

Electronic supplementary information

Insights into the Mechanism and Origin of Solvent-Controlled Chemodivergence in
the Synthesis of Au-Catalyzed Bicyclo[2.2.1]heptanes from 3-Alkoxy-1,6-Diynes: A
DFT Perspective

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I. Calculated IRC results for TS1

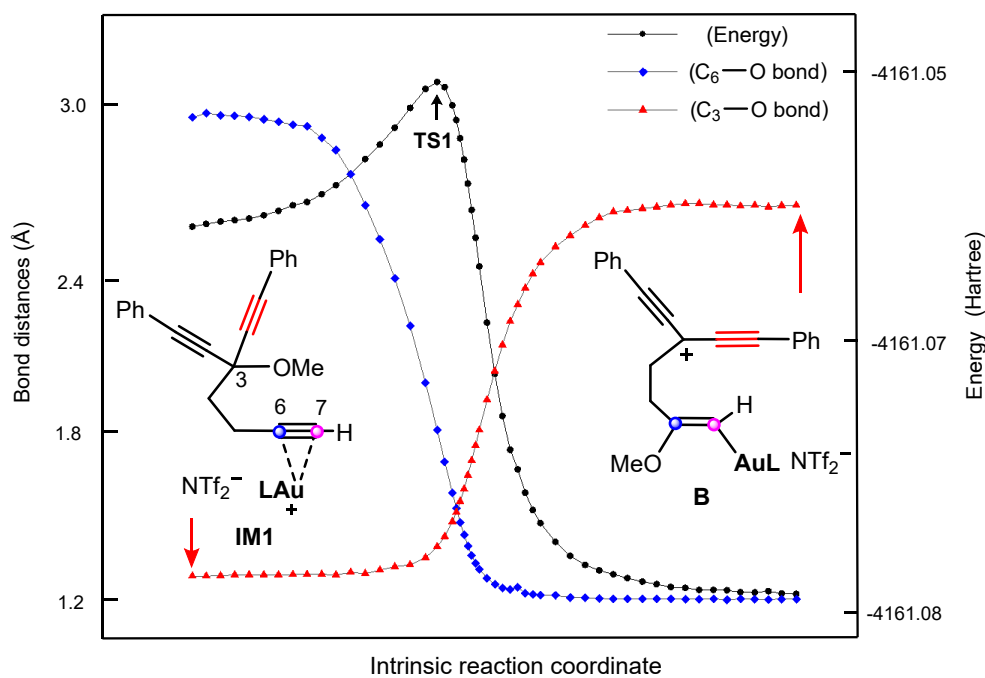


Fig. S1 IRC calculation results for transition state TS1.

II. Calculated results for the formation of cyclopentane D

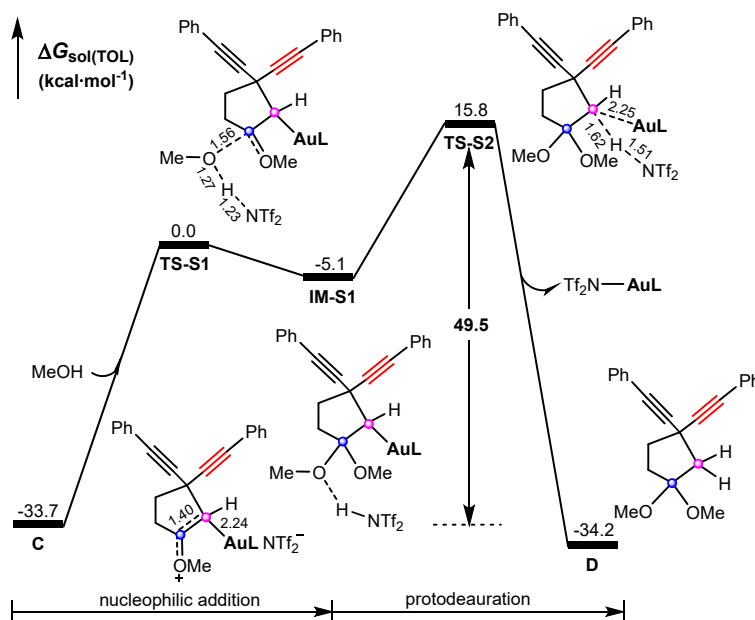


Fig. S2 Calculated free energy profile for the formation of cyclopentane D. Bond distances (black values) are in Å.

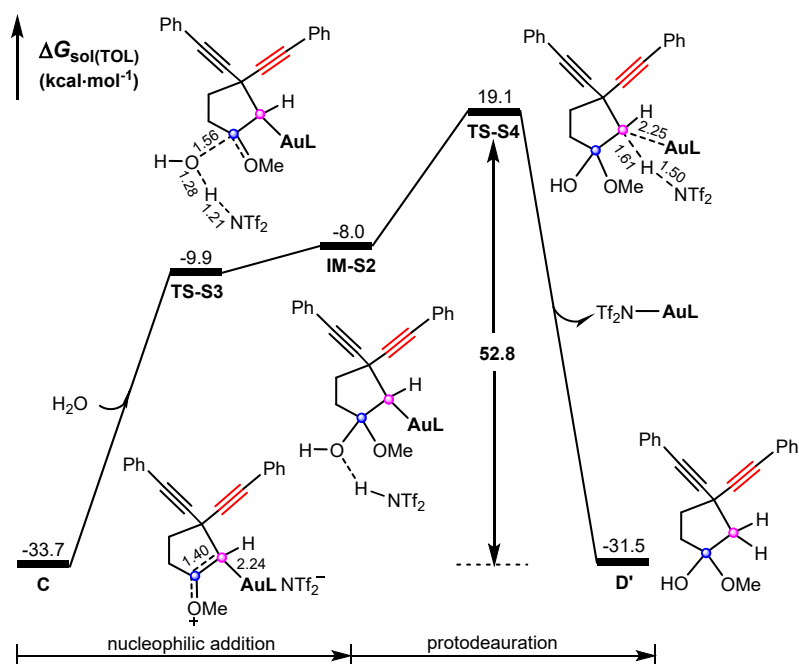


Fig. S3 Calculated free energy profile for the formation of another cyclopentane **D'**. Bond distances (black values) are in Å.

III. Calculated results for the protodeauration process at the C₅ position in **IM3**

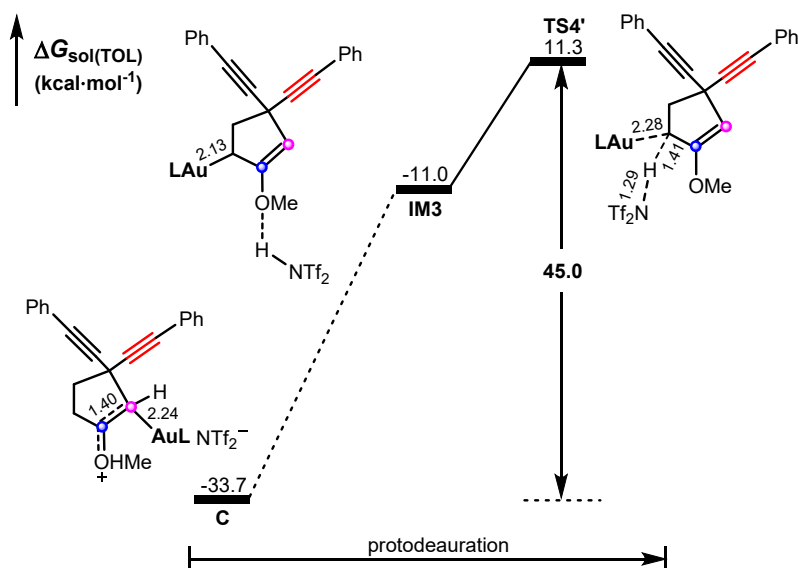


Fig. S4 Calculated free energy profile for the protodeauration process at the C₅ position in **IM3**. Bond distances (black values) are in Å.

IV. Calculated results for the formation of cyclopentene **E_{DCE}** and cyclopentanone

P₂DCE in DCE solvent

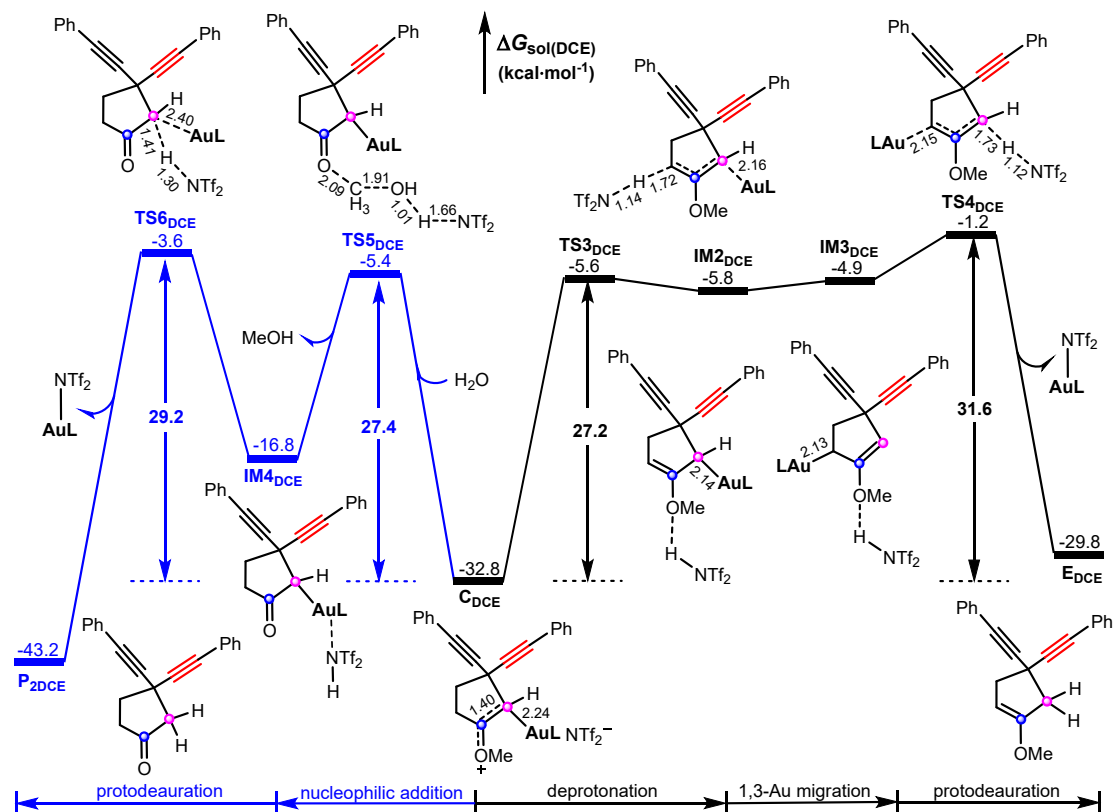


Fig. S5 Calculated free energy profiles for the formation of cyclopentene **E_{DCE}** (the right profile) and cyclopentanone **P₂DCE** (the left profile) in DCE solvent. Bond distances (black values) are in Å.

V. Optimized geometries and calculated the relative Gibbs free energies for key

transition states

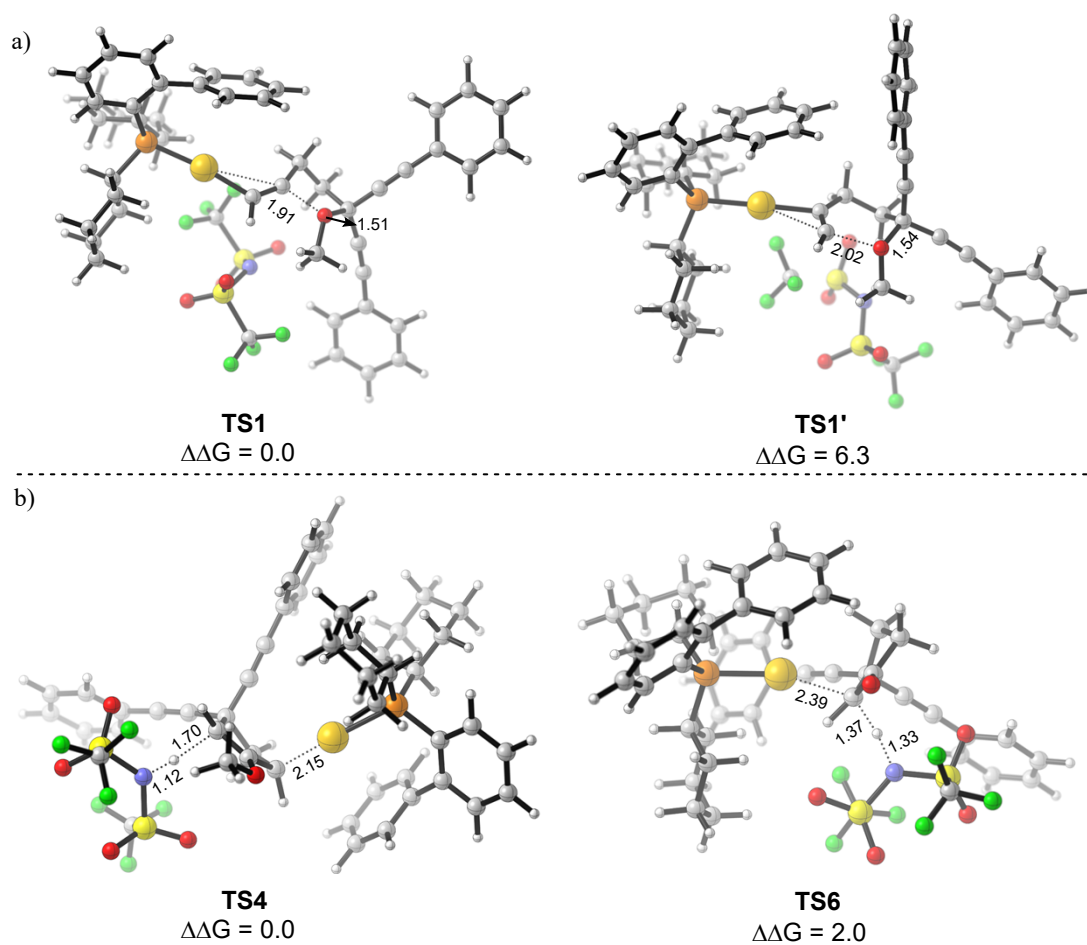


Fig. S6 Optimized geometries and calculated the relative Gibbs free energies for (a) the regioselectivity-determining transition states (TS1 and TS1') and (b) the chemoselectivity-determining transition states (TS4 and TS6). Bond distances are in Å. Gibbs energies are in kcal mol⁻¹.

VI. Thermodynamic data

Stationary point	Thermal correction to Gibbs free energy at B97D/SDD/6-311G(d,p) (in a.u.) (1)	Single-point energy at B97D/def2-TZVP (in a.u.) (2)	Gibbs free energies (G) (in a.u.) (3) (3)=(1)+(2)	Imaginary frequencies
LAuCl	0.424806	-1870.714999	-1870.290193	
R	0.262222	-923.8644314	-923.6022094	
AgNTf₂	0.00176	-1974.534021	-1974.532261	
NTf₂⁻	0.005278	-1827.342046	-1827.336768	
AgCl	-0.02374	-607.5936101	-607.6173501	
H₂O	0.002533	-76.4260548	-76.4235218	
MeOH	0.02702	-115.7062663	-115.6792463	
LAuNTf₂	0.458788	-3237.669934	-3237.211146	
IM1	0.746639	-4161.54027	-4160.793631	
TS1	0.74758	-4161.527926	-4160.780346	-188.26
TS1'	0.748965	-4161.519163	-4160.770198	-208.60
B	0.75111	-4161.562915	-4160.811805	
TS2	0.752999	-4161.562925	-4160.809926	-26.60
C	0.752853	-4161.613945	-4160.861092	
TS3	0.750095	-4161.574944	-4160.824849	-108.58
IM2	0.74984	-4161.577039	-4160.827199	
IM3	0.752273	-4161.577009	-4160.824736	
TS4	0.748443	-4161.571196	-4160.822753	-44.39
E	0.266225	-923.91515	-923.648925	
TS5	0.772026	-4238.016476	-4237.24445	-384.32
IM4	0.72746	-4122.314619	-4121.587159	
TS6	0.719129	-4122.282936	-4121.563807	-1114.93
P₂	0.242671	-884.657744	-884.415073	
TS7	0.756495	-4161.594539	-4160.838044	-115.36
F	0.759529	-4161.619837	-4160.860308	
TS8	0.806589	-4277.333219	-4276.52663	-538.51
TS8'	0.779446	-4238.045532	-4237.266086	-121.83
G	0.806184	-4277.340296	-4276.534112	

G'	0.780653	-4238.052989	-4237.272336	
TS9	0.809625	-4277.334944	-4276.525319	-1033.81
TS9'	0.784681	-4238.050524	-4237.265843	-1044.18
IM5	0.324525	-1039.671647	-1039.347122	
IM5'	0.298791	-1000.393866	-1000.095075	
TS10	0.315328	-1076.799494	-1076.484166	-1368.20
P₁	0.248479	-884.686999	-884.43852	
TS-S1	0.806652	-4277.29307	-4276.486418	-672.30
IM-S1	0.80482	-4277.299544	-4276.494724	
TS-S2	0.801029	-4277.262286	-4276.461257	-1208.60
D	0.319256	-1039.649243	-1039.329987	
TS-S3	0.77277	-4238.019446	-4237.246676	-541.34
IM-S2	0.776238	-4238.01982	-4237.243582	
TS-S4	0.776402	-4237.976759	-4237.200357	-1222.39
D'	0.294542	-1000.364473	-1000.069931	
TS4'	0.746893	-4161.536183	-4160.78929	-1226.97
C_{DCE}	0.75385	-4161.630249	-4160.876399	
TS3_{DCE}	0.747971	-4161.58118	-4160.833209	-241.82
IM2_{DCE}	0.749697	-4161.583128	-4160.833431	
IM3_{DCE}	0.750467	-4161.582327	-4160.83186	
TS4_{DCE}	0.751533	-4161.577465	-4160.825932	-61.28
E_{DCE}	0.266425	-923.918153	-923.651728	
TS5_{DCE}	0.768256	-4238.027654	-4237.259398	-402.67
IM4_{DCE}	0.725429	-4122.321981	-4121.596552	
TS6_{DCE}	0.718882	-4122.294168	-4121.575286	-1204.79
P_{2DCE}	0.242255	-884.660996	-884.418741	
TS4_{gas}	0.748090	-4161.525754	-4160.777664	-694.90
TS6_{gas}	0.722441	-4122.2348	-4121.512359	-906.50

VII. Cartesian coordinates of all structures involved in this work

LAuCl

0 1

C	-1.04138600	2.42890400	-1.01989900
C	0.28569700	1.92892500	-0.95696100
C	1.31301800	2.63036000	-1.62071700

C	1.04411800	3.79274500	-2.34950800
C	-0.26936400	4.26824800	-2.43703300
C	-1.29684800	3.58821200	-1.77715700
C	-2.17775800	1.77087700	-0.31872900
C	-3.18898700	1.13367800	-1.05974800
C	-4.21194400	0.43826700	-0.40638400
C	-4.24295600	0.38157400	0.99228000
C	-3.25568700	1.03703700	1.73793700
C	-2.22920600	1.72981500	1.08619200
H	2.33479100	2.26271300	-1.58543500
H	1.85640200	4.31535100	-2.85241800
H	-0.49241200	5.16663200	-3.01096100
H	-2.31920500	3.95984400	-1.82743300
H	-3.14188700	1.14695700	-2.14742400
H	-4.96811700	-0.08422700	-0.98961700
H	-5.02438900	-0.18308400	1.49729000
H	-3.27599600	0.99749600	2.82611900
H	-1.45530200	2.23140500	1.66400000
P	0.70494500	0.35909400	-0.07613900
C	1.34087900	0.92575300	1.59001500
C	1.20907900	-0.16781000	2.67266300
C	2.76917600	1.50676000	1.52052700
H	0.65699900	1.74520600	1.85748500
C	1.66307700	0.37212200	4.04229000
H	1.82273100	-1.03711200	2.39902700
H	0.16872900	-0.51687000	2.71928500
C	3.20629800	2.03282600	2.90281000
H	3.46778500	0.72068800	1.19808500
H	2.81334300	2.31539900	0.77759800
C	3.09415200	0.93754900	3.97900900

H	1.59760200	-0.42836600	4.79317600
H	0.97318900	1.17223400	4.35849600
H	4.23698600	2.41216800	2.84402600
H	2.56138200	2.88197800	3.18244500
H	3.39001800	1.33721000	4.95981200
H	3.79405200	0.12024000	3.73713000
C	2.12765600	-0.37206200	-1.02937800
C	2.64709800	-1.64689600	-0.32629900
C	1.66298000	-0.69664000	-2.46804900
H	2.94472200	0.36206500	-1.06000200
C	3.77865000	-2.29853100	-1.14491100
H	1.81258200	-2.35662200	-0.21804100
H	3.00749500	-1.40868000	0.68204200
C	2.79620500	-1.35211400	-3.27970500
H	0.81044000	-1.39142000	-2.40595500
H	1.30815700	0.21182300	-2.97206000
C	3.32206500	-2.61806500	-2.57937600
H	4.11753800	-3.21213100	-0.63573700
H	4.63768000	-1.60806500	-1.18397000
H	2.43105000	-1.59393800	-4.28827500
H	3.62271200	-0.63125600	-3.39673300
H	4.15050300	-3.05705900	-3.15443200
H	2.51589500	-3.36863600	-2.54148200
Au	-0.90832000	-1.22544400	0.07066900
Cl	-2.42637900	-3.03338100	0.22553100

R

0 1

C	5.47468300	-2.01634100	0.61388900
C	4.31943200	-1.32541500	0.98832100

C	3.43095500	-0.83784400	0.00102900
C	3.73047300	-1.05765400	-1.36406900
C	4.88849000	-1.75084600	-1.72632700
C	5.76367400	-2.23167200	-0.74159200
H	6.15153700	-2.38788400	1.38206500
H	4.09048200	-1.15625500	2.03859500
H	3.04857800	-0.68437700	-2.12583500
H	5.10899100	-1.91564300	-2.78016900
H	6.66496500	-2.77147800	-1.02858600
C	2.25014100	-0.13336200	0.37953100
C	1.24489900	0.45984600	0.72129800
C	0.01809400	1.19465100	1.07473800
O	0.07154800	1.35821500	2.51582000
C	-1.05662200	2.02107800	3.10559800
H	-0.93906300	1.88868900	4.18770100
H	-1.07049500	3.09899300	2.87561300
H	-2.00957400	1.56689600	2.78801300
C	-1.15595600	0.39411400	0.66482100
C	-2.13711500	-0.24719200	0.33522400
C	-3.27526000	-1.01619600	-0.04778600
C	-4.23529600	-0.48575600	-0.94178800
C	-3.45784700	-2.32303000	0.46331000
C	-5.34632000	-1.24771400	-1.31244600
H	-4.09765400	0.51966600	-1.33561500
C	-4.57395600	-3.07475300	0.08782400
H	-2.71871000	-2.73180200	1.14943600
C	-5.52012900	-2.54165400	-0.79982000
H	-6.07904700	-0.83118400	-2.00225100
H	-4.70495400	-4.07954300	0.48714700
H	-6.38835000	-3.13153400	-1.09032000

C	-0.00338400	2.58982700	0.36783800
H	0.84499300	3.16300300	0.76226600
H	-0.93262300	3.09882300	0.65008900
C	0.07916100	2.50128500	-1.17317400
H	1.01908100	2.00717500	-1.46039000
H	-0.74147600	1.86885500	-1.54525800
C	0.00508000	3.82033800	-1.79904900
C	-0.06037300	4.92712800	-2.28879000
H	-0.11600500	5.89884900	-2.73053700

AgNTf₂

0 1

N	-0.00105000	0.05309700	0.00021600
S	-1.18862500	-0.72031400	-0.89883200
S	1.18501300	-0.72291000	0.89909000
O	-0.87094600	-2.09751900	-1.26943300
O	-1.63909800	0.26345900	-1.89389400
O	1.63890500	0.26082100	1.89276800
O	0.86384100	-2.09877300	1.27155600
C	-2.60531800	-0.79070600	0.39619300
C	2.60110100	-0.79833900	-0.39630700
F	-2.22348000	-1.49188900	1.46742600
F	-2.91153600	0.46799400	0.77696000
F	-3.68483400	-1.35673300	-0.15586500
F	2.90829800	0.45909000	-0.78076900
F	3.68032800	-1.36356800	0.15711300
F	2.21843200	-1.50221600	-1.46539200
Ag	0.00561600	2.22800400	-0.00017400

NTf₂⁻

-1 1

N	0.00001900	-0.00001600	0.85089900
S	1.14426000	-0.87892600	0.08710300
S	-1.14426700	0.87893000	0.08721700
O	0.88224500	-1.28565700	-1.30453300
O	1.64262300	-1.87809300	1.04627200
O	-1.64262300	1.87799500	1.04649600
O	-0.88229900	1.28579700	-1.30438800
C	2.58338500	0.38270800	-0.04238000
C	-2.58337400	-0.38271600	-0.04235100
F	2.22017100	1.46448600	-0.75575000
F	2.97418100	0.78811100	1.18199900
F	3.64235900	-0.19660900	-0.65447300
F	-2.97414500	-0.78823100	1.18199900
F	-3.64236600	0.19664300	-0.65437500
F	-2.22016000	-1.46442600	-0.75582200

AgCl

0 1

Ag	0.00000000	0.00000000	0.63130600
Cl	0.00000000	0.00000000	-1.74537500

H₂O

0 1

O	0.00000000	0.12057500	0.00000000
H	0.75538100	-0.48229900	0.00000000
H	-0.75538100	-0.48230200	0.00000000

LAuNTf₂

0 1

C	-2.54278300	2.54407900	-0.95678600
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C	-2.99723300	1.53437900	-0.06789400
C	-4.16914500	1.75493100	0.68428800
C	-4.87641100	2.95661200	0.58231100
C	-4.40997600	3.96617200	-0.26790800
C	-3.25415100	3.75643900	-1.02564300
C	-1.33381800	2.36591400	-1.80702500
C	-0.17379300	3.11532600	-1.54545700
C	1.00098800	2.87205600	-2.26672600
C	1.02608100	1.88721000	-3.26041900
C	-0.13504800	1.15957100	-3.54958800
C	-1.30978400	1.40030600	-2.83017700
H	-4.52773000	0.99287300	1.37173300
H	-5.77923700	3.10492200	1.17270100
H	-4.94583400	4.91106800	-0.34563600
H	-2.89400200	4.53179800	-1.70003700
H	-0.18336800	3.84962800	-0.74228900
H	1.90411700	3.43050900	-2.03153900
H	1.94865500	1.67506000	-3.79586600
H	-0.11902100	0.39138900	-4.32073000
H	-2.21065200	0.83055800	-3.04865100
P	-2.06722400	-0.03631400	0.18302400
C	-2.88469900	-1.27543200	-0.95144800
C	-1.92727100	-2.41602300	-1.36004500
C	-4.21680700	-1.80540100	-0.37757800
H	-3.11385600	-0.68778300	-1.85169600
C	-2.62157500	-3.38005000	-2.34081500
H	-1.60563100	-2.96754300	-0.46606400
H	-1.02297800	-1.99227900	-1.81551600
C	-4.88754600	-2.76903900	-1.37763600
H	-4.02163000	-2.34311800	0.56211300

H	-4.89060200	-0.96794300	-0.14789500
C	-3.94119800	-3.92102400	-1.76089400
H	-1.93904600	-4.20591600	-2.58725000
H	-2.83379200	-2.84196200	-3.27963500
H	-5.81761600	-3.16203300	-0.94164800
H	-5.16410500	-2.20916700	-2.28584000
H	-4.43054800	-4.58802400	-2.48519400
H	-3.72214600	-4.52207200	-0.86272400
C	-2.38180100	-0.54602100	1.94591600
C	-1.70195900	-1.90379100	2.24044200
C	-1.84908000	0.54854500	2.89995800
H	-3.46590800	-0.66477400	2.08200900
C	-1.90095800	-2.30374900	3.71514100
H	-0.62519100	-1.81532500	2.03050700
H	-2.10165500	-2.68515800	1.58249500
C	-2.04498300	0.13906500	4.37203000
H	-0.77519400	0.68791700	2.70365200
H	-2.34628700	1.50660600	2.70078100
C	-1.37305100	-1.21416900	4.66518800
H	-1.38917100	-3.25851300	3.90321500
H	-2.97509500	-2.46626800	3.90559500
H	-1.63270900	0.92187500	5.02457000
H	-3.12395100	0.06648400	4.58992200
H	-1.54137500	-1.50672800	5.71181100
H	-0.28566500	-1.11101100	4.52325400
Au	0.18235700	0.03918700	-0.06248100
N	2.33410700	-0.10413600	-0.02790900
S	3.09289800	-1.05842800	-1.18862900
S	3.12971000	0.48116300	1.34322100
O	4.53876100	-0.86227000	-1.27508300

O	2.25470600	-1.03292100	-2.39069000
O	2.19365200	0.43463200	2.47250400
O	4.50533600	0.00794300	1.48857500
C	2.80510400	-2.80340800	-0.42817900
C	3.23082100	2.33722200	0.86324500
F	3.24659700	-2.83895600	0.83724000
F	1.48926400	-3.09244600	-0.43889300
F	3.45973000	-3.72002500	-1.15605000
F	1.99493100	2.86607100	0.82082800
F	3.95316600	2.98879800	1.78731500
F	3.81339500	2.47785800	-0.33620700

IM1

0 1

C	4.51635600	1.92434100	-2.00150300
C	4.99726300	0.85556300	-1.19978000
C	6.35940700	0.49775000	-1.27246500
C	7.23611300	1.16635200	-2.13146200
C	6.75719500	2.20053600	-2.94426300
C	5.41073900	2.56971400	-2.87625200
C	3.09771200	2.37732000	-1.96582100
C	2.26068400	2.14160100	-3.07261000
C	0.89936300	2.46009300	-3.00996600
C	0.35934400	3.03153100	-1.85085000
C	1.19421900	3.30501200	-0.76000300
C	2.55560300	2.98015900	-0.81553900
H	6.74271800	-0.31750900	-0.66397900
H	8.28394300	0.87314800	-2.16965000
H	7.42962600	2.72106900	-3.62456500
H	5.03444400	3.38158300	-3.49660100

H	2.67521900	1.66768900	-3.96130500
H	0.25251100	2.23969100	-3.85781600
H	-0.70656400	3.23299300	-1.78798100
H	0.78142300	3.76494700	0.13566700
H	3.19755000	3.17826200	0.04092300
P	3.89930500	-0.11519000	-0.08416100
C	4.12955900	0.65083400	1.60373000
C	2.90961000	0.43501600	2.52599600
C	5.44998800	0.21718000	2.27612600
H	4.19968600	1.72596400	1.37985100
C	3.11355000	1.16500900	3.86634400
H	2.76333100	-0.63757800	2.70825600
H	2.00107600	0.80249200	2.03016500
C	5.63094500	0.95449900	3.61902000
H	5.42718600	-0.86683900	2.46030400
H	6.30024400	0.42495200	1.61172800
C	4.42383900	0.73021800	4.54851700
H	2.25370700	0.97055900	4.52263300
H	3.14573700	2.25163400	3.68092900
H	6.55816200	0.61438700	4.10205600
H	5.74141600	2.03317000	3.42172600
H	4.56350800	1.28018500	5.49015100
H	4.35879900	-0.34026900	4.80384600
C	4.56571700	-1.84825800	-0.08122200
C	3.75519700	-2.71740400	0.90668700
C	4.47378400	-2.41924800	-1.51564100
H	5.61531400	-1.82572900	0.24351500
C	4.20652800	-4.18882200	0.85739400
H	2.69570300	-2.66064700	0.63096900
H	3.84680500	-2.32848800	1.92803500

C	4.92546200	-3.89147000	-1.55410600
H	3.42411000	-2.35410800	-1.84769500
H	5.07332700	-1.81332100	-2.20771700
C	4.11018500	-4.75117400	-0.57138400
H	3.58231600	-4.77754600	1.54402100
H	5.24776200	-4.26522400	1.21207700
H	4.82420400	-4.27635600	-2.57876300
H	5.99450900	-3.94847500	-1.28929800
H	4.45913200	-5.79329300	-0.59544400
H	3.05356900	-4.75358300	-0.88348400
Au	1.67160600	-0.24012200	-0.67170400
C	-0.29482500	7.40632400	0.53463700
C	-1.05665100	6.31731000	0.10369800
C	-1.38625300	5.27867200	1.00579700
C	-0.94219400	5.36379600	2.34682500
C	-0.18299100	6.45926600	2.76703500
C	0.14474200	7.48170100	1.86447200
H	-0.04306000	8.19832800	-0.16919200
H	-1.39384200	6.25146200	-0.92860800
H	-1.19853800	4.56794000	3.04383300
H	0.15212600	6.51603000	3.80184600
H	0.73779600	8.33288400	2.19590100
C	-2.11292200	4.13699800	0.55815800
C	-2.68787900	3.14514600	0.15323200
C	-3.25573800	1.86233100	-0.29615000
O	-2.79007800	1.70063300	-1.65977300
C	-3.32171700	0.55503700	-2.35277300
H	-2.80621400	0.53911600	-3.31994500
H	-3.11796500	-0.38326300	-1.82458100
H	-4.40519000	0.66063400	-2.51738700

C	-4.72867000	1.88695000	-0.21420800
C	-5.94110100	1.79373700	-0.16826800
C	-7.36055900	1.67299400	-0.11003100
C	-7.96213800	0.39236600	-0.07357300
C	-8.18327700	2.82360600	-0.09244500
C	-9.35314300	0.27324800	-0.02049900
H	-7.32941000	-0.49277900	-0.08976600
C	-9.57312000	2.69162200	-0.03695800
H	-7.72035200	3.80813500	-0.12096900
C	-10.16210500	1.41910100	-0.00173200
H	-9.80706200	-0.71635900	0.00646800
H	-10.19846400	3.58331500	-0.02217300
H	-11.24599000	1.32083300	0.04049800
C	-2.74307900	0.71393600	0.63437800
H	-3.19652700	-0.23348900	0.33368000
H	-3.08129600	0.93107000	1.65388100
C	-1.20359700	0.57453300	0.66948300
H	-0.73494600	1.55840800	0.80765100
H	-0.94710600	-0.05548500	1.52924700
C	-0.65751000	-0.06164400	-0.52825000
C	-0.32039400	-0.67707000	-1.54382000
H	-0.36489300	-1.25215400	-2.44793100
N	-2.30598100	-2.54183900	0.38630900
S	-1.87792100	-3.07398500	1.86124500
S	-2.73018500	-3.50715100	-0.86049500
O	-2.33540300	-4.40791000	2.27132500
O	-2.02257100	-1.93867200	2.78898600
O	-2.41148900	-2.79655500	-2.11296400
O	-2.41042400	-4.93789600	-0.75027100
C	0.04642900	-3.24592900	1.66451200

C	-4.64217900	-3.38388900	-0.74763700
F	0.54556300	-4.12025400	2.55599200
F	0.38107300	-3.66199400	0.42518800
F	0.63907500	-2.04642500	1.88208600
F	-5.03786600	-2.10369200	-0.93360000
F	-5.20916100	-4.14757700	-1.69973800
F	-5.07197600	-3.79401600	0.45634700

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C	4.80033600	2.86387000	-0.89115800
C	5.19154400	1.51836800	-0.66584600
C	6.50385800	1.12463200	-0.99967500
C	7.41354500	2.02623600	-1.55948200
C	7.01665700	3.34452200	-1.81193400
C	5.72202200	3.75175100	-1.47978300
C	3.45791800	3.39273300	-0.52560400
C	2.58567500	3.85787100	-1.52623500
C	1.31458400	4.33664700	-1.19246000
C	0.90480800	4.36773100	0.14585300
C	1.76765400	3.91132300	1.15057000
C	3.03753800	3.42793700	0.81686900
H	6.82018500	0.09736600	-0.83946600
H	8.42121000	1.69516100	-1.80618700
H	7.71213200	4.05358100	-2.25860400
H	5.41152400	4.78068700	-1.65560400
H	2.89944000	3.81468200	-2.56785000
H	0.63994600	4.67410200	-1.97767100
H	-0.08454600	4.74175100	0.40244400
H	1.45468900	3.93256200	2.19366700

H	3.70979400	3.07417800	1.59591600
P	4.02474500	0.24360200	-0.01369500
C	4.43850800	0.12765100	1.80546600
C	3.25332400	-0.42073200	2.62607500
C	5.74037300	-0.65008600	2.08698100
H	4.59761400	1.17731000	2.09758000
C	3.58092100	-0.41606200	4.13014300
H	3.03590400	-1.44758700	2.31040500
H	2.35396200	0.17277300	2.41897700
C	6.05249700	-0.64691800	3.59796200
H	5.62289700	-1.68877600	1.74387100
H	6.57687100	-0.20691300	1.52921200
C	4.87310700	-1.20304000	4.41732200
H	2.73641300	-0.84488900	4.68808700
H	3.70513300	0.62525900	4.47200200
H	6.96356700	-1.23311000	3.78712900
H	6.25914200	0.38806400	3.91716300
H	5.10929000	-1.17241500	5.49080600
H	4.71442200	-2.26052500	4.14941700
C	4.51777700	-1.33761200	-0.86426000
C	3.65743100	-2.51041000	-0.34680200
C	4.33356400	-1.16136100	-2.39022200
H	5.57328400	-1.54980100	-0.64319400
C	3.98665100	-3.81301500	-1.10027900
H	2.59924300	-2.26513400	-0.50447200
H	3.80552600	-2.64864800	0.73131700
C	4.66060100	-2.46765500	-3.13861700
H	3.28353300	-0.88863200	-2.58342200
H	4.95950900	-0.33844000	-2.76027200
C	3.80324200	-3.63517900	-2.61750300

H	3.33666500	-4.61651400	-0.72796500
H	5.02942200	-4.10472000	-0.88885800
H	4.49831400	-2.32047200	-4.21631800
H	5.72840000	-2.70748800	-2.99932200
H	4.06085200	-4.56490300	-3.14534900
H	2.74226800	-3.42459900	-2.82390400
Au	1.78038200	0.57854500	-0.46492300
C	-7.10086900	6.77225500	-0.64832300
C	-6.54574600	5.49121100	-0.60535800
C	-5.32799700	5.26711400	0.08006600
C	-4.68316700	6.35475600	0.71519300
C	-5.24795600	7.63149400	0.66581200
C	-6.45605400	7.84448000	-0.01421100
H	-8.03866700	6.93498400	-1.17752000
H	-7.04145100	4.65510100	-1.09456300
H	-3.74714700	6.18407400	1.24395500
H	-4.74565000	8.46237900	1.15903800
H	-6.89325200	8.84126300	-0.04895700
C	-4.76406300	3.95958100	0.12997700
C	-4.30239300	2.83395100	0.15759500
C	-3.74488100	1.48756100	0.24672700
O	-2.85847100	1.33886100	-1.01334600
C	-3.15355300	0.23746200	-1.91916100
H	-2.45294400	0.35609400	-2.75019800
H	-3.00776400	-0.71931500	-1.41460500
H	-4.17989500	0.35391700	-2.28420900
C	-4.76979900	0.46499200	0.29899100
C	-5.52860100	-0.48563500	0.31809600
C	-6.31995200	-1.66750400	0.33014300
C	-7.70507500	-1.64188900	0.04703800

C	-5.68432700	-2.90173400	0.60483000
C	-8.43482600	-2.83337200	0.03925300
H	-8.19141300	-0.69118000	-0.16356300
C	-6.42267700	-4.08595500	0.58312100
H	-4.62155700	-2.90473600	0.82657000
C	-7.79704100	-4.05527800	0.30333100
H	-9.50194500	-2.81083400	-0.17742600
H	-5.92240200	-5.03155600	0.78472900
H	-8.37023300	-4.98142200	0.28965500
C	-2.71818900	1.33504900	1.40785500
H	-2.57761200	0.26814900	1.60491100
H	-3.10663100	1.82420800	2.30758800
C	-1.40430600	1.96580700	0.92167300
H	-1.51582700	3.05233200	0.80375500
H	-0.58806900	1.77160800	1.62598400
C	-1.05820900	1.32568900	-0.35519200
C	-0.21243900	0.70816300	-1.09861600
H	-0.44826700	0.18881000	-2.02411000
N	-1.69845300	-2.30579000	0.03995400
S	-1.11779300	-3.17532900	-1.21913100
S	-1.65475000	-2.81018400	1.58934500
O	-0.17535600	-4.26430900	-0.91913700
O	-0.80167200	-2.22993900	-2.30426800
O	-2.67157900	-2.03932000	2.32641600
O	-1.52534200	-4.25342100	1.83780300
C	-2.72363700	-4.03562600	-1.83054400
C	0.00601300	-2.05110900	2.18283000
F	-3.26625900	-4.78436900	-0.85357300
F	-3.62776200	-3.11118200	-2.21800700
F	-2.44441700	-4.82840400	-2.88215400

F	-0.04895000	-0.70127200	2.14443500
F	0.27394000	-2.42326500	3.45047100
F	1.01074300	-2.46563800	1.39214800

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C	5.41613000	1.27995000	-0.85364400
C	5.31973900	-0.13749700	-0.88379700
C	6.34102500	-0.88176700	-1.50899000
C	7.43300800	-0.24979500	-2.11134300
C	7.51378300	1.14755600	-2.10768200
C	6.51276300	1.89819200	-1.48452700
C	4.39856100	2.14483700	-0.19285900
C	3.59897600	3.00594000	-0.96748600
C	2.58094600	3.75750800	-0.37031300
C	2.35716400	3.66951700	1.00905500
C	3.16550200	2.83663100	1.79281300
C	4.18274800	2.08178500	1.19632700
H	6.28036600	-1.96684400	-1.54197600
H	8.20887900	-0.84746000	-2.58728100
H	8.35488600	1.65097600	-2.58201600
H	6.57702600	2.98512400	-1.46493000
H	3.75655300	3.05133300	-2.04413600
H	1.95027700	4.40376000	-0.97700900
H	1.55850400	4.25184100	1.46320700
H	3.00353700	2.76954600	2.86785900
H	4.80840000	1.43393700	1.80623200
P	3.87433300	-1.03868600	-0.17726100
C	4.42351400	-1.54061900	1.53676900
C	3.23289100	-1.68763500	2.50828400

C	5.33103400	-2.78960800	1.53647500
H	5.03193600	-0.68711300	1.87008100
C	3.73249100	-2.00968900	3.92878600
H	2.57002900	-2.48987900	2.16101200
H	2.63908900	-0.76333200	2.51067000
C	5.81245800	-3.10334100	2.96788000
H	4.76921400	-3.65141400	1.14786400
H	6.19383700	-2.62884700	0.87453100
C	4.62557000	-3.26359600	3.93650600
H	2.87121900	-2.14657400	4.59796000
H	4.30968300	-1.15085900	4.31055000
H	6.42698900	-4.01513800	2.95701900
H	6.45701200	-2.27980900	3.31658700
H	4.99119200	-3.46542400	4.95364700
H	4.02322300	-4.13454500	3.62927100
C	3.65973900	-2.57083000	-1.20705000
C	2.49488300	-3.41602900	-0.64248800
C	3.36509900	-2.16483300	-2.66968900
H	4.58551500	-3.16082700	-1.16010500
C	2.23431900	-4.65645100	-1.51662600
H	1.59268700	-2.79195200	-0.63581400
H	2.69407100	-3.71611800	0.39332800
C	3.09369300	-3.40363800	-3.54435900
H	2.47358900	-1.51584000	-2.67211200
H	4.19679600	-1.57958800	-3.08293000
C	1.94403800	-4.25278400	-2.97228100
H	1.38840600	-5.21873100	-1.09908600
H	3.11675400	-5.31731000	-1.48758800
H	2.86257900	-3.08236900	-4.57037700
H	4.00904200	-4.01689200	-3.59437100

H	1.78372300	-5.14626500	-3.59241300
H	1.01142200	-3.66619900	-2.99864100
Au	1.86752000	0.10664900	-0.19801800
C	0.97833500	7.66313400	-0.72795100
C	0.13748900	6.55950000	-0.89317500
C	-0.44360100	5.93388800	0.23481600
C	-0.17234000	6.44737100	1.52471500
C	0.66718100	7.55392200	1.67710100
C	1.24806200	8.16169800	0.55471700
H	1.42422000	8.13534900	-1.60213500
H	-0.07701600	6.16937600	-1.88617600
H	-0.62229700	5.97002300	2.39321800
H	0.87096600	7.94111000	2.67436200
H	1.90492700	9.02122700	0.67889800
C	-1.25666800	4.77496300	0.07469500
C	-1.91879400	3.76624100	-0.07324800
C	-2.64391100	2.49941800	-0.18133300
O	-2.21367900	1.92664800	-1.51089800
C	-3.00798100	0.78828100	-1.97703100
H	-2.44323700	0.37011700	-2.81668400
H	-3.12928200	0.03608200	-1.19536500
H	-3.98238000	1.14884800	-2.32176000
C	-4.09499200	2.67036000	-0.18652500
C	-5.30867500	2.58621100	-0.16509400
C	-6.71546500	2.36730500	-0.14303400
C	-7.18722400	1.04260000	0.02599400
C	-7.64280800	3.42279200	-0.29775400
C	-8.55951400	0.78648300	0.03554400
H	-6.47088200	0.23329100	0.14120700
C	-9.01401300	3.15326800	-0.28023200

H	-7.27841600	4.43988000	-0.42941900
C	-9.47534300	1.83850700	-0.11531900
H	-8.91071000	-0.23658900	0.15964900
H	-9.72536000	3.96965600	-0.39748500
H	-10.54522700	1.63447300	-0.10589900
C	-2.26747100	1.51849100	0.97824600
H	-2.76007100	0.56234000	0.78084500
H	-2.70730400	1.92308100	1.89736500
C	-0.76124200	1.30472700	1.19079500
H	-0.29560800	2.18832200	1.65078200
H	-0.62385400	0.46844900	1.88452000
C	-0.02637500	1.03927900	-0.08939300
C	-0.32029000	1.23575900	-1.30956200
H	-0.12306400	1.23041100	-2.36477500
N	-3.61527400	-1.83986700	0.38749100
S	-2.65317200	-2.43221700	1.57003800
S	-4.20363300	-2.78612200	-0.81515300
O	-2.99753200	-3.74916700	2.12421800
O	-2.39546600	-1.30817300	2.48605100
O	-4.60383900	-1.89127700	-1.91349000
O	-3.42208200	-3.99942100	-1.11430800
C	-0.92910100	-2.71227300	0.68792300
C	-5.88487600	-3.40976900	-0.11858700
F	-0.71090600	-4.00895500	0.43031500
F	-0.85476900	-2.02303000	-0.46991200
F	0.05829600	-2.27266100	1.50529200
F	-6.63745500	-2.36324600	0.28234400
F	-6.54730900	-4.06674100	-1.09139500
F	-5.70752900	-4.23533900	0.92031200

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C	3.78483800	-2.76591100	-0.04317200
C	3.93171100	-1.48636300	0.55329900
C	4.92783100	-1.30509900	1.53417000
C	5.74821100	-2.35886200	1.94663400
C	5.57459300	-3.62989100	1.38733400
C	4.60221700	-3.82347200	0.40288800
C	2.81990400	-3.05305100	-1.14042100
C	1.77158900	-3.96989200	-0.94622000
C	0.85727300	-4.22582200	-1.97214600
C	0.99102800	-3.58884900	-3.21236500
C	2.04839300	-2.69505900	-3.42309300
C	2.95357700	-2.42479000	-2.39233700
H	5.04791800	-0.33260700	2.00335900
H	6.50593900	-2.18878300	2.71013500
H	6.19564900	-4.46438100	1.71017000
H	4.47460900	-4.80457000	-0.05234000
H	1.65240100	-4.44351000	0.02538300
H	0.03210600	-4.91486900	-1.79880700
H	0.27204600	-3.78482900	-4.00572500
H	2.16183200	-2.19991000	-4.38603500
H	3.77068600	-1.72367100	-2.54977600
P	2.81847900	-0.06214700	0.15144200
C	3.83142300	0.93516400	-1.07606700
C	2.94030200	1.80139700	-1.98971800
C	4.93940300	1.77233700	-0.40564700
H	4.31471500	0.16879100	-1.70082900
C	3.78730300	2.55623100	-3.03069600
H	2.38778700	2.52266600	-1.37660200

H	2.18944100	1.17067200	-2.48344100
C	5.78034600	2.51380500	-1.46298200
H	4.47363400	2.51000700	0.26435400
H	5.58313000	1.12621600	0.20732500
C	4.88992800	3.39540300	-2.35772500
H	3.13589200	3.19680400	-3.64470500
H	4.25622000	1.82669500	-3.71186600
H	6.54877000	3.12375900	-0.96555200
H	6.30611300	1.77417400	-2.08904400
H	5.49840700	3.90786400	-3.11736400
H	4.41945600	4.17305000	-1.73414300
C	2.71641400	0.92465200	1.72545500
C	1.79779100	2.14878600	1.50379500
C	2.16705400	0.03053400	2.85773900
H	3.72245700	1.28374400	1.98917400
C	1.61907700	2.93673200	2.81632100
H	0.81680900	1.80000800	1.15370700
H	2.21328200	2.80577400	0.72841600
C	1.99697500	0.82646700	4.16328100
H	1.18696400	-0.34482100	2.55082100
H	2.82075600	-0.83473700	3.02162500
C	1.07742800	2.03909100	3.94154600
H	0.93851400	3.77917000	2.63789000
H	2.59150800	3.36289600	3.12002100
H	1.57558700	0.16358000	4.93042500
H	2.98414200	1.17016400	4.51988600
H	0.96929700	2.61765800	4.87182200
H	0.08211400	1.67064900	3.65945800
Au	0.70909900	-0.57884800	-0.68952700
C	-7.33277700	0.45333000	-0.05617400

C	-6.07722300	0.86328700	-0.49890500
C	-5.59303800	0.41972100	-1.75846300
C	-6.39828800	-0.43941300	-2.55484100
C	-7.65352700	-0.83726200	-2.09842800
C	-8.12273200	-0.39366400	-0.85070700
H	-7.69349900	0.78297800	0.91648600
H	-5.44734000	1.49735100	0.11623700
H	-6.01862300	-0.78263300	-3.51517900
H	-8.26744400	-1.49784200	-2.70844700
H	-9.10079700	-0.71430300	-0.49500200
C	-4.30555900	0.78328700	-2.18956400
C	-3.15191600	1.03981000	-2.52457000
C	-1.83502700	1.24706400	-2.91356400
O	-2.36382300	-2.02538600	-3.40345700
C	-3.25687900	-2.70619300	-2.49109200
H	-2.69777500	-3.43297600	-1.88558900
H	-3.76232500	-1.99259000	-1.82996600
H	-3.98604700	-3.21831800	-3.12699700
C	-1.07231900	2.18677100	-2.23462900
C	-0.48180500	3.11641500	-1.69268600
C	0.11441100	4.18870700	-1.00566000
C	1.24048700	4.86724400	-1.54157700
C	-0.42658100	4.60385200	0.24045300
C	1.80604300	5.93453700	-0.84636700
H	1.65208200	4.54348500	-2.49430600
C	0.15024200	5.67508300	0.92095400
H	-1.26751500	4.05519100	0.65618400
C	1.26365800	6.34095600	0.38412600
H	2.66824300	6.45381000	-1.26138200
H	-0.26143800	5.98858100	1.87852100

H	1.70982300	7.17487600	0.92380900
C	-1.33382400	0.66975200	-4.24978800
H	-0.71026500	1.41735400	-4.75780300
H	-2.20690800	0.45409800	-4.87652100
C	-0.54558900	-0.62837900	-3.96824900
H	-0.45071500	-1.23231700	-4.88088400
H	0.45153300	-0.38897700	-3.58827600
C	-1.31085300	-1.34394700	-2.87349700
C	-1.07636500	-1.12566700	-1.54142200
H	-1.89146600	-1.40554900	-0.87128100
N	-1.19031500	-0.33354900	2.36377900
S	-1.43353300	-1.72968300	3.18233200
S	-2.31564800	0.45430400	1.50214900
O	-2.82173000	-2.19772300	3.31971400
O	-0.54653800	-1.71240100	4.35528800
O	-1.62448400	1.51164100	0.74532700
O	-3.35055000	-0.35294800	0.83029100
C	-0.60557700	-3.02319000	2.02477300
C	-3.27530500	1.46841400	2.82478800
F	-1.22519400	-3.07434700	0.83086600
F	0.69609400	-2.74106100	1.82967400
F	-0.68928200	-4.24366100	2.59638700
F	-2.43782200	2.30210600	3.47479100
F	-4.21777100	2.22331100	2.20477600
F	-3.88304500	0.67948200	3.72233800

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C	-3.75528300	-2.78912300	-0.00701300
C	-3.91109800	-1.50559100	-0.59215500

C	-4.90125800	-1.32517000	-1.57923000
C	-5.70716000	-2.38355100	-2.00804000
C	-5.52451300	-3.65802300	-1.45954200
C	-4.55809300	-3.85085800	-0.46908700
C	-2.79893300	-3.07592500	1.09774900
C	-1.73713800	-3.97786300	0.90744500
C	-0.83530900	-4.23617000	1.94393200
C	-0.99511200	-3.61719300	3.19019100
C	-2.06499000	-2.73716500	3.39582100
C	-2.95705700	-2.46345500	2.35457800
H	-5.02834400	-0.34943600	-2.03980700
H	-6.46061300	-2.21416800	-2.77589000
H	-6.13429700	-4.49576500	-1.79515500
H	-4.42394600	-4.83475100	-0.02179600
H	-1.59809400	-4.43807400	-0.06790700
H	0.00024800	-4.91363400	1.77454600
H	-0.28663900	-3.81638800	3.99214200
H	-2.19836100	-2.25543700	4.36302600
H	-3.78438600	-1.77350300	2.50808900
P	-2.81780400	-0.07363500	-0.16614400
C	-3.85177300	0.90337200	1.06035100
C	-2.97682000	1.76852400	1.99053000
C	-4.95858000	1.73803200	0.38475100
H	-4.33555700	0.12752800	1.67291800
C	-3.84015600	2.50989800	3.02780900
H	-2.42247600	2.49822500	1.38908600
H	-2.22687500	1.13956300	2.48795600
C	-5.81556900	2.46679000	1.43816100
H	-4.49077600	2.48342900	-0.27516800
H	-5.59150400	1.09200200	-0.23945000

C	-4.94070700	3.34709700	2.34916200
H	-3.19970500	3.14989500	3.65380800
H	-4.31183700	1.77229300	3.69831100
H	-6.58194500	3.07569800	0.93633700
H	-6.34403500	1.71956100	2.05284900
H	-5.56091300	3.84949400	3.10602200
H	-4.46852100	4.13289200	1.73724900
C	-2.70689600	0.92809600	-1.73012700
C	-1.79897800	2.15617800	-1.48716100
C	-2.14136800	0.04722300	-2.86506000
H	-3.71275500	1.28249400	-2.00030000
C	-1.60580100	2.95596200	-2.79041200
H	-0.82041200	1.81116700	-1.12686900
H	-2.22943700	2.80381400	-0.71214200
C	-1.95613200	0.85685100	-4.16015200
H	-1.16454500	-0.33031100	-2.55057600
H	-2.79131500	-0.81733400	-3.04615300
C	-1.04307300	2.06932700	-3.91392300
H	-0.93222800	3.80024400	-2.59507500
H	-2.57576000	3.37981100	-3.10499000
H	-1.52269100	0.20239400	-4.92777000
H	-2.93933300	1.20154800	-4.52653600
H	-0.92079000	2.65564200	-4.83753800
H	-0.05212700	1.70020500	-3.61773800
Au	-0.71094000	-0.57433100	0.69047800
C	7.33023300	0.48567200	0.11251900
C	6.06645200	0.88248700	0.54410800
C	5.56791200	0.41900600	1.79037800
C	6.36693900	-0.44692800	2.58504200
C	7.63075400	-0.83143800	2.14018200

C	8.11447700	-0.36790100	0.90552800
H	7.70192100	0.83116100	-0.85049800
H	5.44147000	1.52202600	-0.07044600
H	5.97610800	-0.80631200	3.53502600
H	8.23997800	-1.49718500	2.74936400
H	9.09919300	-0.67787600	0.55882700
C	4.27229100	0.77028900	2.20967700
C	3.11371900	1.01626800	2.53329300
C	1.78782200	1.20572100	2.90675400
O	2.32792500	-2.07731000	3.39806800
C	3.22110600	-2.74472500	2.47359100
H	2.65407700	-3.43429700	1.83354300
H	3.75274500	-2.01814000	1.84831800
H	3.92798500	-3.29626300	3.10146100
C	1.03025500	2.15776900	2.23590300
C	0.44298700	3.09648500	1.70741400
C	-0.15475000	4.17984400	1.03777200
C	-1.28637400	4.84198700	1.58179200
C	0.38861700	4.62245300	-0.19739200
C	-1.85571100	5.91918900	0.90497300
H	-1.70016300	4.49784400	2.52638100
C	-0.19105600	5.70414500	-0.85916200
H	1.23431300	4.08679900	-0.62053500
C	-1.31065400	6.35312400	-0.31474100
H	-2.72282600	6.42490300	1.32657600
H	0.22307400	6.03856700	-1.80861000
H	-1.75925100	7.19503100	-0.83985500
C	1.28584300	0.63517400	4.24850100
H	0.65224100	1.38115800	4.74618700
H	2.15918900	0.43778300	4.88119500

C	0.51493800	-0.67538200	3.97895000
H	0.43589900	-1.28103000	4.89156400
H	-0.48784600	-0.45323400	3.60319800
C	1.28895300	-1.37279400	2.87931600
C	1.07676900	-1.09995800	1.55177100
H	1.90793400	-1.33878800	0.88533900
N	1.21565600	-0.29880200	-2.39017000
S	1.46486600	-1.69777900	-3.20135600
S	2.32929000	0.48105000	-1.50573300
O	2.85533100	-2.15755300	-3.34233800
O	0.57305500	-1.69072600	-4.37060200
O	1.62693900	1.53112100	-0.74934600
O	3.35367400	-0.33326800	-0.82617200
C	0.64948000	-2.98990600	-2.03317200
C	3.30713200	1.50440000	-2.80745900
F	1.27065700	-3.02568600	-0.83931300
F	-0.65411700	-2.71552100	-1.83871100
F	0.74130900	-4.21478800	-2.59386600
F	2.47782600	2.34005300	-3.46495300
F	4.23958200	2.25681100	-2.16996900
F	3.92871400	0.72058900	-3.69997500
C			
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C	4.13487000	-2.25124500	-1.50326000
C	4.22101900	-1.49551100	-0.30678700
C	5.17181200	-1.86004800	0.66878100
C	6.00770500	-2.96517400	0.48707900
C	5.89206700	-3.73854600	-0.67394300
C	4.96495700	-3.37910800	-1.65520300

C	3.22818900	-1.89813800	-2.62819400
C	2.24253100	-2.80510400	-3.05878300
C	1.42088500	-2.49254600	-4.14596900
C	1.56704400	-1.26976800	-4.81320100
C	2.53870700	-0.35664200	-4.38633400
C	3.36850900	-0.67271200	-3.30498900
H	5.24762700	-1.29298300	1.59290100
H	6.73149400	-3.22740300	1.25706100
H	6.52478200	-4.61291700	-0.81882300
H	4.88579500	-3.96153100	-2.57169400
H	2.11566900	-3.74614600	-2.52661000
H	0.65811800	-3.19881900	-4.46715200
H	0.92220100	-1.03062600	-5.65680600
H	2.66294100	0.59517200	-4.90159500
H	4.14329800	0.02360500	-2.99400100
P	3.07394300	-0.10463800	0.05958400
C	4.03220600	1.44392500	-0.39691200
C	3.09873100	2.60658300	-0.79000400
C	5.03886700	1.85990900	0.69674300
H	4.60683400	1.14838700	-1.28641700
C	3.90572200	3.85009100	-1.20432600
H	2.44287800	2.85219300	0.05349200
H	2.44372300	2.28895400	-1.61214900
C	5.84512100	3.09278200	0.24257600
H	4.49238900	2.11022600	1.61726900
H	5.71407500	1.02381700	0.92560900
C	4.91089500	4.26322600	-0.11350000
H	3.21462400	4.67659200	-1.42670100
H	4.45503000	3.62936600	-2.13480300
H	6.54422200	3.38785800	1.03852100

H	6.44903500	2.82538700	-0.64012400
H	5.49756300	5.13217200	-0.44524600
H	4.35806900	4.56553600	0.79005600
C	2.86329500	-0.10685600	1.90409900
C	1.92112600	1.03910100	2.33711900
C	2.31070100	-1.46853500	2.37449300
H	3.85206100	0.06793000	2.35283100
C	1.75267900	1.03143000	3.86823200
H	0.94212900	0.89101000	1.86079200
H	2.30580600	2.01075200	2.00599900
C	2.11698700	-1.47468200	3.90303400
H	1.34997200	-1.63155600	1.87594500
H	2.97645700	-2.28703800	2.07442100
C	1.20600800	-0.32041300	4.35772100
H	1.08247600	1.84957600	4.15995300
H	2.73167500	1.22724600	4.33880600
H	1.69581700	-2.44015800	4.21055900
H	3.10188700	-1.37683200	4.39169000
H	1.11052600	-0.32051900	5.45375700
H	0.20312000	-0.47173300	3.93557900
Au	0.97949000	-0.11387400	-0.92675600
C	-7.39936400	2.96271900	-0.23850400
C	-6.01088200	2.98647000	-0.38727600
C	-5.40149700	2.32415100	-1.47839200
C	-6.21517800	1.63981900	-2.41059600
C	-7.60283800	1.62310900	-2.25250100
C	-8.19936300	2.28248400	-1.16798200
H	-7.85821200	3.46753300	0.61045800
H	-5.38349200	3.49655900	0.34072800
H	-5.74667500	1.11374500	-3.23995200

H	-8.22021200	1.08572600	-2.97104800
H	-9.28105500	2.25993500	-1.04376100
C	-3.98181000	2.28642000	-1.58707900
C	-2.76831800	2.20406200	-1.61608200
C	-1.32176600	1.93804500	-1.54937000
O	-1.29632100	-1.24069800	-3.33298000
C	-1.47239400	-2.33897800	-2.38387000
H	-0.55619500	-2.44067200	-1.79324300
H	-2.32642500	-2.14040000	-1.73146500
H	-1.65067900	-3.22762800	-2.99350000
C	-0.74490800	2.66932400	-0.41809100
C	-0.27895600	3.31683200	0.49945900
C	0.27182400	4.04637100	1.59133400
C	1.35691100	4.93271700	1.39372900
C	-0.25193800	3.88111300	2.89448800
C	1.90819400	5.62367200	2.47614900
H	1.75905700	5.06578300	0.39195100
C	0.30250500	4.58228100	3.96851700
H	-1.08295400	3.19594700	3.04817300
C	1.38528200	5.45021300	3.76619300
H	2.74434100	6.30218300	2.31237200
H	-0.10763800	4.44483800	4.96794100
H	1.81643200	5.99077800	4.60756400
C	-0.59461000	2.28443600	-2.90146400
H	0.48083900	2.33185100	-2.69242300
H	-0.93309400	3.24264500	-3.30613000
C	-0.90151200	1.08087900	-3.80752200
H	-1.84610600	1.21862900	-4.35609700
H	-0.11530500	0.85232000	-4.53458500
C	-1.10632400	-0.04552300	-2.83514300

C	-1.13640900	0.37996500	-1.49468600
H	-1.69875300	-0.16686200	-0.73972300
N	-2.71290700	-2.84444100	0.63440800
S	-1.28608200	-2.47531600	1.32661600
S	-4.15420800	-2.37519600	1.26444500
O	-1.10050000	-1.06715300	1.73430800
O	-0.24571400	-3.09634600	0.48361500
O	-5.18178300	-3.24712000	0.68145200
O	-4.15427800	-2.08427300	2.70851000
C	-1.20377900	-3.49221700	2.99353400
C	-4.47676800	-0.67553300	0.41771600
F	-1.42639800	-2.70071800	4.05133300
F	-2.10039100	-4.49044800	2.98787600
F	0.03076100	-4.02816700	3.11292900
F	-4.30519000	-0.79162400	-0.92029200
F	-5.73937700	-0.28278400	0.65436400
F	-3.63514300	0.26264200	0.88115800

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C	3.96418300	-3.39375600	-0.49704400
C	4.63149700	-2.36066100	0.21562200
C	5.78859400	-2.67291400	0.95644100
C	6.27502100	-3.98236800	1.02245600
C	5.59581300	-5.00787200	0.35367700
C	4.45415500	-4.71024000	-0.39633400
C	2.77344700	-3.14018000	-1.35537700
C	1.53892000	-3.74994400	-1.06291500
C	0.41169400	-3.48326200	-1.84694100
C	0.49874300	-2.59902500	-2.92888300

C	1.72381600	-1.99475000	-3.23520400
C	2.85486200	-2.27249800	-2.45992700
H	6.30874600	-1.89025200	1.50366200
H	7.17202800	-4.19913100	1.60080500
H	5.95775600	-6.03367100	0.40719200
H	3.93479300	-5.50008700	-0.93696400
H	1.46016400	-4.40998400	-0.20042200
H	-0.54191000	-3.93725200	-1.59032600
H	-0.38435200	-2.37827200	-3.52451200
H	1.80200100	-1.31086300	-4.07929500
H	3.80896000	-1.81988300	-2.71617300
P	3.96028600	-0.64399900	0.25584900
C	4.92770600	0.28177000	-1.05200800
C	4.10362300	1.43966100	-1.65264900
C	6.32552200	0.74349500	-0.58778800
H	5.08201600	-0.46819800	-1.84009100
C	4.87437700	2.10183700	-2.80867200
H	3.89500300	2.18914800	-0.87920600
H	3.13094100	1.06196700	-1.99529500
C	7.07979000	1.41854700	-1.75145000
H	6.22425300	1.46350100	0.23661600
H	6.90217400	-0.11342100	-0.21130600
C	6.26404900	2.58040200	-2.35015100
H	4.29011500	2.94460000	-3.20113700
H	4.99382300	1.37089300	-3.62631600
H	8.05843800	1.77595300	-1.39838800
H	7.27101600	0.66870000	-2.53662800
H	6.81012000	3.03087400	-3.19208400
H	6.13604600	3.36611600	-1.58796300
C	4.46018300	0.05983900	1.90884800

C	3.99889200	1.53354400	2.00136800
C	3.82981600	-0.77285800	3.04803900
H	5.55541500	0.03039000	1.99319400
C	4.34365000	2.13168300	3.37782700
H	2.90948800	1.57348400	1.85191000
H	4.44942100	2.13568600	1.20460500
C	4.16595000	-0.16965600	4.42555300
H	2.73714100	-0.77473300	2.90704500
H	4.16725200	-1.81629900	2.99480800
C	3.72215800	1.30152600	4.51504900
H	3.98938500	3.17177900	3.42502800
H	5.43925700	2.15593500	3.50094000
H	3.68448100	-0.76510100	5.21489200
H	5.25468300	-0.23066100	4.59066900
H	3.99638000	1.72453200	5.49231600
H	2.62393600	1.35051600	4.43404000
Au	1.64738900	-0.42621700	0.16783700
C	-6.14434700	4.47581300	1.24643000
C	-4.95673400	3.96906800	0.71381900
C	-4.34613900	2.82875000	1.28699300
C	-4.95373200	2.21741300	2.40806100
C	-6.14449000	2.72939900	2.93014300
C	-6.74445700	3.85762500	2.35340800
H	-6.60630600	5.35253100	0.79371200
H	-4.49473800	4.43823600	-0.15239400
H	-4.49024800	1.33745100	2.84676900
H	-6.60892400	2.24059600	3.78556400
H	-7.67473300	4.25101400	2.76123100
C	-3.15724300	2.28470100	0.71936500
C	-2.16895900	1.79403200	0.20638400

C	-0.96046300	1.21371400	-0.40279700
O	-1.31948000	-2.35799200	0.44502200
C	-0.78965000	-2.54272000	1.77399100
H	0.29259800	-2.35166000	1.78385200
H	-1.30067000	-1.88185000	2.48397700
H	-0.99002500	-3.58869000	2.02553000
C	0.04735100	2.27121900	-0.54649300
C	0.90813100	3.12798400	-0.63077000
C	1.96738700	4.07699800	-0.69976900
C	2.34358500	4.66048800	-1.93196000
C	2.69229500	4.42046400	0.46684500
C	3.41658600	5.55368400	-1.99236600
H	1.79015500	4.40011300	-2.83209700
C	3.76427700	5.31358500	0.39635200
H	2.40704600	3.97326600	1.41614500
C	4.13346600	5.88170800	-0.83229800
H	3.69693800	5.99315000	-2.94880200
H	4.31363200	5.56695900	1.30243200
H	4.96937300	6.57786700	-0.88448100
C	-1.31665900	0.51148400	-1.76936800
H	-0.37985100	0.41301200	-2.34684100
H	-2.03375100	1.10270200	-2.35075900
C	-1.81705600	-0.84406300	-1.31609400
H	-3.37562100	-0.66282700	-0.69649600
H	-2.13580100	-1.61357100	-2.01444200
C	-1.21762700	-1.13729400	-0.10799300
C	-0.45061700	-0.01291100	0.45632400
H	-0.59926300	0.15395700	1.53010800
N	-4.47456700	-0.69540300	-0.41443400
S	-4.80780200	-1.38031600	1.09528100

S	-5.53785300	-0.68654800	-1.72935300
O	-6.64732200	-1.61844300	-1.53418400
O	-4.71074500	-0.68942100	-2.93611000
C	-6.25335100	1.09375300	-1.58803100
O	-3.67701500	-1.01746200	1.94777600
O	-6.19137500	-1.14779500	1.49494100
C	-4.63079200	-3.30113000	0.74874200
F	-4.04097500	-3.51246600	-0.43506900
F	-3.88422200	-3.84003600	1.72290800
F	-5.83939800	-3.86617000	0.75057500
F	-6.77504200	1.28720200	-0.37836300
F	-5.27382300	1.97550000	-1.81723100
F	-7.20767300	1.23293100	-2.52122200

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C	3.40209700	-2.43906200	-1.25147200
C	3.54554500	-1.80847500	0.01302900
C	4.25901200	-2.46625400	1.03294000
C	4.80802400	-3.73650300	0.82731600
C	4.64361100	-4.37065900	-0.40985400
C	3.94838200	-3.72232200	-1.43571600
C	2.62661600	-1.81501500	-2.36120600
C	1.41409900	-2.40081700	-2.76937500
C	0.61630800	-1.78019200	-3.73450800
C	1.01661400	-0.56850500	-4.30922900
C	2.23570700	0.00705800	-3.93204100
C	3.03920800	-0.61717400	-2.97064600
H	4.36925600	-1.99477800	2.00684900
H	5.35145500	-4.22931900	1.63239400

H	5.05674300	-5.36449800	-0.57733400
H	3.82170100	-4.20880100	-2.40199100
H	1.08024100	-3.32216300	-2.30041900
H	-0.32847900	-2.23600200	-4.01882700
H	0.37940500	-0.07374300	-5.03902800
H	2.56182200	0.94435800	-4.38087000
H	3.98911300	-0.17018000	-2.69082200
P	2.72836800	-0.18898200	0.34502700
C	4.06259800	1.05617600	-0.07890300
C	3.46372500	2.38494600	-0.57994800
C	5.09360100	1.26726900	1.04892100
H	4.59996700	0.59019200	-0.91547500
C	4.58188500	3.34580300	-1.02480300
H	2.87961900	2.85307800	0.22105800
H	2.76436800	2.18516200	-1.40270900
C	6.19946700	2.23901700	0.58799000
H	4.59564900	1.68549900	1.93458700
H	5.53446700	0.30323300	1.34134300
C	5.60257400	3.57434900	0.10469900
H	4.13983500	4.30071700	-1.33884500
H	5.09987700	2.91569100	-1.89891400
H	6.91027700	2.40830600	1.41042400
H	6.76138500	1.77331700	-0.23856800
H	6.40416300	4.24723100	-0.23440200
H	5.09450700	4.07141000	0.94637600
C	2.47612500	-0.09109400	2.19004300
C	1.87987800	1.28905400	2.55552500
C	1.52477500	-1.21585800	2.65252400
H	3.44817900	-0.19590900	2.69288200
C	1.62635700	1.38554300	4.07121500

H	0.92619500	1.41274700	2.02186800
H	2.53682600	2.10223900	2.22702700
C	1.23818800	-1.11913300	4.16276400
H	0.58329200	-1.11651100	2.09191700
H	1.94756200	-2.19703500	2.41159200
C	0.68232400	0.26490900	4.54382100
H	1.19954600	2.37077800	4.31044300
H	2.58747100	1.30805800	4.60734700
H	0.52926700	-1.90886000	4.45079100
H	2.17332200	-1.30091900	4.71949600
H	0.52638800	0.32705300	5.63091800
H	-0.29889100	0.40068000	4.06311200
Au	0.62980200	0.20617000	-0.59646600
C	-7.49155500	2.57222000	0.62442800
C	-6.20597600	2.26958400	0.16837800
C	-5.35987200	3.29410400	-0.32178000
C	-5.84135100	4.62485900	-0.33892900
C	-7.12839200	4.91711300	0.12079600
C	-7.95893700	3.89457900	0.60233000
H	-8.13055000	1.77363200	1.00013500
H	-5.84037600	1.24537900	0.18903800
H	-5.19425700	5.41685700	-0.71170600
H	-7.48469700	5.94645900	0.10354100
H	-8.96152400	4.12693300	0.95907200
C	-4.04672400	2.98470100	-0.78430400
C	-2.92904300	2.70174600	-1.17708600
C	-1.56791400	2.28386500	-1.56495300
O	-2.26702400	-1.25427200	-2.05468700
C	-3.03940600	-1.90342600	-3.07894200
H	-3.97587200	-1.35134600	-3.24504700

H	-2.46964400	-1.95475300	-4.01743800
H	-3.24432700	-2.91432500	-2.71637200
C	-0.60848000	3.22157200	-0.97373500
C	0.16299700	3.98914400	-0.42815600
C	1.09610000	4.81244500	0.26427800
C	1.89479300	5.75737500	-0.42112800
C	1.26694600	4.66118600	1.66186700
C	2.84357700	6.51487600	0.27137300
H	1.76788900	5.87900400	-1.49521200
C	2.21861300	5.42204100	2.34497300
H	0.65480700	3.93506600	2.19130100
C	3.01375200	6.34846300	1.65340300
H	3.45673500	7.23432800	-0.27001800
H	2.34148900	5.29053200	3.41951200
H	3.75757200	6.93828800	2.18727700
C	-1.45585800	2.16510400	-3.13473900
H	-0.38697700	2.22777300	-3.40602600
H	-1.98808200	2.98535300	-3.63396500
C	-2.01750300	0.78539000	-3.40243000
H	-1.90324900	-1.93891200	-0.50853800
H	-2.35219100	0.43906500	-4.37482200
C	-1.92999100	0.05986900	-2.26920200
C	-1.36641000	0.77767200	-1.09797800
H	-1.96313700	0.60293300	-0.19571400
N	-1.86551500	-2.52586000	0.36467700
S	-1.54841600	-4.17474800	0.03125000
S	-2.69147800	-1.90284600	1.72499200
O	-2.29921000	-0.50713400	1.86592800
O	-2.60797800	-2.86644600	2.81340300
C	-4.50572900	-1.87430800	1.06994900

O	-2.44249400	-5.06362400	0.76036400
O	-1.35036900	-4.25077300	-1.41466700
C	0.19676000	-4.33293800	0.81953100
F	0.11624200	-4.18739500	2.14312400
F	0.67098600	-5.54814300	0.52057400
F	0.99166500	-3.39807600	0.30081800
F	-4.55205200	-1.12517600	-0.04050100
F	-4.90845000	-3.11596300	0.78995800
F	-5.28696800	-1.33827600	2.01121100

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C	-3.09942300	-1.89171100	-2.24233300
C	-2.78054100	-2.64697700	-1.08054200
C	-3.77977600	-3.44020600	-0.48426400
C	-5.08023800	-3.47952800	-0.99785300
C	-5.40325500	-2.71135100	-2.12253800
C	-4.41835200	-1.92901900	-2.73332700
C	-2.10871200	-1.01970900	-2.93402000
C	-2.31355300	0.37200700	-2.97959100
C	-1.34862000	1.21656800	-3.53790300
C	-0.16760100	0.68217000	-4.06698900
C	0.03036900	-0.70382900	-4.06074700
C	-0.93649600	-1.54880600	-3.50447100
H	-3.54810800	-4.01704400	0.40815000
H	-5.83577300	-4.09800800	-0.51524800
H	-6.41501700	-2.72340400	-2.52566400
H	-4.65998000	-1.33715800	-3.61505700
H	-3.21189800	0.79107000	-2.53311900
H	-1.50582000	2.29277100	-3.52916400

H	0.59538100	1.34262700	-4.47603100
H	0.94129000	-1.12968700	-4.47934500
H	-0.77683200	-2.62359900	-3.50363000
P	-1.12136600	-2.52729500	-0.27672800
C	-0.17860100	-3.97359000	-1.00650000
C	1.33557500	-3.69339400	-1.08095500
C	-0.47718900	-5.32450000	-0.32315500
H	-0.56264800	-4.04096800	-2.03390600
C	2.05265600	-4.84061100	-1.81521000
H	1.74362900	-3.59909700	-0.06684000
H	1.51323100	-2.73306500	-1.58284500
C	0.25736500	-6.46765400	-1.05392300
H	-0.13583300	-5.28993000	0.72130200
H	-1.56043900	-5.51395500	-0.31418300
C	1.77105400	-6.19452900	-1.13822800
H	3.13290500	-4.64402700	-1.84155300
H	1.69839400	-4.87583000	-2.85958100
H	0.06610100	-7.42024700	-0.53761400
H	-0.15249100	-6.56107800	-2.07317700
H	2.27343400	-7.00766800	-1.68308000
H	2.19212200	-6.17299000	-0.12080300
C	-1.38157500	-2.90104700	1.52900300
C	-0.01024200	-2.86088000	2.24295700
C	-2.33932500	-1.86152100	2.15074600
H	-1.80578700	-3.90987200	1.63944900
C	-0.17054200	-3.08233800	3.75791800
H	0.45162500	-1.87790500	2.06349900
H	0.66972700	-3.61007000	1.82310000
C	-2.49395300	-2.07952400	3.66647600
H	-1.92662600	-0.85878600	1.97024200

H	-3.31943100	-1.90263000	1.66176100
C	-1.12798600	-2.04653900	4.37400800
H	0.81570300	-3.02903100	4.24197700
H	-0.56604700	-4.09607900	3.93861300
H	-3.15962500	-1.30807500	4.07878800
H	-2.97305600	-3.05681800	3.84774200
H	-1.24827100	-2.22850600	5.45217200
H	-0.69106100	-1.04114700	4.25707500
Au	-0.06164000	-0.45876100	-0.43602700
C	9.36533900	3.01936100	-0.07706200
C	8.12801800	2.39330800	0.09683000
C	6.95206400	2.97123900	-0.43941300
C	7.05473200	4.19021100	-1.15149300
C	8.29683100	4.80824000	-1.31941100
C	9.45573300	4.22786100	-0.78318000
H	10.26196800	2.56368700	0.34160900
H	8.05446300	1.45604000	0.64534700
H	6.15368500	4.63983100	-1.56468700
H	8.36076400	5.74699400	-1.86849400
H	10.42152900	4.71394400	-0.91491200
C	5.68547500	2.34068600	-0.25638200
C	4.60315900	1.80659900	-0.09327700
C	3.28422500	1.19008300	0.11267800
O	0.10226400	2.42647500	1.50626300
C	0.32828900	2.81502600	2.87516200
H	0.69635200	1.95200700	3.44727000
H	1.05621500	3.63718700	2.91848300
H	-0.64072600	3.13719000	3.26682100
C	3.46540800	-0.23577200	0.45904500
C	3.66412300	-1.38723000	0.80286800

C	3.88346700	-2.73832700	1.19776900
C	3.33398900	-3.23489400	2.40297200
C	4.63833000	-3.61466700	0.38241800
C	3.52517800	-4.56894700	2.77215000
H	2.74944800	-2.56744000	3.03095600
C	4.82706600	-4.94608100	0.76062200
H	5.06244400	-3.23765700	-0.54597700
C	4.26992000	-5.43068200	1.95341400
H	3.09073600	-4.93734200	3.70084800
H	5.40460700	-5.61045900	0.11920000
H	4.41641400	-6.47061900	2.24204900
C	2.34773700	1.37226800	-1.15120700
H	2.51384200	0.57554300	-1.88270900
H	2.60572600	2.34025800	-1.60622300
C	0.91387400	1.42927300	-0.56580900
H	0.27126300	2.09976100	-1.15235200
C	1.18012700	1.96494700	0.79195900
C	2.46215200	1.88451000	1.20751800
H	2.87107200	2.09438500	2.18882400
N	-2.37241100	2.89051700	0.55706900
S	-2.47143400	4.18417200	-0.54007400
S	-3.58784100	2.29371000	1.59274300
O	-3.84877800	4.33877900	-0.98722100
O	-1.33917600	4.03515500	-1.44801900
O	-2.87157500	1.59565100	2.65788400
O	-4.62170100	3.28968700	1.84039600
C	-2.03149400	5.68447400	0.58710400
C	-4.36719600	0.93727400	0.47083200
F	-2.94177800	5.81949500	1.55265500
F	-0.82525500	5.47128700	1.13130300

F	-2.00014600	6.78390200	-0.17101400
F	-3.40140800	0.16775100	-0.02181700
F	-5.19632100	0.20521700	1.22610300
F	-5.04697100	1.50887600	-0.52649400
H	-1.39011200	2.61053200	0.83670800

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C	4.98754900	-2.76490200	-1.12007600
C	5.23085400	-1.77178300	-0.13387600
C	6.36387200	-1.89704100	0.69529900
C	7.23377000	-2.98540500	0.57913700
C	6.97505400	-3.98063600	-0.37061200
C	5.86144100	-3.86587900	-1.20747800
C	3.83536300	-2.69501900	-2.06149200
C	2.81201400	-3.65810900	-1.99483500
C	1.68584500	-3.55378600	-2.81847500
C	1.56972200	-2.48887100	-3.72057400
C	2.59436400	-1.53833900	-3.81069100
C	3.72295300	-1.64333100	-2.98941100
H	6.56505000	-1.14491600	1.45406300
H	8.10154500	-3.05720400	1.23324300
H	7.63936900	-4.83866000	-0.46375600
H	5.66249500	-4.62848700	-1.95907000
H	2.88493300	-4.46253100	-1.26474300
H	0.88817400	-4.29083700	-2.73812600
H	0.68179100	-2.39617900	-4.34413000
H	2.51205800	-0.70998800	-4.51305900
H	4.51491200	-0.89988200	-3.05172100
P	4.07826900	-0.35110300	0.13360800

C	4.89736000	1.05950100	-0.78156500
C	3.86384300	2.10050500	-1.25745500
C	6.05417200	1.71583700	-0.00107200
H	5.32527500	0.57396300	-1.67190800
C	4.55173400	3.18300200	-2.10907300
H	3.38494800	2.56734700	-0.38781000
H	3.06734100	1.60010200	-1.82526000
C	6.72818200	2.80904700	-0.85516300
H	5.65814300	2.17316300	0.91795300
H	6.79072300	0.95537300	0.29460000
C	5.70203200	3.85267000	-1.33625000
H	3.81199500	3.93307800	-2.41901900
H	4.95391200	2.71761700	-3.02502700
H	7.52642900	3.29360900	-0.27353400
H	7.20349100	2.33673000	-1.73062200
H	6.19660300	4.60756400	-1.96536500
H	5.28291900	4.37834100	-0.46377800
C	4.17203500	0.00629700	1.95878700
C	3.28993800	1.23024600	2.28904800
C	3.68505800	-1.23198200	2.74568800
H	5.21113600	0.23580300	2.23449600
C	3.29198000	1.51052300	3.80310400
H	2.26265300	1.01992800	1.95531000
H	3.62847700	2.11494400	1.73837800
C	3.67296300	-0.95393400	4.26062600
H	2.66403000	-1.47261900	2.40895900
H	4.31410300	-2.10334300	2.52176300
C	2.81566900	0.28032700	4.59596800
H	2.65064000	2.37705500	4.01821900
H	4.31378500	1.77634600	4.12244500

H	3.29698300	-1.83945000	4.79376900
H	4.70609200	-0.78164200	4.60586100
H	2.84484600	0.48485400	5.67627100
H	1.76648700	0.07031100	4.33069300
Au	1.84408500	-0.72021900	-0.37041700
C	-7.20940200	3.51179000	-1.15877500
C	-5.95056700	3.06419400	-0.74956000
C	-5.03834200	2.54066100	-1.69570100
C	-5.42134800	2.48124800	-3.05654700
C	-6.68172400	2.93392900	-3.45516900
C	-7.58065300	3.44898500	-2.50962600
H	-7.90575400	3.90490300	-0.41907300
H	-5.66298300	3.09563200	0.29825000
H	-4.72496900	2.07171300	-3.78571000
H	-6.96552100	2.88056300	-4.50572900
H	-8.56457500	3.79564100	-2.82305400
C	-3.77045000	2.04060700	-1.27771900
C	-2.71365200	1.56427500	-0.90938200
C	-1.47641000	0.90213800	-0.47225700
O	-0.65295200	-2.12509400	1.44927800
C	-1.28595300	-2.00821700	2.73926700
H	-0.97833900	-1.07891900	3.23985900
H	-2.37533000	-2.03308200	2.62491500
H	-0.95122200	-2.87562400	3.31688400
C	-0.45644300	1.93189300	-0.18750700
C	0.30865900	2.84338300	0.07233300
C	1.21199200	3.90515000	0.36381600
C	1.66086100	4.76981900	-0.66261300
C	1.68875800	4.10641500	1.68005000
C	2.56689300	5.79425000	-0.37835800

H	1.29452800	4.62080500	-1.67608300
C	2.59753200	5.13155700	1.95497800
H	1.34613800	3.44573200	2.47252200
C	3.04251500	5.97770200	0.92852500
H	2.90740200	6.44908500	-1.17924700
H	2.95860200	5.27169200	2.97324300
H	3.75102300	6.77588800	1.14551900
C	-0.97645000	-0.13601200	-1.55397000
H	-0.38217000	0.35709900	-2.32950800
H	-1.86632600	-0.58416400	-2.01571600
C	-0.21575800	-1.19447900	-0.73055600
H	-0.23239300	-2.19675600	-1.17755800
C	-0.87630500	-1.13210900	0.57676500
C	-1.68059100	-0.01414400	0.75596400
H	-1.90887800	0.42734200	1.72416400
N	-4.33847100	-0.96064900	0.67373900
S	-4.72915300	-2.30543400	-0.27472600
S	-5.37534300	-0.09832300	1.69603800
O	-5.85670600	-3.04662600	0.28089000
O	-3.45107800	-2.93349700	-0.60596100
O	-4.75076300	1.20316000	1.91562200
O	-6.76917900	-0.26050600	1.29970800
C	-5.35892600	-1.48907000	-1.90612300
C	-5.16667700	-1.04798700	3.36795600
F	-6.30905300	-0.59409100	-1.64302800
F	-4.33521700	-0.89719600	-2.53307700
F	-5.85315200	-2.46350600	-2.68395000
F	-4.01036000	-0.67772400	3.94414600
F	-6.18559000	-0.72112700	4.16996400
F	-5.15641900	-2.36982600	3.16658700

H	-3.26447100	-0.62715200	0.63477300
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C	-5.93842100	-0.67198200	-0.97579700
C	-4.70022100	-0.03906100	-0.83737100
C	-3.71659600	-0.57505300	0.02735500
C	-4.00893100	-1.75869700	0.74627500
C	-5.25019100	-2.38361300	0.60029300
C	-6.21841500	-1.84487500	-0.25962600
H	-6.68671400	-0.24922200	-1.64505200
H	-4.48017300	0.87105300	-1.39263600
H	-3.25470400	-2.17517700	1.41139600
H	-5.46248700	-3.29449000	1.15876900
H	-7.18419000	-2.33591500	-0.37104000
C	-2.44739100	0.06091700	0.17121800
C	-1.35823600	0.58961500	0.29840000
C	-0.04289300	1.22011200	0.45919400
O	1.74209400	4.39087800	-0.33227800
C	2.10785400	4.26497000	-1.71976600
H	2.75958900	3.39227900	-1.88088300
H	1.21949100	4.18820200	-2.36541900
H	2.65610200	5.18068700	-1.96667200
C	1.01108800	0.20378400	0.29395300
C	1.88306700	-0.63358000	0.15422300
C	2.90756500	-1.61328200	-0.00918100
C	3.92955200	-1.75483700	0.95958400
C	2.91534400	-2.46309000	-1.14082300
C	4.92812900	-2.71861800	0.79531300
H	3.92802000	-1.10298400	1.83131100

C	3.91837200	-3.42377000	-1.29524000
H	2.12943100	-2.35964900	-1.88679200
C	4.92684300	-3.55646100	-0.32954800
H	5.70936000	-2.81725600	1.54804200
H	3.91160500	-4.07231000	-2.17044400
H	5.70620000	-4.30721800	-0.45271900
C	0.13199400	1.93751700	1.86587700
H	0.51748700	1.23184600	2.61352600
H	-0.85383900	2.28790500	2.21515300
C	1.06146300	3.08057800	1.54534000
H	1.58556300	3.66704100	2.29585900
C	1.08998900	3.33255900	0.22426700
C	0.19921400	2.39178700	-0.56849500
H	-0.75490700	2.88233900	-0.81917200
H	0.64236100	2.01633500	-1.49766900

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C	-1.39813900	-3.14319800	-1.70387500
C	-0.52409900	-3.50913000	-0.64731900
C	-0.81758500	-4.64795700	0.12851300
C	-1.96304600	-5.41156100	-0.11481500
C	-2.83961400	-5.03797400	-1.13954000
C	-2.55393100	-3.91631400	-1.92195000
C	-1.17164100	-1.96150800	-2.58150400
C	-2.10797200	-0.91051300	-2.59407300
C	-1.91804200	0.20209900	-3.41881000
C	-0.79334400	0.27570800	-4.24985700
C	0.14361600	-0.76464500	-4.24792900
C	-0.04607000	-1.87825300	-3.42104400

H	-0.16205300	-4.93217200	0.94756500
H	-2.17543400	-6.28192200	0.50391100
H	-3.74578600	-5.61181600	-1.32638800
H	-3.23291300	-3.62117000	-2.71981300
H	-2.97765000	-0.96364200	-1.94644400
H	-2.64475700	1.01084100	-3.40688600
H	-0.65191600	1.14079400	-4.89493600
H	1.01797900	-0.71714000	-4.89636800
H	0.66998500	-2.69579100	-3.44381300
P	0.94344800	-2.48576800	-0.22124100
C	2.36733200	-3.30660600	-1.12002600
C	3.50216600	-2.30779600	-1.42602700
C	2.87871300	-4.57514900	-0.40385900
H	1.92752200	-3.62702700	-2.07513200
C	4.63589200	-2.98951200	-2.21235600
H	3.89573800	-1.89788400	-0.48834700
H	3.09903800	-1.45938300	-1.99544000
C	4.00548300	-5.23660200	-1.22201200
H	3.27016500	-4.30662200	0.58722400
H	2.05017100	-5.28165000	-0.25490600
C	5.15315600	-4.24403100	-1.48394300
H	5.45359600	-2.27206700	-2.37575800
H	4.25888900	-3.28078200	-3.20683300
H	4.37698000	-6.12312100	-0.68794500
H	3.59697200	-5.58295400	-2.18549500
H	5.94774900	-4.72595300	-2.07207000
H	5.59353400	-3.94375000	-0.51943000
C	1.22276800	-2.70523400	1.60669200
C	2.50865600	-1.97398600	2.05665100
C	-0.00336300	-2.16551500	2.37444800

H	1.34388400	-3.77718800	1.81609100
C	2.69828000	-2.10722100	3.57976600
H	2.42829900	-0.91016000	1.78814700
H	3.39042100	-2.36667400	1.53753900
C	0.19196000	-2.27693900	3.89663900
H	-0.14245800	-1.10690100	2.10460700
H	-0.90860600	-2.69700200	2.06826800
C	1.47938200	-1.56391800	4.34557700
H	3.61290400	-1.57680500	3.87440500
H	2.84254800	-3.17089200	3.83380600
H	-0.68662300	-1.85392300	4.40417200
H	0.25026400	-3.34158500	4.17829800
H	1.62455500	-1.67996500	5.42953900
H	1.38141700	-0.48421300	4.14284000
Au	0.86912100	-0.19737300	-0.59129300
C	2.51242100	8.57122600	-0.24048000
C	2.36554000	7.21067000	-0.52311700
C	3.27853100	6.26861600	0.00823700
C	4.33785800	6.72657200	0.82700900
C	4.47449600	8.08939000	1.10406000
C	3.56506600	9.01566200	0.57280200
H	1.80299100	9.28640300	-0.65470400
H	1.54814200	6.86231500	-1.15219400
H	5.04182500	6.00481000	1.23694700
H	5.29329200	8.43016500	1.73647900
H	3.67534500	10.07672200	0.79212400
C	3.12826700	4.87900300	-0.27652500
C	3.00225500	3.69253000	-0.52097900
C	2.75731500	2.27100500	-0.82322000
O	-0.66301000	2.74564900	-1.86430900

C	-1.75136000	2.67179600	-0.10265300
H	-1.39882700	1.65866000	0.06391100
H	-1.15936400	3.51643300	0.22274200
H	-2.63073100	2.83113500	-0.71483500
C	3.69507900	1.43689300	-0.06500300
C	4.49110800	0.75083600	0.54857300
C	5.39913100	-0.07539800	1.27203600
C	6.19519100	-1.03189000	0.59816600
C	5.50685700	0.03450500	2.67803700
C	7.06190000	-1.86054900	1.31572900
H	6.12143900	-1.11753100	-0.48317500
C	6.37968500	-0.79593000	3.38622300
H	4.89852100	0.77049100	3.19987700
C	7.15573400	-1.74878500	2.71074000
H	7.66835200	-2.59300000	0.78467200
H	6.45132800	-0.70187700	4.46889000
H	7.83274800	-2.39592900	3.26642200
C	2.84937000	2.01015400	-2.37512100
H	2.90700300	0.92348900	-2.51755700
H	3.73513900	2.48399400	-2.81030000
C	1.51710600	2.55044700	-2.91754800
H	1.58759900	3.61721900	-3.17601600
H	1.14429300	2.01302900	-3.79515900
C	0.54432600	2.43409700	-1.74833200
C	1.23969900	1.95797200	-0.56068100
H	0.86909900	2.33308100	0.39762200
O	-2.80750000	2.74903200	1.51855600
H	-3.56595800	2.11678900	1.28013800
H	-2.34262300	2.25857100	2.21681300
N	-4.58436300	0.89269500	0.88628500

S	-5.75074600	1.10591900	-0.26179800
S	-4.51467600	-0.31563900	1.99612700
O	-6.50472800	-0.09751000	-0.62642500
O	-5.14197900	1.95912800	-1.29365600
O	-3.50915600	0.12654300	2.98144400
O	-5.78750600	-0.89633700	2.43004800
C	-6.98585800	2.25873900	0.64694400
C	-3.61198900	-1.68761000	1.01131600
F	-7.51325800	1.63819900	1.71066400
F	-6.34756300	3.37019000	1.05540400
F	-7.97078900	2.60459900	-0.19927300
F	-2.43766700	-1.20104200	0.56120900
F	-3.37248900	-2.73965300	1.81442100
F	-4.34686000	-2.09318700	-0.03177800

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C	5.36307800	1.43708800	-1.11603300
C	4.76943200	0.23915400	-1.59675400
C	5.26304400	-0.34389300	-2.78077700
C	6.31140800	0.24555500	-3.49508000
C	6.87637200	1.44180900	-3.03733800
C	6.40210500	2.02703600	-1.85929500
C	4.91654400	2.09706700	0.14374500
C	4.25059000	3.33471700	0.09288900
C	3.76387000	3.92734300	1.26321800
C	3.94281700	3.29240100	2.49824700
C	4.62004000	2.06818000	2.56154800
C	5.10846500	1.47706500	1.39154700
H	4.81508400	-1.25804400	-3.16251900
H	6.67647800	-0.22320800	-4.40788300

H	7.68525000	1.91611500	-3.59146600
H	6.84565500	2.95090900	-1.49102300
H	4.07251600	3.80671400	-0.87147800
H	3.20205500	4.85548200	1.19814000
H	3.55020000	3.74560600	3.40697700
H	4.76836700	1.57164200	3.51981700
H	5.64525600	0.53337300	1.44557200
P	3.32290900	-0.51195600	-0.73080700
C	4.07991000	-1.78621700	0.41228900
C	3.19923700	-2.04045900	1.65299300
C	4.47294300	-3.09554700	-0.30363100
H	5.01028900	-1.30982000	0.75018000
C	3.90291600	-3.01066200	2.61947600
H	2.23640600	-2.46761700	1.34728400
H	2.97489700	-1.08659900	2.14893000
C	5.16386700	-4.05906300	0.68282000
H	3.57310500	-3.58233300	-0.70564900
H	5.13759200	-2.87513100	-1.15135600
C	4.27583300	-4.32662800	1.91262800
H	3.24930200	-3.21028300	3.47913600
H	4.82053900	-2.53463400	3.00508300
H	5.40742800	-5.00118000	0.16975900
H	6.11590600	-3.61204100	1.01400900
H	4.78873900	-5.00477100	2.61062200
H	3.35039200	-4.82961100	1.58836200
C	2.37850300	-1.44812800	-2.03563300
C	1.20039200	-2.21562800	-1.39292700
C	1.84986900	-0.47692800	-3.11372100
H	3.05124100	-2.18267200	-2.50224100
C	0.42928300	-3.00217000	-2.47047000

H	0.52993500	-1.49290000	-0.90658500
H	1.55366200	-2.89762000	-0.61154400
C	1.06462600	-1.24404700	-4.19601700
H	1.19224100	0.25673400	-2.62253800
H	2.67688100	0.08303800	-3.56942200
C	-0.08081800	-2.07413200	-3.58689100
H	-0.41298200	-3.53439300	-2.00686100
H	1.09814600	-3.76514600	-2.90333800
H	0.66925100	-0.53466700	-4.93754800
H	1.75751100	-1.91735200	-4.72831200
H	-0.58362300	-2.66033700	-4.36977000
H	-0.83186300	-1.39454100	-3.16411200
Au	1.81010400	0.95137200	0.23426300
C	-6.93423200	1.77059300	1.82685800
C	-5.60076900	1.63506800	2.22310400
C	-4.58337700	2.38023800	1.57495100
C	-4.94793100	3.27152900	0.53348300
C	-6.28609400	3.39914600	0.14887700
C	-7.28234400	2.64930600	0.79022800
H	-7.70315300	1.18184000	2.32478400
H	-5.32461500	0.94137600	3.01294400
H	-4.17108800	3.83940100	0.02679500
H	-6.54793800	4.07566000	-0.66268700
H	-8.32188600	2.74423700	0.48055900
C	-3.20990600	2.17223200	1.89591800
C	-2.03194000	1.93088800	2.09072100
C	-0.60746100	1.55492400	2.13823000
O	0.74117100	4.40482500	0.36958800
C	-0.52073100	0.09836400	2.28711500
C	-0.41861300	-1.11132100	2.37709900

C	-0.25851900	-2.52536200	2.42283600
C	0.36635700	-3.15007700	3.52740300
C	-0.69007000	-3.32641900	1.33887700
C	0.56148500	-4.53352900	3.53963900
H	0.70067000	-2.53716200	4.36217900
C	-0.48985100	-4.70906800	1.36042700
H	-1.17655700	-2.85256700	0.49109600
C	0.13908600	-5.31843500	2.45655400
H	1.04869600	-5.00077600	4.39458300
H	-0.82757000	-5.31323300	0.51912900
H	0.29475500	-6.39637900	2.46916400
C	0.18757200	2.30762500	3.26986200
H	1.14328300	1.77996000	3.38216500
H	-0.35313500	2.28600500	4.22284600
C	0.41988500	3.70960100	2.69567500
H	-0.42819500	4.37762800	2.91091200
H	1.33252800	4.19567800	3.05870500
C	0.46706100	3.51472300	1.16807800
C	0.09986400	2.10876000	0.84482500
H	-0.54890200	2.06528800	-0.03221800
H	-4.77048200	0.81707000	-0.13321000
N	-4.53498200	0.04469400	-0.76850500
S	-4.14909700	0.49510800	-2.37254900
S	-4.34698100	-1.48376800	-0.01243000
O	-4.94791100	1.67752800	-2.66964600
O	-4.12108900	-0.69818400	-3.20333400
O	-3.39829800	-2.29106900	-0.76507900
O	-4.25568100	-1.23145400	1.41843300
C	-2.32188700	1.09816600	-2.15401400
C	-6.10254400	-2.20367500	-0.33265600

F	-1.66410900	0.25710500	-1.35270100
F	-1.73818100	1.13371100	-3.35516200
F	-2.34387700	2.32146600	-1.62104600
F	-6.30868600	-2.32677500	-1.64390300
F	-6.17308200	-3.40020100	0.25843700
F	-7.01137100	-1.37846400	0.19895900

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C	4.18523800	-3.04240400	-0.34693400
C	4.26750700	-2.03574900	0.65077800
C	5.02845400	-2.27355700	1.81289600
C	5.68852700	-3.49150000	2.00281500
C	5.58371200	-4.49637400	1.03414200
C	4.83990400	-4.26797400	-0.12778800
C	3.42570100	-2.84578500	-1.61475500
C	2.22220100	-3.54067100	-1.82983000
C	1.46276600	-3.29939300	-2.98044800
C	1.89718600	-2.36521700	-3.92898800
C	3.10782000	-1.68691200	-3.73490300
C	3.86938200	-1.93096200	-2.58684300
H	5.09622200	-1.51252400	2.58606200
H	6.26954700	-3.65633000	2.90877800
H	6.08364700	-5.45295200	1.17877000
H	4.76641700	-5.04131000	-0.89087700
H	1.85905600	-4.23167500	-1.07222800
H	0.51381500	-3.81317700	-3.10604300
H	1.29777400	-2.16820500	-4.81647800
H	3.46125500	-0.97100100	-4.47597300
H	4.81850300	-1.41901800	-2.44769600

P	3.35424000	-0.44837800	0.48718900
C	4.54861800	0.71592800	-0.34628100
C	3.83864900	1.82273300	-1.15193800
C	5.59320100	1.28428700	0.63837100
H	5.08234700	0.07055200	-1.05619400
C	4.87653100	2.69227400	-1.88597900
H	3.24634400	2.45554600	-0.48054100
H	3.13471400	1.36822800	-1.86234800
C	6.61284400	2.16267400	-0.11394300
H	5.08888000	1.89516400	1.40053800
H	6.10858800	0.46302400	1.15668500
C	5.90670600	3.27972000	-0.90419200
H	4.36054700	3.49689500	-2.42631000
H	5.40076300	2.07496500	-2.63474800
H	7.32998900	2.58866100	0.60259200
H	7.18510000	1.53016700	-0.81213200
H	6.64642000	3.88702400	-1.44577300
H	5.38686300	3.94915800	-0.19974600
C	3.03171700	0.17326200	2.21132700
C	2.34464600	1.55721500	2.14430300
C	2.14979500	-0.83512900	2.98343200
H	4.00076100	0.28885200	2.71743300
C	2.01728300	2.07432400	3.55683500
H	1.41181200	1.46262900	1.57017700
H	2.97272500	2.28261000	1.61553700
C	1.81909900	-0.30880000	4.39292800
H	1.21070400	-0.97972400	2.42976100
H	2.64594800	-1.81198600	3.04652000
C	1.14124200	1.07147100	4.32747200
H	1.51042700	3.04675700	3.47565300

H	2.95763000	2.24288500	4.10824600
H	1.16576500	-1.03068300	4.90214800
H	2.74875100	-0.23293700	4.98217900
H	0.93590700	1.44401600	5.34157500
H	0.17473700	0.96540200	3.81309900
Au	1.29305900	-0.59022500	-0.49056200
C	-7.59503100	1.68919100	-1.87442700
C	-6.27900900	1.23603900	-1.99529000
C	-5.20432500	2.06164900	-1.59161200
C	-5.48101700	3.34466000	-1.06381800
C	-6.80110500	3.78758100	-0.94893900
C	-7.86167600	2.96360600	-1.35393100
H	-8.41580900	1.04130400	-2.17933300
H	-6.06475200	0.24095700	-2.37523000
H	-4.65449600	3.97609500	-0.74329700
H	-7.00384300	4.77590900	-0.53789100
H	-8.88990200	3.31006800	-1.25770100
C	-3.85886500	1.60185500	-1.69385700
C	-2.71151400	1.20460100	-1.75840700
C	-1.31125800	0.74842400	-1.80038700
O	-1.10576900	-2.88801800	-1.22640800
C	-0.45431700	1.89525200	-1.47685700
C	0.22920100	2.85157200	-1.16062300
C	1.04470000	3.93892100	-0.73653800
C	1.09586600	4.29313700	0.63264700
C	1.83930600	4.65706200	-1.65997100
C	1.93283500	5.32576000	1.06243200
H	0.48347100	3.74517200	1.34472800
C	2.67058200	5.69039500	-1.22057700
H	1.80041900	4.38849100	-2.71363400

C	2.72548800	6.02545200	0.14038200
H	1.96606700	5.58593700	2.11955100
H	3.28041900	6.23390600	-1.94088700
H	3.37672200	6.83006000	0.47863500
C	-0.96519000	0.11409000	-3.20473900
H	0.13031700	0.11897100	-3.29727700
H	-1.40697500	0.69206800	-4.02313000
C	-1.46991200	-1.32969500	-3.09865800
H	-2.56180400	-1.37716900	-3.22574000
H	-1.00408400	-2.02212500	-3.80702800
C	-1.16944900	-1.74487000	-1.65255400
C	-1.07311400	-0.47930500	-0.86486100
H	-0.71641300	-0.35037600	0.17672500
H	-2.20418900	-0.76060200	-0.14814900
N	-3.18590900	-1.03326400	0.71847600
S	-4.66872300	-1.58979800	0.17741400
S	-2.82730300	-0.54904400	2.26719700
O	-4.58159000	-1.58629000	-1.28533500
O	-5.81115400	-1.01402100	0.88727300
O	-3.77735500	-0.99766500	3.28317300
O	-1.37894900	-0.74909500	2.42797200
C	-4.61245700	-3.45375000	0.66625500
C	-3.01453600	1.36061800	2.15102500
F	-4.34062800	-3.59764400	1.96890700
F	-5.82200000	-3.98182000	0.40425400
F	-3.68688400	-4.08868000	-0.05691600
F	-4.22202400	1.69533400	1.69322300
F	-2.83561100	1.88476900	3.37674800
F	-2.06837400	1.85410900	1.32889400

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C	-5.49797100	-1.68312100	-0.02272500
C	-4.44415700	-0.76592800	0.01336300
C	-3.10446600	-1.22001800	0.03413400
C	-2.85040300	-2.61200700	0.01827300
C	-3.91180900	-3.51999600	-0.01836100
C	-5.23691600	-3.06104300	-0.03852600
H	-6.52541000	-1.32189600	-0.03913900
H	-4.64321700	0.30422000	0.02308700
H	-1.82066100	-2.96391300	0.03391300
H	-3.70404200	-4.58916900	-0.03101800
H	-6.06054000	-3.77313600	-0.06681000
C	-2.02245500	-0.29044000	0.06906200
C	-1.09000300	0.49120500	0.09480700
C	0.01695400	1.46268400	0.12242300
O	-1.75951000	4.36242000	-1.12206000
C	1.30361200	0.76294000	0.06285200
C	2.37508100	0.18664200	0.02630300
C	3.63121100	-0.48952500	-0.01707800
C	4.36825100	-0.71080900	1.17048900
C	4.15429800	-0.95731700	-1.24587700
C	5.59553800	-1.37737600	1.12433200
H	3.96785700	-0.35537900	2.11809800
C	5.38268000	-1.62277700	-1.28064500
H	3.58897200	-0.79213200	-2.16115600
C	6.10663100	-1.83598500	-0.09853800
H	6.15355500	-1.54162600	2.04526300
H	5.77505000	-1.97825200	-2.23251100
H	7.06325100	-2.35563300	-0.13014400

C	-0.10106100	2.38185300	1.40524900
H	0.85498600	2.90903900	1.52255600
H	-0.28798900	1.78267900	2.30196500
C	-1.22490400	3.37075100	1.05894600
H	-2.21431800	2.95053200	1.29509700
H	-1.14597100	4.34178300	1.56272400
C	-1.15282700	3.54354500	-0.46591300
C	-0.16631600	2.50983000	-1.02813800
H	0.79259700	3.02508500	-1.19580600
H	-0.50385100	2.07978600	-1.97623400

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C	2.38538800	5.23248100	-0.84400100
C	1.48469000	4.19788800	-1.10740000
C	1.53204200	3.50693700	-2.34177600
C	2.49397300	3.89039100	-3.30423000
C	3.38837500	4.92938100	-3.03236800
C	3.34213300	5.60044500	-1.80176100
H	2.33954200	5.75266300	0.11197900
H	0.74368200	3.90854100	-0.36895600
H	2.53397000	3.36238600	-4.25502900
H	4.12720800	5.21279100	-3.78077300
H	4.04350500	6.40695000	-1.59279500
C	0.64946400	2.41265400	-2.57622200
C	-0.09683100	1.46170800	-2.71014300
C	-0.99400500	0.32247900	-2.81918600
O	-4.42766000	-0.91649500	-3.03107600
C	-5.15887700	-0.27265300	-1.94303900
H	-4.59313100	-0.33967700	-1.00971100

H	-5.34892300	0.77886000	-2.18528200
H	-6.09839400	-0.82784700	-1.86568600
C	-0.67735000	-0.83059300	-1.83440100
C	-1.37344600	-1.90748000	-1.87848200
C	-1.95561700	-3.12160100	-1.44434900
C	-2.35221900	-4.13361800	-2.34962000
C	-2.09101000	-3.33509900	-0.04927100
C	-2.86839300	-5.33587800	-1.86698500
H	-2.25551300	-3.95596300	-3.41777300
C	-2.58764200	-4.55191900	0.41874300
H	-1.79168700	-2.54632900	0.63397000
C	-2.98016900	-5.55200200	-0.48341900
H	-3.18273100	-6.10893800	-2.56634300
H	-2.68404400	-4.71196500	1.49153300
H	-3.38092500	-6.49394700	-0.11177000
C	-1.04400200	-0.35305100	-4.23456100
H	-0.15344100	-0.95816900	-4.43671100
H	-1.11535900	0.44255000	-4.99574900
C	-2.32602000	-1.14118200	-4.12699500
H	-2.59384100	-1.99629300	-4.73936600
C	-3.17813100	-0.51361000	-3.25180200
C	-2.50451900	0.67889900	-2.59653900
H	-2.75169800	1.60171800	-3.14458100
H	-2.75219500	0.81922100	-1.54274100
C	3.33031000	-3.22333000	1.26167900
C	3.38984300	-1.92568400	1.83257200
C	4.00665600	-1.75600200	3.08856000
C	4.54460500	-2.84252000	3.78442400
C	4.46119200	-4.12714900	3.23508400
C	3.85737600	-4.30900300	1.98780400

C	2.72332600	-3.49571000	-0.07122100
C	1.56252500	-4.28485300	-0.15901200
C	0.95686700	-4.52122400	-1.39674700
C	1.49946900	-3.96725100	-2.56280000
C	2.66600400	-3.19616500	-2.48901000
C	3.27908900	-2.96868000	-1.25187400
H	4.05415900	-0.76866800	3.53994500
H	5.01636300	-2.68472800	4.75309600
H	4.86760100	-4.98308800	3.77205800
H	3.79975700	-5.30390600	1.54888700
H	1.12200800	-4.68689400	0.75159600
H	0.04704800	-5.11429600	-1.44576900
H	1.01311000	-4.13447700	-3.52269000
H	3.09863300	-2.76706700	-3.39185400
H	4.18879500	-2.37564100	-1.19874200
P	2.67313500	-0.45045000	0.99219500
C	4.13704500	0.28056900	0.07320400
C	3.71258600	1.02800200	-1.20612200
C	5.03261800	1.15602200	0.97534000
H	4.72426100	-0.60064900	-0.22172800
C	4.94829800	1.53181000	-1.97345800
H	3.07724900	1.88022300	-0.93682700
H	3.10603600	0.36777300	-1.84017900
C	6.26147700	1.66078300	0.19149600
H	4.45659700	2.02348900	1.32937800
H	5.35433000	0.58656700	1.85886400
C	5.83814100	2.41576700	-1.08216600
H	4.62295200	2.08927000	-2.86172300
H	5.53350100	0.66363300	-2.32156400
H	6.86978000	2.30792700	0.84042300

H	6.88854900	0.79838200	-0.08858500
H	6.72652900	2.74837300	-1.63892000
H	5.27341200	3.31865400	-0.80041500
C	2.21022800	0.73670400	2.33661800
C	1.61766200	2.02320700	1.71622700
C	1.19348800	0.09756100	3.30554800
H	3.12500900	1.00588900	2.88435900
C	1.25892600	3.02758200	2.82933600
H	0.71328900	1.75432400	1.14922000
H	2.32041200	2.47673100	1.00677600
C	0.83719500	1.09228700	4.42743700
H	0.28745100	-0.16050300	2.74088600
H	1.59427000	-0.82986400	3.73535200
C	0.28844300	2.41050700	3.85264400
H	0.81488600	3.92869500	2.38356500
H	2.18652000	3.33961200	3.33925300
H	0.09301000	0.63693100	5.09594700
H	1.73980400	1.29531100	5.02952400
H	0.08948600	3.12633800	4.66365200
H	-0.67162000	2.20401700	3.36464000
Au	0.85339300	-0.78434700	-0.40178200
N	-3.35219900	1.16164100	0.67330500
S	-3.00645700	0.36680400	2.05261500
S	-4.06186700	2.63342100	0.59594300
O	-2.99129900	1.14248500	3.30229600
O	-1.88615800	-0.54897700	1.76922100
O	-4.63972300	2.75684900	-0.75253400
O	-4.83380900	3.07782900	1.76391900
C	-4.52029500	-0.80350500	2.20174600
C	-2.52514500	3.77839500	0.52679000

F	-5.66182500	-0.09833300	2.25814700
F	-4.58012600	-1.63556700	1.13773800
F	-4.40835200	-1.55021200	3.31738500
F	-1.74625200	3.44594300	-0.52331400
F	-2.90952700	5.05993700	0.38890500
F	-1.79181300	3.66561400	1.65144600

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C	2.17902200	5.34475500	-0.93596800
C	1.35250200	4.24731300	-1.18676700
C	1.41949200	3.57145700	-2.42906100
C	2.32977200	4.02932900	-3.40888400
C	3.15141100	5.12992400	-3.14830300
C	3.08296800	5.78915600	-1.91257500
H	2.11781100	5.85331000	0.02544200
H	0.65568000	3.89629300	-0.43188200
H	2.38744200	3.51131900	-4.36437200
H	3.85089300	5.47145900	-3.91019000
H	3.72689100	6.64441400	-1.71281000
C	0.60349200	2.42502200	-2.65396000
C	-0.09126400	1.43390300	-2.77802500
C	-0.94819900	0.26846100	-2.83208900
O	-4.25600800	-1.16176300	-2.74890800
C	-5.17824600	-0.36426600	-1.90324000
H	-4.65732900	-0.05673000	-0.99616500
H	-5.50419600	0.50443200	-2.48250900
H	-6.01004600	-1.03968500	-1.69439100
C	-0.60562600	-0.91143500	-1.85232100
C	-1.36705200	-1.96452500	-2.29098800

C	-1.68007500	-3.23236300	-1.62788200
C	-2.04695100	-4.37574100	-2.36911900
C	-1.59934400	-3.33601600	-0.22240800
C	-2.29211400	-5.59490000	-1.72857500
H	-2.11439900	-4.32059300	-3.45453200
C	-1.84313900	-4.55422600	0.41416000
H	-1.36470100	-2.45127700	0.36089400
C	-2.18410900	-5.69126700	-0.33384100
H	-2.56271900	-6.47046700	-2.31772800
H	-1.78102200	-4.61090600	1.50031200
H	-2.37790100	-6.63953300	0.16612700
C	-1.05962700	-0.50446900	-4.18182800
H	-0.10969900	-0.96412200	-4.47637700
H	-1.46245100	0.11995200	-4.99173300
C	-2.05224500	-1.55214600	-3.64336000
H	-2.42405700	-2.35896100	-4.27425800
C	-3.06291200	-0.72464800	-2.95524600
C	-2.46133000	0.58449700	-2.53578600
H	-2.86025100	1.39340300	-3.17012300
H	-2.64702800	0.83613400	-1.48828300
C	3.48945000	-3.04882400	1.26498600
C	3.42169500	-1.77453800	1.88544200
C	3.98893600	-1.60396900	3.16391200
C	4.59835700	-2.66850100	3.83527300
C	4.64004500	-3.93270700	3.23605500
C	4.08869800	-4.11448500	1.96450400
C	2.93986900	-3.31962600	-0.09343100
C	1.84880200	-4.19432600	-0.23526800
C	1.29384000	-4.44166700	-1.49371600
C	1.81856900	-3.81347300	-2.62908100

C	2.91578900	-2.95259400	-2.50238300
C	3.47819100	-2.71306900	-1.24374200
H	3.94108900	-0.63414600	3.65212800
H	5.02783500	-2.51064700	4.82356700
H	5.10351600	-4.77215600	3.75260000
H	4.12833200	-5.09217600	1.48640900
H	1.41549600	-4.65410900	0.65070800
H	0.43446800	-5.10125300	-1.57950300
H	1.37048700	-3.99055800	-3.60594500
H	3.33461600	-2.46291100	-3.38078900
H	4.33701700	-2.05326600	-1.15462600
P	2.60939600	-0.34018500	1.05658100
C	4.05580200	0.49954000	0.19543600
C	3.61919600	1.22591400	-1.09117700
C	4.87091700	1.41880000	1.12738000
H	4.70929600	-0.33715400	-0.08779900
C	4.83699200	1.82206800	-1.81971500
H	2.91369300	2.02575500	-0.83628700
H	3.08064300	0.52820000	-1.74547600
C	6.08444100	2.00836200	0.38006500
H	4.23420200	2.24422200	1.47633700
H	5.20453400	0.85988800	2.01341600
C	5.64472400	2.75060700	-0.89585300
H	4.49856300	2.36842200	-2.71008000
H	5.48756100	0.99883000	-2.16197300
H	6.63599000	2.68474800	1.04988100
H	6.77054600	1.18994000	0.10598500
H	6.52289600	3.14873900	-1.42549600
H	5.01515100	3.61065400	-0.61774400
C	2.06676000	0.79817400	2.41516300

C	1.41876300	2.06352700	1.80511300
C	1.06960500	0.09381700	3.35903300
H	2.95832300	1.10553400	2.98052100
C	0.99520700	3.03006700	2.92809500
H	0.53916100	1.76034900	1.21718000
H	2.11025300	2.56284800	1.11451500
C	0.64206200	1.05097200	4.48796300
H	0.18803900	-0.20497400	2.77646100
H	1.51263800	-0.81754800	3.78154800
C	0.03719100	2.34911400	3.92351100
H	0.51962200	3.91966400	2.49213200
H	1.89862300	3.37166200	3.46220800
H	-0.08938800	0.54799300	5.13644000
H	1.52178000	1.29140000	5.10971700
H	-0.21304600	3.04066300	4.74154800
H	-0.90239100	2.10329300	3.41316000
Au	0.82703500	-0.74953500	-0.39789600
N	-3.38880100	1.05456700	0.65112000
S	-3.14080800	0.20194900	2.02311300
S	-4.14536100	2.50162200	0.55898200
O	-3.28988800	0.92144700	3.29612900
O	-1.96375500	-0.65522400	1.81358300
O	-4.68573300	2.60688400	-0.80860800
O	-4.96842400	2.92068700	1.70055500
C	-4.60993100	-1.03212600	1.93811700
C	-2.64283600	3.69046100	0.53799900
F	-5.77823100	-0.37810400	1.79335200
F	-4.45543300	-1.86305400	0.88287700
F	-4.65672600	-1.76982800	3.06051200
F	-1.81150800	3.36680800	-0.47424200

F	-3.05904500	4.95730700	0.36620000
F	-1.95947200	3.61068400	1.69439500

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C	0.77035300	5.87783400	-1.75458500
C	0.32142000	4.56393600	-1.59890200
C	0.57688400	3.59637900	-2.60023700
C	1.29262100	3.98582800	-3.75658000
C	1.73330900	5.30399400	-3.90526900
C	1.47782700	6.25425000	-2.90608200
H	0.56630000	6.61139000	-0.97558500
H	-0.23525400	4.27162700	-0.71058600
H	1.49421500	3.24548600	-4.52847000
H	2.28301700	5.58881200	-4.80154000
H	1.82559400	7.27959700	-3.02353500
C	0.13407700	2.25334000	-2.43105100
C	-0.24312100	1.10788600	-2.26185300
C	-0.69859400	-0.24024500	-1.98935500
O	-2.38535200	-2.62817800	-0.01456600
C	-2.43267400	-2.14486300	1.34497300
H	-1.43849800	-1.78306100	1.64389600
H	-3.18036000	-1.35653500	1.46669200
H	-2.71058000	-3.00778800	1.95781700
C	0.37689700	-1.27368400	-1.54208200
C	-0.20074700	-2.49261300	-1.73918200
C	0.28651900	-3.81932700	-1.33366900
C	0.00398500	-4.94956500	-2.13160300
C	1.03845200	-4.01588000	-0.15570500
C	0.48003500	-6.21908900	-1.78618200

H	-0.57807600	-4.82221100	-3.04386200
C	1.51179200	-5.28405500	0.19354500
H	1.24163900	-3.16471400	0.48902400
C	1.24034200	-6.39327300	-0.62105100
H	0.25760900	-7.07318100	-2.42567600
H	2.08579700	-5.41027100	1.11168600
H	1.60650800	-7.38179700	-0.34587600
C	-1.44908000	-1.00034900	-3.12047000
H	-0.81100300	-1.16204200	-3.99616400
H	-2.38964200	-0.51291700	-3.40579800
C	-1.62673700	-2.27472200	-2.27780700
H	-2.11737000	-3.14227100	-2.72620100
C	-2.37621500	-1.70755000	-1.02849700
C	-1.75112800	-0.30335200	-0.82119700
H	-2.49211400	0.48519100	-0.94737000
H	-1.25529900	-0.19218700	0.14487200
C	5.39056000	-1.56566400	1.02296100
C	4.76778200	-0.55806500	1.80813700
C	5.21079200	-0.34766300	3.12922600
C	6.23741200	-1.12038000	3.68128200
C	6.83330100	-2.13028600	2.91630700
C	6.40867700	-2.34676300	1.60166700
C	4.98259800	-1.84150500	-0.38403800
C	4.32392000	-3.04410200	-0.69605600
C	3.83443200	-3.27308200	-1.98657400
C	4.00930100	-2.30721300	-2.98418300
C	4.68950700	-1.11799000	-2.69123200
C	5.17563500	-0.88668300	-1.39963200
H	4.73820000	0.41557200	3.74306400
H	6.56142200	-0.93893900	4.70516800

H	7.62745800	-2.74435500	3.33888000
H	6.87457200	-3.12364100	0.99699800
H	4.14892200	-3.77614900	0.08925900
H	3.28518800	-4.18813800	-2.19689500
H	3.60595400	-2.47429900	-3.98160100
H	4.82834600	-0.36263500	-3.46356100
H	5.69413700	0.04232700	-1.17147700
P	3.34785100	0.41935100	1.14921000
C	4.12271100	2.00698100	0.53573700
C	3.25660200	2.67519400	-0.55334800
C	4.49654300	2.98657700	1.66708700
H	5.05700300	1.66928100	0.06284600
C	3.95168700	3.93396800	-1.10167800
H	2.28049200	2.95398200	-0.13619200
H	3.05435500	1.95765800	-1.35896800
C	5.18248400	4.24422900	1.09556500
H	3.58415200	3.29201600	2.20039800
H	5.15614900	2.49154000	2.39418700
C	4.30100300	4.91878800	0.02824000
H	3.30354300	4.41464800	-1.84340100
H	4.88014900	3.63484500	-1.61729100
H	5.40835700	4.94538200	1.91270900
H	6.14359500	3.95392100	0.64019600
H	4.80717000	5.80561000	-0.38084800
H	3.36709400	5.26755000	0.49978500
C	2.29241100	0.83076500	2.63423400
C	1.11417200	1.74174400	2.21069800
C	1.76677800	-0.48921100	3.24539000
H	2.89811800	1.36642300	3.37915200
C	0.15030000	1.99248900	3.38681600

H	0.56854600	1.25797400	1.38670500
H	1.49155500	2.69693500	1.82606200
C	0.80961200	-0.22285500	4.42106700
H	1.22798800	-1.04110000	2.45845300
H	2.60531100	-1.12078000	3.56686200
C	-0.36488000	0.67107200	3.98434600
H	-0.68909300	2.61384200	3.04391900
H	0.67534400	2.56178900	4.17186400
H	0.43843600	-1.17985200	4.81629200
H	1.36173100	0.27348200	5.23621700
H	-1.03480600	0.87125200	4.83287800
H	-0.95574400	0.13779800	3.22341300
Au	1.92727400	-0.60560300	-0.38565400
N	-5.09400300	0.16646500	0.07807500
S	-6.07618800	-0.51991100	1.24692800
S	-4.87720700	1.82527000	-0.07728800
O	-6.16845100	0.28583600	2.46497700
O	-5.71050000	-1.93996600	1.27671400
O	-4.25810000	2.02154500	-1.39029700
O	-6.04268400	2.59631100	0.34793700
C	-7.82100700	-0.49862300	0.42809900
C	-3.47030300	2.21422700	1.24767000
F	-8.30775700	0.73894800	0.35024900
F	-7.73664700	-1.02414900	-0.80814800
F	-8.63661900	-1.25763500	1.17477700
F	-2.36398100	2.62688300	0.60810800
F	-3.88854800	3.17686800	2.07113400
F	-3.17171500	1.11834300	1.96503700
C	-4.68094100	-2.54447300	-1.75526400
H	-5.70114200	-2.16127000	-1.83738500

H	-4.35163100	-2.94367400	-2.71982800
H	-4.61183600	-3.29906100	-0.96593000
O	-3.84808100	-1.39548500	-1.42710700
H	-4.41270700	-0.65364300	-0.69726700

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C	4.01485600	5.89418700	0.78733800
C	3.01900200	4.91487700	0.81878500
C	2.28845200	4.59813700	-0.35172400
C	2.58935700	5.28743300	-1.54980500
C	3.58677000	6.26648700	-1.57087100
C	4.30251700	6.57483200	-0.40499000
H	4.57021700	6.12605100	1.69529700
H	2.79518700	4.38445100	1.74255600
H	2.03324400	5.04642600	-2.45384700
H	3.80674800	6.78961800	-2.50058000
H	5.08000000	7.33711800	-0.42561600
C	1.27356000	3.59802000	-0.31516600
C	0.41125900	2.73916200	-0.26342100
C	-0.58438300	1.69477100	-0.13010100
O	-2.86827600	-0.20174600	1.78335100
C	-2.75308000	0.00021400	3.21527600
H	-1.69411700	0.03938400	3.50495600
H	-3.27167600	0.91836300	3.51634700
H	-3.23667500	-0.86867000	3.66741900
C	-0.07669100	0.22521800	-0.29416400
C	-1.20002200	-0.51705600	-0.50905200
C	-1.33588000	-1.97382700	-0.61914500
C	-2.32406400	-2.53431700	-1.45628400

C	-0.48524300	-2.85305400	0.08412700
C	-2.43854300	-3.91925300	-1.61135800
H	-3.00103200	-1.87804400	-1.99982400
C	-0.59470900	-4.23738400	-0.07397600
H	0.25547600	-2.43797300	0.76351100
C	-1.56844000	-4.77923700	-0.92638200
H	-3.21012100	-4.32589600	-2.26429500
H	0.07353700	-4.89709400	0.47961700
H	-1.65874100	-5.85868700	-1.04246400
C	-1.79743300	1.70050400	-1.10788300
H	-1.49077400	1.55506000	-2.14823800
H	-2.40874100	2.61212600	-1.03621000
C	-2.41911200	0.42291700	-0.50733300
H	-3.35105300	0.04332900	-0.92595400
C	-2.53485300	0.81200300	0.98013700
C	-1.32412800	1.72678500	1.26536500
H	-1.63575000	2.74179400	1.53706100
H	-0.68536100	1.32627600	2.05771600
C	4.32664800	-2.89305400	-1.57878200
C	4.84158200	-2.32320200	-0.38399000
C	5.87764300	-2.98763700	0.30252600
C	6.39273500	-4.20208600	-0.16167800
C	5.86436700	-4.77947100	-1.32254700
C	4.84189400	-4.12783000	-2.01808600
C	3.24963700	-2.24231500	-2.37640500
C	1.98576800	-2.85151900	-2.47332600
C	0.93785500	-2.21039300	-3.14202900
C	1.14477700	-0.95900100	-3.73421400
C	2.40770200	-0.35651000	-3.66846400
C	3.45564000	-0.99568000	-2.99667900

H	6.27655400	-2.56391800	1.22120400
H	7.19386600	-4.69663700	0.38581800
H	6.24933100	-5.73033200	-1.68866200
H	4.43637600	-4.56584000	-2.92893500
H	1.81264700	-3.80563200	-1.98025700
H	-0.04485000	-2.67550700	-3.16857900
H	0.32234300	-0.45062900	-4.23506700
H	2.57518700	0.61635000	-4.12879300
H	4.43334300	-0.52231400	-2.93575800
P	4.13537900	-0.76964700	0.32121200
C	5.31067800	0.56877200	-0.25001100
C	4.61433800	1.94392200	-0.32712700
C	6.62399400	0.63164300	0.55573300
H	5.56261400	0.26646600	-1.27758100
C	5.56953000	2.99403500	-0.91910500
H	4.30425800	2.26053400	0.67817700
H	3.69820000	1.86649800	-0.92623600
C	7.56712400	1.70358600	-0.02999100
H	6.39694300	0.88479100	1.60192400
H	7.11818500	-0.35023500	0.55203200
C	6.87494900	3.07794500	-0.10790500
H	5.07002400	3.96900700	-0.94823300
H	5.80838000	2.71355400	-1.95883300
H	8.48191200	1.76384600	0.57815200
H	7.86999600	1.39537400	-1.04420200
H	7.55433600	3.82095700	-0.55099000
H	6.63935000	3.42239600	0.91303900
C	4.30925600	-0.94649200	2.16878700
C	3.82499700	0.34535500	2.86908300
C	3.47204700	-2.16188800	2.63194600

H	5.36550900	-1.10793600	2.42679400
C	3.85342000	0.18876600	4.40159900
H	2.79497200	0.55785100	2.54238900
H	4.44347600	1.19968600	2.56616000
C	3.50046700	-2.30852100	4.16421700
H	2.43244100	-2.00955600	2.30001000
H	3.83428200	-3.08052600	2.15191400
C	3.01559200	-1.02057700	4.85381400
H	3.48222700	1.11175600	4.87097100
H	4.89578700	0.05155300	4.73420300
H	2.87713300	-3.16371400	4.46342500
H	4.53118800	-2.52742500	4.48990300
H	3.06060600	-1.13030300	5.94712600
H	1.96021500	-0.84641600	4.58538200
Au	1.88955700	-0.29950800	-0.09374400
N	-5.87091200	0.43355700	0.33484300
S	-6.42761400	1.10555500	-1.07085300
S	-6.61393100	-0.78986600	1.18476000
O	-7.21651300	0.22741500	-1.93427600
O	-5.27552600	1.86322200	-1.59561200
O	-6.11684900	-0.68943100	2.56140300
O	-8.04132900	-0.93931500	0.89458900
C	-7.61177000	2.47905800	-0.43700400
C	-5.76562000	-2.35767400	0.44618600
F	-8.65338900	1.95969900	0.21783100
F	-6.92595600	3.29085000	0.39317700
F	-8.05181000	3.19366000	-1.48448400
F	-4.51404000	-2.46232500	0.90209100
F	-6.46683400	-3.43941400	0.82357700
F	-5.74527200	-2.29241600	-0.89515800

O	-3.89714800	1.83662400	1.11559900
H	-4.73829700	1.19833100	0.87655100
H	-3.87929600	2.46569300	0.37141000
G			
01			
C	-0.72172500	5.69984900	-2.03653800
C	-0.86334500	4.30967800	-2.00295200
C	-0.69246800	3.60159500	-0.78985500
C	-0.38343800	4.32780600	0.38479600
C	-0.24277900	5.71703100	0.34117800
C	-0.40881200	6.40907100	-0.86769900
H	-0.85370900	6.23148500	-2.97821500
H	-1.10321700	3.75578100	-2.90866400
H	-0.25489100	3.78809400	1.32101900
H	-0.00215800	6.26263100	1.25283700
H	-0.29603700	7.49181700	-0.89812200
C	-0.81705100	2.18395800	-0.75273500
C	-0.92548200	0.97102300	-0.73281500
C	-1.08828200	-0.46592800	-0.64741000
O	-2.16491800	-3.37381500	1.07847400
C	-2.70060200	-3.19945700	2.40210200
H	-2.25994300	-2.32216600	2.90008800
H	-3.79410200	-3.08845100	2.37765800
H	-2.43014900	-4.10555800	2.95574700
C	0.21400700	-1.32070900	-0.56605200
C	-0.18765300	-2.59368100	-0.84511000
C	0.61487500	-3.82013300	-0.79920800
C	0.37882500	-4.87196900	-1.71181400
C	1.67053900	-3.97455700	0.12574300

C	1.19424000	-6.00893100	-1.73244900
H	-0.43243300	-4.78055300	-2.43309300
C	2.48476000	-5.10996300	0.10740200
H	1.84265400	-3.19031600	0.85908500
C	2.25906200	-6.13109600	-0.82789400
H	1.00222200	-6.79885600	-2.45854800
H	3.29499400	-5.20237900	0.83089700
H	2.89394500	-7.01638500	-0.84193500
C	-1.84095700	-1.18511400	-1.80911300
H	-1.29999600	-1.09624100	-2.75763000
H	-2.87934700	-0.85656900	-1.92736600
C	-1.68796600	-2.57836200	-1.16363900
H	-2.07498600	-3.44469100	-1.70542500
C	-2.42712900	-2.32769200	0.19250800
C	-1.94258600	-0.90705700	0.60423300
H	-2.77349600	-0.22210400	0.78809900
H	-1.31310900	-0.94103700	1.49815200
C	5.80168300	-0.94283900	-0.78843200
C	5.57734000	-0.10105400	0.33337300
C	6.62914400	0.11829700	1.24521400
C	7.87666900	-0.49054700	1.07432500
C	8.08915600	-1.34182900	-0.01646800
C	7.05814200	-1.56138000	-0.93489700
C	4.74305600	-1.22328600	-1.79893300
C	4.19684700	-2.51559900	-1.88807100
C	3.13340100	-2.78054900	-2.75648800
C	2.60901800	-1.75766300	-3.55477300
C	3.16715900	-0.47383600	-3.49816300
C	4.23061500	-0.20811700	-2.62842500
H	6.47250300	0.75776200	2.11050100

H	8.67260500	-0.30595300	1.79454700
H	9.05355200	-1.82899000	-0.15467000
H	7.21915300	-2.21295800	-1.79269100
H	4.57379400	-3.30067500	-1.23621300
H	2.69248000	-3.77422800	-2.77575400
H	1.76005600	-1.95640100	-4.20700400
H	2.76347200	0.32670800	-4.11669800
H	4.65559900	0.79228700	-2.58019000
P	3.92098500	0.65765000	0.63892300
C	4.07639200	2.37421500	-0.09156600
C	2.70032300	2.94996700	-0.48625000
C	4.88676100	3.34783600	0.78833900
H	4.64862000	2.20622000	-1.01551800
C	2.85726100	4.32218500	-1.16472100
H	2.07198100	3.05907800	0.40675700
H	2.17776900	2.24593000	-1.14609000
C	5.02715000	4.71759400	0.09258800
H	4.37159100	3.48561500	1.75033400
H	5.87976900	2.92709500	1.00247000
C	3.64905900	5.29795600	-0.27588100
H	1.86592900	4.73059000	-1.39570000
H	3.39234300	4.19122900	-2.12056700
H	5.57763200	5.41056400	0.74631800
H	5.62397400	4.59206600	-0.82595000
H	3.76629700	6.26718900	-0.78278700
H	3.07697100	5.48316600	0.64841400
C	3.78954900	0.83761600	2.49049500
C	2.48183300	1.57916800	2.85581300
C	3.81160800	-0.57029300	3.12908000
H	4.63777200	1.42613900	2.86824900

C	2.29375200	1.64827500	4.38378900
H	1.63227700	1.04454900	2.40384300
H	2.48826700	2.59146300	2.43368200
C	3.62290100	-0.49187900	4.65523600
H	2.99020900	-1.15916500	2.69043000
H	4.74928600	-1.08635000	2.88363900
C	2.32014600	0.24470500	5.01478800
H	1.34486500	2.15535400	4.61237000
H	3.10219600	2.25746900	4.82192200
H	3.62003000	-1.50675800	5.07919000
H	4.47784300	0.04431100	5.10038200
H	2.20738500	0.31439100	6.10672400
H	1.46403200	-0.33565100	4.63333200
Au	2.01582700	-0.49244000	-0.06242700
N	-5.31112400	-0.01837100	0.04191700
S	-5.95104000	0.53350400	-1.43400100
S	-5.79423000	0.41443900	1.60921700
O	-7.29025600	1.07882000	-1.25586100
O	-5.63155900	-0.50837300	-2.40886900
O	-4.68852300	0.05627800	2.49288800
O	-6.42701600	1.72575300	1.60300600
C	-4.78321400	2.03339500	-1.81084100
C	-7.16429900	-0.89642900	1.93957700
F	-5.40091200	2.81567300	-2.70280700
F	-4.54385300	2.71865500	-0.69282400
F	-3.63903300	1.57915800	-2.32560600
F	-7.64651000	-0.71232300	3.17230500
F	-8.14393800	-0.77359300	1.04219800
F	-6.62183400	-2.12224900	1.84590600
C	-4.53549700	-3.36303900	-0.58764800

H	-5.60757800	-3.22843100	-0.40901400
H	-4.34806100	-3.41839600	-1.66864500
H	-4.18789500	-4.27993900	-0.09520800
O	-3.88057700	-2.21696900	-0.00868900
H	-4.68029400	-0.89114700	-0.01652700
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C	-0.87521600	5.64892000	-2.01082100
C	-0.99998800	4.25697900	-1.98379900
C	-0.82153800	3.54551100	-0.77380800
C	-0.52278000	4.26999400	0.40453800
C	-0.39857100	5.66094800	0.36741700
C	-0.57177300	6.35644000	-0.83846000
H	-1.01270000	6.18325200	-2.95017100
H	-1.23215100	3.70440400	-2.89233700
H	-0.38900400	3.72770200	1.33850500
H	-0.16518700	6.20515700	1.28177900
H	-0.47190200	7.44058000	-0.86384000
C	-0.92730700	2.12608500	-0.74355200
C	-1.01502500	0.91142800	-0.72945800
C	-1.14775400	-0.52920200	-0.65298800
O	-2.10445600	-3.47881600	1.05964900
C	-2.60183800	-3.33184500	2.40168700
H	-2.16339300	-2.45211200	2.89797500
H	-3.69767900	-3.24511800	2.41074100
H	-2.29588600	-4.23900100	2.93467800
C	0.17440000	-1.35561500	-0.59371500
C	-0.19779600	-2.63396800	-0.88865300
C	0.63289100	-3.84219300	-0.86237600

C	0.42258400	-4.88158700	-1.79510300
C	1.68848000	-3.99004100	0.06332300
C	1.26241100	-6.00009400	-1.83337000
H	-0.38798100	-4.79375500	-2.51784900
C	2.52738200	-5.10695500	0.02725600
H	1.84079900	-3.21543100	0.81106400
C	2.32660200	-6.11548300	-0.92713600
H	1.09043500	-6.78046200	-2.57462700
H	3.33721900	-5.19506600	0.75169000
H	2.98103900	-6.98606700	-0.95533100
C	-1.89745100	-1.25474100	-1.81170400
H	-1.37142900	-1.14455400	-2.76628900
H	-2.94438500	-0.95069500	-1.91508600
C	-1.70314900	-2.64954700	-1.18080700
H	-2.09135400	-3.52191100	-1.71893400
C	-2.42053600	-2.43335700	0.19180800
C	-1.98103300	-0.99867100	0.60383100
H	-2.83558000	-0.34298400	0.78692500
H	-1.34761100	-1.00794500	1.49512200
C	5.76723000	-0.85844300	-0.76549600
C	5.50780000	-0.04339800	0.36844700
C	6.54150200	0.18321200	1.29897000
C	7.80585000	-0.39139600	1.13323700
C	8.05499000	-1.21259100	0.02727600
C	7.04122200	-1.44078200	-0.90818200
C	4.72494200	-1.15543900	-1.78871100
C	4.20971800	-2.45959600	-1.88950500
C	3.16176400	-2.74529900	-2.77009200
C	2.62184800	-1.73109200	-3.56899400
C	3.14896800	-0.43482700	-3.50014600

C	4.19721100	-0.14864100	-2.61841400
H	6.35765600	0.80089300	2.17464200
H	8.58719600	-0.20242600	1.86815600
H	9.03345200	-1.67160300	-0.10815900
H	7.22925500	-2.07183300	-1.77576200
H	4.59839100	-3.23915500	-1.23787100
H	2.74534800	-3.74917600	-2.79964000
H	1.78448200	-1.94634900	-4.23091300
H	2.73308200	0.35896300	-4.11927300
H	4.59861600	0.86090600	-2.56119200
P	3.83354800	0.68115900	0.65665400
C	3.96780900	2.40345100	-0.06502000
C	2.58659100	2.95843100	-0.47127200
C	4.75347500	3.38594700	0.82734000
H	4.55190900	2.24961100	-0.98400800
C	2.72735800	4.33704000	-1.14036100
H	1.94637500	3.05121700	0.41497600
H	2.08392500	2.24979000	-1.14149700
C	4.87869400	4.76097700	0.13924700
H	4.22660500	3.51114900	1.78468100
H	5.75097600	2.98048600	1.04987700
C	3.49504300	5.32110800	-0.23952300
H	1.73156200	4.73051400	-1.37834100
H	3.27323000	4.22025500	-2.09196400
H	5.41200400	5.45950500	0.80124800
H	5.48598200	4.64918200	-0.77419800
H	3.60161800	6.29430300	-0.74116500
H	2.91161200	5.49350900	0.68018200
C	3.67385600	0.85238600	2.50685100
C	2.34967300	1.57303800	2.85516900

C	3.71037900	-0.55772500	3.14029500
H	4.50710700	1.45337000	2.89792000
C	2.13266000	1.62771800	4.37979400
H	1.51503100	1.03192900	2.38369900
H	2.35093300	2.58895200	2.44179500
C	3.49110000	-0.49143400	4.66293700
H	2.90961700	-1.16103700	2.68348500
H	4.66252500	-1.05411300	2.91054800
C	2.16896800	0.22020100	5.00114800
H	1.17221900	2.11890400	4.59432600
H	2.92361300	2.24546000	4.83742700
H	3.49804900	-1.50878800	5.08085200
H	4.32749800	0.05712600	5.12781700
H	2.03283200	0.27990700	6.09100200
H	1.33061300	-0.37142200	4.59812600
Au	1.95846500	-0.49880100	-0.07396400
N	-5.38260000	-0.19333100	0.00348600
S	-6.02318600	0.36916700	-1.47089800
S	-5.87651900	0.21186100	1.57864000
O	-7.36784400	0.89822000	-1.28841800
O	-5.68770700	-0.65818600	-2.45550500
O	-4.77295200	-0.15828100	2.45966200
O	-6.50732300	1.52390100	1.58285700
C	-4.87231100	1.89003900	-1.82250300
C	-7.24756400	-1.10534700	1.88351100
F	-5.50983400	2.68909300	-2.68470300
F	-4.62453100	2.54754100	-0.69017200
F	-3.73139600	1.46090200	-2.36503700
F	-7.70977900	-0.95640100	3.12902300
F	-8.23970100	-0.94549900	1.00636200

F	-6.71149500	-2.32658200	1.74158500
O	-3.87620800	-2.39682800	0.00031700
H	-4.76831200	-1.06180200	-0.06355600
H	-4.13477700	-3.19430800	-0.48485900

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C	2.78284800	5.68848600	0.99462000
C	1.75653900	4.76797300	1.22497400
C	2.02183200	3.55545700	1.90184400
C	3.34141100	3.30011200	2.34799700
C	4.36113200	4.22505600	2.11040100
C	4.08832500	5.42131100	1.43059500
H	2.56286300	6.61492300	0.46539300
H	0.74747600	4.97218000	0.88113900
H	3.55181700	2.36859600	2.86957000
H	5.37256600	4.01182100	2.45466600
H	4.88631200	6.13832400	1.24304400
C	1.00205400	2.58069000	2.10136700
C	0.16618100	1.70651500	2.24692600
C	-0.71471800	0.57215900	2.44149300
O	-1.26374400	-2.73853800	3.49554800
C	-0.14661100	-3.46569500	4.02097000
H	0.77919300	-3.20591000	3.48642000
H	-0.01126500	-3.27745800	5.09688800
H	-0.36712300	-4.52755700	3.85775100
C	-1.14306700	-0.20705500	1.13896200
C	-2.17476400	-1.02139200	1.57889900
C	-2.86664700	-2.09326300	0.86246300
C	-4.24707400	-2.30750600	1.07545700

C	-2.18845000	-2.94297100	-0.03525800
C	-4.93291000	-3.30497900	0.37950600
H	-4.78743400	-1.65302700	1.75371400
C	-2.87250500	-3.95106500	-0.71909100
H	-1.11708300	-2.82802800	-0.16978000
C	-4.24820600	-4.13244100	-0.52243300
H	-6.00280400	-3.43505400	0.53726200
H	-2.32771300	-4.60181700	-1.40208900
H	-4.78048300	-4.91746300	-1.05863500
C	-2.08651600	0.78698200	3.13542200
H	-2.74772500	1.44208200	2.56465400
H	-1.99065700	1.13388300	4.17126600
C	-2.47970200	-0.70185500	3.03246200
H	-3.46365900	-1.00771800	3.39131400
C	-1.29453200	-1.36103100	3.83540600
C	-0.06771400	-0.51987400	3.37928900
H	0.42090800	-0.05657600	4.24267200
H	0.65809200	-1.11780600	2.82346900
C	1.99282900	-2.86197600	-2.93967400
C	2.95790500	-2.48767300	-1.96724300
C	4.13205400	-3.25846600	-1.83886300
C	4.34847100	-4.39310900	-2.62588100
C	3.37763000	-4.78713300	-3.55420200
C	2.21725300	-4.02417500	-3.70566500
C	0.75739100	-2.07841000	-3.21171100
C	-0.50590300	-2.68547200	-3.09316500
C	-1.67014800	-1.96494600	-3.37492900
C	-1.58948600	-0.62809500	-3.78364900
C	-0.33719000	-0.01630000	-3.91046700
C	0.82708000	-0.73614500	-3.62806200

H	4.88521100	-2.98673700	-1.10439500
H	5.26533300	-4.96829800	-2.50473000
H	3.52800300	-5.67643300	-4.16485000
H	1.47021300	-4.30865100	-4.44514800
H	-0.56954800	-3.71884000	-2.75665400
H	-2.64007700	-2.43909900	-3.24724600
H	-2.49386600	-0.06042400	-3.98814500
H	-0.26842200	1.02378600	-4.21910100
H	1.79688200	-0.26114400	-3.74935700
P	2.65832400	-1.08791100	-0.80309300
C	3.59962100	0.36477700	-1.50672400
C	3.03860400	1.70202100	-0.97866000
C	5.12766100	0.25842600	-1.32248700
H	3.39571200	0.31515000	-2.58593800
C	3.76787800	2.89369900	-1.62448700
H	3.15741500	1.75553300	0.10899300
H	1.96435700	1.75755400	-1.17713000
C	5.83051800	1.45913100	-1.98949000
H	5.36999100	0.25805000	-0.24963700
H	5.49843000	-0.68451700	-1.74907800
C	5.29251100	2.79261000	-1.43791300
H	3.38832900	3.82664900	-1.18740700
H	3.53638800	2.91450600	-2.70304600
H	6.91697400	1.38490200	-1.83229200
H	5.65442400	1.41811600	-3.07713400
H	5.79502300	3.63822200	-1.93049800
H	5.52509000	2.85899000	-0.36301100
C	3.52827300	-1.59558200	0.77228500
C	3.49838700	-0.45431500	1.81267200
C	2.85493100	-2.86577600	1.33797000

H	4.58007000	-1.81346600	0.54042000
C	4.15928500	-0.89933600	3.13249000
H	2.45615500	-0.16105200	1.99592400
H	4.01679800	0.42978800	1.42622200
C	3.51765200	-3.30633300	2.65640200
H	1.79182800	-2.64201900	1.51730900
H	2.89173800	-3.67931100	0.60156900
C	3.50478400	-2.17158900	3.69669300
H	4.09604600	-0.08182500	3.86576400
H	5.22992100	-1.09170200	2.95065700
H	2.99948900	-4.19343200	3.04946900
H	4.56061100	-3.60270400	2.45592700
H	4.01989400	-2.48999300	4.61470000
H	2.46444800	-1.94334500	3.97121500
Au	0.47557500	-0.63149800	-0.14978900
N	-2.54823600	1.49506400	-0.48384500
S	-1.76802200	2.51873900	-1.56737200
S	-4.21752500	1.48836900	-0.30240000
O	-2.48740700	2.64906400	-2.83646200
O	-0.35280200	2.15954900	-1.52560600
O	-4.49377300	0.84199800	0.98071200
O	-4.81686100	2.77721500	-0.65109400
C	-1.85598700	4.26294900	-0.71087000
C	-4.82696600	0.22462400	-1.63298500
F	-2.94697100	4.93102200	-1.08162900
F	-1.83627900	4.12777600	0.62274000
F	-0.76665300	4.95029600	-1.10260400
F	-6.03819000	-0.21507000	-1.25546600
F	-4.92327400	0.81069600	-2.83111500
F	-3.98280800	-0.80800600	-1.70855500

C	-2.58809800	-1.75165700	5.83660600
H	-2.40656300	-1.76988100	6.91812800
H	-3.48012900	-1.13682500	5.63404400
H	-2.76056100	-2.77573100	5.47423300
O	-1.41258700	-1.17729500	5.24478800
H	-1.87587400	0.68808300	0.20949400

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C	4.37052300	4.35181700	1.66765100
C	3.35748400	3.45860400	2.02501500
C	2.02668200	3.66932100	1.58866200
C	1.74175800	4.80737000	0.80002700
C	2.76157900	5.69671300	0.44976900
C	4.07836000	5.47283300	0.87630300
H	5.39048000	4.17295300	2.00636400
H	3.58112300	2.58522200	2.63366400
H	0.72339200	4.97884800	0.46565000
H	2.52727500	6.56640100	-0.16293800
H	4.87034200	6.16532500	0.59465800
C	1.01696900	2.71924400	1.91612100
C	0.19847300	1.85761900	2.18291100
C	-0.63974800	0.72274400	2.51368400
O	-1.01111100	-2.51823000	3.82277700
C	0.18143500	-3.16484800	4.28822700
H	1.04706500	-2.89552800	3.66483700
H	0.39237300	-2.91119000	5.33813300
H	-0.00038400	-4.24273300	4.20123600
C	-1.12106900	-0.16162700	1.29900100
C	-2.10694400	-0.96199400	1.85422100

C	-2.81598300	-2.09268800	1.25404800
C	-4.18450400	-2.29647300	1.54092600
C	-2.16562900	-3.00988400	0.40358100
C	-4.88778200	-3.35442500	0.96156200
H	-4.70310300	-1.58977700	2.18257400
C	-2.86607600	-4.08049000	-0.15833800
H	-1.10296400	-2.89636800	0.20941300
C	-4.23062100	-4.25398700	0.10952500
H	-5.94938500	-3.47640900	1.17258400
H	-2.34248800	-4.78458900	-0.80361600
H	-4.77522200	-5.08714600	-0.33351700
C	-1.97110900	0.95040900	3.27699800
H	-2.68684000	1.54537500	2.70682100
H	-1.82269000	1.37027000	4.27885300
C	-2.32226600	-0.55319900	3.30272300
H	-3.26569700	-0.86417800	3.76070400
C	-1.06731800	-1.12196400	4.06644500
C	0.09919500	-0.27637100	3.48464100
H	0.61983400	0.26400900	4.28193300
H	0.81211400	-0.88532500	2.92548000
C	1.86282700	-3.12289900	-2.66588700
C	2.86776900	-2.62892800	-1.79184000
C	4.06134200	-3.36414300	-1.63663600
C	4.26133700	-4.57639400	-2.30349100
C	3.25537400	-5.08299100	-3.13479300
C	2.07391800	-4.35865900	-3.31086700
C	0.59590200	-2.39653900	-2.95084700
C	-0.64301700	-3.01545200	-2.70443700
C	-1.83926100	-2.34876000	-2.98414300
C	-1.81685000	-1.05616400	-3.52137400

C	-0.59013800	-0.43375700	-3.77844000
C	0.60624100	-1.09949600	-3.49655700
H	4.84186400	-3.00140400	-0.97281200
H	5.19312800	-5.12289300	-2.16490400
H	3.39395400	-6.03126000	-3.65242900
H	1.29859200	-4.73391400	-3.97702700
H	-0.66213100	-4.01238200	-2.26767500
H	-2.78782000	-2.82806900	-2.75552900
H	-2.74644400	-0.52962800	-3.72233100
H	-0.56439400	0.57418400	-4.18545200
H	1.55398000	-0.61662500	-3.71764600
P	2.59528600	-1.11529000	-0.77369900
C	3.44302800	0.27602800	-1.69323900
C	2.86538200	1.64912400	-1.29091000
C	4.98231900	0.23323800	-1.59049800
H	3.18256500	0.09643100	-2.74580300
C	3.50952600	2.77064000	-2.12531000
H	3.05488900	1.84347200	-0.22931000
H	1.77896500	1.64414200	-1.41849000
C	5.60598200	1.37053800	-2.42608400
H	5.28733200	0.35266800	-0.54061800
H	5.35748800	-0.74088900	-1.93585700
C	5.04466300	2.74295700	-2.00896900
H	3.11618600	3.74006000	-1.79174800
H	3.22312300	2.64353200	-3.18300800
H	6.70069200	1.35023300	-2.31729500
H	5.38140600	1.19589300	-3.49116800
H	5.49054400	3.53760200	-2.62542400
H	5.32587000	2.94686000	-0.96311200
C	3.58361900	-1.40202500	0.78610700

C	3.55565500	-0.14129100	1.67938500
C	3.01794200	-2.62440700	1.54253700
H	4.62857400	-1.59704000	0.50752400
C	4.30021200	-0.38455400	3.00546900
H	2.51494000	0.14392200	1.88343400
H	4.01596100	0.70355000	1.15791500
C	3.77482700	-2.85988100	2.86315500
H	1.95471300	-2.43461100	1.75473500
H	3.06247300	-3.52100000	0.91068900
C	3.74449800	-1.60717200	3.75702700
H	4.22724400	0.51586300	3.63308700
H	5.37029300	-0.54649700	2.79307300
H	3.33288900	-3.71800600	3.39036700
H	4.82185900	-3.12211800	2.63803000
H	4.31947700	-1.78208900	4.67824400
H	2.70526300	-1.40520600	4.05619100
Au	0.43597200	-0.65806200	-0.03878400
N	-2.64051800	1.41587200	-0.34519800
S	-4.29896700	1.38757700	-0.07899600
S	-1.94566700	2.35061700	-1.55934000
O	-4.94421500	2.63825500	-0.48018000
O	-4.49482500	0.82448800	1.25713500
O	-0.52395800	2.01594600	-1.57613300
O	-2.74261300	2.36001200	-2.78830300
C	-4.94209600	0.02497700	-1.29356200
C	-2.00878400	4.15992100	-0.84834000
F	-5.13763600	0.53804900	-2.51261000
F	-4.06060600	-0.97675100	-1.36690100
F	-6.10727200	-0.43950100	-0.81570500
F	-0.96276200	4.82576000	-1.37341900

F	-3.13535200	4.78032000	-1.19455900
F	-1.89288700	4.13553300	0.48641100
O	-1.14485300	-0.85678200	5.46493200
H	-1.91773800	0.65783200	0.35403500
H	-1.93679600	-1.31970000	5.77896400

IM5

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C	6.49924500	-0.70296800	1.35291900
C	5.12703200	-0.44433400	1.29688500
C	4.44279400	-0.47644400	0.05811500
C	5.17316900	-0.77498400	-1.11726700
C	6.54527500	-1.03117900	-1.05041700
C	7.21345800	-0.99691600	0.18224800
H	7.01276200	-0.67555400	2.31325200
H	4.57079600	-0.21711800	2.20454600
H	4.65241500	-0.80260100	-2.07269900
H	7.09512000	-1.25902600	-1.96280900
H	8.28277300	-1.19824500	0.23017400
C	3.04126800	-0.21486200	-0.00666300
C	1.84382800	0.00289600	-0.07081500
C	0.42072900	0.27555500	-0.14817200
O	-2.52219700	1.57479600	1.03503200
C	-2.56999200	2.44369200	2.17323800
H	-1.60180900	2.48297200	2.70005500
H	-2.86383500	3.46381400	1.88788000
H	-3.32386600	2.01406300	2.84391200
C	-0.52219800	-0.88003000	0.21263400
C	-1.73497200	-0.61485300	-0.32476900
C	-2.97793100	-1.37810300	-0.19385000

C	-4.23151700	-0.74474500	-0.33184500
C	-2.95058600	-2.76691200	0.06636500
C	-5.41794100	-1.47449200	-0.20062600
H	-4.26425100	0.32858000	-0.50090000
C	-4.13682100	-3.49314700	0.19683900
H	-1.98955300	-3.27311100	0.14874100
C	-5.37756900	-2.85047400	0.06353700
H	-6.37676000	-0.96628600	-0.30048000
H	-4.09573100	-4.56396900	0.39470000
H	-6.30225400	-3.41798600	0.16216900
C	-0.15932000	0.64328300	-1.55066500
H	-0.02460000	-0.16785400	-2.27510200
H	0.26654400	1.57088600	-1.94469200
C	-1.61549900	0.74111100	-1.03465500
H	-2.40366000	0.97977000	-1.75397500
C	-1.48983800	1.82181000	0.11174700
C	-0.04957100	1.54102100	0.67988500
H	0.62903100	2.38089900	0.49180600
H	-0.06560600	1.33155100	1.75312000
C	-0.90877400	3.71607900	-1.36631200
H	-1.19194900	4.77411500	-1.43570900
H	0.17298800	3.65676800	-1.15536100
H	-1.11275600	3.23171000	-2.33569700
O	-1.70240200	3.17153700	-0.31857300
H	-0.25460600	-1.69004700	0.88524800

IM5'

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C	6.71695100	0.40305900	0.16415200
C	5.34652400	0.67680300	0.15947000

C	4.40844000	-0.37192600	0.00462900
C	4.88417100	-1.69698800	-0.14376400
C	6.25645200	-1.95984900	-0.13695200
C	7.17765100	-0.91338400	0.01626300
H	7.42813100	1.21961800	0.28302500
H	4.98687900	1.69782000	0.27353500
H	4.16727500	-2.50735500	-0.26275300
H	6.60816900	-2.98443000	-0.25197400
H	8.24655300	-1.12236200	0.02036400
C	3.00768500	-0.10145400	-0.00324900
C	1.80964100	0.12124600	-0.01453700
C	0.38644600	0.39688800	-0.02996300
C	-0.54739800	-0.79350000	0.22029500
C	-1.77559300	-0.47121400	-0.24930700
C	-3.02283800	-1.23473100	-0.14116300
C	-4.27358400	-0.58107100	-0.20181200
C	-3.00574800	-2.63785300	0.03389200
C	-5.46559500	-1.30449200	-0.07822200
H	-4.30489700	0.49956200	-0.32283200
C	-4.19649600	-3.35665800	0.15292700
H	-2.04952200	-3.15861600	0.05653900
C	-5.43334700	-2.69350600	0.09943100
H	-6.42026700	-0.78134700	-0.12037700
H	-4.16352000	-4.43817600	0.28056300
H	-6.36113700	-3.25670600	0.19025900
C	-0.23083600	0.94202300	-1.36484600
H	-0.08795200	0.24429900	-2.19820800
H	0.14485100	1.93972300	-1.62182400
C	-1.67275500	0.94902200	-0.81435300
H	-2.47808000	1.24092800	-1.49232100

C	-1.49576900	1.92906600	0.42134600
C	-0.08313000	1.53199800	0.96714300
H	0.59345700	2.39156300	0.91288000
H	-0.13402500	1.17265900	1.99989100
C	-2.59665500	3.81740700	-0.59573800
H	-2.41902000	4.89539000	-0.68685400
H	-2.74341200	3.39432300	-1.60325800
H	-3.49540700	3.64351200	0.01210500
O	-1.42357400	3.28195200	0.03751100
H	-0.26296500	-1.67258300	0.79241500
O	-2.54491500	1.81816500	1.38500300
H	-2.67250700	0.87592400	1.56486300

TS10

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C	-6.57459900	-0.61065000	-1.29526400
C	-5.19378800	-0.39960200	-1.25476400
C	-4.49831100	-0.45117000	-0.02293000
C	-5.22557100	-0.71995900	1.16128000
C	-6.60635900	-0.92875000	1.10980500
C	-7.28582100	-0.87627100	-0.11602400
H	-7.09703900	-0.56845600	-2.25022600
H	-4.63973800	-0.19414000	-2.16890400
H	-4.69582100	-0.76127300	2.11123000
H	-7.15414000	-1.13384800	2.02880300
H	-8.36188700	-1.04073200	-0.15203200
C	-3.08738300	-0.24275700	0.02423800
C	-1.88229700	-0.06802400	0.06832600
C	-0.44764300	0.13708000	0.11207500
C	0.43110200	-1.07690700	-0.23246300

C	1.67249700	-0.84858000	0.25334800
C	2.88858700	-1.64646600	0.08347300
C	4.15824800	-1.03039700	0.09824100
C	2.81809500	-3.04559900	-0.10043500
C	5.32038900	-1.78974600	-0.07575900
H	4.22010500	0.05042200	0.20302800
C	3.98086100	-3.80076700	-0.27185000
H	1.84509400	-3.53516900	-0.08919000
C	5.23816600	-3.17669600	-0.25945900
H	6.29203900	-1.29660100	-0.07270200
H	3.90906900	-4.87964500	-0.40657100
H	6.14408200	-3.76743700	-0.38969000
C	0.18441200	0.53156100	1.49023000
H	0.01228700	-0.23929000	2.24972700
H	-0.15105300	1.51415200	1.83943300
C	1.63058000	0.52634200	0.94662300
H	2.45367200	0.73722900	1.63261000
C	1.51363300	1.52797200	-0.22445900
C	0.08238400	1.32543300	-0.79337300
H	-0.54155300	2.21488000	-0.66571000
H	0.12226400	1.04940600	-1.85195800
C	2.31887100	3.49099500	1.48263700
H	2.32410000	4.57770400	1.65990300
H	2.18713600	2.97865800	2.44618000
H	3.28510900	3.19673700	1.03856500
O	1.23343100	3.17332900	0.60649600
H	0.10852600	-1.89213800	-0.87410800
O	2.53872700	1.74120500	-0.99101400
H	2.29023000	2.80410900	-1.51945400
O	1.83039900	3.94492400	-1.59256200

H	1.45709600	3.76040700	-0.45291400
H	2.55365600	4.58710900	-1.60035600
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C	-6.19983500	-0.57759400	-1.29918200
C	-4.83954600	-0.26204200	-1.24889800
C	-4.15076200	-0.26249300	-0.01230800
C	-4.86291700	-0.58688000	1.16699400
C	-6.22356500	-0.89983700	1.10563300
C	-6.89686200	-0.89632600	-0.12465200
H	-6.71767800	-0.57343700	-2.25749000
H	-4.29648100	-0.01349300	-2.15888300
H	-4.33855200	-0.58880100	2.12079600
H	-6.76078600	-1.14632000	2.02060600
H	-7.95735500	-1.14060600	-0.16785200
C	-2.76281500	0.06593700	0.04165700
C	-1.57885900	0.35068700	0.08090700
C	-0.17425000	0.70920800	0.11355500
C	0.84293000	-0.40729600	-0.17955300
C	2.04942900	-0.01977800	0.29858800
C	3.35731700	-0.65523100	0.11613100
C	4.54193700	0.11031200	0.17169300
C	3.46018600	-2.04310400	-0.12928200
C	5.78941600	-0.49248000	-0.02600800
H	4.47998000	1.18346400	0.34224500
C	4.70696300	-2.64176300	-0.32092800
H	2.55486600	-2.64794400	-0.15227200
C	5.87813500	-1.86901600	-0.27103100
H	6.69282200	0.11509000	0.01072400

H	4.76872100	-3.71403700	-0.50367200
H	6.84983500	-2.33859400	-0.41818700
C	0.40403300	1.23458900	1.47296100
H	0.31123300	0.49293900	2.27471400
H	-0.04933400	2.18868200	1.77528400
C	1.85286300	1.36328000	0.94493000
H	2.64009100	1.70194500	1.62197000
C	1.62708400	2.28163700	-0.28520800
C	0.22762400	1.90888500	-0.82842900
H	-0.44935700	2.76426500	-0.69324700
H	0.25267900	1.64109100	-1.88999300
H	0.62125100	-1.27437700	-0.79507100
O	2.38837700	3.11074500	-0.73188800

TS-S1

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C	3.83984800	-3.12418100	-1.26184200
C	4.13680100	-2.42376600	-0.06148000
C	4.95876400	-3.03846900	0.90528000
C	5.46200000	-4.32942800	0.72173700
C	5.13796800	-5.03682700	-0.44169100
C	4.33993100	-4.43454200	-1.41692200
C	3.05222700	-2.55373300	-2.38949900
C	1.95367000	-3.26329900	-2.90958900
C	1.24201800	-2.77346500	-4.00816000
C	1.61565400	-1.56423200	-4.60679400
C	2.70051800	-0.84320500	-4.09378200
C	3.41621800	-1.33771300	-2.99917400
H	5.19899200	-2.51130400	1.82533000
H	6.09378000	-4.77928600	1.48627100

H	5.51377900	-6.04745500	-0.59542600
H	4.11042400	-4.97014500	-2.33685800
H	1.65140500	-4.19474800	-2.43427200
H	0.38298400	-3.32562400	-4.38312900
H	1.06108900	-1.18200700	-5.46221800
H	3.00038600	0.09794700	-4.55265700
H	4.28045300	-0.79109900	-2.63642900
P	3.42525200	-0.76000300	0.30222700
C	4.78416400	0.42721500	-0.20941100
C	4.21063000	1.78183900	-0.67077900
C	5.89071400	0.59609300	0.85224000
H	5.25369700	-0.06005100	-1.07516200
C	5.33575600	2.69720700	-1.18653400
H	3.70128000	2.27151400	0.16795800
H	3.44887500	1.61858700	-1.44486700
C	7.00420500	1.52256500	0.32278000
H	5.46541400	1.03585500	1.76503900
H	6.30827500	-0.38527500	1.11963200
C	6.43353700	2.88206600	-0.12331900
H	4.91254900	3.66926900	-1.47292600
H	5.78086200	2.24842700	-2.09104300
H	7.76966500	1.66153400	1.10063400
H	7.49664200	1.03706800	-0.53606900
H	7.23926500	3.52172600	-0.51292000
H	6.00086300	3.39782500	0.74905200
C	3.31875200	-0.66225600	2.15975700
C	2.79765400	0.72836500	2.58548400
C	2.38640400	-1.76355000	2.70748300
H	4.32673800	-0.79419000	2.57796300
C	2.72394000	0.82247500	4.12206200

H	1.80180600	0.87904900	2.14753200
H	3.43809300	1.52685800	2.19481800
C	2.30436000	-1.68609800	4.24488300
H	1.38885200	-1.61729100	2.26905300
H	2.73528600	-2.75717400	2.39813300
C	1.85128400	-0.29416100	4.72482400
H	2.33048400	1.80733200	4.41315800
H	3.74544400	0.74738300	4.53128400
H	1.61544600	-2.45832700	4.61743600
H	3.29963100	-1.90868400	4.66473300
H	1.88262500	-0.24598500	5.82329100
H	0.80756600	-0.13280200	4.42663500
Au	1.30030000	-0.31599000	-0.52722900
C	-6.93325800	2.18488400	-0.92222100
C	-5.55947200	1.94615400	-0.99705700
C	-4.69895600	2.88949200	-1.61074300
C	-5.25603000	4.07344600	-2.14578000
C	-6.63298500	4.30425400	-2.06506400
C	-7.47613100	3.36389400	-1.45518700
H	-7.57932000	1.45031400	-0.44360800
H	-5.13109900	1.04101000	-0.57759400
H	-4.59982800	4.80351600	-2.61642800
H	-7.04963100	5.22233700	-2.47807300
H	-8.54765500	3.54972100	-1.39300800
C	-3.30346600	2.60882400	-1.67831300
C	-2.14642900	2.23428100	-1.65808300
C	-0.78861400	1.66116500	-1.67955100
O	-1.13312000	-1.99400700	-2.16752300
C	-1.09381900	-2.79769000	-0.97642400
H	-0.24055100	-2.52362900	-0.34150900

H	-2.02852200	-2.70869100	-0.41577100
H	-0.97958600	-3.83113800	-1.32098500
C	0.14086000	2.60802100	-1.05751000
C	0.90651100	3.36612700	-0.49134000
C	1.83313900	4.18199400	0.21768200
C	2.65017900	5.11829500	-0.45750900
C	1.97964700	4.03200400	1.61778700
C	3.59426700	5.86989300	0.24747800
H	2.53919100	5.23916100	-1.53339000
C	2.92697900	4.78716900	2.31354900
H	1.35141500	3.31332200	2.13861800
C	3.74087000	5.70497400	-1.63249700
H	4.22074900	6.58409000	-0.28557500
H	3.03110200	4.66000100	3.39042700
H	4.47981700	6.29095700	2.17734400
C	-0.41577100	1.27455400	-3.14815500
H	0.64877000	1.01107900	-3.16303400
H	-0.60717500	2.09110900	-3.85385000
C	-1.28829100	0.03339600	-3.40589100
H	-2.26181000	0.34268600	-3.79796600
H	-0.83231100	-0.66406000	-4.11301900
C	-1.45202200	-0.65504300	-2.02588300
C	-0.72849400	0.22507500	-0.99932400
H	-1.27238100	0.25477200	-0.05469900
O	-2.95689200	-0.59729200	-1.59546800
N	-3.75768600	-0.82396700	0.77055700
S	-3.29624000	0.27293800	1.97979800
S	-4.57225500	-2.24963100	1.12602300
O	-4.21088000	0.24669100	3.11769100
O	-2.94694900	1.51040000	1.29067700

O	-4.39417700	-3.13084600	-0.03136100
O	-4.33279600	-2.70997000	2.49309400
C	-1.59522800	-0.47571400	2.61935800
C	-6.41459300	-1.69034500	1.02740700
F	-1.71146300	-0.82885200	3.90198300
F	-1.23848500	-1.54734400	1.89644300
F	-0.65444500	0.47052900	2.49912400
F	-6.68155700	-1.27966400	-0.22741700
F	-7.18856600	-2.74365000	1.32076700
F	-6.66688400	-0.69386600	1.87572600
H	-3.29666100	-0.70754200	-0.37296500
C	-3.92108000	-1.18390600	-2.49972100
H	-4.82927500	-1.37097200	-1.92284100
H	-4.14205900	-0.47780100	-3.30974900
H	-3.53649200	-2.12984000	-2.89946100

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C	3.87308500	-3.06658800	-1.33145200
C	4.12474000	-2.43052300	-0.08524900
C	4.88121000	-3.11139200	0.89006400
C	5.36750700	-4.40285800	0.66726500
C	5.09293000	-5.04386600	-0.54620100
C	4.35675300	-4.37694300	-1.52850900
C	3.13760400	-2.42882800	-2.45882200
C	2.03105100	-3.08057600	-3.03328400
C	1.36079200	-2.52133900	-4.12465100
C	1.78521500	-1.30053500	-4.66241700
C	2.88233100	-0.63902800	-4.09771500
C	3.55511500	-1.20216500	-3.00954800

H	5.07607700	-2.63988600	1.84978200
H	5.94724800	-4.90460000	1.44071800
H	5.45658800	-6.05361400	-0.73171800
H	4.16168500	-4.86186400	-2.48388900
H	1.68612500	-4.01914900	-2.60368000
H	0.49165300	-3.02739800	-4.53842900
H	1.26023300	-0.86250000	-5.50970100
H	3.22304000	0.31061900	-4.50829900
H	4.42860700	-0.70103400	-2.60686200
P	3.41773500	-0.77270100	0.31395400
C	4.78692100	0.42871200	-0.13993800
C	4.21313000	1.78318100	-0.60158300
C	5.86637500	0.59223600	0.95046300
H	5.28696000	-0.04087400	-0.99737000
C	5.34322400	2.71498500	-1.07618500
H	3.67415400	2.25778800	0.22754400
H	3.47644200	1.61856100	-1.39932500
C	6.98507400	1.53232200	0.45641300
H	5.42071300	1.01794700	1.85952000
H	6.28496400	-0.38934900	1.21547700
C	6.41393500	2.89330700	0.01538000
H	4.91974700	3.68791600	-1.35939800
H	5.81309600	2.28235100	-1.97591000
H	7.73303600	1.66645100	1.25184800
H	7.49852800	1.06095700	-0.39790700
H	7.22324500	3.54493900	-0.34581600
H	5.95639300	3.39317000	0.88416700
C	3.29209200	-0.71564200	2.17181500
C	2.77526800	0.66966400	2.62189500
C	2.34405100	-1.81703500	2.69122200

H	4.29574600	-0.86249500	2.59645600
C	2.70438700	0.73400600	4.16028100
H	1.78000200	0.82840000	2.18639200
H	3.41443700	1.47582600	2.24578500
C	2.25960200	-1.77402800	4.22985000
H	1.35076500	-1.64635700	2.25203500
H	2.67811000	-2.80845800	2.35984800
C	1.82418900	-0.38786300	4.74196600
H	2.31982900	1.71564800	4.47312000
H	3.72610600	0.64289900	4.56559000
H	1.56016800	-2.54556000	4.58412400
H	3.25102000	-2.01993300	4.64558200
H	1.85914300	-0.36436500	5.84113600
H	0.78101100	-0.20916000	4.45166000
Au	1.29869600	-0.31773500	-0.53413300
C	-6.96113600	2.19846700	-0.96205600
C	-5.58949500	1.94328400	-1.02201900
C	-4.71153400	2.87250900	-1.63216900
C	-5.25050700	4.05899000	-2.18077700
C	-6.62536500	4.30600900	-2.11585900
C	-7.48538800	3.37995700	-1.50764800
H	-7.62135000	1.47455400	-0.48634900
H	-5.17735600	1.03362500	-0.59606700
H	-4.58119300	4.77775200	-2.65017600
H	-7.02746800	5.22558100	-2.53984700
H	-8.55527100	3.57828900	-1.45746400
C	-3.31778200	2.58091200	-1.68479300
C	-2.15885600	2.21162400	-1.66256400
C	-0.79299000	1.65740900	-1.67801400
O	-1.04370200	-1.99827300	-2.24427200

C	-1.04940700	-2.82544900	-1.07467800
H	-0.23737600	-2.54980100	-0.38575900
H	-2.01471700	-2.77683700	-0.55860000
H	-0.89009200	-3.85058000	-1.42917100
C	0.11508900	2.60595800	-1.02733100
C	0.87215400	3.35897200	-0.44280100
C	1.78788200	4.16994300	0.28576800
C	2.62394600	5.10223000	-0.37202900
C	1.90398800	4.02089800	1.68895400
C	3.55568300	5.85046800	0.35274400
H	2.53742300	5.22252600	-1.45020300
C	2.83860400	4.77340900	2.40480200
H	1.26066900	3.30635100	2.19713900
C	3.67076200	5.68747400	1.74100000
H	4.19670000	6.56125000	-0.16745400
H	2.91804100	4.64764600	3.48400300
H	4.39956300	6.27148000	2.30137000
C	-0.39255800	1.30258300	-3.14716800
H	0.67636300	1.05671500	-3.14687100
H	-0.58092000	2.13062900	-3.84084100
C	-1.24240200	0.05457400	-3.44448800
H	-2.20700100	0.35780200	-3.86337900
H	-0.75549800	-0.62290800	-4.15033100
C	-1.44799500	-0.66066200	-2.07642200
C	-0.72608800	0.21072700	-1.02372700
H	-1.29115900	0.22294500	-0.08911300
O	-2.88238600	-0.66231400	-1.66518600
N	-3.80462600	-0.81650800	0.81790300
S	-3.29225600	0.27741200	2.02828900
S	-4.60547600	-2.27951000	1.13006400

O	-4.20362500	0.21460400	3.16338000
O	-2.95919000	1.51557100	1.33893000
O	-4.39359000	-3.13367900	-0.03678900
O	-4.36413900	-2.72809800	2.49723700
C	-1.58770200	-0.50170600	2.61623600
C	-6.44157700	-1.70708900	1.01645100
F	-1.69426700	-0.88618000	3.88906800
F	-1.26049900	-1.55429600	1.85726800
F	-0.64876200	0.44229900	2.50459700
F	-6.67444900	-1.25061100	-0.22485200
F	-7.22160700	-2.76634800	1.25754600
F	-6.69325500	-0.74341000	1.90013900
H	-3.35805200	-0.72683200	-0.17045300
C	-3.82150400	-1.22858600	-2.59702100
H	-4.73785000	-1.43750600	-2.03791300
H	-4.04823600	-0.51254500	-3.39992900
H	-3.43279400	-2.16453500	-3.01980000

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C	4.27528200	-1.56278000	-0.84963500
C	4.19154400	-0.31142900	-0.17942900
C	5.21170900	0.05681800	0.72277800
C	6.28830600	-0.78991000	0.99573000
C	6.35661000	-2.03771300	0.36768700
C	5.36535300	-2.40671200	-0.54227400
C	3.32930800	-2.05190200	-1.89038500
C	2.86964800	-3.38401800	-1.84223900
C	2.12329200	-3.92061700	-2.89340200
C	1.79673600	-3.13448800	-4.00497400

C	2.22160000	-1.80370000	-4.05481900
C	2.98309700	-1.26956900	-3.00952100
H	5.16188400	1.00857800	1.24409300
H	7.05733800	-0.47779000	1.70048000
H	7.18254900	-2.71655200	0.57508000
H	5.43610700	-3.36337100	-1.05626000
H	3.09881900	-3.99078300	-0.96908500
H	1.77880300	-4.95181800	-2.83610300
H	1.20236800	-3.55192600	-4.81547600
H	1.97755600	-1.18087100	-4.91462500
H	3.35822600	-0.25627700	-3.09762900
P	2.76700300	0.83080000	-0.37531800
C	3.25608100	2.02637500	-1.73942700
C	2.02098300	2.45135400	-2.55956000
C	4.09472500	3.23132300	-1.25599200
H	3.91647200	1.43951200	-2.39175800
C	2.41685400	3.37476300	-3.72463200
H	1.30137300	2.96031900	-1.90394300
H	1.51880700	1.55173300	-2.94106000
C	4.47756600	4.12566300	-2.45375000
H	3.52477200	3.83062500	-0.53453200
H	4.99962200	2.87260700	-0.74559500
C	3.22893800	4.58531700	-3.22963600
H	1.51317900	3.70481700	-4.25726500
H	3.02809600	2.80246800	-4.44219000
H	5.04993300	4.99300600	-2.09452900
H	5.13533700	3.55840400	-3.13231400
H	3.52130600	5.22065700	-4.07791100
H	2.59671100	5.19871200	-2.56597000
C	2.67462600	1.82799000	1.18893500

C	1.55107200	2.88239700	1.10815000
C	2.42713000	0.92435800	2.41493100
H	3.63137900	2.35635200	1.30344400
C	1.58868900	3.76721300	2.36763200
H	0.58847800	2.36201500	1.04268600
H	1.63497000	3.50445600	0.21081100
C	2.43625500	1.76741700	3.70479700
H	1.44567500	0.44873500	2.29023500
H	3.17115300	0.12276700	2.48171400
C	1.41977000	2.92446300	3.64491100
H	0.80110600	4.52654700	2.30430000
H	2.55629200	4.29668000	2.40040900
H	2.22514500	1.11713300	4.56482000
H	3.44881000	2.18046100	3.84879900
H	1.52037900	3.56147800	4.53606200
H	0.40350700	2.51019000	3.65824100
Au	0.66665300	-0.13677200	-0.66895700
C	-8.20390600	-0.76872000	-0.61620300
C	-6.81656500	-0.61187300	-0.66904900
C	-6.24515000	0.42361000	-1.44819200
C	-7.10046800	1.29288900	-2.16553600
C	-8.48694100	1.12680200	-2.10486000
C	-9.04404700	0.09753000	-1.33192900
H	-8.63137500	-1.56849500	-0.01243700
H	-6.15918200	-1.27786700	-0.11379100
H	-6.66509200	2.09178600	-2.76332600
H	-9.13501700	1.80351800	-2.66083300
H	-10.12515100	-0.02776100	-1.28666400
C	-4.82928700	0.57121000	-1.49968800
C	-3.61407100	0.61385900	-1.52510700

C	-2.14477500	0.71543300	-1.51809300
O	-0.68005100	-2.62700400	-2.33642700
C	-0.61879300	-3.50231800	-1.20028700
H	0.10587400	-3.11619900	-0.47728700
H	-1.60521100	-3.61749700	-0.73482600
H	-0.27394500	-4.47731000	-1.56294600
C	-1.82035600	1.92698900	-0.75676200
C	-1.66201900	2.98600800	-0.17794800
C	-1.46728600	4.19667200	0.54542000
C	-0.77188700	5.28196000	-0.03741900
C	-1.96140300	4.32915400	1.86468300
C	-0.57332700	6.46248100	0.68301100
H	-0.39662400	5.18641700	-1.05476200
C	-1.76069800	5.51534100	2.57539400
H	-2.49060700	3.49488000	2.31814100
C	-1.06693000	6.58469600	1.99036700
H	-0.03481000	7.29023200	0.22316400
H	-2.14398200	5.60389700	3.59102700
H	-0.91022800	7.50597000	2.54960600
C	-1.58789900	0.79051800	-2.98694400
H	-0.60276400	1.26700400	-2.93505800
H	-2.23954800	1.40838600	-3.61420800
C	-1.45753700	-0.66886200	-3.47420100
H	-2.21228700	-0.90886200	-4.22971600
H	-0.47008900	-0.84948200	-3.91124000
C	-1.62753600	-1.58698000	-2.23081300
C	-1.50494100	-0.64666600	-0.98963700
H	-2.17212000	-1.03343700	-0.21766700
O	-2.95198400	-2.13193000	-2.10653800
N	-0.64977100	-1.70374500	1.66405900

S	-1.99467700	-1.46196000	2.62413700
S	0.69029500	-2.51009500	2.26962000
O	-2.07152500	-2.38339800	3.76095900
O	-3.14053900	-1.26228500	1.73219500
O	1.72233100	-2.44332300	1.22820600
O	1.02101500	-2.16830900	3.65602400
C	-1.65024800	0.28803700	3.33635500
C	0.11721600	-4.39136400	2.29577300
F	-0.69628000	0.24788700	4.27358500
F	-1.25212300	1.08970500	2.33158300
F	-2.77631900	0.78543800	3.87214400
F	1.03201300	-5.11680300	1.62824000
F	0.04457500	-4.82455500	3.55544700
F	-1.07453000	-4.54755500	1.70010300
H	-0.60684500	-1.03730500	0.30907900
C	-3.36743300	-3.02388300	-3.14278800
H	-4.32978900	-3.43430500	-2.81441000
H	-3.51703500	-2.50536500	-4.10520200
H	-2.64578200	-3.84282000	-3.28647600

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C	-3.66668100	3.98908800	1.27954300
C	-2.72441200	2.96290900	1.17070000
C	-2.53593400	2.29334000	-0.06162700
C	-3.31675400	2.68050400	-1.17677000
C	-4.25734900	3.70695900	-1.05691600
C	-4.43649700	4.36456600	0.16885700
H	-3.80147100	4.49695800	2.23373100
H	-2.12630200	2.66738700	2.03057200

H	-3.17486900	2.16903800	-2.12710300
H	-4.85265400	3.99497600	-1.92253500
H	-5.17077000	5.16407100	0.25754500
C	-1.58183800	1.23940400	-0.17694600
C	-0.77779000	0.33075300	-0.26800300
C	0.17374400	-0.78605800	-0.39636500
O	-1.01453400	-4.15696500	0.03018400
C	-0.84670000	-4.72562600	1.33563400
H	0.04253800	-4.31801500	1.84617000
H	-1.72964300	-4.55010000	1.96836700
H	-0.70819600	-5.80262100	1.18350600
C	1.54629600	-0.28232400	-0.27158300
C	2.68980500	0.12191700	-0.16658200
C	4.02655800	0.60171000	-0.02921500
C	4.99638100	0.33384600	-1.02428700
C	4.40233100	1.35792200	1.10655200
C	6.30299700	0.80859800	-0.88181300
H	4.71205700	-0.24635800	-1.90022000
C	5.71150000	1.82810500	1.23894900
H	3.65893000	1.56835500	1.87312100
C	6.66584300	1.55675600	0.24763400
H	7.03999900	0.59532200	-1.65501100
H	5.98724100	2.40945900	2.11788000
H	7.68514100	1.92531500	0.35456900
C	-0.07087500	-1.55897300	-1.74047800
H	0.77020700	-2.25031600	-1.88531800
H	-0.12506500	-0.87812500	-2.59727900
C	-1.37217100	-2.32890800	-1.47202300
H	-2.22823500	-1.65519200	-1.59940800
H	-1.50229900	-3.19719900	-2.12647100

C	-1.29358700	-2.75330000	0.02423000
C	-0.14267700	-1.91317600	0.64973400
H	-0.40138800	-1.51060700	1.63293400
O	-2.46872900	-2.45134500	0.77049300
C	-3.66153500	-3.07604500	0.27971200
H	-4.45369800	-2.82555100	0.99509400
H	-3.94305500	-2.69083500	-0.71477100
H	-3.54767200	-4.16935600	0.21979000
H	0.75137100	-2.54191200	0.73579600

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C	3.58971400	-3.72596200	0.36343300
C	4.39134200	-2.60569700	0.71222500
C	5.59341800	-2.81758800	1.41884600
C	6.00043700	-4.09940400	1.79909300
C	5.19793500	-5.20143800	1.48104100
C	4.00982200	-5.00930700	0.77295700
C	2.32524000	-3.63401800	-0.41622400
C	1.14601200	-4.20788000	0.09637700
C	-0.04056800	-4.17883400	-0.64043000
C	-0.06840500	-3.57893400	-1.90502600
C	1.09415200	-2.99731400	-2.42341100
C	2.28263900	-3.02642200	-1.68536200
H	6.21539100	-1.97019200	1.69521100
H	6.93369200	-4.23287700	2.34428000
H	5.49813000	-6.20604100	1.77577600
H	3.39279600	-5.86536100	0.50445000
H	1.16424300	-4.66350500	1.08521300
H	-0.94962300	-4.60489400	-0.22319000

H	-0.99622800	-3.55400900	-2.47216400
H	1.08049300	-2.52324500	-3.40407400
H	3.18636000	-2.59763600	-2.10881200
P	3.87505900	-0.87946100	0.31945900
C	4.82296400	-0.46643700	-1.24536000
C	4.08145200	0.59718000	-2.08102400
C	6.29650900	-0.08491500	-0.98994000
H	4.82704800	-1.40858100	-1.81280000
C	4.82969700	0.87958900	-3.39609900
H	3.99456100	1.52406400	-1.50058100
H	3.05749900	0.25501700	-2.28340000
C	7.02191700	0.19250800	-2.32194700
H	6.34059900	0.81940000	-0.36708000
H	6.80336100	-0.89149400	-0.44186500
C	6.29338700	1.27880500	-3.13463000
H	4.30890700	1.67149900	-3.95280600
H	4.80991900	-0.02684400	-4.02415500
H	8.06037700	0.49381400	-2.12017200
H	7.06148600	-0.73791000	-2.91215600
H	6.81624400	1.45592100	-4.08607600
H	6.31110100	2.22531100	-2.57044000
C	4.59293800	0.16976300	1.68535500
C	4.31622400	1.66760300	1.41614800
C	3.97758800	-0.26015000	3.03701200
H	5.68144200	0.02260200	1.71486900
C	4.86073900	2.53103500	2.56892200
H	3.23125500	1.82033800	1.32383800
H	4.76124200	1.98605800	0.46648200
C	4.50853300	0.61307700	4.18912000
H	2.88332600	-0.15006100	2.96865500

H	4.18576500	-1.32008300	3.23407300
C	4.25375200	2.10687200	3.91798300
H	4.64397000	3.58764400	2.36317100
H	5.95798700	2.42785900	2.61377800
H	4.03393000	0.30611300	5.13252200
H	5.59270200	0.44466900	4.30102000
H	4.66576600	2.71943200	4.73345300
H	3.16611600	2.28566000	3.89132700
Au	1.61204500	-0.34230200	0.27344800
C	-4.73632400	5.76441200	1.91315600
C	-3.63576600	4.98320600	1.55169200
C	-3.70009000	4.14942200	0.41046200
C	-4.88728900	4.12106800	-0.35763100
C	-5.98259600	4.90300300	0.01648600
C	-5.91216400	5.72664100	1.14920600
H	-4.67766000	6.40222300	2.79413200
H	-2.72228000	5.00516700	2.14308200
H	-4.94084800	3.46965500	-1.22564700
H	-6.89585200	4.86398300	-0.57475700
H	-6.76946000	6.33374900	1.43681900
C	-2.58726000	3.33187700	0.04891800
C	-1.64898400	2.61077400	-0.24927600
C	-0.51589900	1.72340000	-0.58288400
O	-1.42609800	-1.69025100	0.58627100
C	-1.10485400	-1.87524700	1.97619600
H	-0.05003400	-1.62631900	2.16780800
H	-1.75997400	-1.26783300	2.61370900
H	-1.27709500	-2.93541200	2.18382000
C	0.67380900	2.56740500	-0.73896200
C	1.66429600	3.26131100	-0.87757500

C	2.85945100	4.01942000	-1.03560500
C	3.51533600	4.07190800	-2.28845100
C	3.43400900	4.70014300	0.06312500
C	4.71643100	4.77122500	-2.42969200
H	3.07838400	3.55009700	-3.13667400
C	4.63514300	5.39791300	-0.08751700
H	2.93399400	4.66430400	1.02831700
C	5.28408600	5.43294300	-1.33053200
H	5.21203800	4.79746500	-3.39913700
H	5.06830700	5.91367600	0.76854500
H	6.22146500	5.97578400	-1.44339600
C	-0.82343600	0.88284200	-1.87733300
H	0.14372200	0.55868500	-2.27937900
H	-1.34437000	1.48214100	-2.63178700
C	-1.63647800	-0.34060100	-1.39357300
H	-2.69259200	-0.26702300	-1.66594500
H	-1.23186200	-1.26782000	-1.80669700
C	-1.47232000	-0.38872200	0.14066600
C	-0.33031100	0.56484500	0.48291900
H	-0.42415900	0.95831900	1.50413800
O	-2.78723300	0.15051500	0.80326600
H	-2.85202600	1.10480200	0.59159200
N	-4.82966100	-1.03605500	-0.02541700
S	-5.21522900	-2.55883500	0.57628500
S	-5.82622200	-0.06360200	-0.95591800
O	-6.65571500	-2.78918200	0.65246800
O	-4.32362100	-2.79045800	1.71129400
O	-4.93117600	0.92086900	-1.57273800
O	-6.81178300	-0.81300900	-1.72921200
C	-4.56733000	-3.68269500	-0.84169200

C	-6.78862300	0.91902400	0.38921600
F	-5.22935800	-3.42965900	-1.97558900
F	-3.25885200	-3.46657000	-1.03462100
F	-4.75668500	-4.96325600	-0.48642300
F	-5.91183500	1.49138300	1.22791100
F	-7.51663700	1.86953000	-0.21664600
F	-7.59570100	0.10596200	1.07498500
H	-3.82114700	-0.48346900	0.38129300

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C	3.41235000	-3.74880100	0.11733300
C	4.26082400	-2.71096900	0.58586800
C	5.41547100	-3.04897400	1.32097100
C	5.72782300	-4.37893900	1.61637100
C	4.87303200	-5.40099500	1.18670100
C	3.73240000	-5.08277600	0.44588400
C	2.20848100	-3.51543300	-0.72645700
C	0.95957100	-4.02605100	-0.32743700
C	-0.16540700	-3.87401900	-1.14200500
C	-0.05917200	-3.21328900	-2.37195800
C	1.17516800	-2.68900900	-2.77504700
C	2.30048900	-2.83876800	-1.95747600
H	6.07253800	-2.26451000	1.68802100
H	6.62653900	-4.61126800	2.18597000
H	5.09767800	-6.44125600	1.41822100
H	3.07816700	-5.87553200	0.08660200
H	0.87507700	-4.53063600	0.63367700
H	-1.12703600	-4.25494000	-0.81068900
H	-0.93648900	-3.10029600	-3.00663900

H	1.26569500	-2.16922100	-3.72811600
H	3.26170700	-2.45522900	-2.28835600
P	3.84284300	-0.93366600	0.33105700
C	4.88912900	-0.41859300	-1.13704500
C	4.22900200	0.73727300	-1.91704400
C	6.35760100	-0.10864800	-0.77652400
H	4.89706800	-1.30825300	-1.78383300
C	5.04969700	1.08453900	-3.17181400
H	4.15620400	1.62251700	-1.27309400
H	3.20130400	0.45867900	-2.18670900
C	7.16201000	0.24305500	-2.04422600
H	6.39505800	0.74320400	-0.08335300
H	6.81001900	-0.97099700	-0.26668700
C	6.51094400	1.40905100	-2.81214800
H	4.58596900	1.93592100	-3.68880200
H	5.02865700	0.22723700	-3.86582800
H	8.19650400	0.49414600	-1.76674300
H	7.20616400	-0.64290600	-2.69887300
H	7.08746600	1.63284600	-3.72190400
H	6.52938800	2.31400200	-2.18362300
C	4.53814600	-0.05539900	1.82346000
C	4.31933600	1.46949200	1.69100600
C	3.85478700	-0.58405500	3.10471300
H	5.61924100	-0.24666400	1.87707300
C	4.85435500	2.20386700	2.93396100
H	3.24213300	1.66623300	1.58747400
H	4.79950100	1.85948600	0.78664600
C	4.37395400	0.15694700	4.35177200
H	2.76892200	-0.42414900	3.00708400
H	4.01647800	-1.66483600	3.20965600

C	4.18731900	1.67945000	4.21823900
H	4.67965800	3.28380200	2.82435700
H	5.94529000	2.05654600	3.00236100
H	3.85327200	-0.21696000	5.24544300
H	5.44608600	-0.06612700	4.48385900
H	4.59664900	2.19307300	5.10058700
H	3.10915700	1.90629300	4.17846700
Au	1.60644200	-0.30070400	0.23857700
C	-4.65047800	6.04128200	1.75147900
C	-3.53776400	5.26855500	1.40876000
C	-3.64845800	4.26441900	0.41827600
C	-4.89480100	4.05846400	-0.21936100
C	-6.00169900	4.83310200	0.13636700
C	-5.88425600	5.82621600	1.11950000
H	-4.55594800	6.81211300	2.51524000
H	-2.57959400	5.42854100	1.89951700
H	-4.98032900	3.28602400	-0.97887500
H	-6.95782600	4.65884600	-0.35468500
H	-6.74930600	6.42891300	1.39297800
C	-2.52307400	3.45866600	0.06862500
C	-1.57948600	2.74408300	-0.22894100
C	-0.46460300	1.83945100	-0.57774500
O	-1.46902400	-1.58901400	0.48015100
C	-1.13085600	-1.86313400	1.84964100
H	-0.07891000	-1.61010500	2.05294100
H	-1.79078900	-1.31633300	2.53503700
H	-1.28030200	-2.93861300	1.98544400
C	0.74828500	2.65171100	-0.71985000
C	1.76448700	3.30945100	-0.84847600
C	2.99043900	4.02029400	-0.99115300

C	3.51323700	4.30558000	-2.27484700
C	3.72946500	4.41558800	0.14888400
C	4.74206400	4.95678200	-2.40861300
H	2.94858300	4.00415700	-3.15479500
C	4.95805500	5.06528500	0.00529900
H	3.33435900	4.19565500	1.13766600
C	5.47133800	5.33610300	-1.27173400
H	5.13439500	5.16564200	-3.40301300
H	5.51757900	5.35874600	0.89268100
H	6.42974200	5.84174700	-1.38071100
C	-0.80288100	1.03454000	-1.88415400
H	0.14727800	0.64897200	-2.27204300
H	-1.27147800	1.67155900	-2.64268200
C	-1.70122300	-0.13152500	-1.41643000
H	-2.75305900	0.04784800	-1.65286900
H	-1.39370100	-1.07324700	-1.87704000
C	-1.51121400	-0.24593000	0.11726300
C	-0.30927700	0.65044900	0.46134300
H	-0.38802000	1.03114200	1.48951100
O	-2.74471100	0.26924200	0.83050900
H	-2.78728700	1.23219300	0.67901200
N	-4.89370500	-0.97643300	0.13087000
S	-5.11147100	-2.53826400	0.74427500
S	-5.89904100	-0.17970800	-0.95420200
O	-6.52832200	-2.87283600	0.83441900
O	-4.19876900	-2.64788300	1.87717900
O	-5.07928900	0.85033900	-1.59396200
O	-6.71465300	-1.12357800	-1.71154700
C	-4.36395500	-3.64524000	-0.68130400
C	-7.05645900	0.78158400	0.24617300

F	-5.35768700	-4.18106900	-1.39265500
F	-3.57873700	-2.92117900	-1.48636400
F	-3.64140000	-4.62139100	-0.11254100
F	-6.30485100	1.43960600	1.13803000
F	-7.77306700	1.65902300	-0.47195800
F	-7.87371300	-0.06128100	0.87786700
H	-3.95884100	-0.44280100	0.42170700

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C	4.33954100	-1.38393900	-0.79817600
C	4.15913800	-0.17984800	-0.06218300
C	5.10765200	0.17604300	0.91967000
C	6.20878100	-0.63434800	1.20368700
C	6.37623700	-1.83355900	0.50434700
C	5.45574000	-2.19051400	-0.48141400
C	3.47401300	-1.85980800	-1.91288800
C	3.10858200	-3.22062600	-1.97585500
C	2.45180900	-3.73495800	-3.09584300
C	2.12115500	-2.89981300	-4.16972400
C	2.44954100	-1.54238000	-4.11000300
C	3.12089000	-1.02952300	-2.99486700
H	4.98216300	1.08790000	1.49614600
H	6.91946800	-0.33177700	1.97103900
H	7.22415200	-2.48339700	0.71583500
H	5.60537800	-3.10851900	-1.04646000
H	3.34134200	-3.87046600	-1.13523400
H	2.18215400	-4.78949800	-3.12316100
H	1.59959800	-3.30173500	-5.03636300
H	2.20083900	-0.87976900	-4.93813100

H	3.42361200	0.01099700	-3.00108500
P	2.69699000	0.91232900	-0.27028200
C	3.19207100	2.19974700	-1.54753200
C	1.97241700	2.60942000	-2.40014400
C	3.94871700	3.41493600	-0.96413800
H	3.90890500	1.68061500	-2.19819300
C	2.36428400	3.62305000	-3.48969400
H	1.19693900	3.03834400	-1.75000800
H	1.53835900	1.70829600	-2.85512200
C	4.32923600	4.39820000	-2.09039700
H	3.32070600	3.94230100	-0.23513400
H	4.85109700	3.07460500	-0.43710500
C	3.08802500	4.84044000	-2.88705000
H	1.46578300	3.93799500	-4.04002300
H	3.03416600	3.13046300	-4.21403500
H	4.83998800	5.26988500	-1.65622400
H	5.04203600	3.90893700	-2.77405300
H	3.37720900	5.54333100	-3.68149700
H	2.39790800	5.37590200	-2.21359800
C	2.48471400	1.82506700	1.33139400
C	1.31847900	2.83195000	1.24458700
C	2.22011800	0.86100800	2.50631300
H	3.41051600	2.38880100	1.51172600
C	1.27280300	3.66980900	2.53613000
H	0.38408000	2.27123400	1.12190200
H	1.40653000	3.49152500	0.37518800
C	2.15584700	1.65016200	3.82853200
H	1.25853200	0.36361100	2.32326900
H	2.98505100	0.07899200	2.56770100
C	1.10449300	2.77704700	3.77957500

H	0.45189800	4.39358500	2.47395700
H	2.21201200	4.24318500	2.61835900
H	1.93490000	0.95907000	4.65346500
H	3.14923400	2.08691800	4.02640600
H	1.16395700	3.38657800	4.69345100
H	0.10283600	2.33058000	3.75626800
Au	0.66154400	-0.12691900	-0.71602100
C	-8.20246500	-1.18165600	-1.01910300
C	-6.82050100	-0.97625900	-1.00570700
C	-6.25651200	0.12193300	-1.69916500
C	-7.11367100	1.00399100	-2.39875600
C	-8.49456500	0.78872900	-2.40511700
C	-9.04440800	-0.30298600	-1.71735200
H	-8.62458700	-2.03004700	-0.48159600
H	-6.16178200	-1.65245300	-0.46444300
H	-6.68398400	1.85166300	-2.92977900
H	-9.14392300	1.47551600	-2.94709200
H	-10.12121900	-0.46716600	-1.72423000
C	-4.84615200	0.32182600	-1.68791200
C	-3.63409500	0.42191100	-1.67566700
C	-2.17360500	0.60261100	-1.61278400
O	-0.45695100	-2.58575900	-2.56119500
C	-0.39201000	-3.50830000	-1.46353200
H	0.17524300	-3.06484400	-0.63971700
H	-1.39660200	-3.79841900	-1.13093400
H	0.14280600	-4.39270900	-1.82414300
C	-1.94151400	1.78532400	-0.77535300
C	-1.84645400	2.82651500	-0.15236100
C	-1.72880400	4.01826700	0.61759100
C	-1.04288600	5.14345800	0.10318300

C	-2.29076500	4.09299900	1.91392600
C	-0.92209600	6.30696600	0.86713000
H	-0.61239200	5.09185600	-0.89526400
C	-2.16775900	5.26261300	2.66858600
H	-2.81070000	3.22714600	2.31576500
C	-1.48442100	6.37254700	2.15073400
H	-0.38994000	7.16587400	0.45994100
H	-2.60441700	5.30626700	3.66536800
H	-1.38802700	7.28118600	2.74326800
C	-1.57165000	0.80598800	-3.05561500
H	-0.62933900	1.35346400	-2.93853000
H	-2.24774100	1.40653200	-3.67325100
C	-1.30107100	-0.60697100	-3.61800300
H	-2.00203100	-0.86768900	-4.42101700
H	-0.28194500	-0.68169100	-4.01147900
C	-1.46934200	-1.60799000	-2.44174700
C	-1.46728900	-0.74546500	-1.14137200
H	-2.13648800	-1.22609700	-0.42569000
O	-2.75684700	-2.23790700	-2.46420700
N	-0.68119900	-1.78131800	1.53470700
S	-2.07552400	-1.63966400	2.44398300
S	0.64787200	-2.60444300	2.14518000
O	-2.17615200	-2.63681000	3.51333800
O	-3.18557600	-1.40915100	1.51499400
O	1.72550000	-2.44407500	1.16207500
O	0.90594800	-2.35457900	3.56594600
C	-1.81898900	0.06360000	3.29045600
C	0.11318600	-4.49440600	2.01390500
F	-0.87828700	-0.00543100	4.23907100
F	-1.44341000	0.95721800	2.35749300

F	-2.97507400	0.46798800	3.84095700
F	1.04978800	-5.14818800	1.30378200
F	0.03525100	-5.02608000	3.23517600
F	-1.06806200	-4.62587500	1.39272900
H	-0.61978100	-1.09265800	0.19462400
H	-2.84842300	-2.63494100	-3.34301000

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C	-3.85510000	-3.72915200	-1.14160100
C	-2.89644300	-2.71317200	-1.10296500
C	-2.65126000	-2.00731500	0.09879300
C	-3.39400000	-2.34637000	1.25493600
C	-4.35145300	-3.36298400	1.20512400
C	-4.58616300	-4.05756600	0.00947100
H	-4.03300000	-4.26560400	-2.07281000
H	-2.32827100	-2.45495700	-1.99460600
H	-3.20870100	-1.80677300	2.18203600
H	-4.91654200	-3.61413600	2.10193500
H	-5.33324500	-4.84943000	-0.02471100
C	-1.67599400	-0.96727100	0.14464600
C	-0.84834200	-0.07604900	0.18205700
C	0.13986400	1.01386700	0.25105200
O	-0.77886300	4.41378400	-0.33569300
C	1.49479900	0.45654100	0.17102900
C	2.62559200	0.01079100	0.10326400
C	3.94741600	-0.51817600	0.00807400
C	4.90028200	-0.26939600	1.02429600
C	4.32635200	-1.30114000	-1.10835000
C	6.19292600	-0.79058200	0.92230400

H	4.61355600	0.33207200	1.88498700
C	5.62150800	-1.81756700	-1.20038300
H	3.59621100	-1.49608400	-1.89155300
C	6.55883800	-1.56555600	-0.18792800
H	6.91681700	-0.59194500	1.71159100
H	5.89980900	-2.41924000	-2.06472100
H	7.56709800	-1.97041600	-0.26337300
C	-0.08984100	1.87041400	1.54790600
H	0.77533600	2.53614300	1.66800900
H	-0.18225200	1.24019500	2.43944200
C	-1.35488100	2.67559300	1.21750300
H	-2.23867500	2.03610900	1.33271300
H	-1.47491400	3.56624800	1.84334300
C	-1.20724100	3.04909200	-0.28380200
C	-0.13077400	2.08661300	-0.86605400
H	-0.44905800	1.63255400	-1.80913600
O	-2.38613800	2.85478600	-1.05728000
C	-3.52851400	3.59245600	-0.60143400
H	-4.32425400	3.40549900	-1.33212300
H	-3.86574800	3.24658700	0.39047500
H	-3.31475000	4.67101400	-0.55400800
H	0.79789000	2.64808200	-1.02233200
H	-0.60270500	4.60710600	-1.26901600
TS4'			
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C	3.54848900	-3.36085800	-0.50594200
C	4.19995800	-2.25592500	0.10330000
C	5.39319100	-2.47800100	0.82179400
C	5.93317900	-3.76008600	0.95687100
C	5.27422700	-4.85327400	0.38252200

C	4.09452200	-4.64837000	-0.33739900
C	2.30511500	-3.22526000	-1.31308500
C	1.10473500	-3.80088500	-0.85829000
C	-0.08155200	-3.62729300	-1.58067800
C	-0.08123400	-2.88091400	-2.76673000
C	1.11369900	-2.31830800	-3.23387400
C	2.30157900	-2.49345000	-2.51496100
H	5.90405800	-1.64541700	1.29843200
H	6.85714200	-3.90186700	1.51544600
H	5.67811900	-5.85898200	0.48925200
H	3.58312800	-5.49130300	-0.79955900
H	1.09957700	-4.34885000	0.08245500
H	-1.00786800	-4.05934200	-1.20829500
H	-1.00926900	-2.72236200	-3.30969600
H	1.11878300	-1.73854800	-4.15578500
H	3.22865300	-2.05050200	-2.87426800
P	3.51922900	-0.53944500	0.05609800
C	4.49786500	0.32599800	-1.27418000
C	3.70961400	1.50590000	-1.87920600
C	5.90926100	0.75364400	-0.81820200
H	4.60819000	-0.44690500	-2.05059400
C	4.49334200	2.13106000	-3.04649000
H	3.53684700	2.26779700	-1.10930900
H	2.72047400	1.15963800	-2.21071300
C	6.68068800	1.39815500	-1.98815700
H	5.81992900	1.48434900	-0.00054700
H	6.46538400	-0.11263400	-0.43344500
C	5.89712200	2.57543400	-2.59793700
H	3.93197700	2.98486700	-3.44858700
H	4.58770800	1.38829100	-3.85621800

H	7.66772700	1.73309900	-1.63695300
H	6.85344900	0.63564800	-2.76516000
H	6.45309600	2.99987700	-3.44673000
H	5.79365500	3.37203700	-1.84382300
C	3.93879800	0.19341400	1.71405500
C	3.48500200	1.66803900	1.77436000
C	3.24919000	-0.64197400	2.81949500
H	5.02827100	0.16058900	1.85159800
C	3.76121300	2.25598900	3.17101200
H	2.40727500	1.72207000	1.56077500
H	3.99404200	2.26122100	1.00590800
C	3.49677700	-0.03471600	4.21300400
H	2.16695200	-0.65935300	2.61758900
H	3.60076900	-1.68159700	2.78952900
C	3.05401500	1.43791900	4.26504800
H	3.43112400	3.30263600	3.20129300
H	4.84795700	2.25341300	3.35934600
H	2.96074300	-0.62705700	4.96885200
H	4.57141300	-0.09874400	4.45176500
H	3.25811900	1.86510900	5.25751800
H	1.96549600	1.49315200	4.09992700
Au	1.24195900	-0.37803100	-0.16909900
C	-5.99689100	6.48436600	0.65904900
C	-4.81671500	5.73571600	0.68008900
C	-4.84903200	4.34419900	0.42487400
C	-6.09298000	3.72819200	0.14644700
C	-7.26660800	4.48608200	0.12922900
C	-7.22490000	5.86454700	0.38512100
H	-5.95837100	7.55472800	0.85839900
H	-3.86235500	6.21412200	0.89277500

H	-6.12205600	2.65966600	-0.05256500
H	-8.21717500	3.99833900	-0.08376600
H	-8.14269800	6.45099100	0.37136300
C	-3.65284700	3.56728700	0.44679700
C	-2.64834800	2.87987400	0.46217500
C	-1.47248600	1.99648900	0.46884400
C	-0.25128300	2.80058500	0.25848300
C	0.73170000	3.48542400	0.03766500
C	1.87190400	4.29557900	-0.23217900
C	2.25369100	4.57804300	-1.56511100
C	2.64938400	4.82301500	0.82454600
C	3.38788900	5.35066000	-1.82658300
H	1.65628500	4.17806500	-2.38174700
C	3.78681300	5.58819100	0.55453500
H	2.34956000	4.62218600	1.84986700
C	4.16360100	5.85172400	-0.77081700
H	3.67137200	5.55818500	-2.85724100
H	4.37852700	5.98252900	1.37987600
H	5.05003200	6.44897200	-0.97966600
C	-1.60244400	0.89534100	-0.66985800
H	-1.09100900	1.20604400	-1.58364000
H	-2.66854200	0.77543700	-0.89040800
C	-1.03202900	-0.37032900	-0.01183600
H	-0.73465400	-1.30382600	-0.52092700
C	-1.06944500	-0.12305100	1.45494900
C	-1.37414100	1.16101400	1.75504100
H	-2.19469100	-1.17518700	-0.08329000
O	-0.79815500	-1.16557600	2.27106100
N	-3.32752200	-1.79524700	-0.21975800
S	-4.11997100	-2.45344100	1.10340300

S	-3.99508200	-1.78610900	-1.75873200
O	-5.53317100	-2.71718200	0.82180500
O	-3.70062300	-1.72912100	2.30133800
O	-2.95275000	-1.20928000	-2.61468200
O	-4.66325000	-3.03505200	-2.12402600
C	-3.24968200	-4.16089200	1.21862500
C	-5.39151700	-0.41371800	-1.62069000
F	-3.45031100	-4.86686300	0.09759700
F	-1.92903700	-3.98644700	1.39726800
F	-3.75291100	-4.83276300	2.26542200
F	-5.23813700	0.45550000	-2.62889600
F	-6.59647100	-0.97948600	-1.69924700
F	-5.28086600	0.24565200	-0.45543700
H	-1.46992900	1.60797700	2.73618800
C	-0.87480600	-0.88702100	3.67812000
H	-0.62769300	-1.82529100	4.18545900
H	-0.15076600	-0.10435100	3.95490600
H	-1.89101700	-0.56925600	3.94793800
C_{DCE}			
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C	4.03937100	-2.40123400	-1.54883400
C	4.15263600	-1.71024100	-0.31456700
C	5.02323300	-2.20873300	0.67646300
C	5.75365900	-3.38359700	0.47312800
C	5.60878400	-4.09137600	-0.72648600
C	4.76058700	-3.59980000	-1.72275100
C	3.21226800	-1.91430500	-2.68563700
C	2.17801600	-2.71762300	-3.20197600
C	1.41395100	-2.27868900	-4.28800100
C	1.66869200	-1.03005100	-4.87034500

C	2.69265100	-0.22117400	-4.36136700
C	3.46511000	-0.66357400	-3.28067200
H	5.12058500	-1.68925400	1.62576800
H	6.41920000	-3.74803900	1.25410800
H	6.15922100	-5.01672100	-0.89040400
H	4.66159300	-4.13422000	-2.66628500
H	1.96865000	-3.67967100	-2.73715300
H	0.60939800	-2.90410400	-4.66924700
H	1.06663600	-0.68800900	-5.71013900
H	2.89751500	0.75032600	-4.80944100
H	4.27419000	-0.04355700	-2.90343100
P	3.12898900	-0.23236900	0.08047800
C	4.21708700	1.24720200	-0.27640100
C	3.37880100	2.49080600	-0.64167900
C	5.21559300	1.53293800	0.86658700
H	4.79608500	0.94658100	-1.16064900
C	4.28584300	3.69273400	-0.96141600
H	2.71713700	2.74040700	0.19614000
H	2.73183700	2.25993600	-1.49945500
C	6.11713800	2.72971800	0.50425300
H	4.66165500	1.77107300	1.78545900
H	5.82538300	0.64097600	1.06641100
C	5.27317800	3.97704500	0.18503300
H	3.66243000	4.57713600	-1.16059300
H	4.85432600	3.47845100	-1.88163200
H	6.80679100	2.93407200	1.33626800
H	6.72918500	2.46892200	-0.37479200
H	5.92589300	4.82269000	-0.07750900
H	4.70669600	4.26495600	1.08487200
C	2.83282000	-0.30347500	1.91370300

C	2.00625100	0.91916700	2.37369100
C	2.10410700	-1.61534300	2.27922000
H	3.80966300	-0.27076800	2.41579800
C	1.74914400	0.84712000	3.89058700
H	1.04607800	0.92106500	1.83841300
H	2.51763400	1.85596300	2.12540900
C	1.83551100	-1.67999700	3.79508500
H	1.15108800	-1.64209900	1.73642300
H	2.69039500	-2.48659400	1.96121500
C	1.02848800	-0.45825100	4.26910800
H	1.15780600	1.71951800	4.19734400
H	2.71504700	0.90023700	4.42083000
H	1.30281700	-2.60951100	4.03313600
H	2.80027800	-1.70748500	4.32937600
H	0.86728700	-0.50585400	5.35661600
H	0.04118800	-0.47547200	3.78458900
Au	1.06736100	-0.04552600	-0.94568500
C	-7.27539600	3.23776100	-0.24946500
C	-5.88057600	3.21546600	-0.33295600
C	-5.24448800	2.60493100	-1.43952800
C	-6.03688500	2.01796600	-2.45411300
C	-7.43103000	2.04598300	-2.36012200
C	-8.05464800	2.65418700	-1.25997200
H	-7.75521700	3.70543500	0.60910600
H	-5.27181300	3.65389900	0.45529200
H	-5.54952500	1.53582900	-3.29934900
H	-8.03251200	1.58668000	-3.14339800
H	-9.14125300	2.66952100	-1.18865600
C	-3.82257600	2.52622500	-1.49637700
C	-2.61079000	2.41065600	-1.50446200

C	-1.17136100	2.10202700	-1.44451600
O	-1.21900200	-1.01558800	-3.33711500
C	-1.42092100	-2.13788600	-2.42586200
H	-0.52036600	-2.25783500	-1.81391600
H	-2.29463600	-1.95201200	-1.79471700
H	-1.58114800	-3.01006400	-3.06351600
C	-0.57442700	2.77206200	-0.28453700
C	-0.07699900	3.36549800	0.65391500
C	0.52293500	4.03365600	1.76078400
C	1.69035900	4.81391300	1.58171900
C	-0.03074700	3.90930800	3.05621400
C	2.29071800	5.44180100	2.67682400
H	2.11907100	4.91221300	0.58725300
C	0.57464500	4.54641100	4.14336900
H	-0.92528300	3.30590700	3.19690800
C	1.73725300	5.30981600	3.95989400
H	3.19151900	6.03548700	2.52822600
H	0.14179500	4.44032200	5.13698700
H	2.20822900	5.80015900	4.81065400
C	-0.42681900	2.47549700	-2.78099500
H	0.64796900	2.48299600	-2.56155500
H	-0.73581200	3.45586900	-3.15486600
C	-0.75879300	1.31278800	-3.73112100
H	-1.69293400	1.49450300	-4.28484900
H	0.02996500	1.08974100	-4.45716200
C	-1.00286000	0.16101000	-2.79989500
C	-1.03590100	0.54023400	-1.44734600
H	-1.60593300	-0.01933100	-0.70737800
N	-3.04356900	-2.91157500	0.53000700
S	-1.59732300	-2.60209700	1.22803600

S	-4.44123700	-2.30159800	1.12502500
O	-1.36036500	-1.19709800	1.61157200
O	-0.58977100	-3.29694800	0.40717800
O	-5.53426500	-3.08513400	0.52796900
O	-4.45043500	-2.01701800	2.57304300
C	-1.58613200	-3.58818700	2.91614500
C	-4.62108100	-0.57088700	0.29054100
F	-1.75070300	-2.75766400	3.95505200
F	-2.55723700	-4.51702700	2.93246700
F	-0.39779700	-4.21069500	3.04508700
F	-4.35130000	-0.66273100	-1.02763200
F	-5.88777100	-0.14164300	0.44264100
F	-3.79162300	0.32078800	0.84905700

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C	4.07020200	-3.40015800	-0.42423300
C	4.71486000	-2.30815400	0.21691200
C	5.92170800	-2.53272900	0.90980600
C	6.48268300	-3.81155200	0.99267600
C	5.83136900	-4.89488500	0.38928400
C	4.63838300	-4.68483300	-0.30918100
C	2.81688400	-3.25103600	-1.21515800
C	1.65717100	-3.95580300	-0.84044500
C	0.46864700	-3.80590000	-1.56348200
C	0.42106900	-2.94926700	-2.67128800
C	1.57135900	-2.24911900	-3.05741500
C	2.76272800	-2.40592000	-2.33976900
H	6.42372900	-1.70576000	1.40576600
H	7.41656900	-3.95916000	1.53320200
H	6.25241200	-5.89720100	0.45535300

H	4.13689600	-5.52073400	-0.79486400
H	1.68589700	-4.60192500	0.03581200
H	-0.42733800	-4.33375500	-1.24575100
H	-0.50743200	-2.82206000	-3.22351000
H	1.54422100	-1.58174200	-3.91782700
H	3.65487000	-1.87041100	-2.65223900
P	3.97219900	-0.62096900	0.22219400
C	4.85495900	0.28283900	-1.15796900
C	3.96951200	1.39050300	-1.76572600
C	6.24688600	0.81091200	-0.75102000
H	5.00844300	-0.48960500	-1.92471100
C	4.68022400	2.05287800	-2.95941600
H	3.75462300	2.14791000	-1.00164100
H	3.00524900	0.96370000	-2.07405600
C	6.94005700	1.47543200	-1.95686600
H	6.13902500	1.55325700	0.05218100
H	6.86325100	-0.01174300	-0.36248400
C	6.06465700	2.59288200	-2.55576900
H	4.05340400	2.86412300	-3.35509800
H	4.80252300	1.30645600	-3.76216000
H	7.91657600	1.87571300	-1.64607700
H	7.12898200	0.71116300	-2.72862200
H	6.56627900	3.04417300	-3.42486400
H	5.93149300	3.38858100	-1.80466000
C	4.49812700	0.16097900	1.82897800
C	3.98045400	1.61689700	1.89148400
C	3.94080200	-0.66017700	3.01342600
H	5.59541200	0.17771600	1.87423800
C	4.34867700	2.27187500	3.23484200
H	2.88548900	1.61000000	1.78294800

H	4.37838200	2.20982400	1.06074200
C	4.29823500	-0.00026500	4.35896900
H	2.84449900	-0.71316000	2.91137600
H	4.32317300	-1.68910400	2.98132000
C	3.79871500	1.45500800	4.41792900
H	3.95324800	3.29794000	3.25896600
H	5.44608000	2.34046600	3.31751600
H	3.86683900	-0.58808800	5.18259600
H	5.39347300	-0.01269700	4.48650400
H	4.08756700	1.91965600	5.37218900
H	2.69709000	1.45738300	4.37075200
Au	1.65307900	-0.46160100	0.19490000
C	-6.15045300	4.46697900	1.21172200
C	-4.95661700	3.95831000	0.69317800
C	-4.34843900	2.82408800	1.28203000
C	-4.96347400	2.22150300	2.40463300
C	-6.15978500	2.73598900	2.91320400
C	-6.75835400	3.85745000	2.32006700
H	-6.61076200	5.33811000	0.74707100
H	-4.49031300	4.42194600	-0.17378400
H	-4.50127800	1.34811000	2.85800400
H	-6.62792900	2.25671400	3.77204200
H	-7.69205600	4.25312500	2.71743300
C	-3.15250800	2.27727900	0.72966100
C	-2.15773400	1.78256300	0.23103300
C	-0.93846100	1.20516800	-0.36379800
O	-1.34049000	-2.36099600	0.46263100
C	-0.80499300	-2.56205500	1.79001800
H	0.27815700	-2.37726800	1.79701200
H	-1.30686100	-1.90135100	2.50688400

H	-1.01126700	-3.60875200	2.03253000
C	0.06515500	2.27024600	-0.48788200
C	0.91147600	3.14287000	-0.56593600
C	1.95728700	4.10820300	-0.64666400
C	2.31248300	4.68612900	-1.88843900
C	2.68908700	4.46711400	0.51099600
C	3.37514000	5.59080800	-1.96701600
H	1.75620300	4.40976000	-2.78206700
C	3.75039700	5.37203600	0.42156500
H	2.42682800	4.01909500	1.46656400
C	4.09977900	5.93519900	-0.81565000
H	3.64274600	6.02322700	-2.93015000
H	4.30920500	5.63494200	1.31885300
H	4.92937800	6.63766700	-0.88206100
C	-1.27542800	0.51579100	-1.74203800
H	-0.32875100	0.42048200	-2.30400600
H	-1.97912000	1.11657500	-2.33082300
C	-1.78927800	-0.84078100	-1.30748800
H	-3.38780700	-0.65834400	-0.69380700
H	-2.09615600	-1.60761400	-2.01425900
C	-1.21344000	-1.14300200	-0.08760700
C	-0.44357100	-0.02926200	0.49131100
H	-0.59455500	0.12871600	1.56605600
N	-4.49377300	-0.69401200	-0.41882000
S	-4.84002200	-1.37712600	1.08981200
S	-5.54841300	-0.68420300	-1.73630200
O	-6.67788600	-1.59189000	-1.53135400
O	-4.72338600	-0.72480700	-2.94384600
C	-6.22979800	1.11122900	-1.62542400
O	-3.72098700	-1.01073300	1.95472900

O	-6.22926200	-1.13780100	1.47205400
C	-4.66382400	-3.29910300	0.74866900
F	-4.06321100	-3.50923200	-0.42828400
F	-3.93283600	-3.83550000	1.73137800
F	-5.87802200	-3.85416500	0.73523600
F	-6.76057900	1.32466600	-0.42150900
F	-5.22889800	1.96846500	-1.85012000
F	-7.17016900	1.25834100	-2.56923900

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C	3.21153600	-2.72557000	-1.19624200
C	3.46802500	-2.03826900	0.02054000
C	4.19780700	-2.68666600	1.03624600
C	4.65137200	-4.00074400	0.87588200
C	4.37208700	-4.69064600	-0.31066000
C	3.66101400	-4.05326300	-1.33256700
C	2.44049900	-2.11701800	-2.31596800
C	1.23367100	-2.70941100	-2.73340700
C	0.46016400	-2.11612200	-3.73637700
C	0.87950400	-0.92326100	-4.34005100
C	2.08989300	-0.33739200	-3.94773700
C	2.86811700	-0.93550900	-2.94943500
H	4.39817100	-2.17202900	1.97315200
H	5.20961700	-4.48300700	1.67717500
H	4.70861200	-5.71821000	-0.44240600
H	3.44965000	-4.58182200	-2.26125000
H	0.88665600	-3.61603800	-2.24439000
H	-0.47808900	-2.57938100	-4.03376200
H	0.26614600	-0.45206500	-5.10528900

H	2.42951200	0.58647500	-4.41396600
H	3.80825000	-0.47832000	-2.65526500
P	2.77623400	-0.35587100	0.32630400
C	4.17703000	0.79137600	-0.15409100
C	3.65012700	2.15203500	-0.65097500
C	5.24616500	0.94841900	0.94729300
H	4.66047500	0.28279000	-0.99939500
C	4.81417600	3.03699500	-1.13244000
H	3.12168900	2.65929500	0.16486100
H	2.91748700	1.99363200	-1.45384500
C	6.39916400	1.84398600	0.45053900
H	4.79498100	1.40920900	1.83694900
H	5.62913600	-0.03889500	1.24292500
C	5.87390100	3.21055400	-0.02899500
H	4.42550800	4.01519500	-1.44746100
H	5.28400300	2.56580600	-2.01236000
H	7.13827100	1.97534400	1.25493500
H	6.91029600	1.33981400	-0.38627400
H	6.70626400	3.83123700	-0.39312200
H	5.41788300	3.74105100	0.82251900
C	2.56120000	-0.20074900	2.17300300
C	2.05918100	1.22094800	2.51827500
C	1.55532800	-1.25921600	2.67294000
H	3.53378800	-0.35412300	2.66055400
C	1.81967500	1.36162600	4.03266600
H	1.11412100	1.40554900	1.98619500
H	2.77052700	1.98065700	2.17723600
C	1.29195700	-1.11232200	4.18293200
H	0.61242700	-1.12628200	2.12122800
H	1.92451000	-2.26671200	2.45197200

C	0.81489800	0.30854300	4.53365000
H	1.45296900	2.37547300	4.25105300
H	2.77712000	1.23667000	4.56579500
H	0.54532700	-1.85705000	4.49643100
H	2.22267800	-1.32824400	4.73401500
H	0.66608000	0.40519500	5.61945300
H	-0.15882200	0.48873200	4.05031700
Au	0.69098600	0.15478900	-0.59264700
C	-7.24559500	2.93149800	0.60353400
C	-5.97041100	2.58752300	0.14606500
C	-5.09653300	3.58492200	-0.35302000
C	-5.53689700	4.92996800	-0.37892900
C	-6.81432100	5.26303900	0.08241700
C	-7.67325500	4.26793500	0.57353200
H	-7.90643500	2.15437500	0.98606600
H	-5.63723200	1.55253100	0.17078400
H	-4.86951900	5.70114700	-0.75971100
H	-7.14036100	6.30210400	0.05830200
H	-8.66752400	4.53224900	0.93104700
C	-3.79449100	3.22623900	-0.81508800
C	-2.69176300	2.87949800	-1.20191300
C	-1.35601800	2.36811800	-1.57159600
O	-2.33946600	-1.10210500	-2.02414700
C	-3.13763400	-1.71127900	-3.05988300
H	-4.01865800	-1.08630100	-3.26271500
H	-2.54428400	-1.82613200	-3.97611500
H	-3.43602500	-2.69159700	-2.67944400
C	-0.34126300	3.24519700	-0.97773200
C	0.47579700	3.96278100	-0.42882500
C	1.45584400	4.73766400	0.25754000

C	2.29760300	5.63611300	-0.43927300
C	1.62344600	4.58503600	1.65545500
C	3.28378300	6.35295600	0.24530300
H	2.17573200	5.75509000	-1.51423200
C	2.61257200	5.30553100	2.33009500
H	0.98368100	3.88935300	2.19315800
C	3.44822900	6.18901600	1.62903100
H	3.93020800	7.03649600	-0.30359300
H	2.73458200	5.17424400	3.40458300
H	4.22101500	6.74599300	2.15694700
C	-1.23490000	2.22112400	-3.13836500
H	-0.16099900	2.18813700	-3.39635000
H	-1.68743900	3.07703400	-3.65594200
C	-1.91024600	0.89004200	-3.39495300
H	-2.14724900	-1.77209800	-0.49882800
H	-2.25527000	0.55480500	-4.36763400
C	-1.88818200	0.17297300	-2.25187300
C	-1.26729800	0.85719100	-1.08767300
H	-1.87223900	0.73420800	-0.18273200
N	-2.16076400	-2.33849100	0.39537600
S	-1.87775100	-4.00171900	0.12361300
S	-2.99914400	-1.65069200	1.71011100
O	-2.56726100	-0.26215400	1.81893100
O	-2.97055800	-2.57673200	2.83499800
C	-4.79608100	-1.58819400	1.00808400
O	-2.79976900	-4.84168600	0.87892300
O	-1.67578700	-4.13881000	-1.31662000
C	-0.14253000	-4.16916900	0.93408500
F	-0.24205300	-3.97965000	2.25123700
F	0.30947800	-5.40268400	0.68027800

F	0.67271200	-3.26688100	0.39610100
F	-4.77078800	-0.96139400	-0.17507900
F	-5.26166800	-2.82875700	0.85389200
F	-5.56082900	-0.90910300	1.86610900

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C	-3.07737100	-1.85924700	-2.28778200
C	-2.77718300	-2.63094900	-1.13159300
C	-3.78632000	-3.43147600	-0.56149300
C	-5.07949700	-3.46095900	-1.09535500
C	-5.38557500	-2.67416700	-2.21262200
C	-4.39008900	-1.88453600	-2.79738500
C	-2.07524800	-0.98476800	-2.95973700
C	-2.28635700	0.40612600	-3.01581500
C	-1.31563200	1.25260700	-3.56262600
C	-0.12203500	0.72143400	-4.06900500
C	0.08309200	-0.66425700	-4.04992900
C	-0.88971900	-1.51150900	-3.50564600
H	-3.56769700	-4.02373300	0.32369900
H	-5.84239400	-4.08609600	-0.63333400
H	-6.39158000	-2.67741200	-2.63018000
H	-4.61941300	-1.27861800	-3.67293500
H	-3.19514400	0.82308800	-2.58887400
H	-1.48011600	2.32826600	-3.56485900
H	0.64416600	1.38316400	-4.47033600
H	1.00384400	-1.08806900	-4.44862700
H	-0.72330600	-2.58503900	-3.49192500
P	-1.13225400	-2.53273400	-0.29641500
C	-0.18632000	-3.97795100	-1.01981400

C	1.33052600	-3.70720900	-1.06583200
C	-0.50555100	-5.32818500	-0.34469500
H	-0.55192400	-4.03792300	-2.05414300
C	2.05256300	-4.85676300	-1.79206200
H	1.71923900	-3.62079500	-0.04335000
H	1.52195900	-2.74709800	-1.56387500
C	0.23151600	-6.47303800	-1.06962600
H	-0.17858800	-5.29910700	0.70426100
H	-1.59022600	-5.50774400	-0.35098200
C	1.74865700	-6.21122200	-1.12521900
H	3.13503100	-4.66832800	-1.79986600
H	1.71361100	-4.88539900	-2.84143000
H	0.02433300	-7.42673400	-0.56136200
H	-0.16008000	-6.55612000	-2.09688700
H	2.25571200	-7.02569800	-1.66397700
H	2.14890400	-6.19648900	-0.09901000
C	-1.43079100	-2.90911600	1.50129700
C	-0.07381400	-2.88675600	2.24218200
C	-2.38924500	-1.86117500	2.10684600
H	-1.86952000	-3.91250500	1.59725500
C	-0.26508600	-3.11136300	3.75282000
H	0.40290100	-1.90805700	2.07734700
H	0.60418900	-3.64321200	1.83300600
C	-2.57597200	-2.08559000	3.61815300
H	-1.96204800	-0.86205000	1.93880900
H	-3.36020600	-1.89073900	1.59912100
C	-1.22410800	-2.06805000	4.35370800
H	0.71323600	-3.06790200	4.25338400
H	-0.67518700	-4.12120700	3.92083800
H	-3.24462300	-1.31168300	4.02231200

H	-3.06514900	-3.06064500	3.78222000
H	-1.36837800	-2.25332000	5.42855700
H	-0.77416600	-1.06682400	4.24854900
Au	-0.06127200	-0.46598300	-0.42569500
C	9.39354200	2.91311900	-0.10353200
C	8.14580700	2.31067700	0.08382900
C	6.97930900	2.89905300	-0.46284900
C	7.09968000	4.10256900	-1.19906000
C	8.35239900	4.69656600	-1.37992600
C	9.50254100	4.10652600	-0.83364500
H	10.28295400	2.45070300	0.32270000
H	8.05916600	1.38535900	0.65061800
H	6.20643000	4.55986400	-1.62091400
H	8.43117000	5.62315200	-1.94716000
H	10.47610400	4.57359500	-0.97588000
C	5.70202100	2.29149800	-0.26784500
C	4.61054900	1.77800800	-0.09381600
C	3.28357800	1.18005500	0.12054600
O	0.11370800	2.43860300	1.51451800
C	0.34860600	2.86928900	2.87443100
H	0.69364000	2.01701500	3.47501100
H	1.09703300	3.67277100	2.88820000
H	-0.61237900	3.23238600	3.24911700
C	3.44947800	-0.24581800	0.47888000
C	3.63229200	-1.39459000	0.84272400
C	3.82791100	-2.74261600	1.26470800
C	3.24714700	-3.20875500	2.46755900
C	4.58531800	-3.64164000	0.47646100
C	3.41150100	-4.53975700	2.86127100
H	2.65571800	-2.52576300	3.07204100

C	4.74645100	-4.96978700	0.87990000
H	5.02957900	-3.28895800	-0.45206400
C	4.15854900	-5.42555400	2.06987100
H	2.95127000	-4.88745100	3.78525400
H	5.32379000	-5.65372900	0.25942400
H	4.28117100	-6.46333300	2.37664800
C	2.34759100	1.36479100	-1.14258600
H	2.51038300	0.56757800	-1.87450300
H	2.60852500	2.33202900	-1.59832800
C	0.91545900	1.42598200	-0.55296000
H	0.27217000	2.09724100	-1.13833500
C	1.18553300	1.96864700	0.80119400
C	2.47090200	1.89013400	1.21304100
H	2.87863900	2.09674200	2.19591400
N	-2.35321200	2.90573400	0.56750400
S	-2.42819700	4.22217700	-0.49992600
S	-3.58671400	2.30128100	1.57605100
O	-3.80397500	4.41161700	-0.94303800
O	-1.30297000	4.06852800	-1.41684500
O	-2.89389200	1.58249000	2.64246800
O	-4.61676300	3.30269300	1.82645700
C	-1.96065200	5.69727900	0.65212800
C	-4.36263600	0.97137500	0.41872600
F	-2.83794100	5.79077600	1.65233600
F	-0.73358500	5.48461200	1.14121900
F	-1.97439400	6.81519200	-0.07830200
F	-3.39675500	0.20725400	-0.07759400
F	-5.20485900	0.23280100	1.15105200
F	-5.02718400	1.57241200	-0.57189700
H	-1.37368700	2.62055700	0.85768400

TS4_{DCE}

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C	4.58103400	-2.81739200	-1.57866100
C	5.03274400	-1.94078100	-0.55507400
C	6.23931400	-2.23402200	0.11296800
C	6.98175100	-3.37898200	-0.19456200
C	6.51664100	-4.26328100	-1.17578900
C	5.32918000	-3.97897200	-1.85692000
C	3.34687100	-2.56937900	-2.37455500
C	2.27394700	-3.47841700	-2.31164000
C	1.08332100	-3.22001400	-3.00059800
C	0.94988000	-2.05187900	-3.76336800
C	2.02167700	-1.15385300	-3.85249800
C	3.21573800	-1.41452900	-3.16896500
H	6.59949300	-1.56887300	0.89396100
H	7.91027500	-3.58129400	0.33759300
H	7.07799900	-5.16542300	-1.41541600
H	4.97204100	-4.65405700	-2.63348300
H	2.36626000	-4.36814900	-1.69081000
H	0.25179100	-3.91919500	-2.92322300
H	0.01464900	-1.84054900	-4.27984300
H	1.92735700	-0.24583900	-4.44660500
H	4.04492800	-0.71393400	-3.23592400
P	4.05672200	-0.46570300	-0.01357800
C	4.86731900	0.96597500	-0.90178500
C	3.87831200	2.12648300	-1.13405000
C	6.17192400	1.44904900	-0.23505200
H	5.13010900	0.54526900	-1.88329200
C	4.54220900	3.23160900	-1.97522700

H	3.56541800	2.54319100	-0.16898800
H	2.97242500	1.74922300	-1.62850400
C	6.82221800	2.56469600	-1.07792200
H	5.94326300	1.84289700	0.76557500
H	6.86816400	0.60794000	-0.11180300
C	5.84074200	3.72866500	-1.31330300
H	3.83849700	4.06431900	-2.11022100
H	4.77678000	2.82917800	-2.97506400
H	7.73245000	2.92468300	-0.57559300
H	7.12785400	2.14644900	-2.05103700
H	6.31325900	4.50478400	-1.93379500
H	5.59005300	4.18977800	-0.34427100
C	4.39126400	-0.29085300	1.80809500
C	3.66319800	0.96591400	2.33346000
C	3.89303500	-1.55354600	2.54743300
H	5.47066800	-0.17013700	1.97205500
C	3.84112500	1.11163300	3.85482700
H	2.59144100	0.87363800	2.10046300
H	4.02364100	1.86635500	1.82417200
C	4.06235700	-1.40463500	4.07137200
H	2.82625800	-1.69630700	2.30992900
H	4.42931600	-2.44242700	2.18989900
C	3.34705800	-0.14494200	4.59366300
H	3.29512500	2.00112400	4.20055100
H	4.90822400	1.27190200	4.08214700
H	3.67327400	-2.30306500	4.57295800
H	5.13674500	-1.33578100	4.31039300
H	3.50275800	-0.03901900	5.67757300
H	2.26277400	-0.25348600	4.42572300
Au	1.75685300	-0.63453900	-0.28775400

C	-7.29309700	3.64953700	-0.48505400
C	-6.01974000	3.18888400	-0.13791200
C	-5.03279600	3.00222000	-1.13484600
C	-5.35393600	3.29248600	-2.48222400
C	-6.63026500	3.75295800	-2.81839000
C	-7.60428500	3.93118700	-1.82389800
H	-8.04591100	3.78266800	0.29078600
H	-5.77851200	2.96196900	0.89835800
H	-4.60018600	3.14405400	-3.25309500
H	-6.86728800	3.96907000	-3.85940100
H	-8.59898300	4.28534800	-2.09112600
C	-3.75310500	2.47393400	-0.79214900
C	-2.69026200	1.95369000	-0.50644900
C	-1.47262400	1.20664200	-0.15738900
O	-0.77144500	-1.93014700	1.62924800
C	-1.10392200	-1.70480500	3.02055300
H	-0.41250900	-0.96482200	3.44789200
H	-2.13588900	-1.35335700	3.13006800
H	-0.98221000	-2.67158900	3.51802100
C	-0.37983400	2.15229500	0.15076500
C	0.47392400	2.96643000	0.45645200
C	1.48894100	3.90369900	0.80872500
C	1.93020000	4.87228200	-0.12408500
C	2.09087900	3.86142800	2.08828200
C	2.95302100	5.76205500	0.21376200
H	1.47448500	4.90542800	-1.11157300
C	3.11363500	4.75528900	2.41681900
H	1.76401000	3.11346200	2.80634900
C	3.55190400	5.70525200	1.48162600
H	3.29150400	6.49489800	-0.51715400

H	3.57468000	4.70507300	3.40231800
H	4.35351200	6.39626900	1.73852700
C	-1.06515100	0.19186700	-1.29848500
H	-0.45997400	0.68166900	-2.06719200
H	-1.99137700	-0.18211200	-1.75285800
C	-0.34942500	-0.94760200	-0.54164600
H	-0.45992500	-1.92526700	-1.02828300
C	-0.95661400	-0.89669900	0.79247200
C	-1.69804300	0.24827800	1.02850200
H	-1.96944000	0.63728800	2.00499100
N	-4.29449800	-0.80669000	0.50448900
S	-4.61351800	-1.90760400	-0.73534000
S	-5.30581400	-0.56780700	1.84418100
O	-5.65102600	-2.85468200	-0.32451400
O	-3.32280000	-2.33881500	-1.27007700
O	-4.64845500	0.47370000	2.63272700
O	-6.70693000	-0.48307600	1.44351200
C	-5.41250300	-0.78182200	-2.08644900
C	-5.10439700	-2.23963700	2.85650500
F	-6.35168600	-0.01049100	-1.54088100
F	-4.46943700	-0.02774600	-2.65677500
F	-5.96219300	-1.58638600	-3.00637900
F	-4.85500600	-1.92243300	4.13141500
F	-6.23165400	-2.94346800	2.77633600
F	-4.08396200	-2.95745400	2.36822900
H	-3.23216500	-0.47010000	0.65290500

E_{DCE}

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C	-5.92327800	-0.69312000	-1.00574400
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C	-4.68146900	-0.06577800	-0.86783700
C	-3.71492200	-0.58641600	0.02606800
C	-4.02592300	-1.74743500	0.77438700
C	-5.27080900	-2.36660900	0.62808500
C	-6.22269100	-1.84383000	-0.26058600
H	-6.65871800	-0.28331200	-1.69679100
H	-4.44717800	0.82684700	-1.44527000
H	-3.28570200	-2.15178900	1.46248900
H	-5.49841400	-3.25968300	1.20863700
H	-7.19081500	-2.33012800	-0.37182300
C	-2.44336800	0.04675600	0.17087600
C	-1.35602600	0.58080100	0.29725300
C	-0.04313500	1.21690800	0.46028100
O	1.74591000	4.38525000	-0.31814100
C	2.05989600	4.29343800	-1.72574000
H	2.69362700	3.41778000	-1.93093900
H	1.14560100	4.24346400	-2.33483400
H	2.60931200	5.20995400	-1.96589000
C	1.01392900	0.20301000	0.29262400
C	1.88815500	-0.63289900	0.15194700
C	2.91596400	-1.61034600	-0.01271800
C	3.93070300	-1.75771400	0.96357700
C	2.93280400	-2.44938100	-1.15296900
C	4.93284300	-2.71843700	0.79769300
H	3.92216800	-1.11467400	1.84190500
C	3.93936400	-3.40719600	-1.30812500
H	2.15380500	-2.34072700	-1.90551900
C	4.94124500	-3.54617200	-0.33545300
H	5.70869700	-2.82214300	1.55514300
H	3.94104700	-4.04718700	-2.18950200

H	5.72331200	-4.29384300	-0.45976400
C	0.12825700	1.92787400	1.87011000
H	0.50746900	1.21917900	2.61806500
H	-0.85784300	2.28163700	2.21489100
C	1.06321600	3.06912500	1.55488700
H	1.58695200	3.65059000	2.31014400
C	1.08912000	3.32815400	0.23352300
C	0.19609900	2.39259700	-0.56279900
H	-0.75766000	2.88652400	-0.80605100
H	0.63721300	2.02554300	-1.49580000

TS5_{DCE}

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C	-1.56005000	-3.02996600	-1.77126200
C	-0.71037600	-3.44232600	-0.71133500
C	-1.05107400	-4.58524400	0.03969300
C	-2.21872300	-5.30643200	-0.22952500
C	-3.07140900	-4.88610200	-1.25689000
C	-2.73907400	-3.76027000	-2.01548800
C	-1.28477500	-1.84364000	-2.62961400
C	-2.19169100	-0.76647000	-2.64763100
C	-1.95104900	0.35312000	-3.45064200
C	-0.80485700	0.40930000	-4.25418400
C	0.10233700	-0.65782200	-4.24682200
C	-0.13803900	-1.77884100	-3.44265600
H	-0.41261200	-4.91000600	0.85684100
H	-2.46388500	-6.18173900	0.36998400
H	-3.99201300	-5.42871000	-1.46636400
H	-3.39777500	-3.43051600	-2.81711400
H	-3.07653500	-0.80274000	-2.01849800

H	-2.65411900	1.18349700	-3.44099800
H	-0.61738500	1.28281700	-4.87569300
H	0.99656000	-0.62206500	-4.86789900
H	0.55996000	-2.61222400	-3.45477600
P	0.79873900	-2.49271200	-0.25233900
C	2.18674700	-3.37074600	-1.15362200
C	3.36636300	-2.42166300	-1.45034200
C	2.63714300	-4.66241200	-0.43755500
H	1.73535100	-3.66587400	-2.11101300
C	4.47925500	-3.15005700	-2.22516000
H	3.76893700	-2.03350300	-0.50737100
H	3.00561700	-1.55575300	-2.02245500
C	3.74222600	-5.36841200	-1.24794400
H	3.03179200	-4.41476300	0.55743000
H	1.77769100	-5.33256000	-0.29765600
C	4.93427300	-4.42519600	-1.49224400
H	5.32838700	-2.46649600	-2.37360800
H	4.10122300	-3.42514200	-3.22382700
H	4.06876400	-6.27242100	-0.71302900
H	3.32954100	-5.69047000	-2.21809700
H	5.71559400	-4.93926700	-2.07131800
H	5.37352500	-4.14414700	-0.52158800
C	1.05045300	-2.75942000	1.57328400
C	2.36461500	-2.09477800	2.04351200
C	-0.15426000	-2.17960400	2.34526600
H	1.12286700	-3.83890200	1.76185900
C	2.54148400	-2.27519200	3.56291300
H	2.33008200	-1.02178700	1.80356500
H	3.22815400	-2.51248700	1.51447500
C	0.02900400	-2.33327400	3.86580000

H	-0.24340100	-1.11052400	2.09417100
H	-1.07964600	-2.66815200	2.02671300
C	1.34605400	-1.69149800	4.33615100
H	3.47804600	-1.79591600	3.87663900
H	2.63002500	-3.35090700	3.78930600
H	-0.83088100	-1.88193100	4.38240000
H	0.03875800	-3.40608700	4.12017000
H	1.47976700	-1.83889000	5.41813000
H	1.30076800	-0.60442000	4.15494000
Au	0.84993600	-0.19940900	-0.58297000
C	3.17556800	8.43608900	-0.17443900
C	2.90050500	7.09344800	-0.45048900
C	3.76490100	6.07662900	0.02261900
C	4.90636700	6.44079500	0.77678700
C	5.17076400	7.78668800	1.04767500
C	4.30896900	8.78794600	0.57437900
H	2.50349000	9.20940300	-0.54412600
H	2.02110600	6.81812500	-1.03019700
H	5.57392900	5.66250000	1.14217000
H	6.05193700	8.05480300	1.62909700
H	4.51917900	9.83508100	0.78741000
C	3.48626900	4.70493000	-0.25717000
C	3.25138500	3.53428100	-0.50105500
C	2.89663900	2.13421300	-0.80049500
O	-0.47646500	2.83666000	-1.87223400
C	-1.60513500	2.76021600	-0.11168900
H	-1.32031600	1.71718100	-0.01366500
H	-0.95125100	3.53668800	0.26360400
H	-2.45215100	3.02565600	-0.73225500
C	3.76797800	1.24061800	-0.02948500

C	4.51161400	0.50949200	0.59901400
C	5.35418200	-0.36638500	1.34460900
C	6.09251300	-1.38353100	0.69358400
C	5.44828500	-0.24362300	2.75085800
C	6.89107000	-2.25893400	1.43529700
H	6.02511000	-1.48289800	-0.38698800
C	6.25384400	-1.12101700	3.48265900
H	4.88023900	0.53502800	3.25611000
C	6.97364500	-2.13343500	2.83059000
H	7.44978200	-3.04057800	0.92259100
H	6.31416400	-1.01838700	4.56522000
H	7.59607200	-2.81792500	3.40511500
C	2.98171000	1.86005200	-2.35038800
H	2.95658800	0.77148700	-2.48641600
H	3.90359500	2.26436700	-2.78095400
C	1.69832700	2.49796800	-2.90285200
H	1.85106800	3.55882000	-3.15168600
H	1.29908000	1.99592500	-3.78975400
C	0.70861800	2.44828900	-1.74339600
C	1.35891000	1.93375000	-0.54688100
H	1.00465200	2.33333300	0.40758200
O	-2.66429500	2.80404000	1.48065800
H	-3.42139200	2.16429600	1.28035800
H	-2.15253400	2.36267800	2.18076900
N	-4.58496400	1.03551000	0.90988300
S	-5.74591900	1.37604700	-0.20482500
S	-4.60200900	-0.22404500	1.96372400
O	-6.62586400	0.25784900	-0.56671700
O	-5.09539700	2.18198600	-1.24910800
O	-3.61494100	0.11619100	3.00312600

O	-5.91806500	-0.75994700	2.33143600
C	-6.84295100	2.62429500	0.75305100
C	-3.74502000	-1.58553100	0.92675200
F	-7.34241200	2.05398300	1.85946200
F	-6.10936000	3.69512500	1.10053000
F	-7.85506600	3.01996100	-0.03703300
F	-2.55161200	-1.12985500	0.51174100
F	-3.56527100	-2.68236000	1.68289200
F	-4.49527600	-1.90420300	-0.13735500

IM4_{DCE}

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C	5.41545700	-1.32175300	1.11647600
C	4.78874600	-0.13312800	1.57924400
C	5.27698300	0.49166900	2.74451200
C	6.35153400	-0.05025200	3.45889700
C	6.94830700	-1.23921100	3.02110300
C	6.48002600	-1.86449700	1.86045000
C	4.97749300	-2.02147000	-0.12517400
C	4.36194300	-3.28384800	-0.04171600
C	3.87667000	-3.91469500	-1.19331700
C	4.00606200	-3.29363300	-2.44237500
C	4.63620700	-2.04586600	-2.53792200
C	5.12451700	-1.41671700	-1.38690100
H	4.80718500	1.40111700	3.11001700
H	6.71205900	0.45046100	4.35635600
H	7.77741400	-1.67605000	3.57614200
H	6.94839600	-2.78221600	1.50750100
H	4.22729300	-3.74737800	0.93414800
H	3.35786100	-4.86610200	-1.10613200

H	3.61182500	-3.77589300	-3.33520700
H	4.74689000	-1.55990500	-3.50662000
H	5.62305400	-0.45435200	-1.46663300
P	3.31138500	0.55791600	0.71727400
C	4.01456500	1.82326500	-0.46800300
C	3.12361300	2.00217600	-1.71405700
C	4.35494500	3.16926900	0.20526100
H	4.96311600	1.37569200	-0.79269100
C	3.79124800	2.96485900	-2.71349100
H	2.14655500	2.40358700	-1.41851600
H	2.93841200	1.02375800	-2.17827400
C	5.01076000	4.12397900	-0.81318000
H	3.43735100	3.63419400	0.59081700
H	5.02531500	3.00013600	1.05980400
C	4.11540400	4.31719900	-2.05214900
H	3.13224900	3.11029900	-3.58067300
H	4.72664800	2.50956200	-3.08016000
H	5.21655100	5.09165300	-0.33190200
H	5.97894900	3.70172600	-1.12939800
H	4.60512000	4.98798200	-2.77377300
H	3.17271600	4.79834500	-1.74404700
C	2.34765000	1.49210100	2.00812400
C	1.13798600	2.19576300	1.35183400
C	1.85925600	0.53378800	3.11570900
H	2.99924400	2.26036000	2.44804800
C	0.34366300	2.98674700	2.40805900
H	0.49093000	1.43366700	0.89505000
H	1.45999600	2.86528000	0.54725300
C	1.05600000	1.30599100	4.18158900
H	1.22107000	-0.23399300	2.65022700

H	2.70797600	0.01683200	3.58247200
C	-0.12338900	2.07639700	3.55795300
H	-0.52138600	3.46906400	1.93050600
H	0.98578500	3.78731000	2.81142000
H	0.69020600	0.60532500	4.94680400
H	1.73014100	2.01834400	4.68575300
H	-0.63804800	2.66996600	4.32814500
H	-0.85327500	1.35657600	3.16460700
Au	1.83228100	-0.97319300	-0.19410200
C	-6.91024600	-1.87116400	-1.68855900
C	-5.57176000	-1.72153400	-2.06630000
C	-4.56964800	-2.54176200	-1.48693700
C	-4.95105800	-3.52126000	-0.53670900
C	-6.29356100	-3.66677000	-0.17554600
C	-7.27598800	-2.84164900	-0.74400200
H	-7.66729200	-1.22556500	-2.13112400
H	-5.28336500	-0.96356600	-2.79055000
H	-4.18625600	-4.14748200	-0.08263700
H	-6.57202000	-4.41838400	0.56153200
H	-8.31873000	-2.95239100	-0.45042900
C	-3.19317100	-2.31892900	-1.78929300
C	-2.01781100	-2.06441500	-1.98793600
C	-0.60081300	-1.65911300	-2.04784800
O	0.83221700	-4.45507300	-0.26206600
C	-0.55120100	-0.20210300	-2.21939200
C	-0.47402300	1.00731700	-2.34203900
C	-0.33634200	2.42334900	-2.42590800
C	0.19313400	3.03301000	-3.58771300
C	-0.68477900	3.23746000	-1.32218100
C	0.37498000	4.41810600	-3.63639200

H	0.46811400	2.41040200	-4.43700000
C	-0.49922600	4.62114500	-1.38086000
H	-1.08775900	2.77423600	-0.42677600
C	0.03345500	5.21714200	-2.53445900
H	0.79121200	4.87452600	-4.53346800
H	-0.76759800	5.23522400	-0.52202400
H	0.18128400	6.29543200	-2.57495100
C	0.20354100	-2.40201700	-3.18044600
H	1.14176300	-1.84839700	-3.31226000
H	-0.34970800	-2.41040700	-4.12625900
C	0.48685400	-3.78894400	-2.59267000
H	-0.33894600	-4.48807500	-2.79675800
H	1.41461800	-4.24447200	-2.95700300
C	0.53405600	-3.57576700	-1.07070200
C	0.13363600	-2.18230000	-0.75727000
H	-0.49582900	-2.14109300	0.13430800
H	-4.82043600	-0.71538800	0.12981500
N	-4.53693300	0.04597800	0.75785400
S	-4.14694700	-0.41910200	2.35433600
S	-4.30050900	1.56111900	-0.00455600
O	-4.99413800	-1.56443400	2.66575700
O	-4.05849700	0.77141200	3.18650800
O	-3.34701200	2.35025100	0.76161800
O	-4.17973900	1.29646200	-1.43263000
C	-2.35179600	-1.10054500	2.10315200
C	-6.04505100	2.32423900	0.27737100
F	-1.66785800	-0.27033500	1.31359000
F	-1.75864100	-1.19252000	3.29532200
F	-2.44308100	-2.30670800	1.54123900
F	-6.27065000	2.43704500	1.58668400

F	-6.06905300	3.52710800	-0.30084100
F	-6.95910000	1.52659700	-0.28212300

TS6_{DCE}

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C	4.20883400	-3.06654500	-0.26782500
C	4.29510400	-2.01949900	0.68734800
C	5.07185300	-2.20477500	1.84901400
C	5.74336200	-3.41020500	2.07938700
C	5.63604000	-4.45427900	1.15249700
C	4.87574200	-4.27819800	-0.00866400
C	3.43111300	-2.92749600	-1.53229400
C	2.23527500	-3.64787000	-1.70553800
C	1.45168200	-3.45450700	-2.84952200
C	1.85615300	-2.54409800	-3.83498100
C	3.06014800	-1.84275600	-3.68284900
C	3.84493500	-2.03736200	-2.54005200
H	5.14786800	-1.41104900	2.58756800
H	6.33764900	-3.53297200	2.98347700
H	6.14664200	-5.40002100	1.32855900
H	4.79989900	-5.08214900	-0.73936000
H	1.90008100	-4.32291000	-0.92041100
H	0.50673400	-3.98278800	-2.94541800
H	1.23540000	-2.38055000	-4.71449700
H	3.38848600	-1.14328400	-4.45072600
H	4.78327200	-1.49979800	-2.42885000
P	3.37724200	-0.44002200	0.47073800
C	4.56899400	0.69689800	-0.40045000
C	3.85905300	1.77740500	-1.24083200
C	5.60887500	1.29769900	0.57033800

H	5.10544600	0.03115200	-1.08890000
C	4.89804600	2.62421700	-1.99999700
H	3.26747700	2.43005500	-0.58814900
H	3.15812800	1.29967900	-1.93940200
C	6.63053200	2.14909900	-0.20911200
H	5.10038000	1.93387900	1.30818700
H	6.12121100	0.49457900	1.11851700
C	5.92630300	3.24196100	-1.03409900
H	4.38370500	3.41128200	-2.56819600
H	5.42444700	1.98197900	-2.72537900
H	7.34742700	2.59731100	0.49430600
H	7.20006500	1.49335800	-0.88767500
H	6.66647700	3.83324600	-1.59298600
H	5.40477600	3.93030000	-0.34891500
C	3.05310500	0.23641400	2.17364100
C	2.35367900	1.61096100	2.05971400
C	2.18055600	-0.75112100	2.98147500
H	4.02201300	0.37417700	2.67252700
C	2.02478000	2.17413000	3.45364500
H	1.42182800	1.48764500	1.48842900
H	2.97742000	2.32175200	1.50755100
C	1.84840300	-0.17898300	4.37275100
H	1.24224200	-0.92009400	2.43200200
H	2.68554200	-1.72075500	3.07823300
C	1.15754000	1.19224200	4.26036600
H	1.51184200	3.13973600	3.33970700
H	2.96524500	2.36317800	3.99739800
H	1.20571200	-0.88936800	4.91240600
H	2.78007800	-0.07021600	4.95255200
H	0.95050700	1.59836700	5.26152900

H	0.19069700	1.06273400	3.75029300
Au	1.31517000	-0.62559600	-0.49185500
C	-7.54542600	1.78776000	-2.14390100
C	-6.22599900	1.33600300	-2.23991400
C	-5.18067000	2.05672900	-1.61567500
C	-5.49074500	3.23486200	-0.89503300
C	-6.81375300	3.67698500	-0.80532600
C	-7.84465200	2.95777100	-1.42921100
H	-8.34321500	1.22275700	-2.62434600
H	-5.99094100	0.42065900	-2.77752100
H	-4.68950500	3.78480800	-0.40542600
H	-7.04120200	4.58296600	-0.24489900
H	-8.87467500	3.30391100	-1.35511400
C	-3.83260100	1.59930800	-1.69714300
C	-2.68401100	1.20056500	-1.74275700
C	-1.28329500	0.73865500	-1.76192100
O	-1.19532600	-2.89056900	-1.15006200
C	-0.43089000	1.88938800	-1.43888500
C	0.24872500	2.85406600	-1.13803700
C	1.06698100	3.95112100	-0.74223300
C	1.09971700	4.35796700	0.61272800
C	1.88474600	4.62113300	-1.68212000
C	1.94120600	5.39890200	1.01412200
H	0.47695600	3.84165300	1.33949500
C	2.72112400	5.66218400	-1.27067800
H	1.86605800	4.30655200	-2.72347000
C	2.75605500	6.05238700	0.07689400
H	1.96375700	5.69801800	2.06100200
H	3.35248300	6.16571400	-2.00124600
H	3.41276900	6.86129800	0.39367600

C	-0.91964700	0.09444600	-3.15765600
H	0.17730200	0.09109100	-3.22691100
H	-1.34232200	0.66991500	-3.98792600
C	-1.43408000	-1.34610600	-3.05253500
H	-2.51912200	-1.39539200	-3.22955000
H	-0.93541900	-2.04530600	-3.73128700
C	-1.19257000	-1.74574800	-1.59120800
C	-1.06825300	-0.48477800	-0.81887400
H	-0.72856900	-0.36058500	0.22433300
H	-2.25104700	-0.76161900	-0.09775500
N	-3.21822200	-1.01980100	0.72546200
S	-4.71126900	-1.52210400	0.15592400
S	-2.87543700	-0.56126000	2.29176600
O	-4.60709200	-1.52279900	-1.30399100
O	-5.83946300	-0.89699700	0.85037100
O	-3.87830200	-0.98629800	3.26848400
O	-1.44572100	-0.82937300	2.49252800
C	-4.73792600	-3.38884800	0.65113600
C	-2.99735500	1.35469000	2.19681600
F	-4.39753400	-3.54774500	1.93557300
F	-5.98838200	-3.84251500	0.46124700
F	-3.89353600	-4.07423600	-0.12383200
F	-4.19955600	1.71967700	1.74336800
F	-2.80834600	1.85240200	3.42912700
F	-2.04239100	1.82926300	1.38038800

P_{2DCE}

0 1

C	-5.48905800	-1.69852600	-0.00801400
C	-4.43880900	-0.77625600	0.02919300

C	-3.09675700	-1.22580100	0.03501200
C	-2.83590600	-2.61689200	0.00353500
C	-3.89416700	-3.52962600	-0.03377800
C	-5.22191400	-3.07576800	-0.03962600
H	-6.51810300	-1.34170900	-0.01258000
H	-4.64331400	0.29270100	0.05244100
H	-1.80500900	-2.96604200	0.00814300
H	-3.68179800	-4.59763700	-0.05816300
H	-6.04281800	-3.79092900	-0.06853400
C	-2.01836700	-0.29072100	0.07022800
C	-1.09121600	0.49809600	0.09549800
C	0.01311300	1.47352500	0.12521800
O	-1.75485200	4.37113900	-1.13232300
C	1.29902900	0.77079600	0.06831800
C	2.36818800	0.18897200	0.03166200
C	3.62308500	-0.49122000	-0.01332300
C	4.35990300	-0.71616400	1.17438700
C	4.14386000	-0.95681700	-1.24464200
C	5.58626600	-1.38571000	1.12552400
H	3.96212000	-0.36188500	2.12360500
C	5.37130000	-1.62529300	-1.28148100
H	3.57949300	-0.78807900	-2.15998200
C	6.09567400	-1.84265700	-0.09951200
H	6.14456400	-1.55296900	2.04566200
H	5.76234200	-1.97906300	-2.23445100
H	7.05102000	-2.36444300	-0.13288200
C	-0.10763500	2.39447500	1.40609500
H	0.84829000	2.92078000	1.52368000
H	-0.30166400	1.79863900	2.30339100
C	-1.22662100	3.38622300	1.05222000

H	-2.21914100	2.97120400	1.28597900
H	-1.14280200	4.35785500	1.55391300
C	-1.14951200	3.55255200	-0.46953600
C	-0.16548000	2.51839100	-1.02800000
H	0.79378600	3.03523800	-1.18782100
H	-0.49801200	2.08775000	-1.97769800

TS4_{gas}

0 1

C	4.59563600	-2.80275200	-1.56750500
C	5.03668200	-1.94901500	-0.52077000
C	6.23148400	-2.26007900	0.15840300
C	6.97705300	-3.39778000	-0.16408300
C	6.52705300	-4.25530300	-1.17455200
C	5.34919600	-3.95491600	-1.86392100
C	3.36179100	-2.54303400	-2.35896000
C	2.28431400	-3.44497100	-2.29265300
C	1.08786100	-3.17229700	-2.96372000
C	0.95376200	-1.99704600	-3.71295600
C	2.03003200	-1.10683000	-3.80874100
C	3.22962200	-1.38185800	-3.14269800
H	6.57782900	-1.61612200	0.96334900
H	7.89668100	-3.61523600	0.37706700
H	7.09286700	-5.15025900	-1.42925800
H	5.00102100	-4.60891100	-2.66203400
H	2.37631600	-4.33611600	-1.67406700
H	0.25001700	-3.86231900	-2.87914500
H	0.01219700	-1.77345800	-4.21115200
H	1.93482700	-0.19420600	-4.39511400
H	4.06395800	-0.68787000	-3.21540900

P	4.05914000	-0.47692300	0.01724800
C	4.88203900	0.95122900	-0.86768200
C	3.89618400	2.11157000	-1.11045000
C	6.18418200	1.43351100	-0.19567900
H	5.15432300	0.52629400	-1.84580000
C	4.56637000	3.21413900	-1.94894800
H	3.57625200	2.53251200	-0.14998700
H	2.98991500	1.73482000	-1.60348100
C	6.83844700	2.55385900	-1.03014600
H	5.95329200	1.82308600	0.80657300
H	6.88194100	0.59277000	-0.07379600
C	5.85543500	3.71530400	-1.27242400
H	3.86251300	4.04394500	-2.09140500
H	4.81138900	2.81167700	-2.94654800
H	7.74459600	2.91364900	-0.52119200
H	7.15418300	2.13758300	-2.00089100
H	6.33296500	4.49397500	-1.88484900
H	5.58915200	4.17485300	-0.30719500
C	4.39195600	-0.29159700	1.83958100
C	3.66979000	0.97574000	2.34915000
C	3.88002800	-1.54839700	2.58132100
H	5.47179500	-0.17615700	2.01373400
C	3.81825700	1.12426100	3.87358700
H	2.60241400	0.89856200	2.09206500
H	4.04907700	1.87222000	1.84582700
C	4.02275400	-1.38955000	4.10688100
H	2.81777600	-1.69265000	2.32674200
H	4.41931400	-2.44000300	2.23542600
C	3.29775700	-0.12579100	4.60545000
H	3.27739800	2.02105100	4.20809700

H	4.88144900	1.27566300	4.12428500
H	3.62643800	-2.28428500	4.60813400
H	5.09196900	-1.31881600	4.36798800
H	3.42209400	-0.01512000	5.69221900
H	2.21786700	-0.23132200	4.40853900
Au	1.76428600	-0.64361400	-0.25901200
C	-7.32651200	3.40127300	-0.58588200
C	-6.03419200	2.98570200	-0.25776800
C	-5.03882900	2.90078300	-1.25845400
C	-5.36955200	3.24855700	-2.58821900
C	-6.66391400	3.66772500	-2.90506300
C	-7.64668100	3.74379900	-1.90729400
H	-8.08804000	3.44725400	0.19112500
H	-5.78472500	2.70478800	0.76253800
H	-4.60590900	3.17269700	-3.35985500
H	-6.90927900	3.92992700	-3.93364900
H	-8.65698800	4.06327700	-2.15950900
C	-3.74265700	2.40921200	-0.93270900
C	-2.67186200	1.91200500	-0.64409400
C	-1.46528800	1.17334300	-0.25559100
O	-0.76238900	-1.87541900	1.67051600
C	-1.18398700	-1.61040200	3.02675900
H	-0.56510700	-0.80848000	3.45496700
H	-2.23968100	-1.32001400	3.05721000
H	-1.03403800	-2.54610500	3.57223500
C	-0.37159200	2.11352000	0.05444600
C	0.48282600	2.92312800	0.36484300
C	1.49014400	3.86144500	0.72421000
C	1.94362800	4.82893300	-0.20327200
C	2.07418200	3.83284900	2.01195600

C	2.96439100	5.71730100	0.14148900
H	1.49142200	4.86162600	-1.19235800
C	3.09649400	4.72293300	2.34879300
H	1.72375800	3.09778900	2.73224100
C	3.55156200	5.66453200	1.41413700
H	3.30784100	6.45109400	-0.58639900
H	3.54003200	4.68135600	3.34294900
H	4.34935500	6.35729900	1.67761700
C	-1.03510400	0.11700000	-1.34753200
H	-0.41266300	0.57745900	-2.12035400
H	-1.94687600	-0.28257700	-1.80609700
C	-0.32978000	-0.98826800	-0.53314300
H	-0.41077000	-1.98855000	-0.97324900
C	-0.94207500	-0.88755600	0.78656600
C	-1.72853300	0.25249900	0.95871100
H	-1.95648500	0.70335500	1.92204700
N	-4.23166800	-0.80108400	0.54260600
S	-4.53706500	-1.94425900	-0.64748900
S	-5.29538500	-0.40785700	1.78694300
O	-5.57052200	-2.88826600	-0.22523400
O	-3.22748500	-2.37569600	-1.14134500
O	-4.58160800	0.60764400	2.56563100
O	-6.66809200	-0.22280300	1.32982800
C	-5.31282600	-0.90693800	-2.07922800
C	-5.30399600	-2.01182400	2.90984100
F	-6.29676800	-0.13605300	-1.62353800
F	-4.36670900	-0.14916400	-2.65262400
F	-5.79536800	-1.76948000	-2.98863800
F	-5.23107800	-1.61620300	4.19170100
F	-6.41997800	-2.70867400	2.72209600

F	-4.23398600	-2.78270600	2.63657900
H	-3.10591200	-0.39405600	0.67624100

TS6_{gas}

0 1

C	4.16873600	-2.95096700	-0.27132600
C	4.18507200	-1.96370700	0.74817400
C	4.89038600	-2.21334800	1.94203600
C	5.56286900	-3.42299900	2.13995500
C	5.52776000	-4.40731100	1.14577200
C	4.83484100	-4.16855700	-0.04510000
C	3.45205600	-2.75179000	-1.56294300
C	2.26732600	-3.46364300	-1.82006900
C	1.54942400	-3.23843600	-2.99941500
C	2.00139900	-2.29531100	-3.92968000
C	3.18984400	-1.59323700	-3.68975600
C	3.91500500	-1.82739700	-2.51661300
H	4.90266100	-1.46833300	2.73342700
H	6.10057200	-3.59678600	3.07051800
H	6.03861400	-5.35716200	1.29561400
H	4.80864400	-4.92660100	-0.82620000
H	1.88224200	-4.15544300	-1.07441700
H	0.61595200	-3.77108800	-3.15612500
H	1.43141700	-2.10905900	-4.83842300
H	3.55548900	-0.86908800	-4.41651000
H	4.85197200	-1.30319800	-2.34501000
P	3.26884700	-0.38352800	0.55558600
C	4.48834500	0.78515800	-0.23872800
C	3.79548200	1.87124500	-1.08544900
C	5.48638100	1.38031200	0.77813700

H	5.05958300	0.13853100	-0.91784700
C	4.84648000	2.74832500	-1.78953900
H	3.16890600	2.50264400	-0.44496600
H	3.12312500	1.39851000	-1.81446100
C	6.51883500	2.27016000	0.05651400
H	4.94423900	1.98921700	1.51491200
H	5.99628400	0.57333400	1.32415600
C	5.82444800	3.36636100	-0.77360000
H	4.33800500	3.53585700	-2.36021600
H	5.41163800	2.13122700	-2.50815600
H	7.20058000	2.71587700	0.79500900
H	7.12894100	1.64142100	-0.61257500
H	6.57446400	3.98211500	-1.29046700
H	5.26195200	4.03307800	-0.10000600
C	2.89727800	0.24303700	2.26444600
C	2.21387400	1.62638300	2.17407800
C	1.98672100	-0.75201300	3.02100400
H	3.85250700	0.35827900	2.79813300
C	1.89675500	2.16217900	3.58233500
H	1.27891900	1.51788000	1.60767800
H	2.83738500	2.34543800	1.63139400
C	1.66141800	-0.21819200	4.43044600
H	1.05003800	-0.86739300	2.45692700
H	2.46098400	-1.74012100	3.08571500
C	1.01239800	1.17734200	4.36817500
H	1.39875000	3.13833100	3.49299800
H	2.84256000	2.32963900	4.12569700
H	0.99119000	-0.92546100	4.93786600
H	2.59199200	-0.16588800	5.02176600
H	0.83268200	1.55649200	5.38446300

H	0.03969900	1.09269100	3.86567300
Au	1.25360000	-0.52954000	-0.51051000
C	-6.98260700	3.24667000	-1.13400000
C	-5.64328100	2.94251700	-1.38633600
C	-5.27246500	1.63454900	-1.77601300
C	-6.27131600	0.64317600	-1.90626700
C	-7.60730500	0.95877700	-1.64824200
C	-7.96843300	2.25740700	-1.26358700
H	-7.25834900	4.25553000	-0.82910900
H	-4.87057000	3.70042300	-1.27441700
H	-5.97991300	-0.36764600	-2.17860700
H	-8.36693500	0.18340800	-1.73468800
H	-9.01109300	2.49605600	-1.05784400
C	-3.90172700	1.31146900	-1.98681600
C	-2.72465800	1.03582800	-2.10944800
C	-1.30459000	0.64815000	-2.11672500
O	-0.99998900	-2.93158600	-1.30069800
C	-0.48945000	1.82918200	-1.81785700
C	0.16747100	2.78414500	-1.44781400
C	0.93956100	3.85395300	-0.91619400
C	1.82014500	4.60709300	-1.72547800
C	0.86057400	4.14738800	0.46601600
C	2.61907900	5.60442100	-1.16085600
H	1.87598200	4.38900400	-2.79005000
C	1.66446400	5.14475200	1.02172100
H	0.17546000	3.57476000	1.08673600
C	2.55205900	5.87175600	0.21430700
H	3.29918300	6.17268500	-1.79384700
H	1.59901300	5.35504400	2.08830700
H	3.17873400	6.64765300	0.65138900

C	-0.91985500	-0.06885400	-3.46522200
H	0.17685500	-0.06189500	-3.53873100
H	-1.35253800	0.44664700	-4.32924700
C	-1.41984700	-1.50677900	-3.26564300
H	-2.51252900	-1.56239200	-3.38271700
H	-0.95687900	-2.24491900	-3.92821100
C	-1.11457100	-1.82303500	-1.79526000
C	-1.05211200	-0.50354500	-1.09147700
H	-0.69992300	-0.27444700	-0.05475000
H	-2.12971700	-0.66520000	-0.34185500
N	-3.13060200	-0.77008700	0.59281200
S	-4.40109000	-1.81564800	0.29895500
S	-2.74520400	-0.11353600	2.05066500
O	-4.32806700	-2.07719300	-1.14206700
O	-5.65037400	-1.41834600	0.94592700
O	-3.34881100	-0.78275000	3.20328300
O	-1.29167900	0.15220100	2.00404400
C	-3.82237000	-3.46633500	1.17631600
C	-3.51953900	1.63998600	1.94612300
F	-2.50621200	-3.43559800	1.42595200
F	-4.48833900	-3.62051000	2.32496300
F	-4.09634900	-4.49459600	0.36140800
F	-4.82583100	1.56727100	1.69373700
F	-3.31834000	2.26612100	3.12128000
F	-2.90868000	2.33934400	0.97260100