-0.30065800	9.71630800
H	10.80750800	0.86677200	8.37776900
C	8.79327600	-1.43141500	9.86500700
H	7.94298300	-3.15224300	8.88056500
H	9.82051800	0.32654900	10.57563500
H	8.36916700	-1.67400700	10.83488200
C	10.73131000	2.73075700	6.73904600
O	11.92742900	2.73030500	6.80414300
C	12.25501000	4.86534400	3.49127500
C	12.54311400	3.38100600	3.23298100
H	13.61645100	3.24681800	3.05206200
H	12.27077700	2.77187000	4.09731200
H	11.99954100	3.00895700	2.35967700
C	12.82648200	5.71631100	2.34807200
H	13.91774400	5.60236400	2.34049700
H	12.44712100	5.40386900	1.37266600
H	12.60146700	6.77831800	2.47501900
C	12.90390300	5.29297000	4.81829100
H	13.98611200	5.12706500	4.75385100
H	12.74005400	6.35428400	5.02811500
H	12.53580400	4.69737400	5.65642600
C	9.77026400	1.93476200	6.05372600

IM10

C	6.85562400	6.60625900	4.36672600
C	6.55597900	7.83853400	5.04855500
H	6.29849700	7.94854400	6.09191000
C	6.71607500	8.90847100	4.12324000
H	6.60810100	9.96070300	4.34986900
C	7.10000700	8.35580600	2.86730300
H	7.33986100	8.91310800	1.97211700
C	7.18655600	6.94409200	3.00895200
H	7.49158100	6.24882500	2.24260400
C	10.23773100	6.78421600	4.26521200
C	9.91509500	7.12029400	5.62637300
H	9.74840500	6.40113400	6.41562800
C	9.84612500	8.53703400	5.74114200
H	9.58485300	9.09349100	6.63159300
C	10.13409400	9.09254700	4.45994400
H	10.11794400	10.14446100	4.20681100
C	10.38380700	8.02352100	3.55442500
H	10.57323200	8.09871200	2.49564400
C	6.58851100	5.27446400	6.79445000

C	5.44867900	5.79994000	7.40130200
H	4.59815300	6.06652100	6.78888300
C	5.41092200	5.98060700	8.78434900
H	4.51823100	6.38387300	9.25222800
C	6.51847700	5.64166200	9.56807600
H	6.51197900	5.76595600	10.64437000
C	7.63817600	5.12863200	8.93750600
H	8.54025700	4.81616600	9.44661300
C	5.26217600	4.15898500	4.35438300
C	5.67219800	3.40871100	3.07051500
H	4.77818700	2.97263500	2.60891200
H	6.37319700	2.59940300	3.29193800
H	6.13652200	4.07616500	2.33683800
C	4.70030000	3.15638900	5.37339200
H	3.88907700	2.58803000	4.90412400
H	4.28191100	3.65508400	6.25352500
H	5.45221100	2.43960800	5.70537600
C	4.21108100	5.22352800	4.00745300
H	4.56515000	5.91434200	3.23841000
H	3.90821700	5.82108600	4.87338800
H	3.31217400	4.72301400	3.62836200
C	9.76288800	5.09686400	1.95614400
C	8.99847700	4.01857200	1.49270400
H	8.82828500	3.16471900	2.13430300
C	8.47643500	4.07090200	0.19922600
H	7.87888700	3.24847400	-0.18379200
C	8.72998900	5.19369300	-0.58490300
H	8.33881100	5.28187800	-1.59332000
C	9.51420300	6.21412400	-0.04089600
H	9.74552100	7.10377000	-0.62301600
Fe	8.48433700	7.82196400	4.33355700
N	7.63121800	4.97294100	7.60145900
N	10.02276200	6.17377000	1.19462300
P	6.89740500	4.90281000	4.98806900
P	10.37191100	5.05718400	3.70718200
Pd	8.86473600	3.64613100	5.00075700
C	11.31453500	4.39631800	8.47946800
H	11.90408800	5.03252700	7.81599800
H	10.76886400	5.01335000	9.19622200
H	11.98042100	3.70751200	9.00175400
O	10.31468800	3.67562400	7.73677600
H	8.45935300	4.54725100	7.13472100
C	8.44696100	2.08166200	6.46778600
C	7.43276900	1.04742200	6.17439700

C	6.61589600	0.60535100	7.22685300
C	7.24246900	0.48723400	4.90039600
C	5.64120200	-0.36936600	7.02071900
H	6.76873200	1.01315500	8.22316100
C	6.26920900	-0.48727100	4.69391800
H	7.84842700	0.83543300	4.07181000
C	5.46378200	-0.92062000	5.75111600
H	5.02737800	-0.70306100	7.85224800
H	6.13244100	-0.90622100	3.70076900
H	4.70435200	-1.67873600	5.58473700
H	8.26531000	2.55326600	7.42895500
C	10.32802200	0.78279300	5.36123800
C	10.51866200	0.83850000	3.89294700
O	9.86227200	1.55508300	3.14725300
O	11.43270000	-0.03132600	3.44009200
C	11.54806000	-0.14105100	2.01041500
H	10.59184700	-0.43926600	1.57261200
H	11.86203600	0.81243700	1.58120300
H	12.30530900	-0.90546000	1.84078600
C	10.37680400	-0.43566000	5.94410900
H	10.63980600	-1.27842900	5.30935700
C	9.96918000	-0.77154000	7.31477700
C	9.09898200	-1.85926100	7.49617300
C	10.38482100	-0.04122000	8.43915700
C	8.61209000	-2.17605200	8.76139500
H	8.77643200	-2.43170300	6.63104900
C	9.91080500	-0.37136300	9.70722900
H	11.11832200	0.74717300	8.32073100
C	9.01317400	-1.42917800	9.87117900
H	7.92444400	-3.00767400	8.88227300
H	10.25555700	0.18807400	10.57252800
H	8.64421700	-1.68277000	10.86075400
C	10.83743100	2.72941000	6.85711900
O	12.04010000	2.55839200	6.78739500
C	12.25773600	4.84427400	3.55502800
C	12.55620300	3.36521900	3.27567000
H	13.63281700	3.23887400	3.10943300
H	12.27607200	2.74000100	4.12574900
H	12.03099200	3.00951600	2.38399100
C	12.84806700	5.71840600	2.43946000
H	13.93956900	5.60710000	2.45142200
H	12.48913000	5.42458500	1.45072200
H	12.61789900	6.77739100	2.58217900
C	12.88030500	5.24847000	4.90182800

H	13.96598200	5.10311300	4.84693700
H	12.69543300	6.30117700	5.13719300
H	12.51440000	4.62263000	5.71804000
C	9.82244200	1.99427000	6.08915300

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C	9.41217400	4.93118900	5.56403600
H	10.02499100	5.19211400	4.69746900
H	8.84246100	5.79526100	5.90714200
H	10.06448600	4.55881000	6.35896200
O	8.43560000	3.94458000	5.20640000
C	6.64717000	1.89587700	4.87680300
C	5.54034400	0.95547700	4.66405200
C	4.71458700	0.61670800	5.74669600
C	5.28708700	0.37438600	3.41102200
C	3.69246400	-0.31776900	5.59537200
H	4.90349800	1.06369500	6.71860500
C	4.25462500	-0.54614500	3.25656700
H	5.89715400	0.66208500	2.56160800
C	3.46122300	-0.90400500	4.35030600
H	3.07672400	-0.58726600	6.44859500
H	4.06399500	-0.98264900	2.28006500
H	2.66053200	-1.62813300	4.22877000
H	6.43905300	2.74882400	5.51764500
C	8.41381800	0.60868700	3.63407700
C	8.93312300	0.96069500	2.28583500
O	8.75129800	2.04285000	1.75982100
O	9.60618900	-0.04795100	1.68840400
C	10.09125000	0.24803100	0.37223600
H	9.26227900	0.48502600	-0.30057400
H	10.77673100	1.09881400	0.40126900
H	10.60919300	-0.65288400	0.04211900
C	8.35113900	-0.67508200	4.04135300
H	8.66450400	-1.43702900	3.33225900
C	7.83191100	-1.15073600	5.32996100
C	6.95939700	-2.24888600	5.35489100
C	8.17221100	-0.52612600	6.54051000
C	6.39961900	-2.68319300	6.55443600
H	6.69164700	-2.73546900	4.42140900
C	7.62629800	-0.97219500	7.74078400
H	8.87520900	0.30002700	6.52922900
C	6.72969700	-2.04439000	7.75045400
H	5.70660500	-3.51949700	6.55524900
H	7.90310600	-0.48582200	8.67204600

H	6.29914100	-2.38562400	8.68770600
C	8.94536500	2.78332400	4.73882400
O	10.13935200	2.57997000	4.62064700
C	7.90671100	1.77064800	4.41190700

TS7

C	6.00765400	7.59643000	4.76236200
C	5.90535600	8.95230700	5.22789200
H	5.70851900	9.23458700	6.24970900
C	6.18532500	9.81753200	4.13432300
H	6.23469900	10.89740900	4.18071300
C	6.45347200	9.01763800	2.98410400
H	6.73457000	9.38349300	2.00567500
C	6.34185500	7.65137200	3.36280200
H	6.50915600	6.79092300	2.72876500
C	9.39063600	7.28262700	4.67520000
C	9.09301800	7.88426400	5.95027900
H	8.77158200	7.35835900	6.83646300
C	9.22766300	9.29352900	5.82248900
H	9.03086000	10.01803500	6.60081600
C	9.59699400	9.58510800	4.47810000
H	9.73324800	10.57101800	4.05436200
C	9.69671000	8.35640800	3.76532300
H	9.90469500	8.26442600	2.71048300
C	6.33915500	6.31520700	7.37689300
C	6.93421700	5.24986600	8.06266600
H	7.05889300	4.29373700	7.56481900
C	7.36102200	5.44838900	9.37541500
H	7.82715600	4.64087000	9.93223200
C	7.18171500	6.70326000	9.95383800
H	7.50330100	6.90818600	10.96960400
C	6.56688200	7.70227100	9.19512400
H	6.39928100	8.69158600	9.61452900
C	3.89663900	5.86750600	5.79408100
C	3.36101300	5.46531500	4.41063900
H	2.26780400	5.39327800	4.45518700
H	3.74989900	4.49585700	4.09097800
H	3.61350200	6.21270100	3.65011100
C	3.59676900	4.77537800	6.83021900
H	2.51826400	4.57991100	6.84737600
H	3.89839800	5.08101900	7.83713200
H	4.09589500	3.83711800	6.58372600
C	3.26217600	7.19501700	6.23779300
H	3.37405900	7.97070400	5.47585100

H	3.69629900	7.56419800	7.17120700
H	2.18940400	7.03452600	6.39963400
C	9.55108600	5.27146500	2.58379000
C	10.60808400	5.86349100	1.88717500
H	11.25925300	6.57150800	2.38245100
C	10.82516700	5.51698900	0.55197000
H	11.64529200	5.96746700	0.00138900
C	9.99182100	4.58267100	-0.06302200
H	10.13648600	4.28704800	-1.09608700
C	8.96313900	4.02194900	0.68824700
H	8.28835400	3.27089300	0.29174800
C	10.59859500	4.62778200	5.24023900
C	10.29263000	4.63425600	6.74790100
H	11.08144800	4.08582300	7.27605700
H	9.33789700	4.14675000	6.96367800
H	10.26367300	5.64853000	7.15690400
C	11.94394500	5.31633100	4.97952400
H	11.92438900	6.37187700	5.26918400
H	12.24120300	5.24651200	3.92940700
H	12.72373700	4.82031800	5.56958400
C	10.61709700	3.17833600	4.72545600
H	11.37461700	2.60866100	5.27603500
H	10.87075300	3.12315500	3.66203200
H	9.65166800	2.68209700	4.86765200
Fe	7.79366000	8.54198200	4.50825600
N	6.14810400	7.52055800	7.93748900
N	8.76432500	4.37588700	1.96257800
P	5.77369300	6.03237700	5.64381300
P	9.15487700	5.51438700	4.38714800
Pd	7.05941200	4.40457100	4.58875300
C	8.44942000	0.79251200	2.07072700
C	7.74868000	1.58115700	2.68312700
C	5.99807700	2.74785700	4.08294000
C	7.06947000	2.62441900	3.31821500
C	9.25142700	-0.13582500	1.35413100
C	10.46328900	0.28521900	0.76960100
C	8.84886600	-1.47822000	1.20977300
C	11.24963200	-0.61618200	0.05959700
H	10.77439800	1.31957700	0.88409400
C	9.64152700	-2.37174500	0.49607700
H	7.91666600	-1.80211300	1.66071900
C	10.84110500	-1.94537000	-0.07986500
H	12.18325800	-0.28499200	-0.38543800
H	9.32432100	-3.40456100	0.38893900

H	11.45650000	-2.64694700	-0.63474000
C	4.79926700	2.00246300	4.38136600
C	3.91077000	1.64983300	3.34737500
C	4.51326800	1.59815300	5.69809400
C	2.75600600	0.92653400	3.63244300
H	4.13412400	1.95691600	2.33037200
C	3.37030100	0.85345000	5.97265200
H	5.20888900	1.85696200	6.49067500
C	2.48351900	0.52616400	4.94320000
H	2.07106100	0.66705400	2.83084700
H	3.16642200	0.53204900	6.98954500
H	1.58505600	-0.04308000	5.16117600
H	7.83260900	3.71436400	2.78265200

IM11

C	5.96034200	7.38303400	4.45259500
C	5.65453400	8.72562600	4.85991100
H	5.50394100	9.03579500	5.88112300
C	5.66263800	9.54852700	3.69975800
H	5.51516900	10.62030300	3.68730800
C	5.96542000	8.73253100	2.56983100
H	6.07709700	9.07441200	1.54969800
C	6.15441900	7.39907600	3.02489800
H	6.38788900	6.54010200	2.41275300
C	9.33843200	7.90843300	4.61376000
C	8.94974800	9.07886500	5.35435500
H	8.73416000	9.12550300	6.41060900
C	8.83981300	10.16163600	4.43569800
H	8.53909400	11.17044800	4.68425600
C	9.12858200	9.67203100	3.12913000
H	9.09054100	10.24425600	2.21217600
C	9.42920900	8.28417800	3.23094800
H	9.66452000	7.62017400	2.41127400
C	6.24992800	6.19919000	7.16564400
C	6.52417800	5.12307700	8.02278200
H	6.61474200	4.11762200	7.62500900
C	6.68717500	5.37577400	9.38349200
H	6.88679500	4.56215300	10.07437300
C	6.60368000	6.69248100	9.83566700
H	6.73050900	6.93802400	10.88474900
C	6.35825600	7.69926400	8.90133900
H	6.29754100	8.73984500	9.21107800
C	4.13587300	5.28423700	5.33967700
C	3.67820100	5.24011200	3.87228800

H	2.64988300	4.86135600	3.83984500
H	4.29593700	4.57773500	3.26310900
H	3.68187000	6.23418200	3.41703000
C	4.01576300	3.89066600	5.97560900
H	2.96922600	3.56878600	5.92426300
H	4.30128700	3.89906800	7.03221300
H	4.62636700	3.15244600	5.44991600
C	3.28250800	6.29932000	6.11940500
H	3.37582700	7.30963200	5.71026500
H	3.54530200	6.33073600	7.18063700
H	2.22984100	6.00293100	6.04341100
C	10.37334200	5.25275400	3.95502600
C	11.54046200	5.48478600	3.23685000
H	12.08964000	6.41064800	3.36391100
C	11.97775200	4.49670300	2.34705000
H	12.88855400	4.64428400	1.77492700
C	11.23881600	3.32288600	2.20066500
H	11.55789000	2.54101700	1.52026300
C	10.05862300	3.16948200	2.92896200
H	9.41428900	2.30141900	2.83466800
C	10.61308900	6.19456800	6.73612300
C	9.88523200	6.84469000	7.92454000
H	10.50878800	6.74001400	8.82024200
H	8.92600500	6.36421400	8.12595800
H	9.71692100	7.91263900	7.76958400
C	11.92254300	6.93900300	6.44330100
H	11.73937800	7.97499000	6.14130200
H	12.50559300	6.44405300	5.66113900
H	12.53965700	6.95660500	7.34959000
C	10.87951500	4.71198300	7.05113900
H	11.48174100	4.64094800	7.96403500
H	11.43126800	4.21402200	6.24775700
H	9.94629900	4.16226900	7.21720100
Fe	7.51725100	8.64113500	3.94714700
N	6.17290800	7.46564000	7.59517800
N	9.64832600	4.11731500	3.77764200
P	5.94326600	5.83275600	5.38387600
P	9.46592900	6.22192700	5.24082200
Pd	7.74263000	4.63346000	4.66764800
C	6.22991700	-0.40820300	3.32157000
C	6.47407000	0.66778400	3.83710100
C	6.76993500	3.11351000	3.74609100
C	6.77549900	1.92632100	4.41035300
C	5.91577500	-1.61188900	2.63512400

C	5.89996400	-2.85218000	3.30204200
C	5.61000800	-1.56609500	1.25915400
C	5.58461600	-4.01547200	2.60641100
H	6.13490600	-2.88766000	4.36095800
C	5.29515500	-2.73475800	0.57361500
H	5.62530100	-0.60815200	0.74821300
C	5.28183600	-3.96136800	1.24338200
H	5.57454000	-4.96791200	3.12793500
H	5.06055700	-2.69134600	-0.48593300
H	5.03692700	-4.87191900	0.70485200
C	6.33715000	3.29864400	2.35384800
C	5.22552200	2.60253300	1.83547500
C	6.99904000	4.20506600	1.50155200
C	4.80610200	2.80064000	0.52217500
H	4.68719500	1.91398800	2.47546800
C	6.58429400	4.39507700	0.18480800
H	7.84977200	4.76177400	1.88188200
C	5.48317700	3.69448300	-0.31134200
H	3.94112400	2.25908400	0.15009400
H	7.11846600	5.09350000	-0.45356900
H	5.15298300	3.84672900	-1.33435300
H	7.07513100	1.91367200	5.45888300

IM12

C	7.26468700	6.98173700	3.38345600
C	7.56715600	8.37793600	3.52747500
H	7.51409100	8.92154000	4.45747900
C	8.01794300	8.86772200	2.26969800
H	8.36712500	9.87246700	2.07117200
C	7.99015600	7.79267300	1.33220200
H	8.30661300	7.84209400	0.29878000
C	7.52387800	6.63263200	2.01188600
H	7.41127500	5.63966000	1.59782000
C	10.40459900	5.70566300	3.37070000
C	10.34868500	6.59810700	4.49886500
H	9.93880800	6.36207500	5.46917300
C	10.86575700	7.86006800	4.09772500
H	10.91009500	8.74675700	4.71511900
C	11.24492600	7.77081600	2.72766200
H	11.63114100	8.57759300	2.11937500
C	10.96984400	6.44869600	2.27441400
H	11.10844700	6.09888700	1.26251200
C	7.44602200	6.26816700	6.20872400
C	7.86873400	5.26565600	7.09307200

H	7.76096300	4.22221100	6.81266500
C	8.43634600	5.63617500	8.31194600
H	8.77304700	4.88062800	9.01599100
C	8.56740200	6.99224600	8.60515300
H	9.00853500	7.32956500	9.53734800
C	8.10875100	7.91944600	7.66688100
H	8.18445500	8.98685000	7.86214900
C	4.87625400	6.10840000	4.79239100
C	4.19815000	5.59889500	3.51108000
H	3.11181200	5.72358300	3.59375100
H	4.40591900	4.53925800	3.34716000
H	4.53486900	6.16145000	2.63284700
C	4.37646400	5.33580000	6.02264200
H	3.28366500	5.40255300	6.07666800
H	4.78371500	5.75773700	6.94740700
H	4.63963800	4.27796800	5.98038600
C	4.59731500	7.60806200	4.96969600
H	4.87885100	8.18007600	4.08115600
H	5.13266800	8.02380900	5.82741400
H	3.52221800	7.75183400	5.13474000
C	9.93264000	3.45497000	1.70834600
C	11.04363600	3.51533700	0.87196500
H	11.96275100	3.95015400	1.24139100
C	10.96874500	3.00867200	-0.42781700
H	11.83915800	3.05264200	-1.07517400
C	9.77890000	2.44441000	-0.89186300
H	9.69095200	2.04330400	-1.89428300
C	8.69191400	2.38350600	-0.03562000
H	7.73254600	1.95815200	-0.29818300
C	11.14086600	3.04420500	4.35924800
C	10.69372400	2.99040500	5.83284400
H	11.45198000	2.45876400	6.42073500
H	9.73932900	2.46732100	5.93743000
H	10.58409200	3.99355000	6.26010500
C	12.51139600	3.72615400	4.25764000
H	12.50612500	4.72601700	4.69882700
H	12.85667400	3.81690800	3.22239800
H	13.25127300	3.12028500	4.79449300
C	11.20810400	1.62428600	3.77395700
H	11.73895700	0.96093000	4.46529800
H	11.74831000	1.60860100	2.82173800
H	10.21868100	1.19451600	3.60687600
Fe	9.22537100	7.30207800	2.93508600
N	7.55731500	7.57560600	6.49714000

N	8.81129500	2.88109900	1.20848200
P	6.71994800	5.74383900	4.59187100
P	9.75865500	4.01560600	3.47653200
Pd	7.53430900	3.54962500	4.09893400
C	6.07702700	2.08183800	4.46016700
C	7.13653600	1.48003000	4.08426600
H	8.01778700	2.81288200	1.87825800
C	4.73161500	1.96654700	4.97850000
C	4.54097600	1.66983600	6.34019300
C	3.60862800	2.15476400	4.15697100
C	3.25419300	1.57881300	6.86477600
H	5.41099200	1.51898100	6.97190800
C	2.32390500	2.05946900	4.68747100
H	3.74945800	2.37830900	3.10389600
C	2.14188300	1.77854600	6.04305900
H	3.11802900	1.35055700	7.91782100
H	1.46328200	2.20653000	4.04155100
H	1.14009500	1.71102200	6.45592700
C	7.87243700	0.26504800	3.87439400
C	8.66562600	-0.27397200	5.03257400
O	9.46838000	-1.18211600	4.95737900
O	8.38506200	0.37202700	6.18323200
C	9.09273600	-0.11069400	7.33868400
H	8.74620400	0.50502400	8.16827300
H	8.86038900	-1.16344300	7.51354700
H	10.17078300	-0.00084700	7.19768000
C	7.31462300	-0.20904500	1.43689800
C	6.14872400	0.57016900	1.27596200
C	7.86358600	-0.82214200	0.29030700
C	5.57527600	0.74012100	0.01533400
H	5.67665800	1.00856400	2.14414800
C	7.29242600	-0.64637400	-0.96758800
H	8.74687400	-1.44548900	0.40058000
C	6.14489500	0.14038000	-1.11299700
H	4.66672600	1.32756700	-0.08325400
H	7.73125600	-1.13507300	-1.83256500
H	5.68723500	0.26635800	-2.08953800
C	7.97107500	-0.44123600	2.71736700
H	8.65124600	-1.28855000	2.75326800
TS8			
C	7.29618100	6.90971100	3.41128000
C	7.48029200	8.33468900	3.44753700
H	7.37899600	8.94336600	4.33181500

C	7.88658900	8.76092500	2.15267700
H	8.14937800	9.77328000	1.87542300
C	7.95089100	7.61805900	1.30143900
H	8.26549600	7.61243800	0.26641900
C	7.58410200	6.47792800	2.06867100
H	7.55883800	5.45112500	1.72904500
C	10.54408200	5.91263500	3.48725200
C	10.41731100	6.89622200	4.53255100
H	10.03391200	6.71616300	5.52566900
C	10.82034800	8.15668300	4.01350100
H	10.79509400	9.09552400	4.54957300
C	11.19226400	7.97753600	2.65032200
H	11.50297400	8.75653300	1.96717500
C	11.02573600	6.60257800	2.31863400
H	11.17553400	6.17814600	1.33814000
C	7.47952100	6.43763000	6.29152600
C	7.95530800	5.54485500	7.25935400
H	7.93169100	4.47788600	7.06418100
C	8.46421300	6.05481300	8.45377200
H	8.84214500	5.38693700	9.22230700
C	8.48210800	7.43574600	8.63769600
H	8.87346700	7.87974700	9.54704800
C	7.97500700	8.24725400	7.61984800
H	7.96217900	9.32921600	7.72939100
C	4.93996800	6.00027100	4.86178500
C	4.28946300	5.30117700	3.65711100
H	3.20566300	5.46469300	3.68870000
H	4.46842700	4.22370400	3.66825400
H	4.65890700	5.70906700	2.70931700
C	4.47506400	5.35988600	6.17704700
H	3.38042100	5.39288000	6.22845000
H	4.86747700	5.89789200	7.04599200
H	4.77539100	4.31356500	6.24661000
C	4.57906100	7.49449800	4.85595500
H	4.80741800	7.96315900	3.89512100
H	5.10645900	8.04402800	5.64027900
H	3.50112400	7.59481600	5.03181400
C	10.22133400	3.40379000	2.07247400
C	11.34652900	3.56977100	1.26256600
H	12.14715200	4.22514200	1.57754100
C	11.43337100	2.88042500	0.05185000
H	12.30689200	3.00096200	-0.58144300
C	10.39179300	2.03778400	-0.32944800
H	10.41811400	1.48766700	-1.26332200

C	9.30173100	1.90254900	0.52418200
H	8.46021300	1.26267800	0.29072000
C	11.29084400	3.37204100	4.80710600
C	10.93947900	3.72442100	6.26322100
H	11.66222800	3.24726900	6.93579400
H	9.93951200	3.36248600	6.52053900
H	10.97550600	4.80227700	6.44849300
C	12.71033400	3.84938200	4.47732300
H	12.80700400	4.93560100	4.56396300
H	13.01915500	3.55209100	3.47067400
H	13.41680400	3.39011100	5.17912200
C	11.16702400	1.85253100	4.61216900
H	11.84542400	1.34487300	5.30812400
H	11.44387900	1.54279900	3.59931600
H	10.15183900	1.50384000	4.81889100
Fe	9.22240200	7.36146600	2.93242800
N	7.48055600	7.76841900	6.47280800
N	9.23609700	2.56855000	1.68508000
P	6.80894300	5.75125100	4.71543600
P	9.97375500	4.21235700	3.72907400
Pd	7.72199700	3.67115100	4.22055400
C	6.32142900	2.21456500	4.20420400
C	7.25741800	1.65924900	3.46816900
H	8.24329500	2.32833800	2.59446100
C	5.07130000	1.82039600	4.81238800
C	4.90978200	1.89888100	6.20754800
C	4.02189000	1.30668300	4.02798600
C	3.72814100	1.47150000	6.80462400
H	5.72987900	2.28099200	6.80794400
C	2.83183400	0.90348600	4.62898400
H	4.14774100	1.22702000	2.95313200
C	2.68212900	0.98407100	6.01555900
H	3.61747300	1.52303600	7.88361100
H	2.02388600	0.51523300	4.01618800
H	1.75560800	0.66223900	6.48122200
C	7.54953100	0.23060500	3.26473700
C	8.23262200	-0.52616600	4.36226000
O	8.67504300	-1.65215400	4.25656800
O	8.29832400	0.18560400	5.51146700
C	8.91584500	-0.50031200	6.61335800
H	8.88551200	0.20316300	7.44530700
H	8.35996700	-1.40902200	6.85443300
H	9.94661300	-0.76729300	6.36709100
C	6.54795200	-0.09112900	0.93676400

C	5.92294000	1.15878100	0.73055100
C	6.54391600	-1.01472100	-0.12915000
C	5.33472400	1.46561100	-0.49369300
H	5.89936000	1.88611100	1.53097200
C	5.95880500	-0.70298000	-1.35310600
H	7.01154400	-1.98494200	0.01479100
C	5.35153100	0.54060000	-1.54091600
H	4.85269900	2.42978700	-0.62857300
H	5.97061500	-1.43179600	-2.15781400
H	4.88828300	0.78394100	-2.49226900
C	7.22743900	-0.49165300	2.16476100
H	7.53280700	-1.53483100	2.20315500

IM13

C	7.21002300	6.79114700	3.49793100
C	7.40793200	8.20643700	3.35582000
H	7.63872300	8.87671800	4.16820500
C	7.31345800	8.53078600	1.97410900
H	7.46410400	9.51310500	1.54616500
C	7.06088100	7.33105800	1.24569500
H	6.97841100	7.24393500	0.17070300
C	6.99990800	6.25672400	2.17576500
H	6.84594000	5.21303400	1.94057800
C	10.43978600	5.93995500	2.77394000
C	10.63538300	7.27196700	3.28602600
H	10.69490000	7.55222700	4.32656800
C	10.65701700	8.16733000	2.18019100
H	10.75729400	9.24241500	2.24212200
C	10.45037100	7.41298200	0.98903800
H	10.37215800	7.81378100	-0.01256200
C	10.31017700	6.04249300	1.34782600
H	10.10448600	5.22563500	0.67101900
C	8.10815400	6.48237600	6.31245100
C	8.42266000	5.66861700	7.41046900
H	8.07569200	4.64147600	7.44830300
C	9.19533100	6.20139000	8.44031400
H	9.44559800	5.59830600	9.30794000
C	9.64982900	7.51490500	8.32606700
H	10.26141200	7.96983500	9.09809500
C	9.29979000	8.24088900	7.18680700
H	9.63645600	9.26685100	7.05813700
C	5.26618100	6.13802900	5.57987700
C	4.28477100	5.53255700	4.56399100
H	3.27008300	5.85291900	4.82779000

H	4.29657000	4.44207700	4.59245600
H	4.48414100	5.88087800	3.54477600
C	5.02908000	5.51608700	6.96533500
H	4.00680300	5.75730200	7.27810000
H	5.70951000	5.91874400	7.72217200
H	5.11388700	4.42962600	6.93850100
C	5.07487600	7.66345800	5.66332700
H	5.11673700	8.13569200	4.67896500
H	5.81787200	8.14228900	6.30885100
H	4.08400300	7.86218200	6.08769200
C	10.01334800	3.03201000	2.66612200
C	10.79026700	2.62676900	1.58715400
H	11.63299200	3.22616000	1.26217300
C	10.45533800	1.43383500	0.93787900
H	11.04325200	1.08789600	0.09324500
C	9.36151800	0.69601700	1.38575200
H	9.07395500	-0.23118600	0.90228100
C	8.61571400	1.17059300	2.46612700
H	7.73403500	0.65554000	2.83042300
C	11.61811400	4.13874600	4.87007400
C	11.82796200	5.33589300	5.81257900
H	12.59394000	5.07435500	6.55211700
H	10.91582600	5.59807700	6.35446900
H	12.18256200	6.21638300	5.27115500
C	12.87675900	3.91658600	4.02058400
H	13.07295100	4.76835400	3.36029100
H	12.80214700	3.01039300	3.41233400
H	13.74481400	3.79961800	4.68050000
C	11.28073400	2.88172200	5.69212900
H	12.11997700	2.65280400	6.35936600
H	11.11326300	2.00730500	5.05466500
H	10.38685800	3.02992800	6.30789300
Fe	8.84534100	7.16029500	2.29538700
N	8.53692300	7.74748000	6.20159700
N	8.93989600	2.31082500	3.08645000
P	7.03058400	5.77774600	4.99163800
P	10.11483200	4.48787200	3.78814400
Pd	7.90315500	3.75468500	4.39847300
C	6.28614700	2.63421400	4.86114700
C	6.14639900	2.37464700	6.17523900
H	6.81244900	2.88038000	6.87141000
C	5.62202200	1.92836700	3.75959000
C	5.25915400	2.59755500	2.57805500
C	5.41342800	0.53484100	3.82296900

C	4.68772800	1.91143800	1.50965700
H	5.41761400	3.66802800	2.51389100
C	4.84453400	-0.15213000	2.75138900
H	5.70791200	-0.00717900	4.71592800
C	4.47946900	0.53207000	1.58963500
H	4.40211000	2.45299200	0.61225700
H	4.69169700	-1.22530800	2.82278700
H	4.03777800	-0.00373100	0.75493200
C	5.19219600	1.46661200	6.82452500
C	3.78856800	1.47789900	6.31076400
O	3.28714500	2.40605300	5.70520800
O	3.12520800	0.34212300	6.60423000
C	1.75398300	0.30735400	6.17183100
H	1.37473400	-0.66425900	6.48732500
H	1.18417300	1.11555800	6.63684700
H	1.70044200	0.41118900	5.08528000
C	6.79703000	0.68862300	8.60727200
C	8.02158100	0.80186900	7.91678200
C	6.83693400	0.47667400	9.99865700
C	9.23274500	0.74261600	8.60196000
H	8.01975500	0.90129700	6.83719800
C	8.04804100	0.43057800	10.68349900
H	5.90275800	0.36197300	10.54193100
C	9.25187400	0.56957900	9.98819000
H	10.16590600	0.81512100	8.04949500
H	8.05456500	0.27759300	11.75854900
H	10.19731200	0.52312600	10.52059300
C	5.49326000	0.76371000	7.94614400
H	4.68366200	0.22879200	8.43499800

IM14

C	7.51461900	6.77870900	3.92251100
C	7.76933200	8.12723400	4.34669900
H	7.66721700	8.47390800	5.36218100
C	8.26369100	8.86102100	3.23165400
H	8.59532800	9.89077400	3.25119400
C	8.30329100	7.99145000	2.10186600
H	8.65847000	8.24752900	1.11260700
C	7.83802000	6.71377100	2.52078400
H	7.75806000	5.82916600	1.90665700
C	10.70064800	5.59884300	3.67978200
C	10.47532800	6.08798300	5.01862500
H	9.97208600	5.54151100	5.80387000
C	10.95051300	7.42347200	5.09584600

H	10.86998400	8.07060700	5.95813700
C	11.47684200	7.78196300	3.82090000
H	11.87616000	8.74872200	3.54495200
C	11.33579300	6.66623600	2.94822800
H	11.64146500	6.65950200	1.91342500
C	7.23392600	5.60717200	6.61882700
C	7.09386300	4.50242700	7.47098100
H	6.84369500	3.53060100	7.06416300
C	7.25176700	4.68120100	8.84398700
H	7.11944700	3.84255500	9.52102400
C	7.57738100	5.95237400	9.31516700
H	7.71859900	6.14424500	10.37385800
C	7.71540000	6.98814400	8.38965600
H	7.96948200	7.99314800	8.71943900
C	5.06205100	5.46153200	4.64517500
C	4.37349100	4.39698700	5.50975300
H	3.28973500	4.45714300	5.34946600
H	4.55881400	4.55872800	6.57551800
H	4.69480800	3.38560200	5.25755200
C	4.59254000	6.86051700	5.06963300
H	3.50004800	6.91699600	4.98731700
H	5.01870500	7.64329600	4.43618600
H	4.86318400	7.07796500	6.10741000
C	4.73267500	5.21730100	3.16271400
H	5.11373300	4.24805800	2.82508800
H	5.15361600	5.99683300	2.51969100
H	3.64463500	5.22320600	3.02426100
C	9.61788600	3.99817100	1.46443200
C	10.23527300	4.66773900	0.40931800
H	11.11917800	5.25710300	0.59879100
C	9.71839200	4.57942800	-0.88483100
H	10.20660000	5.11028500	-1.69627700
C	8.58125900	3.80850300	-1.13727100
H	8.16037900	3.72329300	-2.13195000
C	7.99176900	3.14492500	-0.07477300
H	7.10818500	2.52196000	-0.13799400
C	11.68661700	2.88675400	3.19508900
C	12.05938900	2.63949500	4.66852500
H	12.96262000	2.01981700	4.71346500
H	11.26457500	2.11943100	5.20665800
H	12.27537500	3.58024600	5.18674200
C	12.84332000	3.59499700	2.47806400
H	13.09486500	4.54891000	2.94884300
H	12.62849300	3.77029800	1.41833200

H	13.73311700	2.95556600	2.52206000
C	11.36651700	1.56328100	2.48781500
H	12.23394200	0.89671400	2.55450200
H	11.14872800	1.71275000	1.42392500
H	10.52284200	1.05278000	2.95161600
Fe	9.47594100	7.21134700	3.63690900
N	7.53927500	6.83345800	7.07047400
N	8.51793900	3.26314500	1.15770600
P	6.94832700	5.30387600	4.81795800
P	10.10764500	3.94180400	3.26807900
Pd	8.10087500	3.27631400	4.27156600
H	8.00004100	2.76446000	1.91369900
C	6.15216800	1.21538600	10.61884000
C	6.41739600	1.00797800	9.26765400
C	5.50481700	1.45670600	8.29104500
C	4.32149700	2.10180200	8.69935200
C	4.06568500	2.30136600	10.05302800
C	4.97910500	1.86411800	11.01595400
H	6.85897500	0.86465300	11.36529900
H	7.32575600	0.50650600	8.94912400
H	3.61888600	2.44522500	7.94713000
H	3.15113600	2.80060000	10.35901100
H	4.77473000	2.02146300	12.07065700
C	5.83553000	1.33520800	6.91318800
C	6.22054600	1.36874600	5.76082900
C	6.83200200	1.47113300	4.48133200
C	8.20634300	1.10701000	4.27379800
H	8.42274200	0.72787100	3.27794900
C	9.09474200	0.58446700	5.33146900
C	9.90817400	-0.52554900	5.05149500
C	9.20170300	1.18291700	6.60166300
C	10.79837900	-1.02417500	6.00211900
H	9.83489600	-1.00558000	4.07897200
C	10.09135700	0.68626700	7.55024500
H	8.60532300	2.05687300	6.83323200
C	10.89477600	-0.41948100	7.25568800
H	11.41438300	-1.88597500	5.76303200
H	10.16457800	1.16990200	8.52033500
H	11.58957700	-0.80344600	7.99636200
C	6.00109400	1.56215500	3.26119400
O	6.44897200	1.69710500	2.11374100
O	4.69160500	1.47466400	3.50591400
C	3.81248100	1.55092800	2.36963700
H	4.03100500	0.74361900	1.66741400

H	2.80879600	1.44422900	2.77840900
H	3.92133900	2.51506600	1.86766300

TS9

C	7.16716700	6.83640200	3.77176600
C	7.38555800	8.21808700	4.09419100
H	7.54091200	8.59796000	5.09175800
C	7.45116100	8.95029400	2.87575800
H	7.66186500	10.00784400	2.78627100
C	7.26701600	8.04019000	1.79236600
H	7.30503900	8.28857600	0.74024600
C	7.09261800	6.73700400	2.33559700
H	6.94790800	5.81891800	1.78129600
C	10.34743500	6.03059000	3.14509000
C	10.52970100	7.08370000	4.10953100
H	10.44718900	6.98448100	5.18138100
C	10.75056200	8.29818900	3.40131500
H	10.88376100	9.27333900	3.84980600
C	10.68835100	8.02008800	2.00504800
H	10.77075100	8.74527700	1.20677700
C	10.43487400	6.62827200	1.83949500
H	10.29143000	6.11830500	0.89783700
C	7.62886100	5.64618500	6.46279800
C	7.57961400	4.55965400	7.34839700
H	7.11254100	3.62980100	7.04656500
C	8.15021800	4.69463100	8.61108100
H	8.10808400	3.87074200	9.31768800
C	8.77588600	5.89888300	8.93405700
H	9.24169300	6.05246200	9.90198400
C	8.79254800	6.91627900	7.97833900
H	9.27462500	7.86752300	8.19232600
C	4.97157500	5.68336500	5.20222300
C	4.42671000	4.56592700	6.10079300
H	3.36749100	4.77071700	6.30046300
H	4.93789200	4.53198900	7.06699500
H	4.49551400	3.58518100	5.63268400
C	4.78071100	7.03633200	5.90743600
H	3.71227800	7.17824000	6.11033600
H	5.11611300	7.87345400	5.29089600
H	5.31029700	7.07592200	6.86418600
C	4.23263800	5.68493800	3.85373000
H	4.44731800	4.78497200	3.27250900
H	4.49713000	6.55497200	3.24721400
H	3.15202700	5.71799400	4.03648200

C	10.49631900	3.39241700	2.00585100
C	11.58542800	3.68921900	1.18524000
H	12.18842500	4.56810900	1.37758000
C	11.88059400	2.83721100	0.11930500
H	12.72365200	3.05072200	-0.53047000
C	11.08978800	1.70867100	-0.10025800
H	11.29237300	1.02661500	-0.91835600
C	10.01997800	1.47306500	0.75866800
H	9.36541300	0.61502500	0.64906600
C	11.37297000	3.78254100	4.75795500
C	10.83055000	4.01547400	6.17726000
H	11.60431100	3.75080900	6.90784400
H	9.95154800	3.39592000	6.37179600
H	10.54984600	5.05752400	6.35423100
C	12.66984800	4.57379400	4.53645200
H	12.55298500	5.64109000	4.73241800
H	13.04987800	4.45408600	3.51697400
H	13.43645100	4.18544900	5.21773100
C	11.65897400	2.28522400	4.55665700
H	12.30202200	1.93564200	5.37284500
H	12.18639400	2.09562400	3.61708200
H	10.75327400	1.67722000	4.57221200
Fe	8.90943800	7.46591200	2.92861500
N	8.22608100	6.80774800	6.76740800
N	9.74639500	2.30386200	1.76954800
P	6.82060800	5.41193800	4.82524100
P	9.99417200	4.30200800	3.54310700
Pd	7.80332800	3.46394800	3.90491700
H	8.66557600	2.16618000	2.70210900
C	6.99813500	0.90427500	10.04788700
C	7.01045700	0.87856300	8.65626900
C	5.91318100	1.38306700	7.92835300
C	4.80190400	1.89539500	8.62669700
C	4.79972000	1.91487900	10.01838700
C	5.89632000	1.42559300	10.73295400
H	7.84486500	0.50852000	10.60115100
H	7.85517700	0.46291300	8.11654700
H	3.95411000	2.27597300	8.06710600
H	3.93919000	2.31177300	10.54843400
H	5.88890100	1.44157000	11.81851600
C	5.97196600	1.44194800	6.50955200
C	6.09724000	1.61640100	5.31222000
C	6.37119200	1.88585700	3.94336300
C	7.55967700	1.31052200	3.29451100

H	7.32626000	1.09485300	2.24954600
C	8.35891800	0.23506200	3.95024100
C	8.60389000	-0.94967700	3.24298900
C	8.88246900	0.36023200	5.24564600
C	9.34047000	-1.98763500	3.81461400
H	8.19171800	-1.06853200	2.24337600
C	9.61466200	-0.67611000	5.82058100
H	8.72159300	1.28090500	5.79530100
C	9.84732900	-1.85447700	5.10757200
H	9.51200300	-2.90051800	3.25214900
H	10.01590600	-0.55956300	6.82359200
H	10.41992700	-2.66052200	5.55590800
C	5.23978400	2.17135900	3.00171300
O	5.37653900	2.32325700	1.80066700
O	4.05351100	2.22128000	3.63047500
C	2.90496000	2.42218400	2.78483900
H	2.81287500	1.59666100	2.07571700
H	2.05201300	2.44737200	3.46172900
H	2.99175700	3.36193700	2.23569700

IM15

C	8.05329900	6.69715800	4.46810300
C	8.58975300	7.57790600	5.47263200
H	8.68486500	7.34965600	6.52419100
C	9.02055400	8.77195000	4.83034100
H	9.50881200	9.60744900	5.31372500
C	8.75154300	8.65058800	3.43573600
H	9.00337100	9.37491700	2.67313900
C	8.15575900	7.38005100	3.20598500
H	7.86422900	6.98355000	2.24600000
C	10.88607600	5.54762000	3.11033600
C	11.10378200	5.44535200	4.53200400
H	10.71039200	4.66594700	5.17026100
C	11.81808300	6.60118000	4.94826800
H	12.09261100	6.84159600	5.96659700
C	12.05193400	7.41845000	3.80175100
H	12.53466700	8.38673800	3.80156100
C	11.48966000	6.77425900	2.66566800
H	11.44855700	7.14738400	1.65454400
C	7.76585200	4.75411700	6.51103800
C	7.06352400	5.28076100	7.59761700
H	6.19323000	5.90647800	7.44985200
C	7.50911000	4.99261200	8.88877600
H	6.97248000	5.37557300	9.75065800

C	8.64073900	4.20067200	9.04908200
H	9.00586800	3.93086300	10.03325600
C	9.28566500	3.73192900	7.90319300
H	10.16632800	3.10038600	7.98186400
C	5.47473700	5.38090300	4.55503200
C	5.17184300	5.17739600	3.05773400
H	4.10769200	5.36910800	2.87571300
H	5.40134300	4.16138800	2.72921400
H	5.74451900	5.86753600	2.42995600
C	4.65409500	4.39012200	5.39599500
H	3.59237600	4.53154800	5.15911100
H	4.77723500	4.55911200	6.46808700
H	4.90457300	3.35138700	5.19064600
C	5.10666100	6.82535100	4.94145100
H	5.59121100	7.55875000	4.29326800
H	5.36981900	7.06889400	5.97424000
H	4.02168300	6.94583600	4.83941600
C	9.03450700	5.18783100	0.83552400
C	7.78508800	4.70408500	0.42483200
H	7.33003600	3.85394200	0.92473600
C	7.14107100	5.34088900	-0.63686400
H	6.17286900	4.98938500	-0.98068100
C	7.76091400	6.43264200	-1.24101800
H	7.29416000	6.96272300	-2.06464200
C	9.01285900	6.83281400	-0.76692800
H	9.53397400	7.67307600	-1.21967700
C	11.10516100	3.17321600	1.38915300
C	11.84438800	2.39720100	2.49166300
H	12.58565200	1.73434800	2.03053600
H	11.17148800	1.77516100	3.08932900
H	12.37691500	3.07145900	3.17060300
C	12.11444600	3.97994900	0.55560200
H	12.70956700	4.64837300	1.18408300
H	11.62380600	4.58229700	-0.21340100
H	12.80113000	3.28426400	0.05855100
C	10.32264700	2.21106300	0.48129600
H	11.01473100	1.47823000	0.05098500
H	9.83735300	2.73813100	-0.34568900
H	9.54990500	1.65679900	1.02503900
Fe	9.99886100	7.09704400	4.05585800
N	8.86647300	3.99823900	6.66369400
N	9.64521400	6.22709900	0.24452100
P	7.33781100	5.05810300	4.74128100
P	9.88420300	4.34331000	2.23311200

Pd	8.25059700	3.26589200	3.55761200
H	8.92006000	1.57575400	3.08100400
C	7.65865400	1.01454500	10.36367000
C	7.65475200	0.94998800	8.97362100
C	6.59786100	1.53306500	8.24496600
C	5.54726300	2.16659400	8.93531300
C	5.56345800	2.22770300	10.32529600
C	6.61872700	1.65621600	11.04264300
H	8.47246100	0.56017500	10.92127600
H	8.45940600	0.46059600	8.43410700
H	4.73289700	2.60814600	8.36998200
H	4.74954600	2.71610200	10.85298800
H	6.62456000	1.70162800	12.12755000
C	6.63985300	1.52171500	6.82869100
C	6.75119800	1.54416700	5.61828000
C	7.04054000	1.60929200	4.23780300
C	8.26617700	0.86657800	3.73102300
H	7.97457800	0.15166100	2.95574700
C	9.15487900	0.26547100	4.78505800
C	9.07731900	-1.10489900	5.05073800
C	10.01940000	1.06437400	5.54132400
C	9.84737100	-1.66998100	6.06775900
H	8.40633700	-1.73028100	4.46775800
C	10.79692600	0.49836600	6.55084000
H	10.05594900	2.13388400	5.35687900
C	10.71053700	-0.87006700	6.81895400
H	9.77732000	-2.73464900	6.26830000
H	11.47679900	1.12282500	7.12390000
H	11.31856800	-1.31218200	7.60253300
C	5.93968700	1.62684700	3.22422100
O	6.15375000	1.67754800	2.01984000
O	4.71419300	1.57914200	3.75949800
C	3.61368200	1.61660300	2.82862900
H	3.70010800	0.80074600	2.10862100
H	2.71923900	1.50363400	3.43932100
H	3.60129100	2.57146500	2.29789000

IM16

C	7.54158000	6.89783500	4.24093900
C	7.97435500	8.11067400	4.88664100
H	8.16999500	8.23296500	5.94085900
C	8.17865900	9.09925300	3.88408400
H	8.54577200	10.10235000	4.05469200
C	7.87626800	8.52181900	2.61750700

H	7.97305600	9.00818700	1.65633800
C	7.48453600	7.17123100	2.82774800
H	7.24132600	6.46040400	2.05439300
C	10.45948900	5.76911000	3.09801000
C	10.72940400	6.16460200	4.45299500
H	10.51321300	5.57297800	5.33170000
C	11.26439200	7.48362200	4.42835900
H	11.52093800	8.07754600	5.29544000
C	11.33645200	7.91055000	3.06956000
H	11.66068100	8.88367700	2.72574800
C	10.84682400	6.85964700	2.24543000
H	10.76206100	6.87321100	1.16912900
C	7.89713700	5.46597500	6.70829400
C	7.39973500	6.40290800	7.62180100
H	6.60828800	7.08586700	7.34258100
C	7.95346600	6.45292500	8.90193000
H	7.58338200	7.16854100	9.62981500
C	8.98424300	5.57433500	9.22727600
H	9.44148200	5.57957500	10.21106000
C	9.42208700	4.67835200	8.25038800
H	10.22458200	3.97456000	8.45664200
C	5.41185000	5.04942400	4.99589600
C	4.98593400	4.83990200	3.52951500
H	3.90695300	4.64836400	3.49895600
H	5.48107700	3.97289200	3.08181900
H	5.17851900	5.73030000	2.92343900
C	5.04438400	3.80737800	5.82286300
H	3.95380700	3.75455000	5.92026100
H	5.46664200	3.84237300	6.83332900
H	5.36900900	2.89074200	5.32644000
C	4.69621800	6.28584800	5.56368000
H	5.04366200	7.21538700	5.10268000
H	4.81172300	6.36103500	6.64792100
H	3.62257100	6.19433400	5.36143500
C	9.36394700	4.41562000	0.84854100
C	7.99602000	4.48340500	0.56214600
H	7.26462800	4.30947200	1.34408900
C	7.59805300	4.75369600	-0.74669700
H	6.54396300	4.81182300	-1.00092500
C	8.57895900	4.93101800	-1.72074400
H	8.31735000	5.13365800	-2.75391800
C	9.91945300	4.83317600	-1.34059200
H	10.71450500	4.95773400	-2.07166800
C	11.59540900	3.20487500	2.56808500

C	11.57762700	1.98194700	1.63964800
H	12.58549100	1.54980600	1.63047000
H	11.32841200	2.25756800	0.61150200
H	10.89864000	1.20883500	1.99359000
C	11.84910000	2.76946800	4.02402600
H	11.07377200	2.09420300	4.39254800
H	11.91674300	3.63086200	4.69623900
H	12.80643000	2.23697800	4.07147100
C	12.72104900	4.15107700	2.10859700
H	13.65657700	3.57874000	2.10071800
H	12.85476600	4.99529500	2.78786100
H	12.53726400	4.52880400	1.10105100
Fe	9.37198100	7.41324800	3.56394100
N	8.89588200	4.62226300	7.02245800
N	10.31148300	4.58675500	-0.08485400
P	7.29776900	5.26511500	4.97233400
P	9.91751400	4.12016100	2.58109800
Pd	8.26194000	3.20637100	4.02710200
C	12.11354600	-2.37104600	6.38549600
C	11.05120700	-1.64321200	5.85870700
C	11.14571700	-1.08858400	4.56694000
C	12.32463500	-1.28171400	3.81896500
C	13.38106500	-2.01053700	4.35548100
C	13.27951100	-2.55655700	5.63799300
H	12.03236100	-2.79760200	7.38075600
H	10.14029700	-1.49874000	6.43091500
H	12.39572700	-0.85797400	2.82251400
H	14.28542400	-2.15666500	3.77240100
H	14.10548300	-3.12658100	6.05234200
C	10.07240100	-0.33014000	4.02923000
C	9.17599300	0.35005000	3.56683500
C	8.17165200	1.20680900	3.03304100
C	7.84292100	-0.01458300	0.85584700
C	6.52318500	-0.37841000	0.55855500
C	8.87345900	-0.92618800	0.59274700
C	6.23947400	-1.62962300	0.01015300
H	5.71795800	0.32222900	0.76022200
C	8.59129300	-2.17601100	0.04397000
H	9.90059600	-0.65522900	0.81784400
C	7.27252800	-2.53222400	-0.24629800
H	5.21235500	-1.89690100	-0.22120600
H	9.40050000	-2.87158100	-0.15858300
H	7.05274100	-3.50587500	-0.67405200
C	6.75436300	0.93200400	3.49647800

O	5.79259400	1.57887900	3.10594500
O	6.65982600	-0.06499700	4.38225500
C	5.33167200	-0.37417900	4.84909800
H	4.91837400	0.47096100	5.40552600
H	4.68182300	-0.60701600	4.00342900
H	5.45147700	-1.24014600	5.49810900
C	8.14627900	1.32718200	1.49170400
H	9.09477300	1.70973000	1.12489400
H	7.36903700	2.04243000	1.22562000
C	7.90601700	2.23151800	5.72808200
O	7.94159300	1.68940000	6.73087600

TS10

C	7.60244500	6.85017900	4.02711600
C	7.82039000	8.16981500	4.55620200
H	7.79957300	8.43069000	5.60284800
C	8.08212400	9.03950300	3.46229200
H	8.32589700	10.09082100	3.53815100
C	8.02454900	8.27821400	2.25723400
H	8.21810300	8.65027100	1.26022500
C	7.72521100	6.93002100	2.59639100
H	7.64459600	6.09658200	1.91292700
C	10.81498900	5.98374100	3.25639200
C	10.81397700	6.39810600	4.63479200
H	10.53176900	5.78136500	5.47614200
C	11.18411100	7.77037900	4.68769200
H	11.23188800	8.37846800	5.58075400
C	11.41453600	8.21910400	3.35400500
H	11.66872800	9.22807700	3.05814000
C	11.19418200	7.12538900	2.46984000
H	11.24649400	7.16505800	1.39186900
C	7.78134000	5.63868900	6.65391500
C	8.70418500	4.79602000	7.28083500
H	9.12388700	3.95100800	6.74700200
C	9.05896600	5.06338100	8.60422600
H	9.77143300	4.42775800	9.12124100
C	8.47818200	6.15355100	9.24686100
H	8.72118200	6.39708900	10.27580300
C	7.56213700	6.93495800	8.53710500
H	7.08401000	7.79229200	9.00470300
C	5.37674800	5.15777300	4.90940600
C	4.98340000	4.51047700	3.56946900
H	3.88993500	4.48825000	3.49395400
H	5.34196400	3.47923000	3.49418900

H	5.36286100	5.08054800	2.71419800
C	4.92832000	4.27055200	6.07997100
H	3.83898200	4.15927400	6.03335500
H	5.17829300	4.71790100	7.04616900
H	5.35926900	3.26885200	6.03392300
C	4.73857300	6.55321800	5.03493800
H	4.97505100	7.18481600	4.17426400
H	5.06824100	7.06342200	5.94303600
H	3.64952600	6.43294500	5.07719400
C	9.84406000	4.52752600	0.94139500
C	10.75049500	4.91722500	-0.05014300
H	11.77294700	5.17025700	0.20264000
C	10.31444300	4.97148600	-1.37467100
H	10.99694800	5.26891200	-2.16505600
C	8.99389800	4.63362300	-1.66361000
H	8.61527100	4.65660600	-2.68001400
C	8.15921400	4.25902200	-0.60898600
H	7.12213300	3.98699600	-0.78858600
C	11.75251500	3.21591700	2.87192900
C	11.55137900	2.01462900	1.93579200
H	12.37473300	1.30626700	2.07986600
H	11.53978900	2.31415600	0.88365700
H	10.62480700	1.47927700	2.15844600
C	11.77106400	2.73654300	4.33705900
H	10.85335900	2.19452500	4.59284000
H	11.88889300	3.57410400	5.03405400
H	12.61196600	2.05039600	4.49015500
C	13.06918900	3.93416500	2.54773300
H	13.90539500	3.24713000	2.72522200
H	13.21790300	4.81656100	3.17654100
H	13.12430600	4.24474000	1.50022200
Fe	9.47038400	7.48204200	3.53243100
N	7.21645300	6.69054800	7.26883000
N	8.56642200	4.20613700	0.66455800
P	7.26097900	5.32470600	4.91795100
P	10.24490300	4.35485000	2.73037800
Pd	8.35711400	3.49454500	3.99307900
C	12.92694700	-1.88400300	5.84126000
C	11.67192500	-1.33066500	5.60617000
C	11.25323100	-1.06555400	4.28732600
C	12.11271800	-1.37784200	3.21437500
C	13.36314300	-1.93525500	3.46053000
C	13.77495900	-2.18632900	4.77252300
H	13.24370200	-2.08504200	6.86013200

H	11.00472900	-1.09890100	6.43014400
H	11.78139600	-1.18924800	2.19848500
H	14.01711200	-2.17961700	2.62888100
H	14.75163100	-2.62151200	4.96085200
C	9.98755700	-0.47215600	4.04084400
C	8.91229500	0.05258800	3.81343800
C	7.71746700	0.74999800	3.52837500
C	7.28740500	0.16639900	1.13430300
C	5.98150500	-0.21834400	0.80417000
C	8.36556300	-0.53590200	0.57889200
C	5.76008900	-1.28488700	-0.06735300
H	5.14292600	0.31464900	1.24095500
C	8.14476200	-1.60124000	-0.29184600
H	9.38102100	-0.24305400	0.83169800
C	6.83976000	-1.97929200	-0.61572600
H	4.74347100	-1.57247400	-0.31915400
H	8.98847700	-2.13588400	-0.71858700
H	6.66599700	-2.80970300	-1.29359000
C	6.40900700	0.19385100	4.05415500
O	5.33431400	0.70974500	3.80670700
O	6.58156100	-0.87042400	4.83575700
C	5.38085200	-1.40964900	5.42484200
H	4.91335700	-0.66068900	6.06849900
H	4.67991200	-1.70824300	4.64260100
H	5.70781000	-2.27133000	6.00461500
C	7.54682900	1.30357200	2.10217100
H	8.43995100	1.84810700	1.79978100
H	6.71252300	2.00738300	2.09652800
C	7.56356300	2.17425600	5.12048300
O	7.36305000	1.76865200	6.19392400

IM17

C	7.73133100	6.40914300	5.00449500
C	8.21949600	7.52253000	5.77528800
H	8.73682700	7.45444000	6.72026400
C	7.92675200	8.71698300	5.06274600
H	8.20591000	9.71675200	5.36695500
C	7.25461900	8.36425000	3.85638900
H	6.94063300	9.04678800	3.07834900
C	7.13017900	6.94866800	3.81342200
H	6.69677300	6.38162900	3.00522200
C	10.13019200	6.20629000	2.67121000
C	10.87493300	6.39211800	3.89149600
H	11.12107900	5.61368600	4.59899100

C	11.17243900	7.77539600	4.02417100
H	11.68468200	8.23659400	4.85773700
C	10.62451000	8.45453900	2.89556900
H	10.64505400	9.52328000	2.72857400
C	9.99211300	7.49723700	2.05517300
H	9.43687000	7.68602500	1.15002600
C	8.70661500	4.79116100	7.10684800
C	10.08106800	4.54258500	7.15727500
H	10.60501700	4.19409800	6.27385700
C	10.74684700	4.72191800	8.36818200
H	11.81474900	4.53948600	8.44124700
C	10.01406800	5.12352300	9.48356000
H	10.48905000	5.26866800	10.44813900
C	8.64094300	5.32879500	9.33734500
H	8.02990900	5.63232600	10.18383400
C	5.99333100	4.22810500	5.83467700
C	5.33407100	3.95466300	4.47391900
H	4.28162300	3.69579600	4.64027800
H	5.81218700	3.11812600	3.96069300
H	5.35476800	4.82696800	3.81615300
C	5.89407800	2.96393800	6.70151500
H	4.83865100	2.80236600	6.95050200
H	6.45264400	3.05432100	7.63531100
H	6.24056600	2.07820200	6.16383100
C	5.28150700	5.40473400	6.52940300
H	5.29067300	6.30588400	5.91076100
H	5.74135600	5.63255800	7.49111500
H	4.23503500	5.12050300	6.69352700
C	7.90097500	4.89662300	1.26125000
C	6.88410500	3.94048300	1.35517400
H	7.01795800	3.06480600	1.97861600
C	5.69798000	4.14357200	0.64935300
H	4.89249800	3.41992500	0.71168500
C	5.57535200	5.29585700	-0.12360200
H	4.67038300	5.50543900	-0.68452400
C	6.65209400	6.18601900	-0.17046700
H	6.59702300	7.08976800	-0.77298900
C	10.64149000	3.90635700	0.92561900
C	10.02900500	2.62190600	0.34303300
H	10.74205000	2.16796300	-0.35581600
H	9.10868800	2.83145600	-0.21133600
H	9.80505900	1.89010500	1.12376700
C	11.96701500	3.60203100	1.64468500
H	11.83977100	2.85015100	2.42738300

H	12.39475400	4.50628100	2.09057000
H	12.69204500	3.21944700	0.91586500
C	10.87963500	4.93146700	-0.19363300
H	11.54794000	4.49067200	-0.94362400
H	11.35671400	5.83841000	0.18837900
H	9.95050700	5.22054700	-0.69181700
Fe	9.11570300	7.43231200	3.92198500
N	7.99704800	5.17597300	8.17455000
N	7.79433900	5.99831700	0.49978600
P	7.80586900	4.67164400	5.49965600
P	9.44866800	4.60326800	2.21613600
Pd	8.97615100	3.20151000	4.16556400
C	3.12653500	1.24103500	1.65063600
C	4.14755000	1.10314000	2.58768200
C	5.44696900	0.76117700	2.16910500
C	5.70053700	0.55563400	0.79925100
C	4.67287300	0.69288400	-0.12949100
C	3.38534200	1.03695600	0.29230500
H	2.12570000	1.50190100	1.98077100
H	3.95167500	1.25358900	3.64374300
H	6.70260200	0.28886600	0.47926800
H	4.87538100	0.53023400	-1.18357600
H	2.58527400	1.14031200	-0.43429900
C	6.50688200	0.63505400	3.11374000
C	7.42297400	0.52562000	3.90135400
C	8.56425000	0.38034600	4.79979000
C	8.02123700	-2.12739300	5.17848300
C	8.95331900	-3.14129000	4.92921800
C	6.67292400	-2.36534200	4.87951600
C	8.55322200	-4.35711700	4.37509300
H	9.99765900	-2.97842000	5.17851500
C	6.27016800	-3.57668600	4.31948900
H	5.93402500	-1.59851200	5.09316800
C	7.21081800	-4.57566800	4.06225200
H	9.28829200	-5.13638700	4.19546700
H	5.22088600	-3.74483400	4.09510000
H	6.89756900	-5.52281700	3.63323200
C	9.80204500	0.38964400	3.91053700
O	10.21915600	1.45067900	3.42278100
O	10.38561400	-0.76297800	3.70965300
C	11.56331200	-0.77677700	2.86143500
H	11.30994400	-0.38657300	1.87450400
H	12.34960500	-0.16993300	3.31432000
H	11.85440500	-1.82363200	2.80766600

C	8.44360700	-0.81130500	5.78874000
H	7.71550900	-0.49634500	6.54207500
H	9.40148800	-0.90849100	6.30780200
C	8.73767500	1.77890900	5.60136300
O	8.84807100	1.76801900	6.79311800

IM17-CO

C	9.12870000	6.48153000	4.53689300
C	10.11443400	7.05593200	5.41461700
H	10.43243200	6.64093800	6.35952700
C	10.62805800	8.23004200	4.79842000
H	11.41565500	8.85675400	5.19450500
C	9.96976900	8.40057500	3.54575600
H	10.17212400	9.17601100	2.81935000
C	9.04913300	7.33081000	3.37699700
H	8.42918300	7.17074700	2.51070300
C	11.17923100	4.99583500	2.31593400
C	11.79496900	4.69534900	3.58508700
H	11.46876000	3.93054300	4.27616000
C	12.80674400	5.66349500	3.82042200
H	13.41638000	5.73636300	4.71096700
C	12.83214800	6.56177400	2.71172800
H	13.46490400	7.43427000	2.61688900
C	11.83959300	6.15518300	1.77860800
H	11.56070500	6.65252900	0.86338300
C	8.89482300	4.43354700	6.47418200
C	8.42633500	4.68496300	7.76319100
H	7.53759100	5.27507400	7.93602600
C	9.12266400	4.14241400	8.84527900
H	8.77298300	4.31358700	9.85872500
C	10.26022300	3.37875100	8.60427200
H	10.82568900	2.93366800	9.41598600
C	10.65874000	3.18955700	7.27905900
H	11.54099900	2.59986200	7.04148000
C	6.40481200	5.73356900	5.19943300
C	5.81254100	6.06885100	3.81877700
H	4.79730500	6.45892300	3.95754900
H	5.74895700	5.18206200	3.18712800
H	6.38802600	6.83447800	3.29408100
C	5.49356000	4.69272600	5.87177400
H	4.53265400	5.16768700	6.10210100
H	5.90093800	4.28667100	6.79960300
H	5.29037600	3.86066100	5.19400600
C	6.48462900	7.03151300	6.02497600

H	7.08455200	7.79068100	5.51718200
H	6.90386500	6.88794600	7.02263200
H	5.47000600	7.42811900	6.14757200
C	8.66144700	5.26000200	0.82716100
C	7.28073300	5.04808500	0.83693000
H	6.86152700	4.20275800	1.37043400
C	6.45700200	5.95562000	0.16690000
H	5.38130400	5.82511700	0.16804000
C	7.04739200	7.03283600	-0.48768900
H	6.44873800	7.76876400	-1.01446600
C	8.44072800	7.14838000	-0.46045300
H	8.93922100	7.96862200	-0.97198000
C	10.35842400	2.92735100	0.35569000
C	11.54843700	2.11520800	0.89032600
H	11.89805200	1.43574900	0.10430200
H	11.29093000	1.50438900	1.75706900
H	12.38350500	2.76560200	1.16694500
C	10.81978500	3.73539100	-0.86794000
H	11.60665000	4.44860600	-0.60554800
H	10.00084600	4.28873900	-1.33208700
H	11.22778600	3.04315700	-1.61415400
C	9.18743100	2.00583800	-0.02602900
H	9.50899900	1.31201500	-0.81166500
H	8.33734800	2.57766600	-0.41495400
H	8.83189900	1.41474600	0.82445300
Fe	10.93374600	6.55327800	3.59229000
N	9.99538100	3.69796600	6.23804700
N	9.23694700	6.28539300	0.17713200
P	8.12816600	5.01407600	4.89113800
P	9.75046400	4.07811100	1.72831100
Pd	8.52703900	3.04305100	3.58655600
C	3.65522800	3.88482600	-1.04929400
C	4.34007000	3.18805800	-0.05798200
C	4.16966500	3.53521800	1.29631800
C	3.29550000	4.58466300	1.63510600
C	2.61616900	5.27813100	0.63613300
C	2.79576900	4.93269900	-0.70622200
H	3.79054900	3.61121000	-2.09114300
H	5.00902300	2.37256200	-0.31299500
H	3.15642000	4.84420500	2.67906700
H	1.94178700	6.08556600	0.90462200
H	2.26246800	5.47375300	-1.48183400
C	4.88698200	2.82516700	2.30155600
C	5.52622800	2.18718900	3.11079600

C	6.12744900	1.30383400	4.09969500
C	4.02633800	-0.10623900	4.39463600
C	2.87768700	0.47028200	3.83870600
C	4.23240500	-1.48477800	4.24476800
C	1.95935100	-0.30998700	3.13725000
H	2.70342200	1.53593700	3.95715200
C	3.31546900	-2.26652900	3.54202300
H	5.11302100	-1.94465800	4.68448100
C	2.17853000	-1.68006600	2.98304900
H	1.07090900	0.15060600	2.71512100
H	3.48304700	-3.33502900	3.44153500
H	1.46181200	-2.28894600	2.44000200
C	6.82969800	0.09004100	3.45957900
O	7.47519600	-0.69638000	4.11858000
O	6.64533600	0.00731600	2.14078100
C	7.17573400	-1.18177500	1.51604700
H	6.67585100	-2.06263500	1.92383900
H	6.95774900	-1.06888300	0.45533300
H	8.25135700	-1.25577500	1.69053200
C	5.05398200	0.74365800	5.09767400
H	4.59092400	1.60050600	5.59456200
H	5.59736900	0.17238500	5.85276500
C	7.25151000	2.06148500	4.90930900
O	7.33790600	1.98793500	6.09773200
C	9.54503900	1.35779900	3.61168200
O	10.33762200	0.57102600	3.85012300

TS11

C	6.69735900	10.48876000	5.59741600
C	7.82043900	10.91177500	6.39293100
H	8.23074700	10.38501600	7.24138300
C	8.33942100	12.11488100	5.83398500
H	9.20973700	12.65062500	6.18854600
C	7.55406600	12.44958200	4.69340200
H	7.72125400	13.28318100	4.02509500
C	6.55016100	11.45337900	4.53923400
H	5.82891800	11.40877000	3.73811600
C	8.35476900	9.23475000	2.91603800
C	9.00916600	8.65573800	4.06308500
H	8.64892000	7.79702800	4.61386000
C	10.14909300	9.44749300	4.37150000
H	10.82329200	9.29369000	5.20334500
C	10.21184900	10.51470600	3.42642000
H	10.94027200	11.31473900	3.42314500

C	9.11959400	10.38424900	2.52394000
H	8.84813800	11.05492000	1.72417300
C	6.17645200	8.41395100	7.47427800
C	6.30295800	9.22797700	8.60554000
H	6.09002000	10.28582500	8.53914800
C	6.71817300	8.67067600	9.81514900
H	6.80293100	9.29250500	10.70102300
C	7.01990200	7.31349300	9.86770400
H	7.32671100	6.83187300	10.78833300
C	6.88546400	6.57025800	8.69947800
H	7.09541600	5.50552300	8.68392900
C	3.90382600	9.89227300	6.18564100
C	3.23050100	10.10644700	4.81812400
H	2.23654400	10.54358500	4.97625100
H	3.11023400	9.16544600	4.27709500
H	3.79454300	10.79864000	4.18766200
C	3.04723600	8.94709500	7.03697800
H	2.05353800	9.39092000	7.17375500
H	3.48221500	8.78752500	8.02738400
H	2.91670400	7.96942000	6.57528300
C	4.03084600	11.24677600	6.90144200
H	4.67347400	11.94509300	6.36112400
H	4.40670500	11.14676800	7.92283900
H	3.03245200	11.69469600	6.97312300
C	5.85060400	9.96376000	1.53690800
C	4.45200200	9.87542100	1.51014700
H	3.95170400	9.03014400	1.97183100
C	3.72740800	10.89425000	0.89213700
H	2.64298400	10.85133900	0.85196700
C	4.42091100	11.96794500	0.33731700
H	3.90010300	12.78756700	-0.14671400
C	5.81555000	11.96740500	0.41312100
H	6.39267700	12.78480100	-0.01324800
C	7.18677800	7.42716300	0.91513800
C	8.00329800	6.26445200	1.50467700
H	8.26159500	5.56143300	0.70360300
H	7.42891600	5.71901000	2.25982200
H	8.93756900	6.61381200	1.95644200
C	8.00012500	8.15490900	-0.16405000
H	8.95255800	8.52343800	0.22980800
H	7.45449800	9.00578400	-0.58125500
H	8.22040800	7.45824000	-0.98213700
C	5.86475600	6.89573500	0.33700000
H	6.08334100	6.16139800	-0.44732300

H	5.26984600	7.69564400	-0.11536500
H	5.25879100	6.40174800	1.10389900
Fe	8.38980000	10.56223000	4.45007900
N	6.47401400	7.10227900	7.54032100
N	6.52345300	10.98980700	0.99086300
P	5.59125200	9.06034500	5.82965900
P	6.77214800	8.59033400	2.34374900
Pd	5.57929500	7.51259400	4.11910700
C	3.82195500	6.74143100	11.57179900
C	3.47299200	6.68276400	10.22499500
C	3.89284600	5.59897000	9.43446800
C	4.64908200	4.56646700	10.02372400
C	4.98945300	4.63113000	11.37205400
C	4.58308200	5.72068600	12.14777900
H	3.49381300	7.58162300	12.17652600
H	2.87547900	7.46849900	9.77578400
H	4.96393700	3.72946700	9.40790500
H	5.56861600	3.82944800	11.82083200
H	4.84757000	5.76770600	13.19992000
C	3.62685700	5.54960100	8.03569900
C	3.50772700	5.47264200	6.83425100
C	3.47207500	5.31547600	5.38726600
C	4.08586500	2.79327500	5.47246200
C	4.03836200	2.32923300	6.79408200
C	5.05965400	2.27766000	4.61032700
C	4.96735500	1.39605800	7.25188500
H	3.26792900	2.69964800	7.46277600
C	5.98598200	1.33688600	5.06365800
H	5.09233000	2.61938200	3.57956800
C	5.94911600	0.90123300	6.38908700
H	4.91256100	1.03792700	8.27635200
H	6.73031000	0.93917000	4.37955200
H	6.66531600	0.16500500	6.74213200
C	2.38495900	6.21507100	4.75414400
O	2.54670500	6.92487500	3.78305900
O	1.22546200	6.07721100	5.40133800
C	0.11943200	6.84378000	4.88086000
H	-0.07475500	6.56854100	3.84204200
H	-0.72817700	6.59097500	5.51569900
H	0.34564200	7.91086200	4.94082300
C	3.10777400	3.83035000	4.98516200
H	3.04009700	3.80720900	3.89360700
H	2.11069000	3.64461900	5.39331700
C	4.80462000	5.73883200	4.73884100

O	5.12596100	5.41216800	3.58507700
C	7.24350300	4.68171000	5.32353900
H	7.06653700	4.47807000	4.26694500
H	7.99906000	5.46607100	5.42942000
H	7.55081000	3.76451100	5.82761200
O	6.00420500	5.11088600	5.91077100
H	6.16654400	5.94365200	6.49959500

IM18

C	6.79772900	10.53317400	5.59047700
C	7.97408300	10.92430700	6.32267300
H	8.43138300	10.37871200	7.13517000
C	8.48183100	12.12690700	5.74940100
H	9.38021600	12.64332100	6.06008800
C	7.63890200	12.48854900	4.65970600
H	7.78356400	13.32644500	3.99158400
C	6.61105900	11.51039000	4.55012000
H	5.85200100	11.48256300	3.78374700
C	8.30592200	9.26592700	2.80279400
C	9.04391100	8.69478500	3.90069700
H	8.73399900	7.82537400	4.46430700
C	10.19084200	9.50101100	4.13896600
H	10.92215600	9.35310900	4.92245100
C	10.17405900	10.57365400	3.19828500
H	10.88826300	11.38512500	3.15058400
C	9.02630100	10.42800300	2.36926400
H	8.69049000	11.09770900	1.59355800
C	6.23888200	8.51252200	7.50201700
C	6.52929800	9.26899900	8.63734900
H	6.50723400	10.34800600	8.57250900
C	6.83411100	8.63774300	9.84550700
H	7.03422900	9.23512200	10.72958700
C	6.87251900	7.24452600	9.91941400
H	7.08029700	6.72471300	10.84613400
C	6.61083000	6.52177300	8.76901200
H	6.61184600	5.44201500	8.71336500
C	4.01389100	9.94571800	6.27813200
C	3.30542700	10.25796700	4.94734800
H	2.31970400	10.68799100	5.16620700
H	3.16499700	9.35521400	4.34958900
H	3.85293900	10.98783900	4.34676200
C	3.17124000	8.93321200	7.06432800
H	2.17524500	9.35517500	7.24608500
H	3.61370600	8.69884200	8.03730200

H	3.04559500	7.99591600	6.52153400
C	4.17800300	11.23599900	7.09179800
H	4.82950700	11.95842900	6.59386100
H	4.56943700	11.04492200	8.09506200
H	3.19309500	11.70162600	7.21846200
C	5.73349200	9.93725900	1.55188700
C	4.33615100	9.82182600	1.58860400
H	3.87780400	8.96084900	2.06456000
C	3.56292300	10.83072500	1.01606700
H	2.47872800	10.76521000	1.02445600
C	4.20687700	11.92598000	0.44297500
H	3.64739500	12.73951700	-0.00717700
C	5.60274800	11.95449600	0.45619400
H	6.14243000	12.78958600	0.01476900
C	7.09474000	7.42971800	0.86171600
C	7.96480500	6.28784700	1.41555100
H	8.19405400	5.58381100	0.60604900
H	7.44310800	5.74063500	2.20655000
H	8.91598600	6.66133900	1.80991400
C	7.83549700	8.17427700	-0.25623500
H	8.79540600	8.56874100	0.09220200
H	7.24876300	9.01049300	-0.64735200
H	8.03577100	7.48281500	-1.08425200
C	5.75824900	6.86428300	0.35309800
H	5.95282900	6.12880400	-0.43682000
H	5.12466500	7.64869200	-0.07402100
H	5.20469900	6.36599600	1.15572600
Fe	8.43073900	10.59473400	4.34560500
N	6.30935000	7.16624900	7.62738900
N	6.35741900	10.98547000	0.98804600
P	5.67731100	9.11419100	5.81974400
P	6.70738200	8.57150300	2.31556800
Pd	5.63921700	7.53926500	4.19541700
C	3.55113300	6.70283000	11.54843100
C	3.28137300	6.63059800	10.18388300
C	3.72547300	5.52703400	9.43323100
C	4.41890000	4.48583200	10.08428700
C	4.68173900	4.56539300	11.44955900
C	4.25660200	5.67684700	12.18370200
H	3.20368800	7.55789100	12.12073300
H	2.72893600	7.42170400	9.68843800
H	4.74445000	3.62864800	9.50182600
H	5.21205400	3.75688600	11.94414300
H	4.45931200	5.73495000	13.24886600

C	3.56827300	5.47509000	8.01769500
C	3.57603400	5.40459800	6.80893500
C	3.66858900	5.26424200	5.35974500
C	4.15181900	2.72238100	5.47818900
C	3.95655600	2.23288300	6.77671800
C	5.20281200	2.20536900	4.71240200
C	4.81432400	1.27025300	7.30841100
H	3.12572100	2.60549900	7.36798200
C	6.06151400	1.24081200	5.24119900
H	5.34791700	2.56708900	3.69793500
C	5.87480100	0.77689500	6.54431600
H	4.64310500	0.88976100	8.31189800
H	6.86871000	0.84399200	4.63201200
H	6.53690600	0.01981600	6.95428400
C	2.67627500	6.21994000	4.66748200
O	2.93531600	6.99577500	3.77023200
O	1.44966200	6.06635800	5.18069700
C	0.41751500	6.88991700	4.60318800
H	0.32388200	6.68534000	3.53435900
H	-0.49526400	6.61924700	5.13161100
H	0.65401500	7.94601700	4.75349400
C	3.25793600	3.79758400	4.91932900
H	3.28188400	3.78646400	3.82560400
H	2.22421900	3.65272400	5.24293500
C	5.11549500	5.53676200	4.87313600
O	5.41180100	5.41931900	3.64987300
C	7.34338900	4.77347300	5.36821400
H	7.28462400	4.04810900	4.55725000
H	7.84564300	5.67965800	5.01183700
H	7.87932400	4.34335200	6.21562400
O	6.03185000	5.08278800	5.85817800
H	6.10317300	6.55904800	6.80780300

6a

C	3.77213000	6.39446800	11.48075700
C	3.69794700	6.41015000	10.09041400
C	4.05462800	5.26867400	9.34977500
C	4.48642400	4.11393100	10.03054900
C	4.55763500	4.10860500	11.42072900
C	4.20150200	5.24596100	12.14990300
H	3.49491000	7.28092200	12.04421200
H	3.36585100	7.29920600	9.56389100
H	4.75807100	3.23512200	9.45475800
H	4.89250500	3.21378100	11.93791800

H	4.25861000	5.23752800	13.23463900
C	3.98166300	5.26307600	7.92603800
C	3.93457700	5.21645200	6.71767500
C	3.88377600	5.02542100	5.27243500
C	3.99892800	2.48443100	5.69681800
C	3.45164100	2.06161300	6.91519900
C	5.17312000	1.87464600	5.23800700
C	4.06484900	1.05726700	7.66387700
H	2.54293800	2.53115200	7.28083300
C	5.78887100	0.87021500	5.98596400
H	5.60596900	2.20132900	4.29875900
C	5.23969700	0.46020400	7.20174800
H	3.62275100	0.73940700	8.60441100
H	6.69890100	0.40594900	5.61584700
H	5.71902400	-0.32356600	7.78182800
C	2.95700100	6.06624700	4.60743900
O	3.25815200	6.72849600	3.64045300
O	1.76002800	6.10710300	5.21226900
C	0.81360700	7.02240900	4.63393000
H	0.61257400	6.75533000	3.59335700
H	-0.08753600	6.92801400	5.23926500
H	1.20174300	8.04313200	4.67267500
C	3.33481000	3.59620100	4.92067700
H	3.46993600	3.46047700	3.84476100
H	2.26406500	3.60959700	5.13788500
C	5.26800200	5.23468300	4.61710600
O	5.69731200	4.57004700	3.70178600
C	7.16830300	6.60307000	4.55890300
H	7.85387300	5.75373900	4.61178000
H	7.01562000	6.87956500	3.51270200
H	7.55294200	7.44710900	5.13078000
O	5.91095700	6.26896000	5.16910900

IM19

C	6.87432000	6.37649600	3.81315100
C	6.81736100	7.73446800	4.28653300
H	6.74193200	8.01887300	5.32357700
C	6.96724000	8.59933700	3.16751800
H	7.01819600	9.67930800	3.20818000
C	7.10611300	7.79929000	1.99482000
H	7.27666100	8.16337100	0.99065300
C	7.04239100	6.43336300	2.38467900
H	7.14271200	5.58050500	1.73029700
C	10.18274200	6.05512400	3.32901900

C	10.03971400	6.61670900	4.64512500
H	9.82287600	6.06946200	5.54892100
C	10.17596900	8.02766100	4.54044000
H	10.06677600	8.73233000	5.35349200
C	10.41336600	8.35240800	3.17241100
H	10.52251000	9.34871300	2.76529600
C	10.42632000	7.14519600	2.42178500
H	10.56842100	7.05613500	1.35609000
C	7.56840100	5.13034200	6.37363400
C	8.27456500	4.09129600	6.99048300
H	8.35366400	3.11708600	6.52236200
C	8.87651400	4.33174200	8.22673500
H	9.43009300	3.54193800	8.72578800
C	8.75573500	5.59541400	8.79900200
H	9.21362400	5.83153500	9.75399900
C	8.01612000	6.56357300	8.11450200
H	7.88558700	7.55896800	8.53315000
C	4.94174800	4.67310200	5.11836200
C	4.72130700	3.51961600	6.10707300
H	3.65121600	3.43464900	6.32964500
H	5.24575900	3.69356400	7.05211500
H	5.04703300	2.56168200	5.70476400
C	4.40906600	5.96988300	5.75055000
H	3.34930300	5.82585800	5.99481300
H	4.48015100	6.81521300	5.06248600
H	4.93926700	6.23068100	6.66959200
C	4.21462500	4.42524400	3.78592000
H	4.56966000	3.52875600	3.27584500
H	4.33625700	5.27859800	3.11076500
H	3.14168700	4.30133900	3.97550600
C	10.03491800	4.34764700	1.06233500
C	8.87777400	4.02077300	0.35080300
H	7.99535600	3.67982100	0.87910500
C	8.89721300	4.11554600	-1.03941300
H	8.01115300	3.87552200	-1.61988000
C	10.07512700	4.51317700	-1.66808600
H	10.13888300	4.59700900	-2.74805600
C	11.18687200	4.80112200	-0.87307800
H	12.12851000	5.10606000	-1.32343900
C	11.66934300	3.56456700	3.48666200
C	11.52421200	3.33139000	5.00167100
H	12.43935800	2.86051500	5.38073300
H	10.67816800	2.67973300	5.23522100
H	11.38699200	4.27120300	5.54522100

C	12.83607000	4.53316500	3.22471600
H	12.70602200	5.47458800	3.76559800
H	12.93561400	4.75522300	2.16115700
H	13.76345500	4.06637600	3.57828100
C	11.92034200	2.23139400	2.76664600
H	12.86335800	1.80909500	3.13446200
H	12.00995000	2.36889300	1.68600100
H	11.13331200	1.49876800	2.95965300
Fe	8.60637200	7.32239100	3.36254500
N	7.42996700	6.34396100	6.93310900
N	11.17147500	4.73096900	0.46240100
P	6.79565100	4.81486000	4.72431300
P	10.03273600	4.30768100	2.90635700
Pd	8.18206000	3.07962300	3.65408800
H	9.15708900	2.14119500	2.85390800
C	6.78383900	1.29824800	4.11957800
C	8.02372600	0.70474600	3.87402100
C	5.62988600	1.20841800	3.20991000
C	5.72842500	1.49398500	1.83728300
C	4.38480600	0.82110800	3.73083400
C	4.60995100	1.40052400	1.01346100
H	6.67670700	1.82156200	1.42649600
C	3.26899700	0.71624300	2.90263300
H	4.29226500	0.59909300	4.79004600
C	3.37677900	1.01086000	1.54259000
H	4.69791200	1.63595600	-0.04312400
H	2.31480400	0.41084200	3.32064900
H	2.50551300	0.94003800	0.89897300
H	6.57984000	1.50441200	5.16515500
C	8.92795100	0.57609300	5.08192100
O	8.64707300	0.98038200	6.19617600
O	10.07280500	-0.04648800	4.78365500
C	10.93592200	-0.34149100	5.89901400
H	10.42070800	-1.00864000	6.59353400
H	11.80583000	-0.83161800	5.46480300
H	11.22345500	0.57823500	6.41162900
C	8.23770100	-0.28632700	2.76557300
C	8.19542100	-1.61659100	3.02330200
H	8.44364300	-2.27178800	2.19364100
C	7.96881500	-2.29524700	4.30069800
C	7.02529600	-1.87444400	5.25396100
C	8.74980100	-3.43244500	4.58132100
C	6.89516400	-2.54973300	6.46511500
H	6.36520900	-1.04672700	5.02906100

C	8.63275000	-4.09311600	5.80029400
H	9.46438100	-3.78102700	3.84064100
C	7.70663200	-3.64975900	6.74859300
H	6.15490400	-2.21890400	7.18716600
H	9.25346100	-4.95946500	6.00737200
H	7.60650600	-4.17029100	7.69612400
C	8.62613600	0.13224800	1.39565500
O	8.38163700	-0.80871500	0.47182400
O	9.13349800	1.20749600	1.10668300
C	8.82764700	-0.50364300	-0.86260100
H	8.33923400	0.40361500	-1.22552700
H	9.91084400	-0.36104300	-0.87883100
H	8.54072200	-1.36465100	-1.46464700

TS12

C	6.89749000	6.41055100	3.80699000
C	6.85187600	7.76061300	4.30389500
H	6.76874900	8.02649300	5.34525700
C	7.01765200	8.64278400	3.20100900
H	7.07947100	9.72129400	3.26053700
C	7.15498300	7.86161800	2.01557200
H	7.33557800	8.24100200	1.01886300
C	7.07424700	6.48970900	2.38074200
H	7.17192500	5.64853700	1.71136700
C	10.19795400	6.05176900	3.35080400
C	10.05804100	6.61123600	4.66856000
H	9.82863200	6.06431800	5.56985800
C	10.21759400	8.02042500	4.56941200
H	10.11687500	8.72414400	5.38441400
C	10.46565100	8.34588400	3.20350300
H	10.59165000	9.34171200	2.80010700
C	10.46297200	7.14084900	2.44914600
H	10.60740900	7.05216800	1.38369200
C	7.53934000	5.13437700	6.36588000
C	8.25936200	4.09723700	6.97004400
H	8.36778900	3.13619100	6.48092500
C	8.83666200	4.32205600	8.22071000
H	9.40023400	3.53329200	8.71007300
C	8.67808400	5.56900500	8.81987800
H	9.11535400	5.79285700	9.78739800
C	7.92758200	6.53623700	8.14609900
H	7.76813500	7.51847700	8.58517800
C	4.93479400	4.69501000	5.05296200
C	4.70680200	3.56200400	6.06344400

H	3.63005000	3.42491900	6.21697000
H	5.15629000	3.79638700	7.03364600
H	5.11304600	2.61179500	5.71949100
C	4.37595900	6.00144700	5.64086500
H	3.31676900	5.84777700	5.88164900
H	4.43968400	6.82599800	4.92708000
H	4.89604200	6.29795000	6.55489600
C	4.24475900	4.40823200	3.70882100
H	4.61616700	3.49918200	3.23482700
H	4.38319800	5.24302700	3.01361200
H	3.16722300	4.28685500	3.87200900
C	9.99863100	4.35029600	1.07981300
C	8.82889100	4.03082500	0.38528600
H	7.95257500	3.69423500	0.92684200
C	8.82724600	4.12597200	-1.00491600
H	7.93086300	3.89140300	-1.57164600
C	9.99775100	4.51683700	-1.65156900
H	10.04540800	4.60109800	-2.73235000
C	11.12333300	4.79692400	-0.87354700
H	12.05991600	5.09599500	-1.33821900
C	11.66232800	3.55212100	3.47736600
C	11.54162800	3.32035400	4.99487100
H	12.46182000	2.84765700	5.35934300
H	10.69837100	2.67171100	5.24598400
H	11.41666600	4.26157600	5.53916600
C	12.83159600	4.51296000	3.19805300
H	12.71776500	5.45403000	3.74302500
H	12.91484600	4.73664400	2.13346600
H	13.76138900	4.03853600	3.53496700
C	11.89668200	2.21908100	2.75232000
H	12.84091600	1.78960600	3.10863200
H	11.97464300	2.35868000	1.67111500
H	11.10788500	1.49074400	2.95175300
Fe	8.64178100	7.34374100	3.38333300
N	7.36505000	6.33124400	6.95056900
N	11.12822800	4.72591400	0.46206600
P	6.79346700	4.84154400	4.70039400
P	10.01984100	4.30671100	2.92408900
Pd	8.15164200	3.08916800	3.68080400
H	9.09058400	2.02329700	2.96531600
C	6.82186000	1.31707500	4.13567700
C	8.07487500	0.73279900	3.85979800
C	5.65292100	1.19410200	3.24847400
C	5.72368000	1.44929200	1.86763300

C	4.42054300	0.80730100	3.79897000
C	4.59195000	1.32661700	1.06632500
H	6.65992900	1.77782100	1.43071700
C	3.29069000	0.67528300	2.99386500
H	4.34856800	0.60852000	4.86433000
C	3.37140400	0.93924000	1.62586500
H	4.65943600	1.53821100	0.00320100
H	2.34686300	0.37179900	3.43618000
H	2.48964500	0.84631900	0.99959300
H	6.62636000	1.47350100	5.19161100
C	8.97765800	0.56959200	5.07059700
O	8.70514200	0.96970600	6.18741500
O	10.10956900	-0.06911800	4.76305800
C	10.97459000	-0.38424400	5.87211900
H	10.45307000	-1.04851800	6.56456900
H	11.83486500	-0.88388500	5.42977400
H	11.27768500	0.52822400	6.38872000
C	8.25618600	-0.27453100	2.75678900
C	8.19165100	-1.60291000	3.01592000
H	8.42185900	-2.26062600	2.18300200
C	7.96556900	-2.27922500	4.29427200
C	7.03867900	-1.84367600	5.25684700
C	8.73093100	-3.42915700	4.56645900
C	6.90996300	-2.51706800	6.46922300
H	6.38871800	-1.00675800	5.03765100
C	8.61559700	-4.08812300	5.78648000
H	9.43226600	-3.78893600	3.81852500
C	7.70649300	-3.63003800	6.74428000
H	6.18229200	-2.17472700	7.19867100
H	9.22421400	-4.96449400	5.98714800
H	7.60756600	-4.14922600	7.69266800
C	8.64257900	0.14564300	1.38801000
O	8.42411700	-0.79930600	0.46255200
O	9.12644700	1.23360000	1.10761400
C	8.86593800	-0.48045300	-0.87018000
H	8.35997100	0.41810400	-1.23062700
H	9.94606500	-0.31605500	-0.88371800
H	8.59772500	-1.34494700	-1.47582000

IM20

C	6.90527800	6.43158400	3.77799500
C	6.81509300	7.77533400	4.29015800
H	6.70489000	8.02798200	5.33214800
C	6.96909200	8.67275300	3.19824300

H	6.99676600	9.75194100	3.26954000
C	7.14809500	7.90839500	2.00759000
H	7.33337300	8.30330400	1.01783400
C	7.10199200	6.53080200	2.35589300
H	7.23382300	5.69992200	1.67970800
C	10.23250000	6.18317800	3.35305900
C	10.05629400	6.71175300	4.67943100
H	9.83329900	6.13852700	5.56625800
C	10.16932300	8.12737100	4.61016400
H	10.03757700	8.81178400	5.43713800
C	10.42121900	8.48704800	3.25335600
H	10.51732900	9.49430000	2.87054800
C	10.47092200	7.29664400	2.47701600
H	10.62725800	7.23197900	1.41145000
C	7.53997100	5.13683400	6.33489100
C	8.28825400	4.11569100	6.93087400
H	8.42572600	3.16232200	6.43433400
C	8.85639600	4.35029900	8.18392500
H	9.44378500	3.57602100	8.66820700
C	8.65850800	5.58742200	8.79206300
H	9.08798000	5.81725600	9.76163500
C	7.87890600	6.53634900	8.12546900
H	7.68741700	7.50946600	8.57164600
C	4.94386700	4.66738100	4.99157200
C	4.73727900	3.53959600	6.01215100
H	3.66324500	3.36201800	6.13967800
H	5.15201700	3.80615000	6.98947000
H	5.19097300	2.60415800	5.68955000
C	4.35584600	5.97049500	5.56105300
H	3.30259600	5.79009500	5.80839000
H	4.39385000	6.78411700	4.83313000
H	4.87082500	6.29434600	6.46856600
C	4.27111800	4.35269100	3.64550600
H	4.64242500	3.43033300	3.19992000
H	4.42154200	5.17022600	2.93219800
H	3.19135800	4.24207600	3.80067100
C	10.01964600	4.49377200	1.05901700
C	8.88087600	4.08056400	0.36132300
H	8.02201400	3.69895400	0.90109000
C	8.88385600	4.14676800	-1.03116700
H	8.01144700	3.83622900	-1.59869900
C	10.02715200	4.61018100	-1.67723700
H	10.07766400	4.67697300	-2.75912900
C	11.12262300	4.98814800	-0.89672500

H	12.03720000	5.34894500	-1.36164900
C	11.66634000	3.64630900	3.42427000
C	11.55617200	3.36929800	4.93511800
H	12.48316500	2.89765300	5.28390000
H	10.72349600	2.70152600	5.17581700
H	11.42023300	4.29253700	5.50768500
C	12.85152800	4.58943400	3.15922300
H	12.76347500	5.51451300	3.73607700
H	12.92190200	4.84890300	2.10151800
H	13.77836000	4.08795300	3.46460700
C	11.86334700	2.33009600	2.65776000
H	12.79210100	1.85760100	2.99947000
H	11.94533400	2.50123100	1.58140800
H	11.05153600	1.61834200	2.82453800
Fe	8.62973300	7.42206700	3.39403600
N	7.32643500	6.32273900	6.92664700
N	11.12438900	4.93936000	0.43945600
P	6.79801900	4.86185600	4.66464600
P	10.02955000	4.44603500	2.90438500
Pd	8.10827600	3.20431000	3.69179400
H	9.01299200	1.56603200	3.28016700
C	6.99881100	1.47722500	4.14231100
C	8.32018600	0.80359600	3.81488900
C	5.81671000	1.21489400	3.29164200
C	5.81655100	1.46397500	1.90619700
C	4.64000500	0.71820000	3.87512000
C	4.67703700	1.23796600	1.14036800
H	6.70895700	1.85974500	1.43471100
C	3.49897300	0.48713100	3.10801100
H	4.61843800	0.51014100	4.94095000
C	3.51106300	0.75068600	1.73826100
H	4.69472200	1.44610900	0.07441600
H	2.60104300	0.10226100	3.58185400
H	2.62189300	0.57702300	1.14021300
H	6.79150500	1.43415600	5.20784300
C	9.12709000	0.50335800	5.08611600
O	8.87956900	0.97578600	6.17784200
O	10.17460300	-0.27769700	4.82697200
C	10.97259500	-0.65528400	5.96858000
H	10.35249600	-1.20421300	6.68047100
H	11.76067200	-1.29101600	5.56883400
H	11.39128100	0.23258400	6.44695200
C	8.29316900	-0.31842600	2.79049000
C	8.07031200	-1.62507800	3.05724300

H	8.17456800	-2.29467900	2.20829900
C	7.81626800	-2.29484600	4.32961900
C	7.13727400	-1.70760000	5.41173700
C	8.29789400	-3.61059400	4.47494300
C	6.98335700	-2.39780000	6.61121600
H	6.69358900	-0.72827900	5.30365100
C	8.15557800	-4.29438500	5.67803200
H	8.80331800	-4.08474300	3.63808100
C	7.50172600	-3.68678200	6.75320300
H	6.45074600	-1.93081600	7.43413300
H	8.54535200	-5.30289100	5.77603500
H	7.38244600	-4.22162800	7.69051800
C	8.64778500	0.09507700	1.41272900
O	8.48115200	-0.86166300	0.49050200
O	9.05869100	1.21603200	1.13522600
C	8.84778500	-0.50334600	-0.85388600
H	8.25316200	0.34834000	-1.19275400
H	9.90833500	-0.24550800	-0.90335300
H	8.63537600	-1.38623200	-1.45522300