

Supporting Information

**Mechanism and Origins of Ligand-controlled
Regioselectivity of Copper-Catalyzed Borocarbonylation of
Imines with B₂pin₂ and Alkyl Iodides: A Computational
Study**

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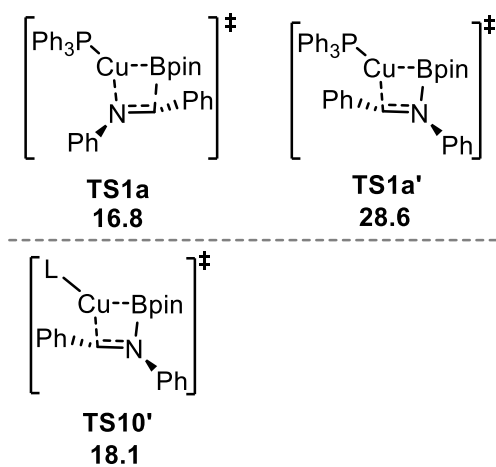
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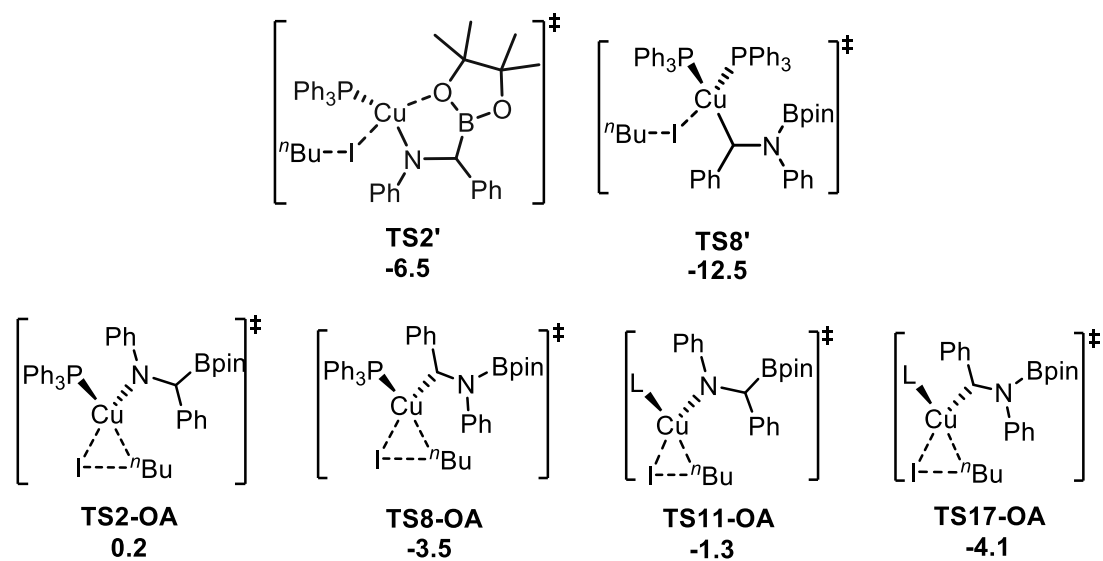
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1. Other possibilities of the migratory insertion into the Cu-B bond



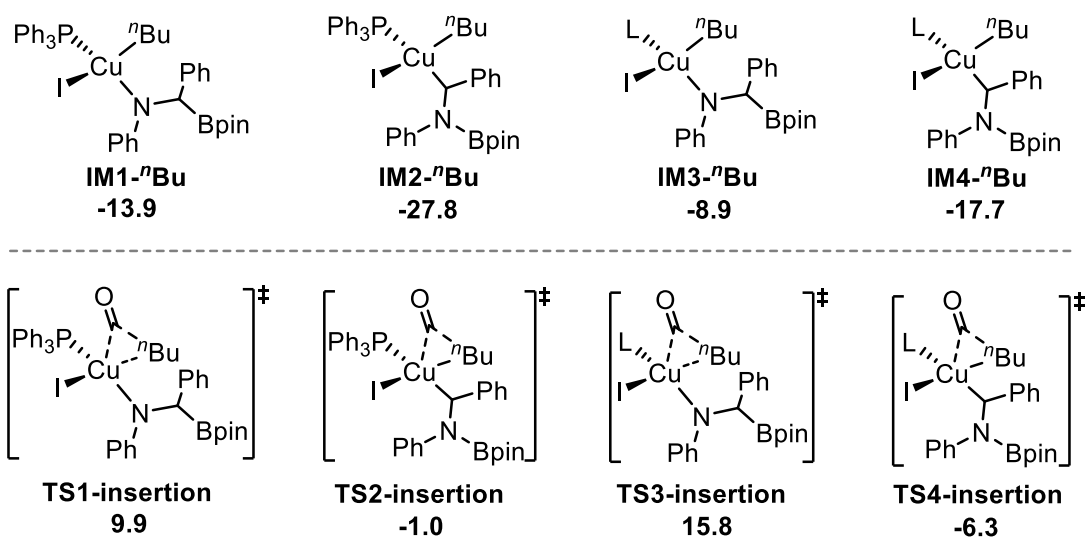
Scheme S1. Other possibilities of the migratory insertion into the Cu-B bond. The Gibbs free energies are given in kcal/mol.

2. The alternative pathways of the C-I bond cleavage



Scheme S2. The alternative pathways of the C-I bond cleavage. The Gibbs free energies are given in kcal/mol.

4. Other possibilities for the formation of acyl-copper(III) species after halogen-atom abstraction



Scheme S4. Other possibilities for the formation of alkylacyl-copper(III) intermediates and amidoacyl-copper(III) intermediates after halogen-atom abstraction. The Gibbs free energies are given in kcal/mol.

5. Calculated overall energy profiles of the Cu/^{Me}IMes-catalyzed reaction

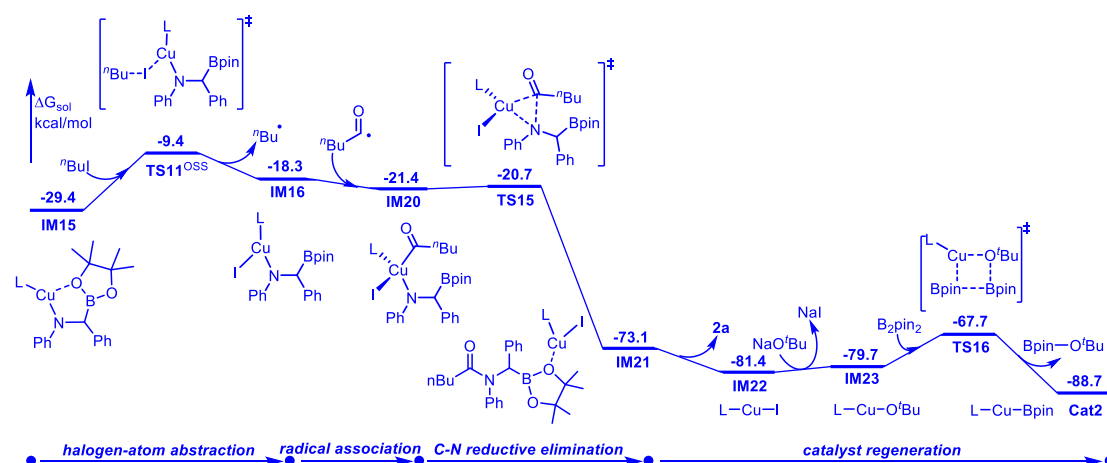


Figure S1. Calculated energy profile leading to α -boryl amide **2a**. The Gibbs free energies are given in kcal/mol.

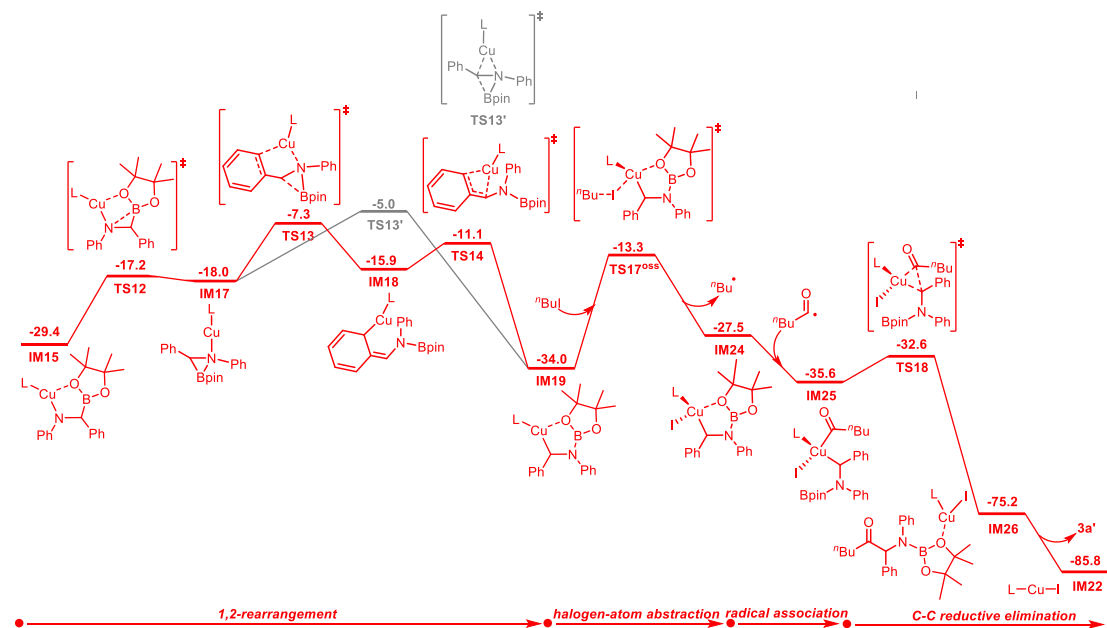


Figure S2. Calculated energy profile leading to α -amino ketone **3a'**. The Gibbs free energies are given in kcal/mol.

6. Visualization of AIM critical points for IM2 and IM15

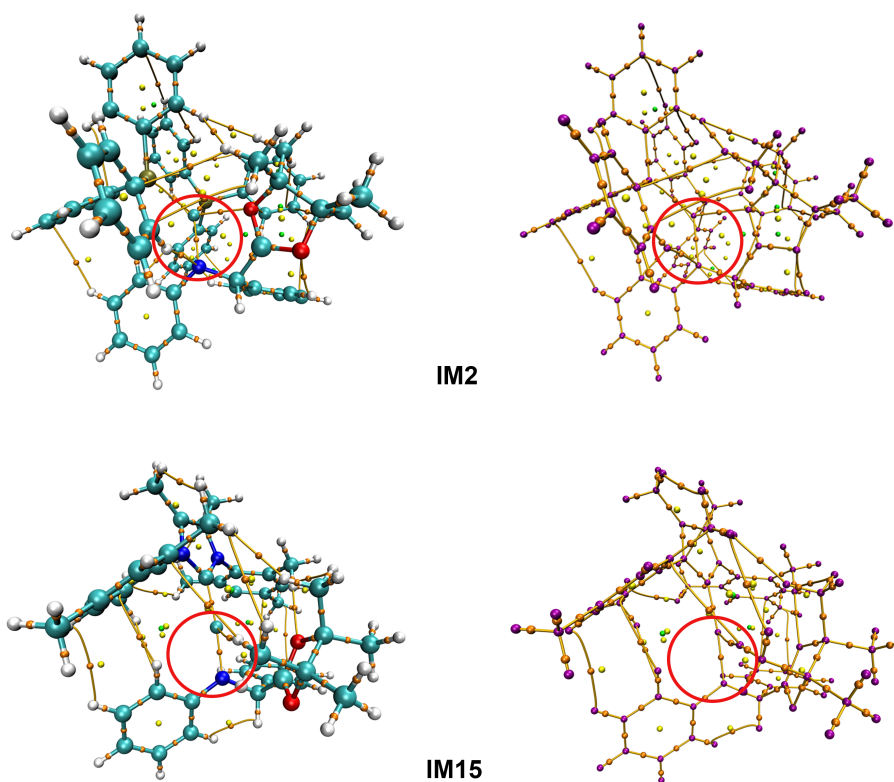


Figure S3. Visualization of QTAIM critical points for IM2 and IM15. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP) and green to cage critical points (CCP). Yellow lines indicate bond path. The red circle identifies the relevant area about Cu-N bond.

7. Table of calculated energies and energy corrections

Stationary point	Single-point energy-B3LYP-D3(BJ)-SMD 6-311+G(d,p)&SDD (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
Cat1	-2682.0603328	0.650083
1a	-556.9589831	0.165677
CO	-113.3452463	-0.014102
ⁿBuI	-169.3421885	0.090691
ⁿBu	-157.8500659	0.088608
ⁿBuCO	-271.2317246	0.097381
PPh₃	-1036.6016028	0.228341
NaO^tBu	-395.4954949	0.091253
NaI	-173.8152557	-0.024046
B₂pin₂	-822.8687219	0.318391
Bpin-O^tBu	-644.6602391	0.269493
2a	-1239.7355704	0.464218
3a'	-1239.7423895	0.463815
IM1	-3239.052228	0.844185
TS1	-3239.0372863	0.849837
TS1'	-3239.0145525	0.848249
IM2	-3239.0999892	0.847783
IM3	-3239.1068859	0.846143
TS2^{OSS}	-3408.4169497	0.952148
IM4	-3250.5638462	0.843525
IM5	-2485.185968	0.711588
TS3	-2485.1849436	0.712398
IM6	-2485.2655189	0.712247
IM7	-2282.1515955	0.477766
IM8	-2503.8267035	0.597359
TS4	-3326.7157711	0.951704
TS5	-3239.0792095	0.849007
IM9	-3239.0818259	0.847877
TS6	-3239.0670363	0.845314
TS6'	-3239.0609666	0.845473

IM10	-3239.0847096	0.848747
TS7	-3239.0800228	0.849600
TS8^{OSS}	-2371.8039963	0.696952
IM11	-2213.9492671	0.584421
IM12	-2485.2131899	0.711980
TS9	-2485.210535	0.711731
IM13	-2485.2703311	0.711659
Cat2	-1612.0540123	0.564321
1a	-556.9590114	0.165677
CO	-113.3451074	-0.014102
ⁿBuI	-169.3420306	0.090691
ⁿBu	-157.8509179	0.088608
ⁿBuCO	-271.2309037	0.097381
NaO^tBu	-395.4895567	0.091253
NaI	-173.8041159	-0.024046
B₂pin₂	-822.8665074	0.318391
Bpin-O^tBu	-644.659438	0.269493
2a	-1239.7348021	0.464218
3a'	-1239.7414224	0.463815
IM14	-2169.0381427	0.756897
TS10	-2169.0205985	0.759739
IM15	-2169.0862613	0.759458
TS11^{OSS}	-2338.4112677	0.868014
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IM18	-2169.0633085	0.757959
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TS1a	-2202.3906686	0.587225
TS1a'	-2202.3699413	0.585167
TS10'	-2169.0082997	0.757099
TS2'	-2371.7867832	0.697717
TS8'	-3408.4280661	0.959057
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TS11-OA	-2338.4027484	0.872348
TS17-OA	-2338.411168	0.876264
IM1-"Bu	-2371.8058877	0.705020
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TS1-insertion	-2485.1298246	0.707459
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TS4-insertion	-2451.7805223	0.882882
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TS13'	-2169.0438534	0.755864
TS17^{OSS}	-2338.4216193	0.872015
IM24	-2180.5680898	0.755243
IM25	-2451.8303768	0.886016
TS18	-2451.8263261	0.886837
IM26	-2451.8910724	0.883687

8. Cartesian coordinates

1a

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H	-0.08700300	1.39924800	-0.51213800
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CO

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H	1.23496000	1.44706000	2.03667500
H	2.53268200	1.79209000	0.86676100
H	1.07281700	2.80035300	0.89049400
O	1.09695400	1.32575500	-1.31803900
Na	1.52092200	1.98606400	-3.12878800

NaI

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I	0.84990300	0.75682400	0.00000000

B₂pin₂

B	-0.85832800	-2.06973900	1.83909500
C	1.31093300	-2.64816700	1.41884100
C	1.78668400	-3.51845800	2.58642800
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C	1.26731300	-0.20804700	0.55039200
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H	0.56007500	-0.54064700	-0.21541200
C	2.21233700	-0.64621100	2.83204000
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H	2.09299700	-4.04827300	-0.01995500
H	3.15490800	-2.65901500	0.27566800
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B	-2.53921500	-2.21611000	2.02340100
C	-4.56360100	-2.63816600	2.99225100
C	-4.67373800	-4.15583000	3.17165800
H	-5.70809000	-4.49998000	3.06993000
H	-4.31684300	-4.42036100	4.17139700
H	-4.05552300	-4.68431600	2.43970400
C	-4.76339700	-2.17304300	1.50726200
C	-5.17343600	-0.70190700	1.38365800
H	-6.20750800	-0.54267500	1.70631700
H	-5.08603700	-0.39721200	0.33656700
H	-4.51863900	-0.05907600	1.97969500
C	-5.68969600	-3.05096800	0.67338100
H	-5.74450700	-2.66105500	-0.34772800
H	-6.70242000	-3.05267500	1.09243900
H	-5.32984000	-4.08059200	0.62283100
C	-5.43415300	-1.92071300	4.01764800
H	-5.25451200	-0.84372500	4.01363000

H	-5.20831400	-2.29785400	5.01989700
H	-6.49649600	-2.10066100	3.81706100
O	-3.41549500	-2.27501900	0.96641800
O	-3.17144300	-2.29118000	3.24123400

Bpin-O'Bu

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C	-0.63895100	-6.05116700	3.76731300
C	-1.17252600	-6.38173800	2.36972800
H	-1.25744500	-7.46204500	2.21442300
H	-0.48282200	-5.97777600	1.62239900
H	-2.15556100	-5.92912100	2.20671000
C	-1.69257000	-6.31270900	4.90468900
C	-1.05294800	-6.44156400	6.29152100
H	-0.50870900	-7.38522100	6.40090800
H	-1.84212100	-6.40563200	7.04813000
H	-0.36060700	-5.61598700	6.48408200
C	-2.63762100	-7.48101100	4.64779600
H	-3.33908300	-7.57659100	5.48233800
H	-2.07961200	-8.42026600	4.56195100
H	-3.21765800	-7.33212800	3.73467400
C	0.72178700	-6.70177700	3.98440300
H	1.18558200	-6.35715400	4.91087200
H	1.38926500	-6.44728300	3.15501500
H	0.62737100	-7.79268200	4.02295600
O	-2.46043600	-5.08490500	4.90382300
O	-0.47938200	-4.60991300	3.82779600
C	-1.12951600	-1.90918700	2.35073600
C	-1.24338500	-1.71064500	3.86618600
H	-0.55169800	-2.80754100	2.12030100
H	-2.12675100	-2.00841800	1.90845200
H	-0.63366000	-1.04759200	1.89038800
C	-2.06566700	-0.46136200	4.18698900
C	0.13722400	-1.63545200	4.52701700
H	-2.17732200	-0.34882300	5.27012400
H	-1.57748000	0.43495000	3.78998000
H	-3.06436800	-0.54093800	3.74595900
H	0.68982200	-0.76516800	4.15617000
H	0.02917500	-1.53664200	5.61258200
H	0.71935500	-2.53520200	4.31267300
O	-1.99833000	-2.80251100	4.44501600

2a

C	-4.01824100	-2.58284400	-6.64334600
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H	-4.98005800	-2.43146200	-6.13861100
H	-4.14090100	-3.40455000	-7.35720000
H	-3.79618700	-1.67309500	-7.21357000
C	-2.90772400	-2.88391600	-5.63403200
H	-3.13844300	-3.81366000	-5.09571900
H	-1.96273400	-3.06205800	-6.16528500
C	-2.70930500	-1.75096900	-4.62392200
H	-3.64982700	-1.56941100	-4.08713900
H	-2.45815800	-0.81889800	-5.14339900
C	-1.59637300	-2.06865100	-3.60782300
H	-0.65843800	-2.25015800	-4.14506200
H	-1.84303500	-2.96690800	-3.03637100
O	-0.81804800	0.14693400	-3.13182500
C	-1.34887200	-0.91393000	-2.68492800
B	-0.59773500	1.23530200	-1.88055600
O	-1.22173100	2.47324600	-2.17152400
C	-0.19181100	3.36848700	-2.62352500
C	1.06799800	2.82836700	-1.85622700
O	0.81156100	1.41742000	-1.80772400
C	-1.36552500	0.35904200	-0.71221400
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C	-0.61143800	0.14929600	0.57268800
C	-1.20371800	0.45945000	1.80075000
C	-0.51704000	0.26173000	3.00085700
C	0.77295300	-0.26614700	2.98580700
C	1.37545500	-0.58087500	1.76370100
C	0.69376900	-0.36794500	0.56773600
H	-2.21565500	0.85696100	1.81537700
H	-0.99446800	0.51201600	3.94436700
H	1.30945200	-0.42708900	3.91686500
H	2.38599300	-0.98039600	1.74362000
H	1.17771200	-0.57371000	-0.38025900
C	2.39976800	3.06268400	-2.56386400
H	2.59298200	4.13422600	-2.69351900
H	3.21458000	2.64065900	-1.96586600
H	2.41593400	2.58145100	-3.54429900
C	1.14287600	3.34052300	-0.41021700
H	0.18343600	3.21123500	0.09935000
H	1.88944400	2.75225000	0.13195700
H	1.42698900	4.39758100	-0.36152000
C	-0.59624400	4.79557900	-2.26501200
H	0.20722800	5.50232100	-2.50371700
H	-1.48415100	5.08435400	-2.83761100
H	-0.83627700	4.88352400	-1.20305100

C	-0.06101300	3.22623200	-4.14686000
H	-1.04175400	3.40374000	-4.59988600
H	0.64924100	3.94819300	-4.56505100
H	0.26074400	2.21734000	-4.41862100
N	-1.66746300	-0.93662200	-1.38905600
C	-2.41831100	-1.97230100	-0.75070900
C	-3.78793100	-2.08658100	-1.00702500
C	-1.79514300	-2.82948600	0.16008100
C	-4.53224800	-3.07753000	-0.36789900
H	-4.25877800	-1.39433100	-1.69838900
C	-2.54807500	-3.81213700	0.80238900
H	-0.73693400	-2.71376700	0.36216500
C	-3.91301500	-3.94092700	0.53787100
H	-5.59475000	-3.16969600	-0.57274500
H	-2.06484700	-4.47862600	1.51051000
H	-4.49369100	-4.70974400	1.03904200
3a'			
C	-0.85299800	1.68223900	-1.03702200
O	-1.35663400	2.71458000	-1.42908400
C	-1.72347500	0.71888600	-0.15912700
H	-2.57203300	0.49549100	-0.81669000
C	-1.05364800	-0.59867300	0.18824700
C	-0.40950600	-0.81271300	1.41084400
C	-1.05882500	-1.63133800	-0.75819700
C	0.22754100	-2.02514700	1.67419400
H	-0.41077800	-0.03006600	2.15945700
C	-0.42054100	-2.84395300	-0.49982200
H	-1.57276100	-1.48333700	-1.70597000
C	0.22883200	-3.04353400	0.71950100
H	0.72157000	-2.17553600	2.63021600
H	-0.43801400	-3.63380000	-1.24558600
H	0.72331700	-3.98803800	0.92757700
N	-2.26848700	1.46089400	0.98329700
C	-3.62093300	1.21289600	1.33814600
C	-4.19179100	-0.05216700	1.12777400
C	-4.41654500	2.22925100	1.89065900
C	-5.52663300	-0.28942100	1.45526000
H	-3.58778500	-0.85994600	0.73042900
C	-5.74376500	1.97660900	2.22746000
H	-3.98955200	3.21003900	2.05266400
C	-6.31227000	0.72001600	2.00926000
H	-5.94620700	-1.27703000	1.28346900
H	-6.34287700	2.77840800	2.65088900

H	-7.35057200	0.53250800	2.26653700
C	0.55818800	1.27070100	-1.39607300
C	1.37478600	2.41720000	-1.98544200
H	0.50410300	0.42322500	-2.09599000
H	1.03143100	0.86951800	-0.49377900
C	2.82996900	2.02633000	-2.25547800
H	0.90031000	2.77156500	-2.90831800
H	1.34094300	3.26202300	-1.28669700
C	3.65948100	3.18522000	-2.81401300
H	3.28663400	1.66370700	-1.32328600
H	2.85953600	1.17986400	-2.95621300
H	4.69784500	2.88625100	-2.99661000
H	3.24299900	3.54712000	-3.76184500
H	3.67185700	4.03109300	-2.11567100
C	-0.65951400	4.12247400	2.88720100
C	0.55677400	3.30450700	2.32551600
C	-0.55978300	4.49818700	4.35959300
H	0.30617800	5.14663100	4.53382800
H	-1.45928700	5.04296100	4.66220600
H	-0.46987000	3.61411000	4.99429800
C	-0.98859200	5.35154200	2.03401800
H	-1.95855400	5.74934700	2.34666900
H	-0.23710200	6.13832700	2.15434600
H	-1.05371500	5.08730000	0.97374700
C	1.64117600	4.13712600	1.65259500
H	2.09460300	4.83318600	2.36705800
H	2.42873700	3.47839000	1.27263100
H	1.24203600	4.70681000	0.81111600
C	1.17238200	2.35601700	3.35878400
H	1.84401400	1.66164700	2.84504900
H	1.74716900	2.90015300	4.11470200
H	0.39854500	1.77146400	3.86646500
O	-0.08115900	2.47724500	1.32071800
O	-1.76196300	3.18873400	2.71963400
B	-1.41574800	2.36731200	1.66976900

Cat1

C	6.99988000	0.45580800	4.97034400
C	8.32903000	0.54766400	4.55482700
C	8.65225800	0.41810800	3.20291700
C	7.64493300	0.19900600	2.25450400
C	6.31329200	0.09355100	2.68422500
C	5.99127300	0.22689700	4.03231200
H	9.11731300	0.71539200	5.28391900

H	9.68910000	0.47440200	2.88635600
H	5.53428500	-0.11989900	1.95686800
H	4.95899300	0.12734000	4.35391700
C	8.07821900	4.25960600	-1.32318900
C	8.30014100	4.09338600	0.04542900
C	8.25802700	2.81844800	0.61100000
C	7.99419800	1.69990400	-0.19216800
C	7.75483300	1.87164500	-1.56523900
C	7.80511200	3.14878500	-2.12406700
H	8.50216800	4.95628700	0.67435300
H	8.41945000	2.69367900	1.67738300
H	7.51219900	1.01459200	-2.18788800
H	7.61825800	3.27428700	-3.18699500
C	12.31584400	-1.56650200	0.25561900
C	12.09091200	-0.19403100	0.38954300
C	10.78819800	0.30374500	0.43881900
C	9.69544300	-0.57114100	0.36137200
C	9.93092200	-1.94527800	0.20406200
C	11.23319500	-2.44231400	0.15868600
H	12.93187100	0.49142700	0.45032700
H	10.61858100	1.37271700	0.52555900
H	9.09686200	-2.62918900	0.09843500
H	11.39107700	-3.50988100	0.03553200
P	7.94934900	-0.01395600	0.45712300
C	2.21025200	-5.56481300	-0.61342800
C	3.08900900	-6.17415100	0.28841900
C	4.25738800	-5.51999000	0.67120300
C	4.55075700	-4.24446100	0.16387400
C	3.67448800	-3.64425100	-0.74795900
C	2.50596700	-4.30518000	-1.13335800
H	2.86550000	-7.16080500	0.68494000
H	4.94674300	-5.99687000	1.36229900
H	3.93554200	-2.68329000	-1.17975600
H	1.83408700	-3.83716600	-1.84727600
C	6.40072900	-3.16400200	5.20338100
C	5.18314100	-3.48954600	4.60771100
C	5.08654600	-3.61067600	3.21966800
C	6.20984800	-3.40281000	2.40734000
C	7.42568200	-3.04440100	3.01800600
C	7.52310600	-2.94171500	4.40200200
H	4.30222700	-3.65545700	5.22208300
H	4.13438200	-3.86859000	2.76874000
H	8.29803800	-2.83236600	2.40803700
H	8.46984000	-2.66094000	4.85256300

C	9.43189900	-6.11196000	-1.11960400
C	9.25637400	-6.05848400	0.26415700
C	8.23809300	-5.27735400	0.81565100
C	7.39087700	-4.53403100	-0.01546400
C	7.56043800	-4.60449200	-1.41119100
C	8.57461400	-5.39052600	-1.95443700
H	9.91003400	-6.62808800	0.91945100
H	8.11321300	-5.24087800	1.89231100
H	6.90267700	-4.03666900	-2.06258000
H	8.69929200	-5.43082700	-3.03308800
P	6.10216800	-3.36176500	0.57766800
Cu	6.54225000	-1.43908900	-0.74094800
B	6.10756900	-1.47244400	-2.72107700
O	6.51178500	-0.53207200	-3.67049200
C	5.92896000	-0.86355400	-4.95640400
C	5.64440200	-2.39356400	-4.80295600
O	5.45592000	-2.52708300	-3.37147200
C	6.84653100	-3.27285600	-5.17128200
H	6.64442700	-4.29822900	-4.84446000
H	7.03131800	-3.28544700	-6.25096200
H	7.75165000	-2.92585000	-4.66342500
C	4.39149700	-2.89605000	-5.51280400
H	4.46903900	-2.75149000	-6.59710300
H	4.26428700	-3.96628800	-5.31985800
H	3.49717600	-2.38108100	-5.15528800
C	6.92070300	-0.49484600	-6.05503900
H	6.54471500	-0.79590400	-7.04019700
H	7.07044500	0.58982300	-6.06660400
H	7.89203800	-0.96641300	-5.89154800
C	4.65357300	-0.02341000	-5.09413000
H	4.91391700	1.03317700	-4.97774300
H	4.17644500	-0.15767400	-6.07133700
H	3.93347900	-0.28164000	-4.31205500
H	8.10869000	5.25358700	-1.76128600
H	6.75169300	0.54669100	6.02408500
H	6.47413300	-3.07064900	6.28316100
H	13.33215200	-1.94853800	0.21476600
H	10.22824500	-6.71643800	-1.54503700
H	1.30185800	-6.07898300	-0.91551300
IM1			
C	6.18551200	0.56245600	4.59747600
C	7.53647800	0.23496900	4.48105100
C	8.07501200	-0.08420900	3.23355300

C	7.26591800	-0.07159900	2.08986300
C	5.90607700	0.26079200	2.21223500
C	5.37373800	0.57346500	3.46122200
H	8.17341300	0.22307700	5.36173500
H	9.12467100	-0.34710700	3.15107300
H	5.26754300	0.27491400	1.33409300
H	4.31835800	0.81539800	3.54598000
C	9.10207100	3.63934300	-1.36519900
C	8.97048600	3.51718600	0.01967700
C	8.61654500	2.29079700	0.58545800
C	8.38290900	1.17818700	-0.23465800
C	8.49625400	1.31407200	-1.62409700
C	8.86757100	2.53370600	-2.18523500
H	9.14304600	4.37690300	0.66160900
H	8.51309800	2.20093600	1.66228400
H	8.27901600	0.46885400	-2.26415200
H	8.96049000	2.61817200	-3.26415700
C	11.91020700	-2.68205400	1.19113400
C	11.90323900	-1.28541300	1.16565900
C	10.71164300	-0.59159900	0.94638300
C	9.51231800	-1.28948200	0.75398200
C	9.53055500	-2.69215200	0.77418700
C	10.71911300	-3.38596000	0.99533600
H	12.82870600	-0.73452200	1.31038800
H	10.71395600	0.49324900	0.91042400
H	8.61606800	-3.24360600	0.57712700
H	10.71453400	-4.47240700	0.99534500
P	7.90084600	-0.46985500	0.41286500
C	1.01096300	-4.37539400	-1.16626800
C	1.88829200	-5.41819100	-0.86128200
C	3.21395900	-5.14323900	-0.52596500
C	3.67406800	-3.82088800	-0.50742400
C	2.79734200	-2.77735700	-0.83899300
C	1.46875500	-3.05677100	-1.15571800
H	1.53836600	-6.44700200	-0.87745400
H	3.89023300	-5.95587300	-0.28042700
H	3.16318400	-1.75471800	-0.84308000
H	0.79748300	-2.24201800	-1.41194700
C	4.82625200	-2.73802800	4.62503400
C	3.70586700	-2.75215000	3.79639300
C	3.84641100	-2.96505900	2.42373400
C	5.11471700	-3.16019700	1.86280000
C	6.23802400	-3.13321200	2.70469100
C	6.09419000	-2.93242900	4.07404900

H	2.71470100	-2.60111200	4.21557500
H	2.96583000	-2.98088500	1.79163100
H	7.23150500	-3.26736100	2.29061400
H	6.97557500	-2.90463600	4.70688100
C	8.00102300	-7.13991300	-0.33919900
C	7.15284000	-7.01623100	0.76405000
C	6.33414900	-5.89421900	0.89669000
C	6.35756100	-4.88291800	-0.07541900
C	7.21102800	-5.01328800	-1.18208800
C	8.02551500	-6.13915900	-1.31271400
H	7.13093100	-7.79251500	1.52411400
H	5.68759400	-5.79407100	1.76262100
H	7.24188200	-4.22977800	-1.93582800
H	8.68487800	-6.22622900	-2.17193400
P	5.35895400	-3.34715400	0.04525000
Cu	6.08357100	-1.31537400	-0.84216800
B	4.93319600	0.22558100	-1.46477600
O	5.00655000	1.01625500	-2.61514600
C	4.23240300	2.22696700	-2.40451600
C	3.19950300	1.77207900	-1.32240700
O	3.93033200	0.72956700	-0.62739100
C	1.94708600	1.11250500	-1.91261000
H	1.37768800	0.65057700	-1.09932000
H	1.29968000	1.83727100	-2.41820000
H	2.21828200	0.32525500	-2.62204700
C	2.80526800	2.84556300	-0.31357600
H	2.31120100	3.69029400	-0.80834200
H	2.10686400	2.42462000	0.41741400
H	3.67674800	3.21915900	0.22827700
C	3.62669200	2.66137300	-3.73446500
H	2.98750000	3.54268200	-3.60395700
H	4.42631900	2.92373700	-4.43491900
H	3.02966900	1.86489800	-4.18513200
C	5.20904500	3.29199200	-1.89271000
H	6.02201100	3.40515300	-2.61486800
H	4.71997100	4.26367600	-1.76176800
H	5.65634700	2.98948300	-0.94159400
C	6.18715200	-1.83505500	-3.68508900
H	6.21257300	-0.74957500	-3.82066200
C	4.87558300	-2.46738900	-3.85159300
C	4.70448600	-3.85742200	-3.76663800
C	3.45200300	-4.42247400	-3.98382900
C	2.36020000	-3.61071000	-4.29998900
C	2.52374200	-2.22645900	-4.39286200

C	3.77253900	-1.65705600	-4.16506100
H	5.56035200	-4.47949200	-3.53125900
H	3.32211200	-5.49679800	-3.89739700
H	1.38297500	-4.05575300	-4.46235600
H	1.67510700	-1.59197700	-4.63394300
H	3.91214500	-0.58203600	-4.20716100
N	7.25985600	-2.51475200	-3.45851400
C	8.49760100	-1.84979100	-3.48265200
C	8.80914900	-0.85296300	-4.42550300
C	9.47648600	-2.23284500	-2.55358300
C	10.05365600	-0.22484600	-4.39689300
H	8.07932200	-0.58969500	-5.18493600
C	10.70785200	-1.58574900	-2.51370600
H	9.24526400	-3.01889300	-1.84588100
C	11.00098100	-0.57430500	-3.43210400
H	10.28306200	0.54225100	-5.13185600
H	11.43364000	-1.87018400	-1.75829200
H	11.96328100	-0.07176100	-3.40428900
H	-0.02310900	-4.59161200	-1.42107600
H	8.64188400	-8.01196400	-0.43675000
H	12.84053100	-3.21897900	1.35413600
H	9.37790000	4.59498800	-1.80279800
H	5.76486400	0.80154300	5.57044200
H	4.71607700	-2.56780800	5.69224700

TS1

C	5.95863200	0.81708300	4.27581100
C	7.34303600	0.65303900	4.19983900
C	7.93942200	0.28453500	2.99328600
C	7.15172100	0.07952300	1.85279700
C	5.75960400	0.22521600	1.94090300
C	5.16847700	0.60032000	3.14581600
H	7.95956200	0.80881100	5.08101400
H	9.01546400	0.15013200	2.93782600
H	5.14540500	0.01796600	1.07109100
H	4.08859100	0.69364100	3.20743100
C	9.26939200	3.66090800	-1.60531000
C	9.01391200	3.59509600	-0.23369300
C	8.59571700	2.39618200	0.34528300
C	8.42403400	1.25395800	-0.44894000
C	8.67592500	1.32725200	-1.82528400
C	9.10383400	2.52315200	-2.39776700
H	9.13746200	4.47813700	0.38738500
H	8.39001000	2.35526800	1.40975200

H	8.53767500	0.45561300	-2.45183900
H	9.30073500	2.55810400	-3.46517600
C	11.74036800	-2.67923400	1.25778300
C	11.80429500	-1.29558400	1.08352100
C	10.65125100	-0.56956700	0.77781600
C	9.42209800	-1.22616600	0.64568900
C	9.36837000	-2.61779700	0.81051800
C	10.51758500	-3.34122300	1.12016300
H	12.75553500	-0.77891600	1.17667400
H	10.71038700	0.50318300	0.62431700
H	8.43443000	-3.14338500	0.64629500
H	10.45718800	-4.42054000	1.22739000
P	7.86323100	-0.35641000	0.22081000
C	1.14611800	-4.64918500	-1.38910100
C	2.07075700	-5.61686300	-0.99358200
C	3.33591800	-5.23679800	-0.54349600
C	3.68609100	-3.88228800	-0.49630400
C	2.75975000	-2.91276600	-0.90924800
C	1.49381000	-3.29791500	-1.34481100
H	1.80839900	-6.67065500	-1.03402700
H	4.05078000	-5.99395500	-0.23891800
H	3.04294400	-1.86614500	-0.90934600
H	0.78920000	-2.54165200	-1.67872000
C	4.62267600	-2.49614300	4.63126900
C	3.52947400	-2.59136600	3.77188200
C	3.72052700	-2.86211700	2.41508100
C	5.01158400	-3.03443400	1.90196000
C	6.10739400	-2.92718900	2.77438200
C	5.91394800	-2.66736100	4.12746300
H	2.52080100	-2.46254600	4.15529600
H	2.86236100	-2.94463600	1.75719700
H	7.11713300	-3.04686200	2.39726700
H	6.77363200	-2.57964800	4.78462400
C	8.10985500	-7.00075700	-0.01758800
C	7.24023400	-6.84732000	1.06530600
C	6.37775400	-5.75208800	1.12109000
C	6.38123400	-4.79876200	0.09209800
C	7.25276800	-4.95956400	-0.99734200
C	8.11130500	-6.05866400	-1.04836700
H	7.23594000	-7.57860400	1.86903000
H	5.71320600	-5.62920100	1.97041100
H	7.26683100	-4.20431800	-1.78150500
H	8.78936300	-6.16819300	-1.89010700
P	5.31800700	-3.30042700	0.10632700

Cu	6.40767300	-1.57022300	-1.04693600
B	5.12423600	-0.03312600	-1.84695200
O	5.31872500	1.15980600	-2.50233300
C	4.44985600	2.17391900	-1.92542500
C	3.33884300	1.31812400	-1.21250100
O	4.01310700	0.03556500	-1.01639500
C	2.10277700	1.04150300	-2.07118400
H	1.46206200	0.32443800	-1.54779700
H	1.52426700	1.95473300	-2.24490500
H	2.36980600	0.60287700	-3.03374900
C	2.90428600	1.84268900	0.15300500
H	2.41036000	2.81569600	0.05218100
H	2.18966200	1.14431700	0.60069100
H	3.74705400	1.95232400	0.83659700
C	3.94505200	3.06139100	-3.05835700
H	3.24836900	3.81850500	-2.68077000
H	4.79238500	3.57797800	-3.51927200
H	3.44087500	2.47856100	-3.83267200
C	5.31244000	2.99174000	-0.96057800
H	6.18093600	3.37722800	-1.50072000
H	4.75495300	3.83648900	-0.54204000
H	5.68670200	2.37890800	-0.13766200
C	5.97580200	-1.43396300	-3.21107300
H	6.18995300	-0.53403200	-3.78943400
C	4.73385200	-2.12147500	-3.67873500
C	4.59390000	-3.51169700	-3.58380700
C	3.44655800	-4.14148900	-4.06066100
C	2.42144900	-3.39469900	-4.64308400
C	2.56098100	-2.00996000	-4.76303900
C	3.71094900	-1.38200700	-4.28894000
H	5.40130200	-4.08469300	-3.14490000
H	3.34634300	-5.21828000	-3.96254100
H	1.52484200	-3.88766600	-5.00849400
H	1.77957500	-1.42112600	-5.23687400
H	3.83603400	-0.30839600	-4.40432200
N	7.06396700	-2.24393900	-2.90548300
C	8.32167600	-1.83635700	-3.32907600
C	8.56405200	-1.02440700	-4.46398600
C	9.45604100	-2.28326700	-2.61108800
C	9.85857100	-0.62539400	-4.80010100
H	7.73509100	-0.70953100	-5.09024800
C	10.74006900	-1.88162100	-2.95209000
H	9.29643600	-2.92263100	-1.75159000
C	10.95844400	-1.03213200	-4.04370800

H	10.00510600	0.00758700	-5.67292500
H	11.57717100	-2.22178700	-2.34694700
H	11.96193800	-0.70966700	-4.30525700
H	0.16350500	-4.94831600	-1.74355400
H	8.78510100	-7.85132900	-0.05509200
H	12.64163800	-3.24075200	1.48724300
H	9.59442300	4.59607100	-2.05325200
H	5.49573300	1.09636400	5.21818300
H	4.47258100	-2.28445700	5.68619000

TS1'

C	6.09541700	0.28785400	-4.71975300
C	7.46566700	0.10307100	-4.52105400
C	7.96320300	-0.12418500	-3.23894900
C	7.09364600	-0.17101000	-2.14205100
C	5.72153400	0.02668300	-2.34815400
C	5.22409900	0.25381600	-3.63081000
H	8.14677500	0.12980000	-5.36742200
H	9.02663300	-0.28246500	-3.09320400
H	5.04981800	-0.01497700	-1.49390700
H	4.15668700	0.38731400	-3.78018300
C	9.47573900	3.62478800	0.78007900
C	8.49512800	3.55708400	-0.21183300
C	7.96910400	2.32392000	-0.59597800
C	8.42086300	1.14298200	0.00803500
C	9.40932100	1.21567200	0.99690000
C	9.93199500	2.44968400	1.37917000
H	8.13752000	4.46534800	-0.68945000
H	7.20353900	2.28353500	-1.36320500
H	9.77808600	0.31371100	1.46634600
H	10.69278800	2.48404100	2.15304100
C	11.21096000	-3.43229000	-0.94145500
C	11.43109000	-2.07046900	-1.16135900
C	10.38927800	-1.15499400	-1.00772800
C	9.11322900	-1.59119500	-0.62433700
C	8.91036500	-2.95752500	-0.38347800
C	9.94549200	-3.87579900	-0.55308000
H	12.41772500	-1.71888900	-1.45037200
H	10.57348100	-0.09671400	-1.16265500
H	7.94232000	-3.29693800	-0.02908000
H	9.76144000	-4.92947000	-0.36212100
P	7.66659000	-0.47210400	-0.41817800
C	0.28565200	-3.28060000	0.21284200
C	0.97069500	-4.49199900	0.09679600

C	2.35420400	-4.50078700	-0.08369900
C	3.06350400	-3.29511400	-0.13528700
C	2.37127900	-2.08180400	-0.01945600
C	0.98777800	-2.07423300	0.14973600
H	0.42796600	-5.43177800	0.14779700
H	2.88377400	-5.44380900	-0.17251600
H	2.93316900	-1.15031400	-0.01860900
H	0.46216400	-1.12909400	0.25125000
C	5.26826300	-3.28766600	-5.02832400
C	4.00737300	-3.37355800	-4.43985700
C	3.87633000	-3.37300600	-3.05014100
C	5.00821700	-3.27704400	-2.22962100
C	6.27208700	-3.17776900	-2.83305300
C	6.40168800	-3.19399100	-4.21920100
H	3.11854500	-3.44355300	-5.06097400
H	2.88994400	-3.44401900	-2.60724100
H	7.16155100	-3.07354500	-2.22386700
H	7.38775600	-3.10581400	-4.66403300
C	6.64216600	-7.16902800	1.25740100
C	6.96209100	-6.76840600	-0.04039600
C	6.39264200	-5.61442700	-0.58308300
C	5.50008500	-4.84246100	0.17348000
C	5.17262300	-5.25859600	1.47428700
C	5.73844300	-6.41377200	2.00859100
H	7.64974500	-7.35837000	-0.64060400
H	6.64056500	-5.32430900	-1.59770300
H	4.47400600	-4.68361400	2.06794300
H	5.47298600	-6.71275900	3.01823200
P	4.87586500	-3.20716300	-0.39400300
Cu	5.82502400	-1.36983300	0.68800400
B	5.23519600	0.13321200	2.01775500
O	6.16468000	1.16007800	2.20804100
C	5.46624000	2.30612000	2.75061100
C	4.21120700	1.64479100	3.41115800
O	3.99824700	0.49536900	2.54889500
C	4.47687300	1.10750500	4.82152000
H	3.62346100	0.49676500	5.13150900
H	4.60862700	1.91744500	5.54717700
H	5.36308200	0.46763200	4.83840400
C	2.94773800	2.49713500	3.40157000
H	3.09295400	3.41659000	3.98098400
H	2.12293000	1.93729500	3.85446200
H	2.65597100	2.76722300	2.38425300
C	6.40491300	3.04052200	3.70333100

H	5.91415600	3.92281600	4.13159600
H	7.29046400	3.37044400	3.15103700
H	6.73857000	2.40014200	4.52256400
C	5.10651200	3.21798800	1.57143300
H	6.02351700	3.47896800	1.03848000
H	4.61905500	4.14090200	1.90446300
H	4.44131800	2.69999700	0.87367600
C	7.16043300	-2.08340800	2.77669800
H	7.23381900	-3.13817200	2.49511700
C	8.38699900	-1.39720200	3.10565600
C	8.39210800	-0.18120500	3.82437900
C	9.58794600	0.40738100	4.21715300
C	10.81435100	-0.18799100	3.90294700
C	10.82616700	-1.39257900	3.18927800
C	9.63313900	-1.99180800	2.80092200
H	7.44527600	0.28222200	4.05705000
H	9.56387700	1.34298300	4.76987900
H	11.74704400	0.27543100	4.21221100
H	11.77051200	-1.86657200	2.93482500
H	9.65284000	-2.92766300	2.25168500
N	5.93862500	-1.54984200	2.94422700
C	4.92892100	-2.44074100	3.39227000
C	5.26909500	-3.41515000	4.35258900
C	3.59051700	-2.35940400	2.97921500
C	4.30987100	-4.29875900	4.84527900
H	6.29071500	-3.46269000	4.71310600
C	2.63931700	-3.24732300	3.47217800
H	3.31045500	-1.61055600	2.25893200
C	2.98881500	-4.23308400	4.39972800
H	4.60313000	-5.04318500	5.58127600
H	1.62065000	-3.17904700	3.10113400
H	2.24474000	-4.93221300	4.77042600
H	-0.79125300	-3.27667700	0.35653100
H	7.08884900	-8.06542200	1.67828500
H	12.02529400	-4.14130600	-1.06187500
H	9.88434200	4.58623500	1.07903300
H	5.70838500	0.45305000	-5.72131400
H	5.36812500	-3.28442400	-6.11007800
IM2			
C	-5.23017600	3.07727200	1.62168500
C	-5.62500200	2.17867900	0.62956400
C	-4.78534500	1.12777800	0.25586600
C	-3.53537300	0.96398100	0.86758800

C	-3.14805000	1.87449200	1.86131400
C	-3.98677200	2.92088300	2.24002000
H	-6.58985300	2.29367300	0.14348500
H	-5.09866500	0.43668100	-0.51908200
H	-2.17500800	1.77282200	2.32890700
H	-3.66724200	3.61765500	3.00997900
C	-3.20741600	-3.76110500	3.46345000
C	-4.17261400	-2.76932900	3.27484700
C	-3.95393800	-1.74701600	2.35086700
C	-2.76180900	-1.70859300	1.61461500
C	-1.78940900	-2.70358000	1.80948100
C	-2.02046100	-3.72781000	2.72802500
H	-5.09657200	-2.79147600	3.84634500
H	-4.70607100	-0.97758700	2.20663400
H	-0.85270700	-2.65365300	1.25535400
H	-1.26662000	-4.49692600	2.87169200
C	-3.97394700	-1.85506200	-3.69165600
C	-4.20038300	-2.63534900	-2.55700700
C	-3.76506800	-2.19915200	-1.30415500
C	-3.09306100	-0.97809300	-1.18154800
C	-2.86593500	-0.19635300	-2.32623200
C	-3.31051400	-0.63062500	-3.57230200
H	-4.71077300	-3.59017900	-2.64546900
H	-3.92905700	-2.81555700	-0.42672200
H	-2.33948600	0.74780200	-2.24200000
H	-3.12789200	-0.01677300	-4.44985900
P	-2.37640200	-0.39006600	0.40016900
C	3.63153200	4.20941500	1.25391600
C	3.93238100	2.87853300	0.94965900
C	3.03689500	2.10747300	0.21229600
C	1.83833000	2.66910600	-0.25899200
C	1.54798100	4.00680500	0.03528400
C	2.43782600	4.76883800	0.79654800
H	4.86201400	2.42939000	1.28654100
H	3.27287000	1.07274000	-0.00238300
H	0.63027500	4.45701900	-0.32806600
H	2.19968700	5.80497400	1.02150700
C	-2.91284900	4.07068700	-2.63421200
C	-1.97705900	3.61377500	-3.56399500
C	-0.84649700	2.91038200	-3.14223000
C	-0.64763400	2.64982300	-1.77976200
C	-1.59252100	3.11766400	-0.85355100
C	-2.71426500	3.82829700	-1.27282700
H	-2.12665700	3.80212000	-4.62364600

H	-0.12891100	2.55024900	-3.87141300
H	-1.46107300	2.89868200	0.19973400
H	-3.44184400	4.16112300	-0.53920100
C	2.92368900	0.20865800	-4.96792600
C	1.92989900	-0.58899000	-4.39610600
C	1.26513600	-0.15752900	-3.24907900
C	1.59192400	1.07423500	-2.66400600
C	2.58766100	1.87237800	-3.24227600
C	3.24964100	1.43956300	-4.39139700
H	1.68372300	-1.55775600	-4.82062100
H	0.52333200	-0.80230500	-2.78818600
H	2.85297500	2.82068300	-2.78509700
H	4.02583200	2.05899200	-4.83238500
P	0.68511100	1.55682500	-1.15323800
Cu	-0.04876600	-0.24844000	0.08266400
B	1.81438900	-1.07160800	2.26622700
O	2.33972700	-1.20121800	3.52441100
C	2.06442800	0.03566400	4.24399200
C	0.80057800	0.58383300	3.48936000
O	0.99761900	0.03677700	2.15201900
C	0.72066900	2.09991200	3.37152000
H	1.60071900	2.51455800	2.87777900
H	-0.15231600	2.37558100	2.77195100
H	0.61478000	2.55965100	4.36048400
C	-0.50400100	-0.00864800	4.02508800
H	-0.74951000	0.39667800	5.01166200
H	-1.32351700	0.22320800	3.34398000
H	-0.44439300	-1.09813000	4.09408000
C	3.29711200	0.92733300	4.07850000
H	3.47183400	1.16888900	3.02776000
H	3.19203600	1.86245900	4.63800100
H	4.17381000	0.39374200	4.45773400
C	1.84171900	-0.29886700	5.71360200
H	2.76879500	-0.69010500	6.14351800
H	1.55811400	0.59852200	6.27501300
H	1.06361000	-1.05381400	5.84170600
C	2.12402600	-2.00259100	1.03869100
H	2.30803300	-3.01956400	1.43212900
C	3.45109700	-1.50357400	0.42951700
C	3.54511100	-1.23308800	-0.93954900
C	4.71064300	-0.69661900	-1.48843700
C	5.80620600	-0.41209600	-0.67147100
C	5.73244800	-0.69573500	0.69462300
C	4.56845700	-1.24285100	1.23821500

H	2.69233000	-1.43394700	-1.56993200
H	4.74827100	-0.48747800	-2.55348800
H	6.71011600	0.01900000	-1.09348400
H	6.58266700	-0.49035100	1.34078100
H	4.51964700	-1.45688200	2.30184800
N	0.98597600	-1.97527200	0.13495100
C	0.87836300	-2.97208800	-0.79867700
C	1.79987600	-4.04275700	-0.96382700
C	-0.23174500	-2.96387300	-1.68801900
C	1.61251700	-5.01127100	-1.94801800
H	2.68519500	-4.09627200	-0.33998800
C	-0.40566600	-3.93380400	-2.66555200
H	-0.95695700	-2.16531100	-1.58971300
C	0.51661700	-4.97685700	-2.81330400
H	2.34970300	-5.80642100	-2.04371500
H	-1.27713300	-3.87257700	-3.31425200
H	0.38467900	-5.73700100	-3.57780600
H	4.32522000	4.80663900	1.83918200
H	3.45016800	-0.13079900	-5.85565600
H	-4.30824300	-2.20099000	-4.66567700
H	-3.38022900	-4.55653300	4.18333000
H	-5.88439900	3.89501100	1.91043600
H	-3.79592200	4.60740500	-2.96912600

IM3

C	2.00438200	5.60163200	-0.77317100
C	2.49307100	4.29901700	-0.66187300
C	1.63631400	3.26290800	-0.28939900
C	0.28570700	3.52008400	-0.01271400
C	-0.19601700	4.83418500	-0.11616000
C	0.65971800	5.86674300	-0.50102000
H	3.53782800	4.07670200	-0.85670200
H	2.01720900	2.25257500	-0.20829100
H	-1.23755300	5.04845300	0.10103500
H	0.27704900	6.88058900	-0.58180000
C	-0.62875800	2.26201200	5.18176900
C	-0.26172400	3.39798100	4.45716600
C	-0.29237600	3.38429200	3.06209500
C	-0.68430500	2.22621600	2.37889400
C	-1.03592400	1.08369900	3.11304400
C	-1.02008900	1.10440600	4.50671800
H	0.05104500	4.29841600	4.97864900
H	-0.00127400	4.26985700	2.50716000
H	-1.31980200	0.17675400	2.59328100

H	-1.30590900	0.21237500	5.05569900
C	-5.12178500	3.03230900	-0.67008600
C	-4.84058100	2.52588800	0.59977400
C	-3.52067700	2.32484300	1.00408300
C	-2.45764600	2.62100400	0.13778800
C	-2.74961000	3.12766100	-1.14096300
C	-4.06968600	3.33965500	-1.53658700
H	-5.65150900	2.28832200	1.28304600
H	-3.31775800	1.92372800	1.99118900
H	-1.93956500	3.35711200	-1.82675400
H	-4.27631500	3.74275700	-2.52448000
P	-0.74009500	2.10700900	0.54639700
C	0.11926500	-5.98152300	-0.61797200
C	-1.08731300	-5.83040500	0.07084300
C	-1.60836700	-4.55728900	0.29485800
C	-0.91922600	-3.42442300	-0.16423700
C	0.29603600	-3.58081700	-0.84171600
C	0.80836100	-4.85747400	-1.07150400
H	-1.62164700	-6.70439000	0.43317100
H	-2.54641100	-4.44033500	0.82876200
H	0.84082200	-2.69991800	-1.16105900
H	1.76018600	-4.96977100	-1.58171700
C	-4.57616300	-1.26110300	-3.49885200
C	-4.14245800	-0.15313900	-2.76863600
C	-3.24676400	-0.32170300	-1.71358400
C	-2.79223700	-1.60061700	-1.35814700
C	-3.23504000	-2.70848300	-2.09359600
C	-4.11833800	-2.53605800	-3.16011900
H	-4.48768800	0.84524700	-3.01868200
H	-2.89221900	0.54399000	-1.16876100
H	-2.87940900	-3.70187300	-1.84333600
H	-4.44819900	-3.40129000	-3.72870300
C	-3.92717700	-1.56091900	3.98788300
C	-4.48354200	-1.01012100	2.83283500
C	-3.82014600	-1.11894500	1.60958300
C	-2.58476000	-1.77500800	1.53150400
C	-2.02801300	-2.32856200	2.69698200
C	-2.70079900	-2.22677600	3.91385300
H	-5.43920700	-0.49493800	2.88023000
H	-4.26108500	-0.68301200	0.71969000
H	-1.06261000	-2.82222300	2.64978100
H	-2.26225800	-2.66406700	4.80685500
P	-1.56448400	-1.72416700	0.00636600
Cu	0.03689800	-0.06267800	0.10540500

B	2.40900300	0.04321800	-1.65232700
O	3.06417200	0.37783000	-2.82233200
C	2.24696600	-0.07347400	-3.92967000
C	0.81129300	-0.09852200	-3.30271500
O	1.11306600	-0.42073100	-1.91689400
C	-0.11830100	-1.16271500	-3.87231100
H	0.26900200	-2.16871500	-3.69850600
H	-1.10279500	-1.09367900	-3.40490100
H	-0.24523600	-1.01701000	-4.95106200
C	0.12137700	1.26812600	-3.29860700
H	0.77240800	2.04056200	-2.87842500
H	-0.18104700	1.56841600	-4.30692800
H	-0.77585100	1.20238800	-2.67591800
C	2.74907600	-1.46825300	-4.31653700
H	3.81873900	-1.40919500	-4.53746300
H	2.61011100	-2.17588800	-3.49318800
H	2.23055700	-1.85477400	-5.19952700
C	2.42074000	0.90165400	-5.08734800
H	1.75519300	0.63984400	-5.91761500
H	2.20864200	1.92715100	-4.77691900
H	3.45199500	0.86232000	-5.45175100
C	1.99176000	-0.24626800	0.76130600
H	2.07352800	0.49031900	1.56769500
C	2.20703800	-1.61368300	1.28309800
C	1.54298500	-2.01978000	2.46297600
C	1.65578100	-3.31598000	2.95136400
C	2.44541600	-4.26354100	2.28734500
C	3.13239500	-3.87069200	1.14003800
C	3.01817300	-2.57066000	0.64573500
H	0.92040000	-1.29420700	2.98310100
H	1.12815900	-3.59360600	3.86220400
H	2.52705400	-5.27868400	2.66457500
H	3.76692400	-4.58414900	0.61848200
H	3.56977700	-2.28190700	-0.24434300
N	2.90371200	0.15557200	-0.33298300
C	4.18648800	0.66353500	0.00059900
C	4.74684200	0.40014800	1.26249600
C	4.90330800	1.49298400	-0.88450700
C	5.98050600	0.94123300	1.62000900
H	4.22266000	-0.24416800	1.95586500
C	6.13638800	2.02649900	-0.51504600
H	4.49351100	1.71358600	-1.86093000
C	6.68733900	1.76002400	0.73936000
H	6.39050400	0.71315800	2.60055600

H	6.66713800	2.66328500	-1.21891300
H	7.64718600	2.18157600	1.02361400
H	0.52571000	-6.97465600	-0.78819700
H	-4.44488200	-1.47381500	4.93883800
H	-6.15032700	3.18886600	-0.98183600
H	-0.60266500	2.27785400	6.26780300
H	2.66800100	6.40993100	-1.06775800
H	-5.26244100	-1.13232400	-4.33125800

TS2^{OSS}

C	1.33809100	4.96962200	-2.64518200
C	0.44559200	4.05406600	-3.20659600
C	-0.15816300	3.08231000	-2.40945400
C	0.10792000	3.02926800	-1.03120200
C	1.00233900	3.95386400	-0.47262300
C	1.61565400	4.91484400	-1.27793300
H	0.23017500	4.07973700	-4.27065700
H	-0.80643600	2.34151200	-2.86493600
H	1.22947800	3.91870000	0.58689400
H	2.31073700	5.62209100	-0.83353100
C	1.43046000	2.23729900	4.05613500
C	0.27918800	2.97368100	3.76306700
C	-0.36600200	2.80526100	2.53830300
C	0.12523400	1.88524100	1.59985400
C	1.26932300	1.13545400	1.90773000
C	1.92367100	1.32218400	3.12515000
H	-0.11173400	3.68491900	4.48548600
H	-1.25394500	3.38527000	2.30848700
H	1.63869600	0.39450700	1.20933700
H	2.81804700	0.74649500	3.33769500
C	-5.08827300	2.73854900	0.64330100
C	-4.45212300	1.76579800	1.41767900
C	-3.10927100	1.47264500	1.20418700
C	-2.37556000	2.15982900	0.22260900
C	-3.01787200	3.13559500	-0.54707500
C	-4.36949900	3.41940300	-0.33804800
H	-5.00776200	1.21570500	2.17053400
H	-2.62980400	0.70457300	1.80272800
H	-2.46538500	3.67827800	-1.30631700
H	-4.85661700	4.17874600	-0.94362900
P	-0.63366700	1.65713200	-0.05720900
C	-1.65864300	-6.02649800	-2.42702100
C	-1.06693200	-5.92854400	-1.16836000
C	-1.19408900	-4.75720000	-0.42308800

C	-1.91799900	-3.66586300	-0.92831500
C	-2.51012800	-3.77236600	-2.19631600
C	-2.38185700	-4.94623600	-2.93616100
H	-0.48825200	-6.75637900	-0.76916600
H	-0.71139400	-4.69459700	0.54676400
H	-3.05150000	-2.93055500	-2.61408200
H	-2.83947700	-5.01010700	-3.91925300
C	-6.23220500	-0.43699600	-0.67607300
C	-5.97203200	-1.33517100	0.36112700
C	-4.68319700	-1.83129700	0.55308600
C	-3.63774600	-1.42814400	-0.28872200
C	-3.90361500	-0.51492800	-1.31921700
C	-5.19589100	-0.03037300	-1.51569500
H	-6.77395200	-1.65126900	1.02312200
H	-4.49462600	-2.51949200	1.36928000
H	-3.09688000	-0.18374600	-1.96433000
H	-5.38271400	0.68138600	-2.31401800
C	-1.62282800	-2.69582200	4.47847500
C	-2.29547400	-3.64594800	3.70369000
C	-2.36996900	-3.49742000	2.31890200
C	-1.76006100	-2.40054500	1.68743300
C	-1.04748800	-1.48221400	2.47039500
C	-0.99633800	-1.61395400	3.85862600
H	-2.76967400	-4.49934700	4.18034800
H	-2.89703100	-4.23655100	1.72398400
H	-0.52769200	-0.66231200	1.99231100
H	-0.45813400	-0.87350900	4.44284300
P	-1.90462200	-2.02439200	-0.10579100
Cu	-0.27053600	-0.49183200	-0.97347700
H	-1.54782800	-6.93448100	-3.01258600
H	-1.57948900	-2.80758800	5.55829300
H	-6.14058600	2.95737200	0.80039700
H	1.93774600	2.37658300	5.00695600
H	1.81887100	5.71679500	-3.27040500
H	-7.23694700	-0.04939600	-0.82102700
I	-0.79748400	-0.42386200	-3.64367900
C	2.81399900	2.56871200	-5.96899600
H	3.90755000	2.65075600	-5.92315700
H	2.40606400	3.13274200	-5.12158400
H	2.48038500	3.05758400	-6.89172300
C	2.36630900	1.10637500	-5.91151300
H	1.27403200	1.04486900	-5.99376000
H	2.77852800	0.55604600	-6.76885600
C	2.78761500	0.42109600	-4.60895900

H	2.35916300	0.96637200	-3.75414000
H	3.88205100	0.52763000	-4.46467700
C	2.40066300	-1.00138300	-4.50241000
H	2.47468900	-1.53087600	-3.56273700
H	2.08469300	-1.57006800	-5.37064400
B	2.28367300	-3.00271200	1.06139200
O	2.39452200	-2.04584200	2.03912400
C	3.11692500	-2.65594200	3.14969500
C	2.83693400	-4.18251700	2.92484600
O	2.66729800	-4.25091500	1.48193200
C	1.62234800	-2.73830200	-0.34647600
H	0.57443700	-2.96885500	-0.11960500
C	1.97432600	-3.67383100	-1.50455700
C	3.03961000	-4.58080800	-1.48087000
C	3.28298500	-5.41834100	-2.57199400
C	2.46547500	-5.36041400	-3.70058200
C	1.39870600	-4.46009900	-3.72982500
C	1.15648400	-3.62684300	-2.64096100
H	3.66792500	-4.65749400	-0.60047800
H	4.11438000	-6.11763900	-2.53552400
H	2.65670300	-6.01311500	-4.54829600
H	0.74715400	-4.40249000	-4.59688200
H	0.33145900	-2.92593600	-2.67868300
C	3.97346300	-5.11300500	3.32716300
H	4.17439500	-5.03489000	4.40151100
H	3.69659500	-6.14860700	3.10720900
H	4.89174700	-4.88389900	2.78208800
C	1.51077800	-4.64974600	3.53298100
H	0.68979700	-3.98438200	3.25283000
H	1.28514700	-5.65066800	3.15302700
H	1.56010700	-4.69782900	4.62537200
C	2.58144600	-2.11462400	4.46834100
H	3.05130100	-2.63742400	5.30916000
H	2.81022900	-1.05029600	4.56275900
H	1.50032300	-2.23513500	4.53834300
C	4.58775400	-2.27209400	2.96718400
H	4.66672000	-1.18170700	2.92377200
H	5.20445000	-2.63421300	3.79575500
H	4.98810400	-2.67055700	2.03027700
N	1.59579000	-1.32196800	-0.73815000
C	2.77302000	-0.68584600	-0.95565500
C	4.06346600	-1.29038100	-0.86491200
C	2.72779600	0.70266900	-1.27783200
C	5.21073100	-0.53731000	-1.05882300

H	4.15088100	-2.35047200	-0.66863300
C	3.88183500	1.44628700	-1.44928800
H	1.75687300	1.16269100	-1.39346400
C	5.13718700	0.83428000	-1.34478000
H	6.18121100	-1.02189100	-0.99112800
H	3.79896200	2.50324400	-1.68570000
H	6.04530800	1.41194600	-1.48855800

IM4

C	5.84635400	2.94065600	1.26787100
C	5.26198500	3.70607300	0.25363100
C	3.96139600	3.43483300	-0.16500500
C	3.23010800	2.39447800	0.43191200
C	3.81864800	1.63261400	1.44918100
C	5.12431600	1.90681400	1.86337700
H	5.82262300	4.51136600	-0.21316200
H	3.51346400	4.02400300	-0.95926400
H	3.26203300	0.81942400	1.90640500
H	5.57168200	1.30423300	2.64866200
C	-1.16346600	5.28320500	1.80200000
C	0.20299100	5.27515900	2.08011400
C	1.03651200	4.32454300	1.48718200
C	0.50508200	3.36353800	0.61914600
C	-0.87612900	3.36518700	0.35647200
C	-1.69824500	4.33038900	0.93213200
H	0.62570300	6.01088300	2.75881500
H	2.09875100	4.32680100	1.70609600
H	-1.30611300	2.59720700	-0.27855400
H	-2.76438400	4.32524600	0.72618900
C	1.84790600	2.87629500	-4.63533800
C	0.96166500	3.63146900	-3.86899500
C	0.83816500	3.39651500	-2.49695000
C	1.59779900	2.39552400	-1.88165400
C	2.48118500	1.63304200	-2.66379200
C	2.61022200	1.87624900	-4.02705900
H	0.36917400	4.41524600	-4.33377400
H	0.15956100	4.00301700	-1.90765000
H	3.07162600	0.84632600	-2.20399000
H	3.28941500	1.27033900	-4.61839800
P	1.51404900	2.00314200	-0.08513700
C	-2.00766800	-5.23161300	-0.71485100
C	-1.10487300	-4.88893200	0.29294100
C	-0.20937600	-3.83840200	0.10778400
C	-0.19487700	-3.12963300	-1.10527600

C	-1.09725400	-3.48295700	-2.11876400
C	-2.00180000	-4.52755300	-1.91942200
H	-1.12197800	-5.41441200	1.24205100
H	0.46057300	-3.54586000	0.91120800
H	-1.09860200	-2.93946500	-3.05781000
H	-2.70253700	-4.78896800	-2.70805500
C	5.22489100	-3.35993000	-1.28958000
C	4.96141400	-2.08297100	-0.79056400
C	3.65290600	-1.60399100	-0.75734500
C	2.59839300	-2.39036100	-1.24196600
C	2.86660800	-3.67790100	-1.72550800
C	4.17598700	-4.15908500	-1.75000400
H	5.76851400	-1.46614400	-0.40575100
H	3.44347600	-0.63276800	-0.32223700
H	2.04838300	-4.30393600	-2.06904800
H	4.37653100	-5.15984700	-2.12265000
C	0.19801400	-0.13897400	-5.54774700
C	1.11111500	-1.17396700	-5.34159200
C	1.34532400	-1.65412500	-4.05251700
C	0.66479300	-1.10481500	-2.95796800
C	-0.24821900	-0.06134500	-3.17159000
C	-0.47863100	0.41561800	-4.46049000
H	1.64628800	-1.60526900	-6.18332200
H	2.06611000	-2.44970500	-3.89545000
H	-0.76386300	0.38949700	-2.33005200
H	-1.15761700	1.24874100	-4.61263400
P	0.91550800	-1.67353800	-1.22889200
Cu	0.61522100	-0.10261200	0.50793500
H	-2.72175900	-6.03412300	-0.55494100
H	0.02633000	0.24482200	-6.54965600
H	1.94093200	3.05903700	-5.70208500
H	-1.81099600	6.02126900	2.26670500
H	6.86331200	3.15085300	1.58793200
H	6.24313800	-3.73859300	-1.30557600
I	1.72082300	-1.39793200	2.62555100
B	-3.30938600	0.14488800	-0.40414100
O	-4.67253500	0.19289400	-0.29947300
C	-5.11954400	1.37899100	-1.02393600
C	-3.94672000	1.59780200	-2.04286900
O	-2.81028800	1.04513000	-1.31520800
C	-2.32039000	-0.80615100	0.39401500
H	-1.73893300	-1.29996400	-0.39217900
C	-2.92050800	-1.93184700	1.22683700
C	-4.06036900	-2.61176700	0.78329700

C	-4.54615600	-3.71472700	1.48524800
C	-3.90126200	-4.14994500	2.64400200
C	-2.76239200	-3.47702600	3.08894600
C	-2.26985000	-2.38012200	2.38289800
H	-4.57218800	-2.27881300	-0.11348900
H	-5.43259900	-4.23143500	1.12656900
H	-4.28266900	-5.00643700	3.19353200
H	-2.24157300	-3.81139700	3.98203200
H	-1.35993000	-1.89131200	2.71441300
C	-4.10450300	0.76055200	-3.31516500
H	-3.16922800	0.77727000	-3.87800000
H	-4.32966900	-0.28288600	-3.07426400
H	-4.90314100	1.15094900	-3.95355600
C	-3.63414800	3.04747500	-2.38881600
H	-3.40052900	3.63644800	-1.50011500
H	-2.76392600	3.08397700	-3.05220900
H	-4.47988300	3.51272400	-2.90679600
C	-5.24038800	2.50125500	0.00994000
H	-5.61138800	3.42480800	-0.44566600
H	-5.94354200	2.19299700	0.78913200
H	-4.27936100	2.70189900	0.49066500
C	-6.47551000	1.08089700	-1.64968700
H	-6.81345700	1.92728600	-2.25787600
H	-6.44227200	0.18888700	-2.27808800
H	-7.21411800	0.91255600	-0.86029900
N	-1.34683600	0.02857900	1.11190100
C	-1.77741000	0.77762100	2.16411700
C	-3.14384500	0.92350100	2.54752100
C	-0.79898100	1.49990700	2.90693100
C	-3.49674100	1.80506700	3.55763200
H	-3.91443600	0.35325700	2.04671700
C	-1.16721200	2.36321400	3.92210200
H	0.24291700	1.33680000	2.66575700
C	-2.51921800	2.53699500	4.24545900
H	-4.54433100	1.91908500	3.82236900
H	-0.40122500	2.91198900	4.46048200
H	-2.80862500	3.22310600	5.03610200

IM5

C	2.63187100	2.55762100	2.27842000
C	3.41564100	1.65920600	1.55513000
C	3.24507800	1.52154900	0.17515500
C	2.29098400	2.29441200	-0.49369000
C	1.51050300	3.20541600	0.23920900

C	1.67772200	3.33527900	1.61467700
H	4.16580600	1.06004700	2.06389400
H	3.84374300	0.80505600	-0.37462900
H	0.76316200	3.80758700	-0.27188300
H	1.06152500	4.03634700	2.16990000
C	3.23851400	6.25557200	-3.93988000
C	3.96348200	5.66730300	-2.89981400
C	3.57733800	4.42753900	-2.39478800
C	2.46244800	3.76235000	-2.93026800
C	1.73620600	4.35913300	-3.96928800
C	2.12727200	5.60133800	-4.47208300
H	4.82672300	6.17640000	-2.48031900
H	4.13478400	3.97674500	-1.57921300
H	0.87719700	3.84707800	-4.38979800
H	1.55922000	6.05578200	-5.27857800
C	4.90790300	-1.04072800	-3.86521000
C	3.81919000	-1.40258300	-3.06778400
C	2.94041400	-0.42991800	-2.59530800
C	3.16100300	0.92364200	-2.90391100
C	4.25014700	1.28349000	-3.70547200
C	5.11870400	0.30112100	-4.18484600
H	3.64142800	-2.44652000	-2.82360900
H	2.09606500	-0.71492900	-1.97789600
H	4.41621200	2.32439400	-3.96137400
H	5.95894200	0.58680200	-4.81147000
P	1.93495500	2.13303700	-2.28791600
Cu	-0.15850600	1.09005900	-2.88579200
H	5.58505600	-1.80221100	-4.24205400
H	3.53895200	7.22381600	-4.33055700
H	2.76169500	2.65413800	3.35247100
I	-0.15644500	1.26058800	-5.51511700
C	-5.49766300	-1.93249500	-1.35290700
H	-4.83835100	-2.06979800	-0.48828600
H	-6.04016400	-2.86949000	-1.52121400
H	-6.22995300	-1.15983000	-1.08960300
C	-4.68473800	-1.53077500	-2.58591600
H	-3.96363000	-2.32267300	-2.82091400
H	-5.34480100	-1.43039200	-3.45854500
C	-3.92581600	-0.22201800	-2.35128800
H	-3.31703600	-0.31918700	-1.45052700
H	-4.62113200	0.60578800	-2.17041200
C	-3.01016700	0.12151500	-3.54024300
H	-3.58021100	0.42678700	-4.42680000
H	-2.38447500	-0.72759400	-3.81378200

O	-2.40656300	2.41274900	-2.90308900
C	-2.14546100	1.28908100	-3.17833600
B	0.40904900	-0.94811900	0.72302500
O	1.65247000	-1.30108600	0.26639100
C	2.10005000	-2.44664400	1.03428000
C	1.23456900	-2.32470900	2.34407000
O	0.06038000	-1.59340500	1.87929800
C	-0.43041500	0.13122700	-0.07737200
H	0.21079100	1.01770000	-0.02521600
C	-1.77808800	0.58263500	0.47433800
C	-2.22829600	1.86205700	0.11934000
C	-3.48448300	2.32399800	0.50600000
C	-4.31514500	1.51370900	1.28267900
C	-3.86203900	0.25824200	1.68798900
C	-2.60205100	-0.19894100	1.29537200
H	-1.58749800	2.49606800	-0.48540200
H	-3.81305900	3.31386200	0.20146900
H	-5.29877700	1.86446200	1.58246500
H	-4.48782800	-0.36937000	2.31688300
H	-2.24813300	-1.15804300	1.65524700
C	0.76911500	-3.65088400	2.93126300
H	1.62656600	-4.26003100	3.23817600
H	0.14891900	-3.46622500	3.81392400
H	0.17714600	-4.21879100	2.21059600
C	1.88168300	-1.45187100	3.42179600
H	2.19584700	-0.48908800	3.00821800
H	1.14667400	-1.25901600	4.20891100
H	2.75034800	-1.94389100	3.87134800
C	3.60577500	-2.32288300	1.23818400
H	3.98761300	-3.15061000	1.84591500
H	4.10498700	-2.35384300	0.26455300
H	3.86920300	-1.38082900	1.72233500
C	1.77901000	-3.68793900	0.19658200
H	2.27770800	-3.59490900	-0.77307400
H	2.13326500	-4.60284800	0.68231000
H	0.70669900	-3.77663900	0.00578000
N	-0.40287500	-0.25297700	-1.50669000
C	-0.78596000	-1.52867600	-1.87394800
C	-1.50361300	-2.42590600	-1.04574400
C	-0.40091200	-2.00656200	-3.15431100
C	-1.81030800	-3.71624900	-1.47629000
H	-1.83970900	-2.10927100	-0.07091600
C	-0.73239100	-3.28525200	-3.58117100
H	0.16811900	-1.35058100	-3.80511000

C	-1.43874200	-4.15960800	-2.74606700
H	-2.36376400	-4.37436800	-0.81070400
H	-0.42122900	-3.60831900	-4.57112800
H	-1.68874800	-5.16240000	-3.07870800

TS3

C	2.53983300	2.62534800	2.24758200
C	3.38499900	1.75538000	1.55895500
C	3.25005800	1.58243900	0.17924800
C	2.27146200	2.29155100	-0.52358800
C	1.42816000	3.17295100	0.17395500
C	1.55960800	3.33796300	1.55004000
H	4.15436400	1.20684800	2.09546300
H	3.89683800	0.88939000	-0.34627600
H	0.66093800	3.72431300	-0.36464100
H	0.89524600	4.01481600	2.07903800
C	3.40146500	6.14584900	-4.05136300
C	3.99226200	5.64754400	-2.88729900
C	3.56892300	4.43095900	-2.35525900
C	2.54999000	3.70008000	-2.98708400
C	1.95722300	4.20660400	-4.15179400
C	2.38594900	5.42494500	-4.68052600
H	4.78018700	6.20814500	-2.39204900
H	4.02307000	4.04973500	-1.44585300
H	1.16945500	3.64638300	-4.64440600
H	1.92025800	5.80982500	-5.58313600
C	5.05639700	-1.10990700	-3.64769200
C	3.85224700	-1.47018200	-3.03760100
C	2.94287200	-0.48900400	-2.64706000
C	3.24243600	0.86759000	-2.85377600
C	4.44844900	1.22607000	-3.46777600
C	5.35103300	0.23722200	-3.86304700
H	3.61097100	-2.51740600	-2.87758000
H	2.01675500	-0.77024900	-2.15938500
H	4.67941400	2.27157700	-3.64312700
H	6.28301900	0.52120100	-4.34364800
P	1.98734900	2.08909400	-2.32515700
Cu	-0.10568900	1.09073000	-2.92373000
H	5.75937600	-1.87664100	-3.96116300
H	3.73023200	7.09603400	-4.46300900
H	2.64212000	2.74947800	3.32174500
I	-0.30202200	1.26482700	-5.53581100
C	-5.65890600	-1.90099200	-1.35174100
H	-5.03702500	-2.04625300	-0.46071100

H	-6.20509800	-2.83143600	-1.54265000
H	-6.39255000	-1.12030500	-1.11753400
C	-4.79194200	-1.50768000	-2.55037100
H	-4.07890100	-2.31292500	-2.76506300
H	-5.41599000	-1.38661500	-3.44638400
C	-4.01316500	-0.21898600	-2.27501600
H	-3.43871100	-0.34042100	-1.35464700
H	-4.69521900	0.62275800	-2.10691700
C	-3.04991300	0.12050400	-3.42826100
H	-3.57679700	0.49699700	-4.31336900
H	-2.46590800	-0.74855000	-3.72831400
O	-2.33228600	2.33535500	-2.64724300
C	-2.13528900	1.22039200	-2.99590500
B	0.35323000	-0.88069400	0.64871300
O	1.59160500	-1.18469800	0.14738000
C	2.09952000	-2.33131900	0.87680300
C	1.26765000	-2.26785300	2.21240300
O	0.06017800	-1.56137200	1.79977500
C	-0.55694400	0.18153200	-0.09981100
H	0.05227200	1.09086900	-0.06924600
C	-1.88617500	0.57063000	0.54202400
C	-2.37574600	1.86413900	0.31027800
C	-3.61594500	2.27229800	0.79767700
C	-4.39053100	1.39337700	1.55646600
C	-3.89481500	0.12165700	1.84456100
C	-2.65207600	-0.28074300	1.35157500
H	-1.77983300	2.55402500	-0.27720700
H	-3.97466500	3.27599600	0.58637300
H	-5.36086800	1.70269500	1.93483200
H	-4.47186100	-0.56062600	2.46309900
H	-2.26258600	-1.25254600	1.62995000
C	0.85799200	-3.62181700	2.77802000
H	1.74117700	-4.21298100	3.04436700
H	0.25894300	-3.47747000	3.68249600
H	0.26156500	-4.18826400	2.05992300
C	1.91901300	-1.40377200	3.29470500
H	2.19290500	-0.42185100	2.89828800
H	1.20142700	-1.25358100	4.10681400
H	2.81433200	-1.88087200	3.70647000
C	3.60551000	-2.16264100	1.04367100
H	4.02797100	-2.99118200	1.62280800
H	4.07989700	-2.15575700	0.05738000
H	3.85163500	-1.22407300	1.54302900
C	1.79753400	-3.56558800	0.02151500

H	2.26709400	-3.43745400	-0.95822400
H	2.19585300	-4.47687900	0.47926000
H	0.72442400	-3.68826100	-0.14299000
N	-0.58087000	-0.19656200	-1.53343000
C	-0.87446600	-1.49925700	-1.89686300
C	-1.57036300	-2.41785500	-1.07546900
C	-0.43624900	-1.97576600	-3.15900200
C	-1.80122300	-3.72869700	-1.49175400
H	-1.95086000	-2.10162100	-0.11753900
C	-0.69367200	-3.27583500	-3.57448200
H	0.10683400	-1.30102900	-3.81314400
C	-1.37450900	-4.17298900	-2.74350700
H	-2.33871200	-4.40277800	-0.82899900
H	-0.34382600	-3.59522300	-4.55263100
H	-1.56562200	-5.19185900	-3.06609100

IM6

C	0.36350600	4.93622700	1.30100000
C	1.75007700	4.80751400	1.20076500
C	2.31017200	4.07021100	0.15764800
C	1.48389400	3.46146000	-0.79733500
C	0.09048700	3.57435100	-0.67797600
C	-0.46357900	4.31461000	0.36501500
H	2.39630100	5.27747100	1.93722700
H	3.38773900	3.95835800	0.09373400
H	-0.55333000	3.05554100	-1.38041500
H	-1.54282800	4.38364400	0.45917900
C	3.53774200	5.56834600	-5.40024800
C	3.30057300	6.01363000	-4.09901300
C	2.86578400	5.11920400	-3.11924600
C	2.66586600	3.77048200	-3.43994600
C	2.89107600	3.32934700	-4.75411900
C	3.33164000	4.22552400	-5.72622600
H	3.45091900	7.05925500	-3.84476300
H	2.67519100	5.47100200	-2.11035600
H	2.71431400	2.28721000	-5.01052200
H	3.50451900	3.87629500	-6.74010600
C	6.03477600	0.60519200	-0.62052500
C	4.86647200	-0.14883100	-0.73888600
C	3.70638400	0.43265100	-1.25023000
C	3.70198400	1.78248500	-1.62951200
C	4.88545900	2.52888200	-1.53132700
C	6.04514300	1.94220500	-1.02533600
H	4.85393300	-1.19449200	-0.44924000

H	2.81841000	-0.17728900	-1.37370600
H	4.90173900	3.56221500	-1.86522900
H	6.95853300	2.52623900	-0.95415400
P	2.13017400	2.51170900	-2.22276000
Cu	0.73590700	1.00480300	-3.14068200
H	6.94020700	0.14969800	-0.22909400
H	3.87431100	6.26712400	-6.16097100
H	-0.07102500	5.50500400	2.11842300
I	0.97972100	-0.95050900	-4.77945900
C	-6.91884200	0.25028000	-2.22991600
H	-6.99549000	-0.39670500	-1.34742500
H	-7.83597500	0.12604400	-2.81610400
H	-6.88431400	1.28852800	-1.87813600
C	-5.67710800	-0.09236800	-3.05661000
H	-5.74731000	-1.12701000	-3.41917400
H	-5.63837700	0.54504900	-3.95025300
C	-4.37821300	0.07249000	-2.26310300
H	-4.41445700	-0.56908600	-1.37294200
H	-4.28863500	1.10675500	-1.90558000
C	-3.13253500	-0.28127900	-3.09650500
H	-3.07884200	0.35378500	-3.98443800
H	-3.18854300	-1.32184700	-3.42478200
O	-1.28187500	1.07305700	-2.40247800
C	-1.86693800	-0.02410400	-2.31222900
B	0.51126200	-2.02318200	-0.13770700
O	1.80653700	-2.29884100	-0.47841500
C	2.10433500	-3.62982600	0.04147900
C	1.05355100	-3.77214100	1.20264200
O	-0.02581800	-2.90221500	0.75495900
C	-0.20579800	-0.71211600	-0.67103300
H	0.51400900	-0.24016100	-1.35422800
C	-0.41470300	0.22740200	0.50533000
C	0.72052800	0.72172100	1.16383300
C	0.59280200	1.53861500	2.28372100
C	-0.67390800	1.87867200	2.76186700
C	-1.80682100	1.40034700	2.10485900
C	-1.67763500	0.57814700	0.98367200
H	1.70972900	0.47444800	0.78669800
H	1.48267600	1.92906300	2.76767300
H	-0.77515500	2.52376200	3.62977700
H	-2.79774600	1.66810300	2.46203800
H	-2.56345700	0.21874700	0.47073000
C	0.48788400	-5.17427700	1.38823800
H	1.28222900	-5.88288200	1.64787500

H	-0.24421700	-5.16885300	2.20161800
H	-0.01516100	-5.52078900	0.48332900
C	1.53994400	-3.19750000	2.53543100
H	1.92635300	-2.18149700	2.40835300
H	0.69532100	-3.15054000	3.22880500
H	2.32253500	-3.81951000	2.98129800
C	3.56119400	-3.66396000	0.48360900
H	3.79957800	-4.62360100	0.95532400
H	4.21061900	-3.54635100	-0.38947400
H	3.78579000	-2.86201800	1.19038900
C	1.86980300	-4.60195800	-1.11737100
H	2.47949400	-4.28771100	-1.96936900
H	2.14739700	-5.62501600	-0.84356300
H	0.82305800	-4.59379400	-1.43286600
N	-1.42245100	-0.98363100	-1.45442600
C	-1.93776700	-2.32757300	-1.47667800
C	-2.81111400	-2.75797100	-0.47788000
C	-1.49418600	-3.20979600	-2.46565500
C	-3.25093800	-4.08102800	-0.47070700
H	-3.11106800	-2.06725300	0.30248200
C	-1.94162400	-4.53155100	-2.45443700
H	-0.80463200	-2.84923600	-3.22469600
C	-2.81711200	-4.96892000	-1.45750300
H	-3.92543700	-4.41987900	0.31012500
H	-1.60258300	-5.21778900	-3.22500700
H	-3.16134900	-5.99921700	-1.44974600

IM7

C	6.97063600	0.43796600	4.91943500
C	8.30181700	0.53196300	4.51085600
C	8.63038300	0.41518000	3.15940600
C	7.62531000	0.20837000	2.20602400
C	6.29159400	0.10262000	2.62699700
C	5.96506800	0.22111400	3.97547900
H	9.08712700	0.69127900	5.24478200
H	9.66832800	0.47312900	2.84686100
H	5.51343900	-0.09143600	1.89336300
H	4.93105800	0.12340200	4.29150800
C	8.08353200	4.35390800	-1.26501700
C	8.31352800	4.15212600	0.09770400
C	8.26759800	2.86431800	0.63184900
C	7.99305700	1.76891100	-0.19963300
C	7.74737700	1.97671400	-1.56534400
C	7.79887500	3.26655700	-2.09324500

H	8.52370700	4.99790000	0.74662000
H	8.43334400	2.71181300	1.69378100
H	7.49457700	1.13443400	-2.20355200
H	7.60295700	3.42023500	-3.15038900
C	12.30634000	-1.52655500	0.20642100
C	12.08532100	-0.15327500	0.33721000
C	10.78421900	0.34859500	0.38646300
C	9.68983300	-0.52440500	0.31149400
C	9.92101900	-1.89977200	0.16065500
C	11.22149200	-2.40021300	0.11402000
H	12.92806700	0.53004400	0.39399200
H	10.61738100	1.41811000	0.47023500
H	9.08513500	-2.58217500	0.05869900
H	11.37765000	-3.46806000	-0.00859400
P	7.95020500	0.04533700	0.40960400
C	2.13301000	-5.58148400	-0.46303000
C	3.11947400	-6.25545600	0.26443500
C	4.32253400	-5.61958600	0.56009500
C	4.54436700	-4.30099100	0.13393400
C	3.55873500	-3.63304800	-0.60293600
C	2.35386700	-4.27493700	-0.89760400
H	2.95101800	-7.27656300	0.59497200
H	5.09234600	-6.14359500	1.11921000
H	3.75079600	-2.62979700	-0.97122300
H	1.59640900	-3.75470300	-1.47636300
C	6.42683600	-3.14018700	5.10950900
C	5.20320500	-3.46148000	4.52437700
C	5.09821300	-3.59220100	3.13763500
C	6.21965600	-3.39561000	2.32219400
C	7.44434900	-3.05073600	2.91951100
C	7.54856800	-2.93654300	4.30196800
H	4.32540200	-3.61782400	5.14530800
H	4.14420400	-3.85205700	2.69144700
H	8.31845800	-2.86868700	2.30233200
H	8.50076000	-2.66611400	4.74703900
C	9.47370900	-6.26174600	-0.95882600
C	9.07613300	-6.32210500	0.37836300
C	8.05132200	-5.49682000	0.84407700
C	7.41973200	-4.59926700	-0.02683900
C	7.81915400	-4.54604200	-1.37311000
C	8.83954700	-5.37655000	-1.83405000
H	9.56417800	-7.01160800	1.06170400
H	7.75631700	-5.53878100	1.88728500
H	7.33920000	-3.84396400	-2.05123100

H	9.14415500	-5.32327100	-2.87515000
P	6.10685900	-3.42582400	0.49417000
Cu	6.52465900	-1.43455600	-0.62206200
H	8.11592500	5.35848700	-1.67756400
H	6.71818100	0.51929300	5.97285100
H	6.50704300	-3.03975000	6.18810800
H	13.32140200	-1.91122200	0.16373700
H	10.27459700	-6.90218300	-1.31762100
H	1.19701800	-6.08111000	-0.69689700
I	5.71490100	-1.23843500	-3.05774400

IM8

C	7.70118700	0.32086000	5.05484500
C	8.95709400	0.21390500	4.45679800
C	9.06746900	0.11083500	3.06814900
C	7.91713300	0.10857900	2.27029300
C	6.65643400	0.19436700	2.88054700
C	6.54977900	0.30963200	4.26320300
H	9.85464500	0.21650400	5.06955100
H	10.04646200	0.03258300	2.60538200
H	5.76021000	0.15587500	2.26688600
H	5.56902300	0.36782000	4.72542900
C	7.34802400	4.35857500	-0.97687500
C	8.17664300	4.11753000	0.12377800
C	8.36995800	2.81392100	0.57629600
C	7.74170900	1.74343300	-0.07928300
C	6.89359100	1.98641000	-1.17055900
C	6.70579100	3.29728500	-1.61533800
H	8.66453600	4.94552700	0.63090200
H	8.99810100	2.62533600	1.44270900
H	6.37291800	1.15311200	-1.64546900
H	6.04924400	3.48575900	-2.46030600
C	12.27347900	-1.31966800	-0.59572100
C	11.93805600	0.03010800	-0.71155100
C	10.65068300	0.46798600	-0.39263000
C	9.68502700	-0.44587100	0.04692900
C	10.02805000	-1.80465600	0.14862500
C	11.31360100	-2.23903600	-0.16457800
H	12.67860400	0.74684100	-1.05558700
H	10.39455100	1.51715500	-0.49411400
H	9.27962700	-2.52729200	0.45661300
H	11.55562500	-3.29535600	-0.08748000
P	7.95255300	0.00461700	0.44090600
C	2.17986400	-5.24826300	-1.06133100

C	3.01711600	-6.03624700	-0.26482600
C	4.24063000	-5.53254300	0.17115200
C	4.63483900	-4.23533200	-0.18895000
C	3.79804400	-3.44846300	-0.99543000
C	2.57105700	-3.95993800	-1.42536100
H	2.71566000	-7.04236300	0.01348300
H	4.89030500	-6.14742200	0.78681700
H	4.12452400	-2.45557700	-1.30683100
H	1.92811500	-3.34930700	-2.05302700
C	5.87971800	-3.04305800	4.96509300
C	4.72284000	-3.21089300	4.20518600
C	4.80727000	-3.38224000	2.82128500
C	6.05460800	-3.37985800	2.18519900
C	7.21340500	-3.18789800	2.95632200
C	7.12715000	-3.03285800	4.33578500
H	3.74925100	-3.21735500	4.68764200
H	3.90404700	-3.52610400	2.23741300
H	8.18648200	-3.16045100	2.47571700
H	8.03114300	-2.87879300	4.91612300
C	9.49449600	-6.69408700	-0.30072100
C	8.68725000	-6.77376200	0.83661000
C	7.69134800	-5.82306800	1.05711900
C	7.48979400	-4.78206100	0.13850900
C	8.30730500	-4.70753800	-0.99851000
C	9.30308900	-5.65963700	-1.21832700
H	8.83667100	-7.57477700	1.55525600
H	7.08366700	-5.87561500	1.95485300
H	8.16524200	-3.89573600	-1.70442700
H	9.93045900	-5.58823900	-2.10219400
P	6.21140500	-3.48384100	0.36023000
Cu	6.55116100	-1.44799500	-0.65180300
H	7.19659000	5.37642800	-1.32630800
H	7.61778000	0.40121100	6.13512000
H	5.81194000	-2.91192900	6.04130900
H	13.27500800	-1.65541400	-0.84950800
H	10.27281200	-7.43335100	-0.46780700
H	1.22669300	-5.64455200	-1.40076200
C	4.28868200	-1.15099200	-4.14276500
C	5.67170700	-1.14006600	-3.45880200
H	3.65375800	-1.92321100	-3.69293400
H	3.80046900	-0.18171200	-3.99380900
H	4.35727000	-1.34696900	-5.22083700
C	6.57605300	-0.10081000	-4.15537200
C	6.31831400	-2.53293100	-3.61145800

H	7.54597800	-0.05421700	-3.64459800
H	6.75154400	-0.33906800	-5.21280200
H	6.11824500	0.89376400	-4.09977900
H	6.40767300	-2.84096500	-4.66161200
H	7.32840400	-2.51519800	-3.17973900
H	5.72850200	-3.28802900	-3.08027000
O	5.49979300	-0.79294400	-2.11581900

TS4

B	-3.81270700	-4.26050700	-1.86113700
C	-3.71612500	-5.54552900	0.09682300
C	-3.05321600	-6.90985900	-0.09634300
H	-3.48267600	-7.65802100	0.57871200
H	-1.98345200	-6.82469600	0.11770200
H	-3.16319300	-7.26128900	-1.12262100
C	-5.19811700	-5.48399900	-0.43553400
C	-6.11151300	-4.57378200	0.39152300
H	-6.29620200	-4.99229400	1.38699900
H	-7.06944200	-4.46514600	-0.12164400
H	-5.68750600	-3.57496600	0.50881600
C	-5.87849400	-6.83894000	-0.62342200
H	-6.88042200	-6.68049500	-1.03469500
H	-5.98179800	-7.36717300	0.33159800
H	-5.32719200	-7.47415500	-1.31950100
C	-3.52706000	-5.09385200	1.54434900
H	-3.88812300	-4.07574600	1.70367900
H	-2.46109100	-5.11931500	1.79443500
H	-4.05405600	-5.76001500	2.23670900
O	-5.05169500	-4.87526700	-1.74140900
O	-3.02525900	-4.59113200	-0.75637000
B	-2.91683900	-4.14308000	-4.05195100
C	-1.51463300	-5.96452200	-4.34851700
C	-1.14888200	-6.57225700	-2.99406800
H	-0.12170200	-6.95221500	-2.98814900
H	-1.82176700	-7.40971500	-2.79039900
H	-1.26393800	-5.83576600	-2.19622900
C	-0.73868200	-4.62898700	-4.63332400
C	-0.65312500	-4.28432200	-6.12765600
H	0.03545100	-4.95057500	-6.65925900
H	-0.28929500	-3.25755500	-6.22800000
H	-1.63221000	-4.34095400	-6.60900000
C	0.65583300	-4.55272200	-4.01905000
H	1.10440900	-3.58181600	-4.24875200
H	1.30429800	-5.33606700	-4.42960500

H	0.62267100	-4.64990700	-2.93425600
C	-1.39298800	-7.01998700	-5.44449800
H	-1.75195000	-6.64550900	-6.40581800
H	-1.99045700	-7.89805700	-5.17795800
H	-0.35095900	-7.33990400	-5.56198500
O	-1.58209500	-3.65358300	-3.99787800
O	-2.89657600	-5.53414100	-4.29647000
C	-3.82902300	0.36258800	2.27430700
C	-4.55872700	1.27138000	1.50728000
C	-5.02934300	0.91048300	0.24393900
C	-4.77423500	-0.36844600	-0.26222300
C	-4.00580700	-1.26613200	0.49818800
C	-3.54397700	-0.90440800	1.76213600
H	-4.75566700	2.26970900	1.88732000
H	-5.58227200	1.62962400	-0.35027500
H	-3.76038900	-2.24225100	0.09170300
H	-2.95353000	-1.61044600	2.33956000
C	-9.53956800	-2.83794800	-0.67609800
C	-8.90848200	-1.96586300	0.21217400
C	-7.67705300	-1.39656600	-0.11665700
C	-7.06294000	-1.69894000	-1.33903500
C	-7.69910500	-2.58209700	-2.22180000
C	-8.93217800	-3.14330200	-1.89656700
H	-9.37207000	-1.72984000	1.16610900
H	-7.18747400	-0.73039500	0.58597900
H	-7.21750500	-2.84627100	-3.15529900
H	-9.40959800	-3.83118200	-2.58867300
C	-6.60236600	2.62051000	-4.48541900
C	-7.33845600	2.36351700	-3.32536600
C	-7.01254700	1.27570400	-2.51617300
C	-5.93306200	0.44460800	-2.84947100
C	-5.21650500	0.69569100	-4.02781300
C	-5.54623200	1.78020800	-4.84079300
H	-8.17257200	3.00591400	-3.05693300
H	-7.60577900	1.06028900	-1.63237700
H	-4.40206000	0.03504100	-4.30785800
H	-4.97953800	1.96210200	-5.74966900
P	-5.43728300	-1.01010800	-1.84761400
C	1.88527700	-2.73251100	-0.87349600
C	2.05658100	-1.70379000	-1.80283300
C	0.94733800	-1.12199000	-2.41726200
C	-0.34287500	-1.57414100	-2.11651400
C	-0.50963300	-2.62158800	-1.20188300
C	0.60028700	-3.18840000	-0.57476700

H	3.05502200	-1.35248200	-2.04914300
H	1.09043000	-0.32607000	-3.14039400
H	-1.49723300	-3.02201100	-1.00823500
H	0.45594100	-4.00373800	0.12906900
C	-2.21712600	3.10958200	-0.32036700
C	-1.56711400	1.99622300	0.21229900
C	-1.43679300	0.82820200	-0.53793400
C	-1.95118400	0.75591700	-1.83998100
C	-2.60899800	1.87976900	-2.36415400
C	-2.74225300	3.04496400	-1.61147300
H	-1.16270100	2.03138900	1.21977400
H	-0.93168300	-0.02999700	-0.10919400
H	-3.00670600	1.85418800	-3.37053000
H	-3.25392700	3.90253700	-2.04007900
C	-0.80021000	0.69377900	-7.07366400
C	-0.30553400	1.38524400	-5.96525800
C	-0.61075400	0.95002500	-4.67605300
C	-1.40808000	-0.18897700	-4.47910300
C	-1.90723700	-0.87489100	-5.59665200
C	-1.60219000	-0.43256100	-6.88532800
H	0.31377900	2.26733100	-6.10394200
H	-0.24773200	1.51018600	-3.82045000
H	-2.52519200	-1.75354900	-5.45211600
H	-1.99371000	-0.97389500	-7.74261600
P	-1.86360500	-0.81260600	-2.81041000
Cu	-3.74821000	-2.32796000	-2.71629300
H	-10.49538700	-3.28387900	-0.41573400
H	-3.46699800	0.64795100	3.25812500
H	-2.31685500	4.01813900	0.26718500
H	-6.86242700	3.46540100	-5.11697700
H	-0.56465700	1.03592400	-8.07782300
H	2.75080800	-3.18210200	-0.39431000
C	-4.45322300	-4.30604900	-6.88081900
C	-4.96418200	-3.72472600	-5.55695100
H	-3.83497300	-3.57097800	-7.40813300
H	-3.85500300	-5.19983500	-6.68924700
H	-5.29205700	-4.58124800	-7.53107500
C	-5.81230700	-4.75967600	-4.81202500
C	-5.76236100	-2.44523500	-5.81605500
H	-6.06348100	-4.41335100	-3.80938100
H	-6.73552900	-4.95398300	-5.37152600
H	-5.26283800	-5.69615400	-4.69893800
H	-6.63841900	-2.64998600	-6.44107900
H	-6.10239200	-2.00470800	-4.87461800

H	-5.13792900	-1.70287700	-6.32493600
O	-3.82499600	-3.30074200	-4.77802400

TS5

Cu	0.04416600	0.35632900	-0.25738200
B	-2.98394700	1.39708700	0.13027700
O	-4.08774200	1.56291900	0.96901100
C	-4.80881700	0.31889300	0.96650000
C	-4.46119100	-0.26424600	-0.45029500
O	-3.13244300	0.25227100	-0.68538300
C	-1.87480500	2.47911900	0.05355100
H	-2.12058300	3.37812600	0.62167600
C	-1.03551900	2.80922600	-1.14533000
C	-1.02248300	1.95258900	-2.25859200
C	-0.14884000	2.17314000	-3.32601900
C	0.71607500	3.26822100	-3.30842900
C	0.68632100	4.14794200	-2.22408700
C	-0.17883600	3.91813200	-1.15308300
H	-1.73456800	1.13677700	-2.26928000
H	-0.14682100	1.49369700	-4.17577600
H	1.40605200	3.43655700	-4.12985200
H	1.34755000	5.01092800	-2.20978400
H	-0.17758200	4.59050700	-0.29965500
C	-4.43863200	-1.78703700	-0.52188700
H	-3.68663200	-2.21253500	0.14514900
H	-5.41815400	-2.19634600	-0.24679300
H	-4.20862700	-2.11138800	-1.53925500
C	-5.35814400	0.29441300	-1.56221400
H	-6.37684800	-0.10469600	-1.50864100
H	-5.40573100	1.38636200	-1.51092500
H	-4.92732800	0.01378300	-2.52851900
C	-6.29008000	0.61109100	1.18792300
H	-6.43616200	1.02788900	2.18960000
H	-6.66491900	1.33703500	0.46311300
H	-6.88604100	-0.30586600	1.10926800
C	-4.26565900	-0.53309000	2.12152700
H	-3.19610700	-0.71307000	1.99752700
H	-4.39550300	0.02017300	3.05621000
H	-4.78454100	-1.49404700	2.20630700
N	-1.24817100	1.40695600	0.90348000
C	-0.92992000	1.67170200	2.22786000
C	-0.64206600	0.57253500	3.07436100
C	-0.85807900	2.95580100	2.81302600
C	-0.30833400	0.74324800	4.41280000

H	-0.71912500	-0.42546500	2.65854700
C	-0.53078400	3.11746300	4.15631100
H	-1.04077600	3.83688800	2.20890900
C	-0.25225300	2.02129000	4.97559200
H	-0.10009800	-0.13276100	5.02407100
H	-0.47599500	4.12400400	4.56454300
H	0.00116800	2.15916700	6.02271200
C	4.11693400	-2.83582500	2.26594100
C	2.79067300	-2.47264200	2.50743700
C	2.27179800	-1.31277800	1.93317600
C	3.07263500	-0.49843500	1.11841000
C	4.40802400	-0.85914100	0.89627600
C	4.92483700	-2.02329700	1.46611000
H	2.14886400	-3.09969900	3.11843600
H	1.23804700	-1.04099800	2.10906100
H	5.03433400	-0.24828200	0.25520800
H	5.95934000	-2.29969000	1.28037700
C	2.68806700	4.46244500	3.25315300
C	2.74493000	3.15277000	3.72816900
C	2.64653400	2.07814000	2.84540500
C	2.49045200	2.30675900	1.47407800
C	2.42701000	3.62595800	1.00029400
C	2.52807300	4.69630500	1.88587300
H	2.85051600	2.96103200	4.79123600
H	2.67420000	1.06562900	3.23024700
H	2.30290000	3.80952000	-0.06039200
H	2.48205400	5.71401400	1.50713600
C	5.06453900	1.85846500	-3.27384100
C	5.41074900	2.31798600	-1.99995900
C	4.57554400	2.06260500	-0.91312700
C	3.38201600	1.34539000	-1.09100900
C	3.03759700	0.90091500	-2.37324400
C	3.87746200	1.14951400	-3.45815900
H	6.33147300	2.87597600	-1.85348800
H	4.84141100	2.42866600	0.07351100
H	2.11036400	0.36267200	-2.52080700
H	3.59917600	0.78826500	-4.44358000
P	2.25684300	0.92623600	0.29162600
C	-0.56498300	-4.55096700	2.30954000
C	0.26555500	-4.95705100	1.26256500
C	0.43020800	-4.14571300	0.13836600
C	-0.22967400	-2.91343000	0.06053900
C	-1.07214600	-2.51723200	1.10986400
C	-1.24113800	-3.33077800	2.22839500

H	0.78838700	-5.90767700	1.32018100
H	1.08044100	-4.46549500	-0.66901400
H	-1.58318300	-1.56268300	1.03973100
H	-1.89255200	-3.00581200	3.03459300
C	3.85318200	-2.58097900	-3.61513700
C	3.81906900	-2.64763900	-2.22173500
C	2.61909200	-2.46397000	-1.53806100
C	1.42957900	-2.21448600	-2.24027400
C	1.46891300	-2.16184000	-3.64154400
C	2.67374800	-2.34227000	-4.32220200
H	4.72791500	-2.82951800	-1.65620500
H	2.61328300	-2.50616500	-0.45699300
H	0.55832000	-1.98001000	-4.20297400
H	2.68760300	-2.29906700	-5.40789800
C	-3.44856800	-3.08078400	-4.24637300
C	-2.94111300	-3.98275300	-3.30894100
C	-1.93526800	-3.58811300	-2.42745100
C	-1.42606200	-2.28318600	-2.47075700
C	-1.93879100	-1.38571400	-3.41610100
C	-2.94152500	-1.78167700	-4.30123300
H	-3.33297300	-4.99474600	-3.25891100
H	-1.55706600	-4.29258600	-1.69465500
H	-1.55966900	-0.37331800	-3.45718100
H	-3.33235700	-1.07120200	-5.02394700
P	-0.09184500	-1.72918100	-1.33114000
H	-0.68732000	-5.18430200	3.18367600
H	-4.23741900	-3.38752200	-4.92716600
H	5.71760200	2.05812600	-4.11902200
H	2.76110100	5.29724100	3.94458500
H	4.51989200	-3.74810700	2.69686400
H	4.79115500	-2.71399400	-4.14636800

IM9

Cu	-0.22660900	0.17338600	-0.05464300
B	-3.10645700	1.53185200	0.54140600
O	-4.23014200	1.48825900	1.42704100
C	-5.35157300	1.02695700	0.67112000
C	-4.94226000	1.40140600	-0.79632700
O	-3.53071800	1.13683000	-0.77917500
C	-1.92152500	2.59538600	0.79708500
H	-1.96164000	3.14500600	1.73712600
C	-1.16226100	3.26780700	-0.26152800
C	-0.73718500	2.61169700	-1.43391300
C	-0.00121200	3.28132300	-2.41171300

C	0.29564900	4.63838900	-2.27138900
C	-0.16901500	5.31945700	-1.14133600
C	-0.87669400	4.64212900	-0.15168400
H	-1.03537000	1.57793300	-1.60622100
H	0.33476200	2.74156200	-3.29228500
H	0.86672300	5.15862400	-3.03479900
H	0.04096700	6.37969200	-1.02137400
H	-1.20349500	5.17329800	0.73884900
C	-5.61162900	0.55905200	-1.87498000
H	-5.41205800	-0.50410300	-1.73359600
H	-6.69682500	0.71364400	-1.86758000
H	-5.23650700	0.85487500	-2.86160400
C	-5.15056800	2.89359200	-1.09865100
H	-6.21201900	3.14710700	-1.19579800
H	-4.71137500	3.51274700	-0.31184600
H	-4.64615100	3.13463400	-2.03986300
C	-6.61024000	1.72288300	1.18384800
H	-6.80948800	1.41157100	2.21493900
H	-6.48706700	2.80828000	1.17945900
H	-7.48450000	1.46355400	0.57449400
C	-5.47243700	-0.49311100	0.86439500
H	-4.60003100	-1.00348500	0.44296000
H	-5.51446600	-0.70652900	1.93745400
H	-6.37536200	-0.90307000	0.39771500
N	-1.70295600	1.10551700	1.02221700
C	-1.45646200	0.70412100	2.35955300
C	-2.19726100	-0.34258100	2.93245900
C	-0.43187100	1.29962900	3.11339700
C	-1.87664400	-0.81655700	4.20483000
H	-3.02322800	-0.76319900	2.37163200
C	-0.11264400	0.81660800	4.38034100
H	0.11163200	2.13590800	2.69159800
C	-0.82418300	-0.25319400	4.93137300
H	-2.46402400	-1.62379300	4.63618300
H	0.69851600	1.28085700	4.93498000
H	-0.57706100	-0.62712600	5.92084300
C	4.06304200	-2.78925400	2.27967100
C	2.75643900	-2.43014100	2.61417600
C	2.17718100	-1.29794900	2.04186000
C	2.90020000	-0.51312100	1.13062700
C	4.21888200	-0.86746100	0.81557600
C	4.79519000	-2.00211100	1.38657900
H	2.17399700	-3.04103700	3.29583700
H	1.15713400	-1.02902500	2.29632800

H	4.78107700	-0.27716100	0.10014400
H	5.81415200	-2.27706200	1.12774100
C	2.70300400	4.53338000	3.09358300
C	3.04469800	3.26057900	3.55484000
C	2.88348100	2.14722000	2.72911900
C	2.37709100	2.30335400	1.43234500
C	2.04551100	3.58432300	0.96803100
C	2.20777000	4.69197700	1.79725200
H	3.43631300	3.13179300	4.56018800
H	3.13793600	1.15907800	3.09702500
H	1.65778200	3.71652900	-0.03485900
H	1.93465100	5.67609300	1.42809500
C	4.39300600	1.81902900	-3.51508600
C	4.90033100	2.23060000	-2.27981000
C	4.19034200	1.96708100	-1.10944100
C	2.96659900	1.28204600	-1.16358100
C	2.45809300	0.89114200	-2.40718100
C	3.16975000	1.15127300	-3.57729400
H	5.84678300	2.76160700	-2.22889000
H	4.57692900	2.30363600	-0.15245100
H	1.50456400	0.38076700	-2.45771000
H	2.76603600	0.83024500	-4.53236500
P	2.00509600	0.88080000	0.34161600
C	0.08977700	-5.13797500	2.34727900
C	0.69267900	-5.39911400	1.11443800
C	0.61552100	-4.46511000	0.08138400
C	-0.06239800	-3.25346300	0.27600900
C	-0.66217000	-2.99936000	1.51536200
C	-0.59109300	-3.93539900	2.54515700
H	1.22666000	-6.33197800	0.95622200
H	1.10284800	-4.67089500	-0.86577600
H	-1.16656600	-2.05589500	1.68858700
H	-1.05217900	-3.70872600	3.50195300
C	3.44093700	-2.44008100	-3.80646200
C	3.58793100	-2.55755500	-2.42360200
C	2.47589600	-2.46546000	-1.58944300
C	1.19746000	-2.25729700	-2.12761700
C	1.05520600	-2.14386700	-3.51836200
C	2.17169300	-2.23599300	-4.35041500
H	4.56966700	-2.71361800	-1.98600600
H	2.60323300	-2.55789800	-0.51869500
H	0.07261900	-1.98699100	-3.95135300
H	2.04670300	-2.15055500	-5.42641100
C	-3.66919900	-3.26392800	-3.80541900

C	-2.70632200	-4.19720000	-3.40906000
C	-1.69107300	-3.81603400	-2.53760700
C	-1.63700600	-2.50231700	-2.04354800
C	-2.62021300	-1.57658200	-2.41413600
C	-3.62520100	-1.96305000	-3.30798200
H	-2.74382600	-5.21581800	-3.78507600
H	-0.93421300	-4.53647100	-2.24375600
H	-2.62759000	-0.57274400	-1.99410500
H	-4.37642000	-1.24169100	-3.60839800
P	-0.22765500	-1.95457900	-1.01011800
H	0.15571200	-5.86723900	3.14993600
H	-4.45500000	-3.55521400	-4.49692000
H	4.94722400	2.02696900	-4.42613700
H	2.82222900	5.39715400	3.74153500
H	4.50948800	-3.68098700	2.71054700
H	4.30900400	-2.50558000	-4.45593600
TS6			
Cu	0.23452100	0.30394400	-0.33616500
B	-3.68620200	1.36151600	0.44654600
O	-4.68072400	1.86027400	1.29991700
C	-5.92959100	1.79363600	0.58677900
C	-5.46514100	1.71488800	-0.91371500
O	-4.22707600	0.98711100	-0.79991500
C	-1.98920200	2.29209400	0.47172600
H	-1.92774500	3.02583600	1.27481300
C	-1.20713600	2.48146800	-0.69294600
C	-1.05486800	1.45885800	-1.69738400
C	-0.24022400	1.67722600	-2.83032000
C	0.44821300	2.86604000	-3.01327800
C	0.27113800	3.89215500	-2.06108800
C	-0.52933900	3.71603400	-0.94964900
H	-1.76569500	0.64164200	-1.71297800
H	-0.17166800	0.88837900	-3.57565300
H	1.09888000	3.01287100	-3.86839300
H	0.78166700	4.84264500	-2.20058300
H	-0.66520600	4.53276600	-0.24362300
C	-6.40555900	0.95197300	-1.84009800
H	-6.57922100	-0.06831100	-1.48950100
H	-7.37369200	1.46025700	-1.91612500
H	-5.96876400	0.89782100	-2.84265000
C	-5.13872500	3.09086000	-1.50979300
H	-6.03961800	3.69256200	-1.67039700
H	-4.45310400	3.63974200	-0.85830500

H	-4.63969500	2.94529000	-2.47282500
C	-6.76341100	3.02322100	0.93320200
H	-7.03539200	2.99887400	1.99357900
H	-6.20329500	3.94263100	0.74961000
H	-7.68762300	3.04943600	0.34391100
C	-6.64326100	0.51734800	1.05124500
H	-6.06755500	-0.37063100	0.77043200
H	-6.72444900	0.53882700	2.14232600
H	-7.65058600	0.42907300	0.62936800
N	-2.36580400	0.93905200	0.86485300
C	-1.92772800	0.37408300	2.05241900
C	-2.67971500	-0.63938800	2.68186900
C	-0.69964800	0.75415900	2.63065300
C	-2.21104800	-1.24588600	3.84357700
H	-3.63433100	-0.92773700	2.25217700
C	-0.23194300	0.12558500	3.78410000
H	-0.14254200	1.57122400	2.18979500
C	-0.97983100	-0.87993900	4.40252500
H	-2.81218200	-2.01845200	4.31683800
H	0.71869400	0.44304400	4.20552900
H	-0.62258000	-1.35650200	5.31070700
C	4.68201400	-2.72703500	1.68993700
C	3.39350800	-2.48547100	2.17297600
C	2.71661000	-1.32639500	1.79772600
C	3.31998800	-0.39901300	0.93533100
C	4.61920200	-0.63637400	0.46976800
C	5.29550300	-1.79778900	0.84640600
H	2.89938500	-3.20835000	2.81409100
H	1.71004300	-1.14782800	2.16056700
H	5.09062500	0.07308500	-0.20178700
H	6.30019300	-1.97984800	0.47453500
C	2.41561500	4.05065900	3.89362400
C	3.08560200	2.83395900	4.02390800
C	3.09704300	1.91999200	2.96817500
C	2.42872000	2.21808200	1.77404700
C	1.75407800	3.44252100	1.64831900
C	1.75496700	4.35503300	2.70066300
H	3.60303200	2.59261900	4.94822600
H	3.62057200	0.97641900	3.07626800
H	1.22573800	3.66840700	0.72770800
H	1.22806500	5.29897400	2.59359500
C	4.78746600	2.74463500	-3.12163700
C	4.88203300	3.35421200	-1.86907000
C	4.14703800	2.85962700	-0.79034000

C	3.29791200	1.76048900	-0.96608900
C	3.19558900	1.16068600	-2.22969300
C	3.94830000	1.64218200	-3.29773500
H	5.53228200	4.21313200	-1.72849400
H	4.22884500	3.33022500	0.18399000
H	2.52611700	0.32157800	-2.37761900
H	3.86470100	1.16247700	-4.26845700
P	2.31021600	1.03003700	0.38658400
C	0.66829300	-5.23454800	2.43424500
C	1.11409300	-5.48052500	1.13255500
C	0.94459200	-4.51662400	0.13930200
C	0.34268200	-3.28942000	0.44745200
C	-0.10659300	-3.04919500	1.75187700
C	0.05065300	-4.02025100	2.74013200
H	1.59022400	-6.42649600	0.88959100
H	1.29359400	-4.71401800	-0.86912000
H	-0.57515300	-2.10345800	1.99646700
H	-0.30342700	-3.81403300	3.74537300
C	3.41641700	-2.07873600	-3.95401200
C	3.69189900	-2.42455900	-2.63013500
C	2.66731600	-2.46993000	-1.68553800
C	1.34605300	-2.17329300	-2.05609000
C	1.07666800	-1.82331700	-3.38950900
C	2.10512200	-1.77931800	-4.33092400
H	4.70852600	-2.64897100	-2.32143000
H	2.90002200	-2.72739600	-0.65930500
H	0.06053400	-1.58831400	-3.68985700
H	1.88004400	-1.50994600	-5.35907500
C	-3.94283500	-3.25937300	-2.73873100
C	-2.77864000	-3.97584600	-3.03768800
C	-1.56302000	-3.60112300	-2.47016400
C	-1.50497900	-2.50177200	-1.59987600
C	-2.67439400	-1.79424600	-1.29520900
C	-3.88977500	-2.17176000	-1.86825800
H	-2.81989800	-4.82470500	-3.71480800
H	-0.65913000	-4.15388500	-2.70890300
H	-2.63987100	-0.94421900	-0.62270100
H	-4.77706000	-1.59190900	-1.63978500
P	0.04312700	-1.96837900	-0.78424100
H	0.80004400	-5.98933400	3.20469300
H	-4.88736600	-3.55044600	-3.19035600
H	5.36358400	3.13011900	-3.95824600
H	2.40472100	4.75755200	4.71827000
H	5.20497200	-3.63777100	1.96798800

H	4.21742100	-2.03956600	-4.68659000
TS6'			
C	1.36505700	3.69891300	-3.41291100
C	2.38245500	4.03427700	-2.51615700
C	2.71961800	3.16827200	-1.47525800
C	2.04321100	1.95080300	-1.31995200
C	1.03488000	1.61604100	-2.23750200
C	0.69523300	2.48227000	-3.27590200
H	2.90861100	4.97947100	-2.61921600
H	3.48495400	3.45984500	-0.76514300
H	0.49240300	0.68428900	-2.12031000
H	-0.10993600	2.21564400	-3.95352800
C	5.11525500	-2.61617500	-0.98750000
C	4.11047200	-2.20592200	-1.86671600
C	3.33326700	-1.09056100	-1.56347200
C	3.53750700	-0.38602300	-0.36771200
C	4.54111000	-0.80728700	0.51480100
C	5.33583300	-1.90956600	0.19526700
H	3.89645400	-2.77326200	-2.76607000
H	2.53474100	-0.80673900	-2.23808400
H	4.68433600	-0.30018500	1.46254300
H	6.11189700	-2.22825300	0.88594600
C	4.09088200	3.64119700	3.33096600
C	4.90107700	3.20195600	2.28019300
C	4.38654000	2.33783700	1.31495100
C	3.05351700	1.90157500	1.39312400
C	2.25383800	2.33834700	2.45733300
C	2.76779100	3.20850400	3.41846800
H	5.93375000	3.53258100	2.21323500
H	5.02013300	1.99338200	0.50332300
H	1.22238700	2.00845700	2.52158600
H	2.13050300	3.54874500	4.22854400
P	2.27346300	0.83598900	0.13066000
C	-3.37516700	2.52256300	-3.56524200
C	-3.24012300	3.56123400	-2.64251800
C	-2.71707800	3.30885000	-1.37352100
C	-2.31879000	2.01233800	-1.01972600
C	-2.46384900	0.96950600	-1.94827200
C	-2.99307600	1.22595000	-3.21204000
H	-3.54007100	4.57074300	-2.90947000
H	-2.60089200	4.12402000	-0.66716200
H	-2.18811600	-0.04028300	-1.66739100
H	-3.10336100	0.41072600	-3.92163400

C	0.27714000	5.55499000	2.21837100
C	0.52110000	5.14341100	0.90616500
C	-0.08258100	3.99200100	0.40850400
C	-0.94629600	3.23505900	1.21750900
C	-1.19433200	3.65711600	2.53045000
C	-0.58359000	4.81133800	3.02614700
H	1.19220600	5.71024000	0.26765000
H	0.11920400	3.68165100	-0.60945300
H	-1.86199800	3.08531500	3.16653300
H	-0.78591200	5.12904200	4.04539400
C	-4.89583000	0.56114500	3.60408500
C	-5.18787800	1.42072300	2.54182100
C	-4.20120400	1.74322500	1.60979500
C	-2.91719500	1.19899300	1.73255800
C	-2.63431500	0.32197900	2.78843000
C	-3.61785000	0.01244300	3.72707000
H	-6.18477000	1.84028900	2.43993300
H	-4.42787500	2.41121700	0.78423000
H	-1.64737200	-0.12675700	2.86424500
H	-3.39102900	-0.66847800	4.54239400
P	-1.55098400	1.61818800	0.59524200
Cu	0.13889000	0.06950900	0.54699600
B	-1.69864800	-2.42862500	0.18208300
O	-2.74624800	-1.56478800	-0.12915600
C	-3.94586900	-2.37169300	-0.24431200
C	-3.36203900	-3.82337800	-0.43374800
O	-2.10884900	-3.74194500	0.29149400
C	-3.00943800	-4.14569900	-1.89022200
H	-2.42412600	-5.06873600	-1.91304700
H	-3.90610000	-4.27805200	-2.50507100
H	-2.38655400	-3.35948400	-2.32613600
C	-4.20402500	-4.93789300	0.17372200
H	-5.19411100	-4.97692500	-0.29485000
H	-3.70978700	-5.89997900	0.00759800
H	-4.33001500	-4.80257400	1.25026500
C	-4.76800800	-1.84889200	-1.41694200
H	-5.66546800	-2.45985100	-1.56546300
H	-5.08240500	-0.81986800	-1.21482700
H	-4.18897400	-1.85072500	-2.34293200
C	-4.72062200	-2.20247100	1.06417900
H	-4.92085500	-1.14065800	1.22542200
H	-5.67507500	-2.73899500	1.04005200
H	-4.13539200	-2.56869800	1.91246500
C	0.04068100	-2.02293200	-0.99284800

H	-0.26354800	-1.14662500	-1.55507700
C	0.58854900	-3.13134400	-1.69250900
C	0.91193100	-2.97918600	-3.07394100
C	1.47956300	-4.00594200	-3.81357000
C	1.76232400	-5.24670900	-3.22482400
C	1.43029300	-5.42642300	-1.87886800
C	0.85263100	-4.40934200	-1.12461700
H	0.70513300	-2.02216100	-3.55260000
H	1.70564700	-3.83939700	-4.86551700
H	2.21191800	-6.04901900	-3.80243000
H	1.61848300	-6.38625200	-1.40133800
H	0.57776700	-4.60118400	-0.09492500
N	-0.34150900	-1.96502800	0.43264700
C	0.47057400	-2.44514400	1.49699000
C	1.83969000	-2.69922300	1.33695900
C	-0.12188100	-2.62877500	2.75932600
C	2.60393000	-3.08186000	2.43839700
H	2.28439200	-2.60004100	0.35793900
C	0.65254500	-3.01490100	3.84912000
H	-1.19201900	-2.47421100	2.86916400
C	2.02562800	-3.23639700	3.69970400
H	3.66410100	-3.27022000	2.29605500
H	0.18003400	-3.14976500	4.81893300
H	2.62855800	-3.54353900	4.54929500
H	-3.77866800	2.72215200	-4.55401500
H	-5.66639000	0.31152800	4.32779800
H	4.49397600	4.31598500	4.08096500
H	5.71234800	-3.49380500	-1.21749900
H	1.09274000	4.38506800	-4.20975400
H	0.75648000	6.44817400	2.60843800

IM10

Cu	-4.21321300	-4.00139400	-0.32058400
B	-0.56760600	-4.67835400	0.02776300
O	-0.70112700	-3.96602000	1.20712900
C	-0.29650200	-2.60217400	0.94542800
C	0.60309100	-2.74926300	-0.33461300
O	0.04858900	-3.93009900	-0.96526500
C	-1.98132700	-6.46161100	0.87977500
H	-1.58438600	-6.75331300	1.84773000
C	-3.32304800	-6.46528100	0.61459300
C	-3.88551300	-6.05058800	-0.67457100
C	-5.21281800	-6.46095400	-1.02076400
C	-6.06480500	-7.03149100	-0.10361300

C	-5.58830400	-7.20894000	1.23780200
C	-4.30405200	-6.91138600	1.59497700
H	-3.18983300	-5.94485600	-1.50017600
H	-5.53327400	-6.30443800	-2.05011700
H	-7.07666600	-7.32161100	-0.37106800
H	-6.27062700	-7.59526100	1.99277800
H	-3.96348500	-7.10240300	2.61028800
C	0.51454100	-1.58959100	-1.31844200
H	-0.50322500	-1.44846900	-1.68199800
H	0.85133300	-0.65778700	-0.85029000
H	1.15766900	-1.78821200	-2.18160000
C	2.06569200	-3.06649100	-0.00653000
H	2.57939900	-2.20276100	0.42790000
H	2.13903200	-3.90428000	0.69400400
H	2.58329500	-3.34782000	-0.92870500
C	0.41748500	-2.06873200	2.18335600
H	0.79034000	-1.05279300	2.00988300
H	-0.28630100	-2.03807300	3.02129700
H	1.25666800	-2.70603600	2.47015900
C	-1.56933700	-1.79769300	0.69354900
H	-2.13307900	-2.20629600	-0.14899200
H	-2.19690700	-1.86429300	1.58212200
H	-1.36235600	-0.74359600	0.48982700
N	-1.02559800	-6.01628600	-0.10683100
C	-0.63644700	-6.89597500	-1.15179600
C	0.48444800	-6.62888000	-1.96118700
C	-1.35689100	-8.07862200	-1.39211300
C	0.85475800	-7.50855800	-2.97701200
H	1.06130000	-5.72923800	-1.79740400
C	-0.98097900	-8.94737900	-2.41433600
H	-2.20679300	-8.31026900	-0.76369800
C	0.12528400	-8.67407800	-3.22004300
H	1.73065200	-7.27800200	-3.57898300
H	-1.56513100	-9.84934000	-2.57843800
H	0.41677700	-9.35606700	-4.01376300
C	-8.45192900	-1.57675900	-2.83154700
C	-8.11056500	-2.76364600	-2.17715800
C	-6.77864800	-3.16916000	-2.12403900
C	-5.76911400	-2.39007200	-2.71642300
C	-6.12217100	-1.21157200	-3.38590600
C	-7.45773000	-0.80905300	-3.44236000
H	-8.87157900	-3.35903200	-1.68171300
H	-6.51761900	-4.08091800	-1.59492400
H	-5.35121100	-0.59718400	-3.83871200

H	-7.72056900	0.11050200	-3.95825100
C	-3.00457300	-6.25919800	-5.39644600
C	-4.22829200	-5.59988000	-5.52054700
C	-4.54658900	-4.54360100	-4.66444600
C	-3.63678900	-4.14547500	-3.67731000
C	-2.40306400	-4.80924600	-3.56088000
C	-2.08873900	-5.85995700	-4.41956200
H	-4.94077300	-5.90898900	-6.28056900
H	-5.50235500	-4.03749000	-4.75764700
H	-1.69587800	-4.52006400	-2.78748400
H	-1.14663300	-6.38310400	-4.29924200
C	-1.53804000	0.87104800	-3.46851100
C	-1.50496300	-0.22998300	-4.32557500
C	-2.26148200	-1.36812400	-4.03986300
C	-3.05159700	-1.41620200	-2.88380400
C	-3.07216600	-0.30887300	-2.02017600
C	-2.32880200	0.83049100	-2.31693800
H	-0.89043700	-0.20518900	-5.22111600
H	-2.23197400	-2.22126300	-4.70914300
H	-3.66574700	-0.34131200	-1.11537100
H	-2.36253200	1.67920800	-1.63996500
P	-4.03143500	-2.89083800	-2.41233500
C	-9.73792200	-3.62083300	1.83812700
C	-9.25735800	-2.36184400	2.20803400
C	-7.90418900	-2.05838400	2.06458500
C	-7.01826300	-3.01450200	1.54626200
C	-7.50508600	-4.27377500	1.17716500
C	-8.85887800	-4.57622400	1.32580800
H	-9.93804000	-1.61417300	2.60577700
H	-7.54303400	-1.07069400	2.33280200
H	-6.82960200	-5.01641000	0.76645400
H	-9.22170300	-5.55815800	1.03451700
C	-5.07345500	1.83702300	0.29341100
C	-5.98772800	0.98910100	-0.33724200
C	-6.05503600	-0.35649000	0.01501000
C	-5.21073400	-0.87756700	1.01188500
C	-4.30935200	-0.01660400	1.65222200
C	-4.23810900	1.33060400	1.29006400
H	-6.64324700	1.36812500	-1.11546600
H	-6.76409000	-1.00326100	-0.48813400
H	-3.66537200	-0.39593100	2.43732800
H	-3.53178900	1.98415800	1.79454800
C	-3.16773200	-3.24913600	5.41539600
C	-4.28922100	-2.41736500	5.32667700

C	-4.93390400	-2.24347300	4.10404000
C	-4.46141900	-2.90288300	2.95892700
C	-3.34893300	-3.74957200	3.05656100
C	-2.70011400	-3.91354100	4.28183300
H	-4.65879000	-1.90489000	6.21054500
H	-5.80300900	-1.59578300	4.03840700
H	-2.97243600	-4.27496500	2.18593600
H	-1.82931000	-4.55988900	4.33487500
P	-5.22831500	-2.69204000	1.31105700
H	-10.79380700	-3.85257600	1.94747100
H	-2.66410000	-3.37776600	6.36958500
H	-0.94748500	1.75451300	-3.69416200
H	-2.76632800	-7.09164700	-6.05254400
H	-9.48758200	-1.25042100	-2.86177900
H	-5.01639700	2.88493100	0.01290400

TS7

Cu	-4.27003300	-4.12547300	-0.37730700
B	-0.50104300	-4.28175100	-0.13728600
O	-0.71971600	-3.42973900	0.93418500
C	0.03629400	-2.21747200	0.69451100
C	1.14803300	-2.71237600	-0.29646200
O	0.48014100	-3.79996400	-0.98572500
C	-2.18079900	-5.75335300	0.78350700
H	-1.80553600	-5.66894300	1.79697000
C	-3.48648600	-6.15490800	0.56726600
C	-4.11589800	-6.28091300	-0.74632500
C	-5.39303900	-6.88021400	-0.87674300
C	-6.14141000	-7.26681300	0.21855000
C	-5.60031500	-7.02052300	1.51462100
C	-4.36199500	-6.46203300	1.69091300
H	-3.49051100	-6.23671300	-1.62949100
H	-5.77078300	-7.04501100	-1.88470400
H	-7.11706700	-7.72916500	0.10402500
H	-6.19260300	-7.26856500	2.39331100
H	-3.97353300	-6.30442200	2.69366000
C	1.59242100	-1.68582000	-1.33207500
H	0.75818700	-1.35842300	-1.95551700
H	2.03137700	-0.80887300	-0.84274200
H	2.35372800	-2.12782900	-1.98292600
C	2.36159000	-3.31762800	0.41624300
H	2.96277600	-2.54920600	0.91300900
H	2.05088700	-4.05468700	1.16335600
H	2.98857200	-3.82750900	-0.32099200

C	0.54094300	-1.69694800	2.03518600
H	1.16847900	-0.80933800	1.89663800
H	-0.31259500	-1.41625800	2.66107700
H	1.11825300	-2.45457700	2.57001200
C	-0.92030000	-1.21706200	0.05150200
H	-1.28396900	-1.59264900	-0.90524000
H	-1.78595300	-1.06914900	0.70192300
H	-0.44749000	-0.24497400	-0.11802300
N	-1.21111000	-5.51119800	-0.26074700
C	-0.81284100	-6.57708600	-1.11717800
C	0.04210800	-6.36284300	-2.21649000
C	-1.29161700	-7.88011700	-0.89735400
C	0.40478200	-7.42064300	-3.04898300
H	0.43000900	-5.37300900	-2.41225400
C	-0.92830400	-8.92638700	-1.74221200
H	-1.94495000	-8.06256300	-0.05427500
C	-0.07915500	-8.71128400	-2.82798600
H	1.07601200	-7.22528700	-3.88228000
H	-1.31897500	-9.92121400	-1.54406300
H	0.20030400	-9.52938300	-3.48563300
C	-8.52872400	-1.59298900	-2.79880000
C	-8.20700600	-2.79636400	-2.16630100
C	-6.88039600	-3.22079200	-2.11351700
C	-5.85754600	-2.44329900	-2.68133800
C	-6.19181800	-1.25016700	-3.33467500
C	-7.52092400	-0.82788200	-3.39046400
H	-8.97907400	-3.39220400	-1.68938700
H	-6.62994200	-4.14817300	-1.60690400
H	-5.41262700	-0.64012500	-3.77823000
H	-7.76808100	0.10357000	-3.89247800
C	-3.30585200	-6.01448000	-5.86740800
C	-4.40703900	-5.16104300	-5.96461300
C	-4.67197600	-4.23768700	-4.95248200
C	-3.83409900	-4.16842100	-3.83236600
C	-2.72826700	-5.02649000	-3.74179100
C	-2.46182700	-5.94374200	-4.75696000
H	-5.06373500	-5.21511600	-6.82868100
H	-5.53062400	-3.57837800	-5.02924700
H	-2.08117300	-4.98537800	-2.87193700
H	-1.61169600	-6.61070000	-4.65795400
C	-1.43249000	0.66190800	-3.21611000
C	-1.19304700	-0.52549600	-3.90916900
C	-2.02318700	-1.63319100	-3.72145800
C	-3.09784000	-1.56442600	-2.82506400

C	-3.32234600	-0.37177800	-2.11823800
C	-2.50442600	0.73563200	-2.32259400
H	-0.36158500	-0.59250300	-4.60527500
H	-1.83166600	-2.54836000	-4.27124800
H	-4.13281400	-0.31085500	-1.40400000
H	-2.70013300	1.64882300	-1.76813700
P	-4.13426600	-3.02841900	-2.43604700
C	-9.86511200	-3.69433100	1.77791100
C	-9.33169500	-2.49250900	2.25152100
C	-7.96867900	-2.23144900	2.11825100
C	-7.12545400	-3.17137300	1.50505600
C	-7.66587400	-4.37370400	1.03414300
C	-9.02960700	-4.63483100	1.17371400
H	-9.97795600	-1.75784800	2.72380600
H	-7.56155400	-1.29093500	2.47577000
H	-7.02220900	-5.11008600	0.56611100
H	-9.43390200	-5.57417500	0.80662700
C	-5.08608700	1.67489400	0.40166300
C	-6.08573500	0.89143800	-0.18066200
C	-6.17445000	-0.46822900	0.11388700
C	-5.26988900	-1.06390500	1.00911400
C	-4.27661300	-0.26964000	1.59695000
C	-4.18193400	1.08887900	1.28921900
H	-6.79285600	1.33168300	-0.87768800
H	-6.95037700	-1.06382100	-0.35296400
H	-3.58159900	-0.71171400	2.30326900
H	-3.40416400	1.68997100	1.75194700
C	-3.27276500	-3.48278600	5.37905500
C	-4.66208700	-3.34244700	5.33474900
C	-5.31157300	-3.15689500	4.11414600
C	-4.57195800	-3.11837000	2.92533900
C	-3.17772800	-3.27246200	2.97071100
C	-2.53322300	-3.44496000	4.19567500
H	-5.24280400	-3.38083600	6.25232700
H	-6.39152800	-3.05707700	4.08657300
H	-2.59209100	-3.29032900	2.05824300
H	-1.45402000	-3.56821000	4.21259900
P	-5.33074100	-2.88680000	1.27653100
H	-10.92820600	-3.89411200	1.88048800
H	-2.77187500	-3.62931700	6.33208400
H	-0.78612400	1.52176300	-3.36767200
H	-3.10940400	-6.73839400	-6.65340500
H	-9.56000500	-1.25300700	-2.83012000
H	-5.01490400	2.73341700	0.16781200

TS8^{oss}

C	-3.13211800	-0.31919200	4.66017500
C	-3.91583000	-0.85044500	3.63471700
C	-3.56971500	-0.62987600	2.29987000
C	-2.43331600	0.12383100	1.98676000
C	-1.64583600	0.65631700	3.02003000
C	-1.99832700	0.43787600	4.34987100
H	-4.79710800	-1.44000900	3.87198900
H	-4.17376200	-1.05446500	1.50466000
H	-0.75332200	1.22679600	2.77598300
H	-1.38492700	0.85516200	5.14311900
C	-4.39718800	-2.39194900	-2.40318100
C	-3.29685200	-2.86883600	-1.68518000
C	-2.56208600	-2.00250100	-0.87931200
C	-2.93354700	-0.65474600	-0.76301400
C	-4.04067400	-0.18211300	-1.47801900
C	-4.76462200	-1.04923900	-2.29941100
H	-3.00126800	-3.91172100	-1.75963600
H	-1.69057500	-2.36729800	-0.34987700
H	-4.33030500	0.86087100	-1.40297500
H	-5.61751800	-0.67385000	-2.85806400
C	-3.17849100	4.70905400	-0.78290300
C	-3.92543500	3.97409700	0.14075900
C	-3.53812500	2.67763400	0.47999200
C	-2.39741900	2.10809900	-0.10294100
C	-1.64253800	2.85792000	-1.01456600
C	-2.03643300	4.15037500	-1.35958700
H	-4.80513500	4.41285000	0.60274700
H	-4.11389800	2.10834400	1.20340100
H	-0.72804500	2.43923500	-1.41949700
H	-1.43934700	4.72740100	-2.05960800
P	-1.85786300	0.40238300	0.27285800
Cu	0.42653500	-0.00186600	0.08258400
B	1.98541000	-1.54975500	-1.89796400
O	2.42863200	-1.88864500	-3.15242100
C	1.35267300	-1.56104800	-4.07860400
C	0.60015000	-0.41599700	-3.32143600
O	0.77962700	-0.85051200	-1.93669000
C	-0.88619300	-0.30307700	-3.62165900
H	-1.42576800	-1.21479300	-3.36346900
H	-1.32227100	0.51815100	-3.04647400
H	-1.03848500	-0.08708900	-4.68506400
C	1.29109600	0.94309800	-3.45140800
H	1.12449600	1.38021300	-4.44090300

H	0.89154700	1.62303300	-2.69450500
H	2.36818500	0.85947900	-3.28038100
C	0.49635000	-2.82102500	-4.23645900
H	1.13749800	-3.64812400	-4.55470400
H	0.02233600	-3.09596000	-3.28883500
H	-0.28822500	-2.67980000	-4.98647100
C	1.96959000	-1.15238100	-5.40884200
H	2.69066000	-0.34220400	-5.28240500
H	2.49088500	-2.00697700	-5.85081300
H	1.19304800	-0.82651400	-6.10964500
C	1.89142500	-1.51739500	0.54694800
H	2.50625500	-1.05228500	1.31252100
C	0.84915900	-2.42451800	1.00309900
C	0.17070800	-2.16210900	2.22210500
C	-0.86295900	-2.97792800	2.65894800
C	-1.23917700	-4.10370200	1.91471200
C	-0.55770100	-4.40029700	0.72916000
C	0.46018800	-3.57144300	0.26754900
H	0.45425600	-1.28766800	2.79991700
H	-1.38614100	-2.72819500	3.57687800
H	-2.04724300	-4.74271400	2.25758100
H	-0.82623600	-5.28484900	0.15695000
H	0.99066000	-3.81706300	-0.64666100
N	2.60839100	-1.83467000	-0.65609300
C	3.89955600	-2.41097000	-0.52274300
C	4.20339300	-3.19454100	0.60030500
C	4.88995400	-2.19363100	-1.49299800
C	5.47299900	-3.75150600	0.74539700
H	3.43966600	-3.37839000	1.34775300
C	6.15046700	-2.76542600	-1.34388000
H	4.66617900	-1.58129300	-2.35791100
C	6.45361100	-3.54418700	-0.22468100
H	5.69037000	-4.35700300	1.62106300
H	6.90655100	-2.58732800	-2.10375400
H	7.44165300	-3.98004200	-0.10987400
H	-3.47762400	5.72108000	-1.04011500
H	-4.96324600	-3.06270800	-3.04345400
H	-3.40235700	-0.49369900	5.69781400
I	1.71477400	2.11263300	0.91111600
C	-2.06201100	4.12265100	3.91969900
H	-2.07661400	3.69096100	4.92708600
H	-2.61569200	3.44438200	3.26084300
H	-2.60878600	5.07354600	3.95391300
C	-0.63262400	4.32722500	3.41330600

H	-0.08629000	4.99299000	4.09604800
H	-0.09072600	3.37403500	3.41357800
C	-0.59185600	4.90667400	1.99447600
H	-1.15555700	5.86122000	1.98845400
H	-1.14821200	4.24702600	1.31848600
C	0.78178600	5.12290500	1.46161600
H	1.61273400	5.32242600	2.13087500
H	0.93439100	5.32448300	0.40722000

IM11

C	4.12718100	3.90109900	-1.73514500
C	3.45498700	2.74260100	-2.13672700
C	3.86595200	1.49745100	-1.66529400
C	4.95108100	1.40402000	-0.77910600
C	5.61844400	2.56526800	-0.37506900
C	5.20556900	3.81057600	-0.85382100
H	2.61670900	2.80842700	-2.82434200
H	3.35971900	0.59163800	-1.99242600
H	6.46710700	2.49538600	0.29793300
H	5.72957600	4.70919800	-0.53987300
C	9.63766500	0.31604300	1.62804900
C	8.52869100	0.26340400	2.47445000
C	7.24755200	0.08931900	1.94662700
C	7.07127200	-0.04328300	0.56308500
C	8.19160300	-0.00922600	-0.28132200
C	9.46588600	0.18283900	0.24792000
H	8.65884800	0.35966900	3.54877300
H	6.38905700	0.05232400	2.60896600
H	8.06483400	-0.13921000	-1.34907400
H	10.32024200	0.22110200	-0.42158900
C	2.52268400	-1.34535800	3.17184600
C	2.96571700	-0.02658100	3.03881200
C	3.83813700	0.31543200	2.00691700
C	4.28082300	-0.66382900	1.10468800
C	3.81901500	-1.98035600	1.23232600
C	2.94577900	-2.31911500	2.26643500
H	2.62498500	0.73576300	3.73377000
H	4.16786000	1.34394300	1.89189600
H	4.11518200	-2.72633400	0.50158000
H	2.58435500	-3.33965200	2.35217400
P	5.44701100	-0.27553200	-0.24784300
Cu	5.37859100	-1.75739100	-1.94426000
B	7.16059000	-3.41411300	-3.62617500
O	7.62142400	-4.69503700	-3.72310400

C	7.70924000	-5.21499000	-2.36188000
C	7.89861900	-3.90744300	-1.50711800
O	7.20678300	-2.91604800	-2.32961800
C	9.35300600	-3.44727800	-1.40627800
H	9.37942000	-2.44422800	-0.97394400
H	9.93491800	-4.11653600	-0.76509800
H	9.82573100	-3.41271900	-2.39255700
C	7.24137000	-3.92940900	-0.13447700
H	7.67841800	-4.71900500	0.48630400
H	7.40410500	-2.97072000	0.36691100
H	6.16596200	-4.10086300	-0.21422300
C	8.87804300	-6.18896800	-2.29926500
H	9.02125700	-6.55213600	-1.27559400
H	8.66948600	-7.05060300	-2.94028500
H	9.80652400	-5.72742300	-2.64174700
C	6.38743400	-5.93017000	-2.07499900
H	6.23864800	-6.70952900	-2.82843100
H	6.39819100	-6.40420700	-1.08827100
H	5.53826800	-5.24100100	-2.12683000
C	6.30286600	-1.26555200	-4.42616200
H	5.32023900	-0.96424500	-4.77593800
C	7.23717100	-0.27985000	-3.99681600
C	6.77860700	1.02789800	-3.67792800
C	7.66112700	2.01569600	-3.26886900
C	9.03342500	1.74716800	-3.17229600
C	9.50754700	0.46876300	-3.49618500
C	8.63216900	-0.53284700	-3.89329700
H	5.71698100	1.24250600	-3.74314300
H	7.27665900	2.99829200	-3.01418300
H	9.72270300	2.52239600	-2.85194500
H	10.57223000	0.25631900	-3.44206900
H	9.01272700	-1.51083900	-4.16644900
N	6.64889100	-2.60556700	-4.68504400
C	6.18388500	-3.15029200	-5.91883500
C	6.32294100	-2.39140000	-7.08755500
C	5.56630000	-4.40553100	-5.97356100
C	5.85486600	-2.88709900	-8.30305200
H	6.80928800	-1.42194700	-7.03445700
C	5.11343300	-4.89786600	-7.19496800
H	5.42253900	-4.97375200	-5.06364500
C	5.25268900	-4.14462600	-8.36310000
H	5.96919400	-2.29139900	-9.20437100
H	4.62921500	-5.86963300	-7.22889800
H	4.88866200	-4.53226700	-9.31010000

H	1.83724200	-1.60874000	3.97247000
H	10.63197700	0.45534800	2.04301900
H	3.81125700	4.87031700	-2.11038500
I	3.33446800	-3.07934800	-2.77283600

IM12

C	3.86146400	2.91842500	1.92501500
C	3.34342800	1.92436300	1.09383800
C	4.20180300	1.08946400	0.37798700
C	5.58909500	1.25723600	0.48738400
C	6.10725300	2.25451800	1.32662800
C	5.24415300	3.08244600	2.04252100
H	2.26953900	1.78545600	1.01109900
H	3.79864700	0.30507000	-0.25245100
H	7.18216800	2.37540000	1.42216700
H	5.64933400	3.85118100	2.69465000
C	7.89269800	2.64993400	-4.23152200
C	7.07092800	3.23223600	-3.26595600
C	6.71967500	2.52115200	-2.11602500
C	7.18108300	1.21218600	-1.92759300
C	7.99606400	0.62691700	-2.91087000
C	8.35881000	1.34492700	-4.04827200
H	6.70190300	4.24460000	-3.40415300
H	6.08327900	2.98171600	-1.36836200
H	8.34521400	-0.39228600	-2.77774100
H	8.99661000	0.88343500	-4.79718900
C	10.42942100	-0.39852700	2.15556000
C	9.17699800	-0.87832300	2.55075700
C	8.06216700	-0.68452900	1.73932200
C	8.18716500	0.01084900	0.52496200
C	9.44088400	0.49344200	0.13389100
C	10.55790200	0.28449300	0.94651400
H	9.06817600	-1.41311900	3.49021400
H	7.09644000	-1.08515700	2.03447000
H	9.54981100	1.03133300	-0.80150400
H	11.52712800	0.66339600	0.63361500
P	6.67862000	0.17706400	-0.49968400
Cu	5.66552000	-1.89978100	-1.14768900
B	5.31988700	-5.67257600	-1.04071400
O	4.27276400	-6.54531000	-0.89645500
C	4.55062200	-7.34720100	0.28401200
C	6.11552700	-7.20952200	0.42939800
O	6.39108500	-5.94670600	-0.23609100
C	6.89609400	-8.27994700	-0.33788000

H	7.95591300	-8.00826300	-0.34438200
H	6.79229100	-9.26528800	0.12746600
H	6.55634500	-8.34723800	-1.37606300
C	6.61848100	-7.10213300	1.86416900
H	6.36889500	-8.00511200	2.43238200
H	7.70754900	-6.99040400	1.86285100
H	6.18689500	-6.23488900	2.36771400
C	4.05566800	-8.76562700	0.02145500
H	4.29856800	-9.42242500	0.86422500
H	2.96805200	-8.75355900	-0.09746400
H	4.49075600	-9.18582600	-0.88790600
C	3.77255200	-6.71834800	1.44146500
H	2.70991200	-6.70143800	1.18099200
H	3.89346300	-7.29609700	2.36367700
H	4.08915200	-5.68732100	1.61982100
C	6.17461600	-3.61556600	-2.33331200
H	6.09048400	-3.31358400	-3.36949300
C	7.55088000	-3.45272900	-1.83345200
C	8.50076700	-2.97461800	-2.76804600
C	9.79579500	-2.65328700	-2.38076300
C	10.17813500	-2.78550700	-1.04140000
C	9.25730400	-3.25975600	-0.10871400
C	7.95720100	-3.58805600	-0.48738900
H	8.20585800	-2.86585300	-3.80881000
H	10.50668400	-2.29526400	-3.12048100
H	11.18093800	-2.51295100	-0.72828300
H	9.54045600	-3.34819700	0.93425100
H	7.25418800	-3.93301700	0.25451600
N	5.27244600	-4.64321300	-2.04869100
C	4.05542100	-4.52620800	-2.81188700
C	4.07044200	-4.79990000	-4.18140000
C	2.89148300	-4.06926600	-2.19242400
C	2.91425000	-4.60936000	-4.93922400
H	4.98384100	-5.16814200	-4.64070100
C	1.73748700	-3.88775300	-2.95415800
H	2.91241100	-3.84045100	-1.13284300
C	1.74629400	-4.15100900	-4.32523800
H	2.92410500	-4.82756700	-6.00340700
H	0.83355200	-3.52463200	-2.47429800
H	0.84599600	-4.00149900	-4.91437100
H	11.29871100	-0.55619700	2.78797700
H	8.16532700	3.20589200	-5.12382400
H	3.18987400	3.56078100	2.48799700
I	4.63815100	-2.70942100	1.19092800

C	5.21074800	1.74611400	-6.82908900
H	4.13190500	1.91934300	-6.92158100
H	5.65181400	1.83557300	-7.82836500
H	5.62332600	2.54605300	-6.20337000
C	5.49740200	0.37652200	-6.20874400
H	5.10694000	-0.41794400	-6.86028100
H	6.58359800	0.22398600	-6.14850400
C	4.89590300	0.23582700	-4.80864500
H	3.80658300	0.34939600	-4.84771400
H	5.27283800	1.04215400	-4.16948600
C	5.23515300	-1.11132000	-4.16234700
H	6.31730400	-1.26852400	-4.13586700
H	4.79863700	-1.94356900	-4.73433400
O	3.64208700	-0.73396700	-2.40783800
C	4.68380800	-1.23506700	-2.75067700

TS9

C	3.80009500	3.15374800	1.24676600
C	3.31938000	2.13746200	0.41997200
C	4.20312400	1.21379200	-0.13823300
C	5.57686700	1.31321400	0.12197800
C	6.05471500	2.32895600	0.96235600
C	5.16724800	3.24726900	1.52090200
H	2.25537400	2.04994800	0.22177000
H	3.82429500	0.40311600	-0.75259400
H	7.11666100	2.39245800	1.18126800
H	5.54000400	4.03137200	2.17391700
C	8.88133200	2.33871200	-4.09101200
C	7.99225500	3.04768700	-3.28228400
C	7.32012200	2.40480800	-2.24011000
C	7.52680400	1.03990500	-2.00561000
C	8.40884800	0.32809900	-2.83373900
C	9.08959500	0.97571700	-3.86231800
H	7.82195800	4.10595500	-3.45833600
H	6.63778800	2.96487600	-1.60983900
H	8.57225500	-0.72996700	-2.66410900
H	9.77613400	0.41286600	-4.48869900
C	10.05386700	-0.78596600	2.40318600
C	8.75049800	-1.24948200	2.60313900
C	7.74706400	-0.94576100	1.68542000
C	8.03948100	-0.16734000	0.55385000
C	9.34343200	0.30799200	0.36446900
C	10.34546300	-0.00364200	1.28540300
H	8.51269300	-1.85672500	3.47195400

H	6.74218600	-1.33000100	1.83338600
H	9.58324800	0.91050200	-0.50421700
H	11.35444300	0.36687200	1.12619900
P	6.69439800	0.10741800	-0.66496200
Cu	5.55227200	-1.87392200	-1.20028900
B	5.21733300	-5.56545200	-1.05253500
O	4.34414500	-6.59732500	-0.81769600
C	4.75125300	-7.23099600	0.42383700
C	6.25934800	-6.78347800	0.56105600
O	6.30883200	-5.56677300	-0.22830800
C	7.24881500	-7.75525700	-0.08775300
H	8.23572100	-7.28370900	-0.11847300
H	7.32653300	-8.69027200	0.47616500
H	6.95402500	-7.99017100	-1.11511200
C	6.69833400	-6.43807600	1.97988600
H	6.60803100	-7.30889700	2.63877400
H	7.74746800	-6.12469000	1.97132200
H	6.10150500	-5.61926200	2.38613800
C	4.54422500	-8.73544300	0.27716000
H	4.89183100	-9.26331100	1.17226300
H	3.47739000	-8.94372700	0.15199600
H	5.07103900	-9.13381300	-0.59252600
C	3.84356700	-6.67879900	1.52528100
H	2.80346600	-6.89160300	1.25978200
H	4.05669900	-7.14937400	2.49078000
H	3.95068900	-5.59571400	1.62449000
C	5.81277300	-3.61235100	-2.61227500
H	5.65951300	-3.47503700	-3.67823400
C	7.26370400	-3.46244700	-2.29917900
C	8.13488000	-3.29705100	-3.39489000
C	9.49465100	-3.05867100	-3.20808000
C	10.01340400	-2.94258100	-1.91557300
C	9.16291600	-3.08681800	-0.81846800
C	7.80763100	-3.35839800	-0.99943700
H	7.73528400	-3.36617600	-4.40313100
H	10.14581600	-2.95303000	-4.07151100
H	11.06862600	-2.73442300	-1.76517600
H	9.54768200	-2.97562800	0.19012200
H	7.17508400	-3.49781800	-0.13285900
N	4.99495300	-4.65436300	-2.14653500
C	3.75525400	-4.81151100	-2.86520600
C	3.77414200	-5.18754300	-4.20979700
C	2.54247400	-4.57859500	-2.21482100
C	2.57510200	-5.32336700	-4.91095300

H	4.72475400	-5.39111200	-4.69608700
C	1.34854000	-4.72664600	-2.91663300
H	2.55548600	-4.25571600	-1.17999900
C	1.35990200	-5.09541700	-4.26406200
H	2.59228000	-5.61985800	-5.95603900
H	0.40565800	-4.53754300	-2.41169900
H	0.42557300	-5.20340100	-4.80769400
H	10.83603700	-1.03111500	3.11632900
H	9.40451500	2.84317100	-4.89824500
H	3.10939100	3.86687100	1.68794500
I	4.30467800	-2.63574300	1.00246200
C	5.04732300	2.67372000	-5.53262800
H	3.96506200	2.74820000	-5.69359600
H	5.54655800	3.18313800	-6.36467000
H	5.28762400	3.21972700	-4.61328700
C	5.49199300	1.21362700	-5.42497200
H	5.27632700	0.68892500	-6.36655200
H	6.57830500	1.17221500	-5.28447100
C	4.80713600	0.48051600	-4.26947400
H	3.71981100	0.47752500	-4.40825600
H	5.00227500	1.01782800	-3.33356600
C	5.28831000	-0.96986500	-4.12620800
H	6.37169200	-1.01405000	-3.99110100
H	5.03431400	-1.53788500	-5.03284600
O	3.39887500	-1.64546600	-2.79985500
C	4.59084000	-1.64399900	-2.95323700

IM13

C	5.09349000	3.93974600	2.31756100
C	4.15892200	3.01013000	1.86386300
C	4.57120300	1.91846000	1.09612600
C	5.92494900	1.75782200	0.77726100
C	6.86309400	2.69296100	1.24218900
C	6.44791500	3.77912300	2.00767600
H	3.10816200	3.12120400	2.11428000
H	3.84725100	1.17614500	0.77511000
H	7.91586700	2.56831200	1.00787900
H	7.17868000	4.49823100	2.36694300
C	8.22842200	2.25315600	-4.08079400
C	7.35178600	2.98416900	-3.27881700
C	6.83184300	2.42410500	-2.11024700
C	7.18209900	1.12094300	-1.73087100
C	8.05483000	0.38587200	-2.55039000
C	8.57757600	0.95126500	-3.71236100

H	7.07034800	3.99522000	-3.55866600
H	6.16014000	3.00604700	-1.48855200
H	8.33900000	-0.62442400	-2.27749500
H	9.26056400	0.37198300	-4.32749000
C	9.94836500	-1.51767700	2.14072000
C	8.64173700	-1.98675700	2.29238100
C	7.60438400	-1.42389900	1.54907100
C	7.86683900	-0.37853900	0.65040600
C	9.17980600	0.09091800	0.50472900
C	10.21511400	-0.47858800	1.24635700
H	8.42794900	-2.79409400	2.98632100
H	6.58849600	-1.79326200	1.66390200
H	9.39696400	0.88700400	-0.19972400
H	11.23035300	-0.11194100	1.12354100
P	6.43511000	0.32918600	-0.24973800
Cu	4.74479900	-1.20807100	-0.41959700
B	5.30680200	-5.39101200	-1.56865600
O	4.64661700	-6.52429200	-1.15320700
C	4.70966200	-6.53175600	0.29855600
C	5.98545500	-5.66006700	0.57712000
O	5.98128100	-4.74881700	-0.55534900
C	7.29428900	-6.45214200	0.48941400
H	8.12892500	-5.74509100	0.45465000
H	7.42775300	-7.11091500	1.35364500
H	7.32734100	-7.05922300	-0.42075900
C	5.93655000	-4.84308100	1.86050800
H	5.83463800	-5.50074100	2.73124800
H	6.87079300	-4.28317500	1.96752400
H	5.10758500	-4.13220600	1.85390800
C	4.80961000	-7.97814900	0.76751300
H	4.94105600	-8.02313900	1.85451800
H	3.88713700	-8.51003800	0.51475700
H	5.64290000	-8.49930500	0.29077700
C	3.42015900	-5.88482500	0.80847500
H	2.56669000	-6.42830900	0.39102300
H	3.35430900	-5.92430200	1.90038800
H	3.34630000	-4.83683700	0.50511700
C	5.99951200	-3.81927100	-3.46246100
H	6.00486500	-3.91402000	-4.55291000
C	7.45859100	-3.70044000	-3.03128400
C	8.44761000	-4.24031600	-3.86129900
C	9.79277600	-4.18353000	-3.49763900
C	10.16332600	-3.58033400	-2.29417800
C	9.18490100	-3.03396700	-1.46188800

C	7.84101400	-3.08693900	-1.83314700
H	8.15831100	-4.71788200	-4.79426200
H	10.54799800	-4.60993500	-4.15180300
H	11.20975400	-3.53758400	-2.00515500
H	9.46125100	-2.56670500	-0.52306900
H	7.08998800	-2.67866600	-1.17033200
N	5.30016800	-4.99039100	-2.93985800
C	4.25380800	-5.47057800	-3.79165500
C	4.56827700	-6.08340300	-5.00978300
C	2.91213100	-5.29918500	-3.43191800
C	3.55277800	-6.51414700	-5.86292700
H	5.61232100	-6.23299000	-5.27202900
C	1.89923000	-5.74595900	-4.27995600
H	2.67624000	-4.81569000	-2.48968400
C	2.21481300	-6.34877400	-5.49923500
H	3.80714500	-6.99219800	-6.80494100
H	0.86075200	-5.61280800	-3.99012900
H	1.42367800	-6.69006300	-6.16068400
H	10.75618200	-1.96159600	2.71537300
H	8.63558000	2.69270400	-4.98671500
H	4.77205500	4.78560400	2.91878700
I	3.03820500	-1.77915100	1.39968000
C	3.80661500	2.19880400	-4.37243300
H	2.74044300	1.95847500	-4.28289900
H	3.90905800	3.00525500	-5.10719800
H	4.14403800	2.58383000	-3.40309700
C	4.61961200	0.96730200	-4.77576800
H	4.29479300	0.61495700	-5.76509100
H	5.67652000	1.24314400	-4.87325200
C	4.48813800	-0.17006300	-3.76051700
H	3.44049700	-0.48511900	-3.67772100
H	4.77360100	0.19725400	-2.76894500
C	5.35045600	-1.37898700	-4.11355900
H	6.41157000	-1.09975000	-4.18525800
H	5.08754700	-1.77271500	-5.10673500
O	4.58406300	-2.45271200	-2.10672200
C	5.24457900	-2.52335300	-3.13718400

Cat2

Cu	0.48007300	0.34947300	-0.55147600
C	0.37566000	-1.61277500	-0.41741200
N	-0.80762400	-2.20909000	-0.10553100
C	-0.64272700	-3.54203300	0.28813100
C	0.69632600	-3.79340700	0.21164100

N	1.28892100	-2.60036300	-0.22713200
B	0.08415500	2.26415100	-0.15120600
O	-0.03124900	3.37511400	-0.98116000
C	-0.38398700	4.53284800	-0.18628800
C	-1.03068000	3.88318300	1.07999700
O	-0.35679000	2.60335800	1.13994800
H	1.96660400	-4.24946200	-2.46746800
C	-4.45948500	-0.09268800	-0.27752300
C	-4.04326200	-0.89230900	-1.34621400
H	-4.65821100	-0.95197600	-2.24077900
C	-2.84276600	-1.60448300	-1.30179600
C	-1.55150900	-0.52468700	2.15438100
H	-0.93849000	0.37599400	2.01961200
C	-2.37186400	-2.41649100	-2.48211400
H	-2.22476100	-3.47249900	-2.22601500
H	5.38810000	-1.24827800	1.30346800
C	5.44410400	-2.03642600	-0.69771600
C	4.67647800	-2.58042800	-1.73300000
H	5.15960500	-2.85723400	-2.66710300
H	-3.95231100	0.60916900	1.69079100
C	3.29860200	-2.76763100	-1.60325900
C	2.74074200	-1.41867000	1.93987100
C	-2.43601300	-0.70899200	0.94828200
H	2.09909100	-2.21072300	2.34288600
C	2.69973800	-2.40408400	-0.39036900
C	3.42866600	-1.84777400	0.66876500
C	4.80452400	-1.67728500	0.49251500
H	-3.09420100	-2.36505500	-3.30135300
H	-1.40885600	-2.04228300	-2.84898600
H	-0.88062900	-1.37347700	2.31193600
H	-2.15577700	-0.38703100	3.05723500
H	3.09074500	-3.50502400	-3.61695000
H	1.68348800	-2.60254300	-3.02022100
H	3.47253100	-1.14547800	2.70513600
H	2.09639500	-0.54989600	1.75538800
C	-3.64741600	-0.01881900	0.85721000
C	2.46895500	-3.31310100	-2.73822500
C	-2.05922700	-1.50422200	-0.14405800
C	6.92577900	-1.80994200	-0.87586300
H	7.45379900	-1.84388800	0.08258200
H	7.36924400	-2.56159200	-1.53725600
H	7.12120700	-0.82626800	-1.32217800
C	-5.74787900	0.69069800	-0.34391300
H	-6.43605300	0.39604800	0.45784100

H	-5.55931900	1.76483800	-0.22853700
H	-6.26013700	0.53996700	-1.29899600
C	-2.52765300	3.58787700	0.90939100
H	-2.85828500	2.95867200	1.74182800
H	-3.12884500	4.50397000	0.90682600
H	-2.71107500	3.03860600	-0.01872900
C	-0.79394200	4.63235500	2.38781500
H	-1.23349400	5.63648500	2.35040400
H	-1.26245700	4.08765400	3.21451300
H	0.27174800	4.72576800	2.60739900
C	-1.31567900	5.42244000	-1.00425600
H	-1.66272500	6.27823800	-0.41234100
H	-0.78152900	5.80811200	-1.87869300
H	-2.18580300	4.86637200	-1.36023500
C	0.91943600	5.28017600	0.12207200
H	1.41944800	5.51948700	-0.82144600
H	0.73767200	6.21421000	0.66574500
H	1.59409500	4.65382200	0.71311100
C	-1.79066500	-4.39166400	0.71346100
H	-2.32410300	-3.94097700	1.55829900
H	-2.51998600	-4.52280600	-0.09454100
H	-1.44105300	-5.38144400	1.01850000
C	1.49782200	-5.01056000	0.52307500
H	2.03464400	-5.38096400	-0.35830000
H	2.24969700	-4.80595900	1.29420600
H	0.84790400	-5.81160900	0.88482700

IM14

Cu	-0.27139300	0.35110800	0.60420900
C	-0.07229100	-1.52450300	1.19268600
N	-0.87030100	-2.59224300	1.44697500
C	-0.18841000	-3.61423600	2.12668000
C	1.08893100	-3.16765800	2.29544600
N	1.13115200	-1.89685300	1.71281100
B	0.27171000	2.27782600	0.55850000
O	0.42346300	3.09189800	-0.57639100
C	1.34648600	4.16442900	-0.26340600
C	1.18869800	4.28731100	1.28668200
O	0.80958600	2.94081800	1.66223200
C	-1.14487900	0.66370300	-1.99745600
H	-0.55319500	1.57903400	-2.08365600
C	-2.52614200	0.85326300	-1.53805300
C	-3.46063400	-0.19254800	-1.53730700
C	-4.76384900	0.03610300	-1.10680800

C	-5.14763800	1.30588700	-0.66610000
C	-4.22133900	2.35251300	-0.66314100
C	-2.91885200	2.12912300	-1.09981100
H	-3.14910300	-1.17247400	-1.87683400
H	-5.48237700	-0.77654500	-1.11406800
H	-6.16623300	1.47976600	-0.32922100
H	-4.51552400	3.34014800	-0.31869400
H	-2.18011100	2.92469800	-1.08028000
H	2.89054200	-3.41086000	0.07579700
C	-4.94986300	-3.01028400	0.47048100
C	-3.95933600	-3.48576500	-0.39263800
H	-4.24870500	-3.98350700	-1.31525400
C	-2.59889900	-3.32234600	-0.11243200
C	-2.79613500	-1.42035900	3.20529100
H	-2.12975100	-2.02399500	3.83295500
C	-1.53875500	-3.74855400	-1.09485400
H	-0.71099800	-4.27609300	-0.60936900
H	3.73687000	1.64393500	3.02269500
C	4.50407800	0.60701000	1.30178600
C	4.29822600	-0.46924200	0.43019300
H	4.99813100	-0.64210300	-0.38338900
H	-5.32103800	-1.93288600	2.29713800
C	3.19817800	-1.31698800	0.56101000
C	1.48071700	0.27201300	3.60679400
C	-3.21527400	-2.16310100	1.96212000
H	1.00553300	-0.63942400	3.98175800
C	2.30028900	-1.06720800	1.61048000
C	2.47864400	-0.01565300	2.51715600
C	3.59204800	0.81197200	2.33880800
H	-1.96106700	-4.40199100	-1.86417400
H	-1.12023200	-2.86081200	-1.58673200
H	-3.66743700	-1.13721300	3.80227900
H	-2.24545400	-0.50890000	2.94385700
H	3.74226700	-2.47501500	-1.16774600
H	2.00390500	-2.27985200	-0.94784600
H	1.96080500	0.78816300	4.44389100
H	0.69598700	0.92888400	3.21355800
C	-4.56049500	-2.33561900	1.63252400
C	2.94963100	-2.43430300	-0.41860000
C	-2.25445400	-2.68296700	1.08439800
C	-6.41239100	-3.22089000	0.16122900
H	-6.81056300	-4.09044100	0.70044400
H	-7.01157100	-2.35361300	0.45927100
H	-6.57445800	-3.39612800	-0.90719200

C	5.67039300	1.54433400	1.10049100
H	6.57222000	1.00400800	0.79243200
H	5.44965100	2.28173600	0.31762100
H	5.90046500	2.09840100	2.01604800
C	2.46408100	4.66026200	2.03685900
H	2.83470900	5.64288200	1.72121000
H	2.25896000	4.70423700	3.11166700
H	3.25025800	3.91987000	1.87348800
C	0.03820800	5.21004400	1.70391100
H	-0.87801800	4.95407700	1.16344300
H	-0.15141500	5.07546100	2.77324200
H	0.27154300	6.26513400	1.52286300
C	0.95379800	5.40401200	-1.05945600
H	1.59334700	6.25595400	-0.79948400
H	1.07038000	5.20589600	-2.12997600
H	-0.08695100	5.68187700	-0.87869000
C	2.73968600	3.68013000	-0.68947000
H	2.71155700	3.41674700	-1.75169200
H	3.50342700	4.45222500	-0.54466900
H	3.02630000	2.78725700	-0.12589100
N	-0.67790300	-0.48875400	-2.34181500
C	0.66483000	-0.58219800	-2.74852600
C	1.67863700	0.29447400	-2.31404900
C	1.00603600	-1.64236700	-3.60542300
C	2.98582000	0.12700700	-2.76411800
H	1.44318300	1.08392700	-1.61071700
C	2.31449000	-1.79730400	-4.05700000
H	0.21992800	-2.32241400	-3.91966600
C	3.31133700	-0.90961300	-3.64230300
H	3.75673100	0.80765400	-2.41343000
H	2.55837000	-2.61396000	-4.73130600
H	4.33315500	-1.03274600	-3.99080500
C	2.26993200	-3.77189300	2.97447700
H	3.11172200	-3.90525200	2.28557400
H	2.62278400	-3.13533700	3.79436400
H	2.01196500	-4.74991600	3.38915500
C	-0.85974500	-4.88095200	2.53347200
H	-1.71394000	-4.68856400	3.19342500
H	-1.24208300	-5.43108800	1.66573800
H	-0.15757900	-5.52914200	3.06437400
TS10			
Cu	0.01200500	-0.35110600	-0.36764400
C	0.43985700	-1.59039300	0.99355000

N	-0.45183900	-2.40271600	1.61378000
C	0.17247700	-3.25117200	2.53846600
C	1.50237900	-2.94688700	2.49133200
N	1.63382100	-1.92561300	1.54040100
B	-0.07585100	1.77861100	-0.16573200
O	0.67042200	2.87314400	-0.53313100
C	0.71363200	3.80405500	0.58353100
C	-0.52283700	3.36072100	1.45212800
O	-0.69816400	1.96553500	1.05467500
C	-0.73597700	0.95367300	-1.86136000
H	-0.14637400	1.68660100	-2.42197200
C	-2.15381100	1.41763500	-1.68879400
C	-3.10300400	0.63038700	-1.02263800
C	-4.40204200	1.09595000	-0.84354500
C	-4.77939900	2.35038500	-1.33478800
C	-3.84479200	3.13356700	-2.01127800
C	-2.53826200	2.66920700	-2.18171600
H	-2.81287200	-0.34410200	-0.64702000
H	-5.12231400	0.48043900	-0.31289300
H	-5.79498900	2.71033300	-1.19340700
H	-4.12890500	4.10566600	-2.40582600
H	-1.80427300	3.28264900	-2.69889700
H	2.83646900	-3.66301500	-0.15878900
C	-4.56501200	-2.28965000	0.68815000
C	-3.68541800	-3.08054800	-0.06102200
H	-4.06789900	-3.65686900	-0.89985300
C	-2.32120800	-3.13438300	0.22687400
C	-2.12659500	-0.62094700	3.11530900
H	-1.38758200	-1.12332700	3.74836800
C	-1.36632900	-3.91886800	-0.63504900
H	-0.66422100	-4.51067200	-0.03746400
H	4.66150600	1.43951400	2.18598700
C	5.09674900	0.21778100	0.46623700
C	4.68764500	-0.88981800	-0.28181000
H	5.24669000	-1.17451300	-1.16916000
H	-4.71840700	-0.88412100	2.30892900
C	3.55599400	-1.63390400	0.06304900
C	2.36839200	0.29355500	3.15152200
C	-2.68949600	-1.53789800	2.05906200
H	2.27179600	-0.50339200	3.89811500
C	2.84088700	-1.23304700	1.19690300
C	3.21324200	-0.13004400	1.97601400
C	4.35477200	0.57852400	1.59700300
H	-1.90953900	-4.59445300	-1.30164100

H	-0.77438700	-3.23291500	-1.25300400
H	-2.92336500	-0.23164500	3.75598900
H	-1.62442200	0.22987600	2.63726900
H	3.85502200	-3.08383700	-1.49795700
H	2.19523600	-2.52078800	-1.34655100
H	2.79962100	1.16835000	3.64659500
H	1.35306100	0.54569200	2.82276100
C	-4.05101300	-1.52495700	1.73825500
C	3.08944700	-2.79316400	-0.77594000
C	-1.85323100	-2.37232200	1.30836700
C	-6.03130400	-2.23907000	0.33384900
H	-6.46524900	-3.24441800	0.28152100
H	-6.60078700	-1.66252300	1.06933000
H	-6.17997700	-1.77139300	-0.64722200
C	6.29224400	1.03344200	0.03772200
H	7.06563200	0.40409700	-0.41494800
H	6.00418200	1.78314000	-0.71074700
H	6.73763000	1.56817500	0.88285200
C	-0.29555200	3.40146000	2.95910000
H	-0.11179900	4.42812900	3.29608800
H	-1.18866900	3.03168400	3.47286800
H	0.55045500	2.77988700	3.25846400
C	-1.82349400	4.08337000	1.09640800
H	-2.02507500	4.04116800	0.02437700
H	-2.65322300	3.58291300	1.60419900
H	-1.80004800	5.13112200	1.41498900
C	0.62549200	5.22023300	0.02547800
H	0.60001800	5.95725900	0.83623600
H	1.50422100	5.42492700	-0.59393400
H	-0.26421000	5.35040500	-0.59387600
C	2.06218300	3.58720200	1.27444700
H	2.86278400	3.75939500	0.54893300
H	2.20190000	4.27301300	2.11672900
H	2.15559500	2.56013500	1.63157400
N	-0.62537500	-0.37856600	-2.33637300
C	0.59889800	-0.71468700	-2.90331800
C	1.79001200	0.05977900	-2.82985800
C	0.68252600	-1.95351400	-3.59472200
C	2.97429000	-0.38735900	-3.42129000
H	1.79466900	1.00751600	-2.30111300
C	1.86447700	-2.37999800	-4.18087400
H	-0.22394400	-2.54855800	-3.66549600
C	3.03020700	-1.60135600	-4.10272100
H	3.86606000	0.23071100	-3.33944900

H	1.88322500	-3.32962300	-4.71147700
H	3.95301000	-1.93708300	-4.56724700
C	2.67903200	-3.50682700	3.21338600
H	3.41219100	-3.92581600	2.51404300
H	3.19633700	-2.73906600	3.80078300
H	2.36566100	-4.30202200	3.89481800
C	-0.59489900	-4.24803000	3.33666800
H	-1.34827900	-3.76201000	3.96784300
H	-1.12469400	-4.95612500	2.68865200
H	0.07735500	-4.81634300	3.98461600

IM15

Cu	0.35567800	-0.13042200	0.67884600
C	1.76435400	1.13438600	0.75260500
N	1.82522800	2.29354900	1.45544200
C	3.05490700	2.94350500	1.28500100
C	3.78910000	2.15453400	0.44693500
N	2.97368300	1.05990800	0.13398400
B	-2.34897700	-0.47739700	-0.76644200
O	-1.97507300	0.83406000	-1.01170800
C	-2.05215600	1.04137500	-2.44775200
C	-1.94374700	-0.42292700	-2.99633000
O	-2.55161200	-1.18934300	-1.92643400
C	-2.36418700	-1.12971400	0.66054100
H	-2.97921300	-2.04011900	0.60818100
C	-2.86165600	-0.28086900	1.81589800
C	-4.01161500	0.50693100	1.67839100
C	-4.50621100	1.24817700	2.75129800
C	-3.85316800	1.21418200	3.98507900
C	-2.69462200	0.44853400	4.12704700
C	-2.20168800	-0.28849500	3.05019000
H	-4.52484500	0.53673100	0.71927500
H	-5.40316600	1.84994300	2.62567600
H	-4.24144200	1.78302800	4.82520600
H	-2.17202600	0.42454600	5.07972200
H	-1.30066500	-0.88510500	3.15120600
H	4.12951000	-0.42991200	1.93172200
C	-1.14683400	3.52611100	4.18833300
C	-0.02251400	2.81373400	4.62037900
H	0.08198600	2.56898400	5.67473900
C	0.95894500	2.38571300	3.72755200
C	-0.53345700	3.63258000	0.42094400
H	-0.97976200	2.74391800	-0.03961900
C	2.12594000	1.54894600	4.18899200

H	2.08098700	1.38428100	5.26890100
H	3.45542800	-1.04983700	-3.91195100
C	3.91271200	-2.31048600	-2.23101500
C	4.01807800	-2.35974800	-0.83694400
H	4.30966900	-3.29054900	-0.35651500
H	-2.17333700	4.31070100	2.47206700
C	3.73193400	-1.25225000	-0.03684600
C	2.85994100	1.32488900	-2.74644200
C	-0.32392800	3.39341400	1.89289600
H	2.35840900	1.12810400	-3.69824900
C	3.34238700	-0.06495400	-0.67737300
C	3.25081200	0.03446700	-2.07162300
C	3.53823700	-1.10500600	-2.82919100
H	2.11699100	0.57059600	3.69349400
H	3.09147000	2.01342200	3.95652600
H	0.40685200	3.83892900	-0.10042600
H	-1.21295100	4.47514700	0.25859900
H	4.44820600	-2.17114700	1.77207000
H	2.78621600	-1.57866400	1.86470600
H	2.19001900	1.92029100	-2.12176400
H	3.74074600	1.94393000	-2.96312200
C	-1.28606900	3.79246400	2.82591200
C	3.78402100	-1.35789300	1.46598100
C	0.79980100	2.71141200	2.37132800
C	-2.17984300	4.00233500	5.17816700
H	-3.14632600	4.16525600	4.69321600
H	-2.32388600	3.27405000	5.98294000
H	-1.87423200	4.94898600	5.64327900
C	4.16705900	-3.54468700	-3.06060200
H	4.32764400	-3.29448000	-4.11377400
H	5.04447300	-4.09370100	-2.70162200
H	3.31172200	-4.23007400	-3.00808100
C	-2.70958100	-0.68460500	-4.28721300
H	-2.32609600	-0.05729700	-5.10026700
H	-2.58853300	-1.73229000	-4.57917000
H	-3.77738200	-0.48890000	-4.16685500
C	-0.49287700	-0.90649500	-3.12355000
H	0.02671800	-0.41103100	-3.95085300
H	0.06640900	-0.73402100	-2.19916800
H	-0.49608000	-1.98426000	-3.30980000
C	-0.92029200	1.96609100	-2.87669000
H	0.03555000	1.61332000	-2.48870000
H	-0.85917200	2.02239800	-3.96953900
H	-1.09246300	2.97720300	-2.49495100

C	-3.41117800	1.69102400	-2.72440200
H	-3.49677300	2.59963800	-2.12072100
H	-3.52382500	1.96253900	-3.77927100
H	-4.22884100	1.01893000	-2.44728400
N	-0.94318100	-1.49004400	0.71831300
C	-0.57949500	-2.77979200	1.04177900
C	-1.39746800	-3.68558900	1.76191800
C	0.70876700	-3.24486300	0.66722200
C	-0.93735700	-4.95691300	2.09988600
H	-2.38288500	-3.37237900	2.09263100
C	1.15922900	-4.51018500	1.01957800
H	1.33291600	-2.58979500	0.06555600
C	0.34269700	-5.38730000	1.74305500
H	-1.59083600	-5.61845000	2.66515400
H	2.15415900	-4.82393200	0.70735100
H	0.69166300	-6.37976800	2.01304600
C	5.17270300	2.29440800	-0.08803900
H	5.77030300	1.40114300	0.12644700
H	5.17873400	2.43558300	-1.17511400
H	5.67084100	3.15481500	0.36615700
C	3.35402200	4.25298200	1.93009800
H	4.36266800	4.58399600	1.66975700
H	2.64677900	5.02510900	1.60510200
H	3.28388900	4.19215100	3.02189600

TS11^{OSS}

Cu	0.46131700	0.45878700	0.27585100
C	1.83376600	1.72024100	-0.27656000
N	1.57702000	2.81956400	-1.03091600
C	2.73453200	3.57179100	-1.27690700
C	3.74933900	2.91366100	-0.64859700
N	3.16844400	1.78749100	-0.04592600
B	-1.21938300	-3.14992000	-1.21402000
O	-2.02819200	-3.29452700	-0.12214700
C	-2.90767700	-4.42276500	-0.38896100
C	-2.08996300	-5.22532700	-1.46496900
O	-1.32652300	-4.16891100	-2.12286400
C	-0.16708400	-1.97071700	-1.34408600
H	0.12959600	-1.87515500	-2.40224200
C	1.02715300	-2.49162100	-0.56350300
C	1.08614000	-2.36637500	0.83272800
C	2.13930400	-2.93328500	1.55056600
C	3.12797300	-3.66329200	0.89060200
C	3.06912100	-3.80652000	-0.49695400

C	2.02890300	-3.22024400	-1.21766900
H	0.30099400	-1.83601700	1.36063400
H	2.17831900	-2.80452300	2.62818700
H	3.94238400	-4.11294700	1.45146200
H	3.83690900	-4.37015300	-1.02071900
H	1.98309200	-3.33571100	-2.29793300
H	2.34958800	1.95712000	2.83293200
C	-2.20381900	3.90487300	-2.55212500
C	-1.75354700	4.41580800	-1.33277100
H	-2.38197800	5.10945500	-0.77953800
C	-0.51591100	4.05073400	-0.79307900
C	0.67835200	1.55626600	-3.44339900
H	1.71239500	1.89076900	-3.58542700
C	-0.06222200	4.56022000	0.55107400
H	-0.04281000	3.74283200	1.28306900
H	5.66943400	-2.03735500	0.10425700
C	5.40780400	-1.11722100	2.03115700
C	4.82414900	-0.04780900	2.71656200
H	4.95725900	0.03419100	3.79267300
H	-1.76007000	2.54157700	-4.15742500
C	4.07122300	0.92699900	2.05596100
C	4.23697300	-0.39570200	-1.53689700
C	-0.15749800	2.59179500	-2.73581900
H	4.76481300	-1.26451500	-1.93813800
C	3.91022800	0.79121500	0.67156800
C	4.47086400	-0.26797100	-0.05309100
C	5.22953300	-1.20616800	0.64794700
H	0.94912600	4.98065000	0.51198800
H	-0.74070300	5.33326500	0.92248800
H	0.25325000	1.31710000	-4.42187400
H	0.71663100	0.63506000	-2.85052200
H	3.65166200	3.03583900	2.32380700
H	3.80504600	2.11229800	3.83215700
H	3.16989100	-0.52272900	-1.74770000
H	4.57200100	0.49442300	-2.08284400
C	-1.39989900	2.98373100	-3.23220100
C	3.43953600	2.07255500	2.80222400
C	0.27371800	3.15808500	-1.52682000
C	-3.53741800	4.31555500	-3.12422200
H	-3.41281500	4.90518500	-4.04127200
H	-4.13573300	3.43444100	-3.37944600
H	-4.10816200	4.92087800	-2.41327400
C	6.17881200	-2.17902600	2.77569700
H	5.50407900	-2.96121800	3.14864800

H	6.91734400	-2.66561400	2.13025200
H	6.70277100	-1.76339700	3.64279900
C	-1.05883000	-6.17705300	-0.85151400
H	-0.45007200	-5.66485500	-0.10007100
H	-1.53667800	-7.04461200	-0.38537800
H	-0.39090300	-6.53141000	-1.64222300
C	-2.93181900	-5.94152500	-2.51210400
H	-2.27779400	-6.44981800	-3.22748100
H	-3.57303100	-6.69475800	-2.04090800
H	-3.56216100	-5.24116100	-3.06376800
C	-4.21697200	-3.84383100	-0.93253200
H	-4.95617300	-4.63031800	-1.11581700
H	-4.62716100	-3.14437700	-0.19964100
H	-4.05052600	-3.29029600	-1.86094400
C	-3.15049400	-5.15863700	0.92255400
H	-3.76390800	-6.05175300	0.75858300
H	-2.21201500	-5.45704700	1.39409800
H	-3.68087600	-4.49975900	1.61634800
N	-0.67259000	-0.71121500	-0.82069500
C	-1.84205000	-0.23982200	-1.34477200
C	-2.47826100	0.85538600	-0.69671500
C	-2.48487200	-0.78183200	-2.49435000
C	-3.68315200	1.35944100	-1.15805700
H	-2.01171800	1.26868400	0.19122100
C	-3.69401600	-0.26367000	-2.94335200
H	-2.02833500	-1.59888200	-3.04182900
C	-4.31017100	0.80312900	-2.28016800
H	-4.14235600	2.19282200	-0.63512500
H	-4.16316000	-0.69747600	-3.82303100
H	-5.26182500	1.19233300	-2.63000200
C	5.20518000	3.20833900	-0.53209800
H	5.50353200	3.33946800	0.51462600
H	5.81493500	2.39420200	-0.94069300
H	5.45207400	4.12507700	-1.07393700
C	2.71045800	4.81810600	-2.09319800
H	2.33651400	4.62449000	-3.10552300
H	2.05812100	5.57902700	-1.64933100
H	3.71639800	5.23787300	-2.17573500
I	-0.46005300	0.84688500	2.76505200
C	-5.73809600	0.33043000	1.67867900
H	-6.21704900	1.25349600	2.02580900
H	-6.45031100	-0.49149700	1.82793600
H	-5.56397400	0.42427200	0.60092700
C	-4.42714800	0.06413700	2.42174300

H	-3.75175800	0.92296900	2.33175400
H	-4.62753100	-0.05744900	3.49531100
C	-3.70114800	-1.18032800	1.89432100
H	-3.38331300	-1.01627000	0.85679900
H	-4.43738100	-2.00970800	1.83510900
C	-2.54660800	-1.62332600	2.71139800
H	-2.54247600	-1.48522700	3.78697500
H	-1.79973800	-2.27587800	2.27754900

IM16

Cu	-0.01729900	-0.32383500	-0.56542500
C	0.92400800	-2.00129300	-0.19398600
N	2.23500700	-2.34387800	-0.16444500
C	2.41272100	-3.71170300	0.09364400
C	1.16241300	-4.23784800	0.22557000
N	0.27403500	-3.16898600	0.04304900
B	-1.42402000	2.87693200	1.84296200
O	-1.68831000	3.45433200	3.05563400
C	-2.17361900	4.80249000	2.77249400
C	-2.70160400	4.66640400	1.29674500
O	-1.87082300	3.59250700	0.77202100
C	-0.60056400	1.52945100	1.68383100
H	-0.58114000	1.01466100	2.65817900
C	0.81190800	1.97280000	1.35069400
C	1.18122500	2.27266100	0.03123500
C	2.46495600	2.73972400	-0.25308500
C	3.37753300	2.95980900	0.77837700
C	3.00789700	2.69104800	2.09768400
C	1.73605600	2.19350600	2.37976200
H	0.46058200	2.15863500	-0.77248400
H	2.74158300	2.93682700	-1.28437400
H	4.37283300	3.33439800	0.55729300
H	3.71319700	2.85853600	2.90751200
H	1.45065400	1.97958700	3.40715100
H	-1.61001500	-2.38431200	3.40883800
C	5.46644800	0.33817200	-0.52811400
C	4.89480800	0.07122000	0.71917900
H	5.28882500	0.56238200	1.60446800
C	3.80875700	-0.79415000	0.85453600
C	3.31756800	-1.87537900	-2.79155700
H	3.19772800	-2.95346900	-2.63393500
C	3.16763500	-1.04898400	2.19480900
H	3.14115100	-2.11792400	2.43842400
H	-3.83502300	-4.12349600	-1.74739700

C	-3.91485100	-3.56609900	0.32942400
C	-3.16267800	-3.14117800	1.42757500
H	-3.66685300	-2.89872000	2.35875900
H	5.38553700	-0.10673600	-2.63172200
C	-1.77764100	-2.98779600	1.34893700
C	-1.17994000	-3.89781500	-2.32705000
C	3.87049200	-1.19063300	-1.56994500
H	-0.80973600	-2.94579600	-2.72865200
C	-1.15430800	-3.27924300	0.12793700
C	-1.87307900	-3.67722500	-1.00728600
C	-3.25710800	-3.81882000	-0.87806400
H	3.70861500	-0.52728200	2.98845700
H	2.13336100	-0.68976200	2.20052300
H	3.97718700	-1.72493900	-3.65080300
H	2.32959200	-1.47274500	-3.04545800
H	-0.54375700	-1.50438200	2.29492600
H	-0.14363400	-3.15367700	2.76625700
H	-0.31646000	-4.56576100	-2.23155100
H	-1.86881000	-4.33042500	-3.05791400
C	4.94530300	-0.30077100	-1.65660900
C	-0.97731700	-2.48469200	2.52284900
C	3.31811000	-1.41276600	-0.30254600
C	6.59810100	1.32742800	-0.65777400
H	7.19754200	1.37492500	0.25739400
H	7.26265100	1.07269400	-1.48980800
H	6.21181600	2.33771000	-0.84814200
C	-5.40724800	-3.75263300	0.44568200
H	-5.91595800	-3.47909700	-0.48473500
H	-5.66019800	-4.79927500	0.66069500
H	-5.81993700	-3.13776400	1.25070500
C	-4.15002500	4.17741000	1.21006800
H	-4.36620500	3.90492900	0.17315700
H	-4.30670300	3.28781700	1.82606200
H	-4.85570800	4.95432000	1.52190500
C	-2.50118700	5.89997800	0.42546100
H	-3.05575500	6.75403400	0.83050000
H	-1.44592500	6.16919900	0.34932100
H	-2.87280900	5.69820400	-0.58358700
C	-0.96138100	5.72923600	2.89738700
H	-0.53379200	5.62105900	3.89868500
H	-0.18813200	5.46595000	2.16918500
H	-1.23951200	6.77754200	2.74989000
C	-3.23427200	5.16165800	3.80481900
H	-2.78069900	5.20553600	4.79994000

H	-3.66921300	6.14302000	3.58501300
H	-4.03692000	4.42164400	3.82833100
N	-1.16592000	0.66201700	0.65797600
C	-2.50627400	0.36456800	0.75479200
C	-3.27228200	0.53384700	1.93741100
C	-3.16142800	-0.12971500	-0.40131100
C	-4.62992300	0.23118100	1.94700400
H	-2.80224400	0.88896100	2.84719400
C	-4.51759700	-0.41386600	-0.37894600
H	-2.58382800	-0.23762700	-1.31425600
C	-5.26505900	-0.23334900	0.79121200
H	-5.19885800	0.36230300	2.86386400
H	-4.99918000	-0.77658200	-1.28220000
H	-6.32849000	-0.45334400	0.80209800
C	0.69011200	-5.62125100	0.51430900
H	0.08205900	-5.65344800	1.42602100
H	0.07095600	-6.01492400	-0.30004200
H	1.54217800	-6.29263800	0.64864300
C	3.76636300	-4.32867100	0.18047400
H	3.68382600	-5.39616800	0.40066400
H	4.31946100	-4.21544800	-0.75912200
H	4.37018400	-3.86183700	0.96729900
I	-0.17867100	0.08110700	-3.19752000

TS12

Cu	-0.05779500	-0.54062200	-0.24304400
C	0.22535300	-1.80148000	1.15707600
N	-0.67357900	-2.69712000	1.63932200
C	-0.11888000	-3.51704100	2.63241600
C	1.18109900	-3.12550300	2.76279300
N	1.36174500	-2.06890600	1.86036900
B	-0.56840700	2.11804900	-1.01230100
O	0.20769700	3.28817000	-1.17865800
C	0.86329800	3.51302400	0.07880400
C	-0.21326000	2.99579100	1.09807700
O	-0.81424100	1.89846400	0.38721000
C	-1.34541000	1.40883500	-2.13558000
H	-1.23260900	1.85438000	-3.12903600
C	-2.63886900	0.67094300	-1.99733800
C	-2.75988800	-0.67447300	-2.37143400
C	-3.99662100	-1.31539700	-2.33398600
C	-5.13401300	-0.62316700	-1.91133800
C	-5.01916500	0.70681100	-1.50488000
C	-3.77903200	1.34599200	-1.54432100

H	-1.87207400	-1.20617600	-2.70155600
H	-4.07484700	-2.35622500	-2.63595200
H	-6.10046200	-1.11844900	-1.89391100
H	-5.89649300	1.24860100	-1.15970500
H	-3.68353200	2.38232600	-1.23181900
H	2.66163100	-3.25740600	-0.01062100
C	-4.70999400	-3.05755900	0.47501000
C	-3.74737700	-3.95820900	0.00628500
H	-4.04960900	-4.76910500	-0.65252800
C	-2.40100800	-3.82954400	0.34507100
C	-2.53228700	-0.63140800	2.46856700
H	-1.78558400	-0.90298100	3.22267200
C	-1.35718200	-4.75146400	-0.23527800
H	-0.82565300	-5.32554000	0.53207300
H	3.98553300	1.30456700	3.49385100
C	4.71079100	0.49514400	1.63576700
C	4.49292100	-0.47399600	0.65481100
H	5.17630300	-0.54394600	-0.18792800
H	-5.02521300	-1.25255000	1.59470400
C	3.40908100	-1.35628700	0.71394200
C	1.77594400	-0.18574300	3.98752800
C	-2.95917700	-1.82245800	1.64786600
H	1.95181300	-0.97148400	4.73232000
C	2.52893300	-1.23613900	1.79658100
C	2.72676000	-0.29338200	2.82001700
C	3.82758600	0.55832200	2.71895800
H	-1.81346000	-5.46159000	-0.93032000
H	-0.59916500	-4.17659200	-0.78090300
H	-3.39284800	-0.18889200	2.97886000
H	-2.08535900	0.14059300	1.82916800
H	4.16039800	-2.69984100	-0.78669300
H	2.61659100	-1.94900200	-1.19642100
H	1.89585500	0.77673600	4.49127100
H	0.73477300	-0.27125000	3.66449100
C	-4.29500800	-1.98818600	1.26936400
C	3.19935800	-2.37718900	-0.37417200
C	-2.03753400	-2.77836700	1.20030300
C	-6.16461300	-3.24214800	0.12262200
H	-6.62370400	-4.02630000	0.73884700
H	-6.73145200	-2.32028900	0.28005900
H	-6.28552300	-3.54009300	-0.92450400
C	5.84497700	1.48153400	1.51055400
H	6.67606100	1.06671400	0.93149600
H	5.50789700	2.39054800	0.99571400

H	6.22641000	1.78283300	2.49177000
C	0.35985300	2.47783800	2.40950900
H	0.87369600	3.27571400	2.95933700
H	-0.44669600	2.09294100	3.04319900
H	1.06672200	1.67015500	2.22485000
C	-1.31590000	4.02787700	1.36462700
H	-1.70861600	4.42076000	0.42219500
H	-2.13580200	3.53721100	1.89902300
H	-0.95701300	4.86575100	1.97270600
C	1.19567100	4.99713000	0.19493100
H	1.60553900	5.23230800	1.18438100
H	1.94545100	5.26629700	-0.55657500
H	0.31125000	5.61517400	0.02444200
C	2.15421500	2.67974600	0.11215900
H	2.76033100	2.93521300	-0.76223100
H	2.74287400	2.87140600	1.01540900
H	1.93839000	1.60914000	0.06442600
N	-0.09364300	0.63218900	-1.77470600
C	0.89296400	0.48255500	-2.77728400
C	1.47297300	1.57858800	-3.44365900
C	1.33201100	-0.80797300	-3.12362500
C	2.46448400	1.37831200	-4.40344600
H	1.16238400	2.58059500	-3.17258600
C	2.33009700	-1.00225300	-4.07846000
H	0.86071500	-1.65827400	-2.63610000
C	2.90565200	0.09246000	-4.72544200
H	2.90477700	2.24051300	-4.89889700
H	2.64807700	-2.01269000	-4.32505900
H	3.68105200	-0.05374200	-5.47230100
C	2.29593600	-3.67236100	3.58739300
H	3.10606300	-4.04784200	2.95080300
H	2.73207100	-2.91953100	4.25165600
H	1.93892800	-4.50211500	4.20278300
C	-0.91847200	-4.53995900	3.36448100
H	-1.79256700	-4.08262800	3.84232900
H	-1.29101100	-5.32989700	2.70314500
H	-0.31075900	-5.00774500	4.14325700

IM17

Cu	-0.02056900	-0.53841400	-0.12336300
C	0.19046000	-1.93408200	1.14396000
N	-0.67927900	-2.76199600	1.77268900
C	-0.02933500	-3.58419400	2.70548300
C	1.29714900	-3.26358900	2.63572200

N	1.39982500	-2.25454800	1.67368100
B	-0.38156100	2.10409300	-0.83181200
O	0.27201500	3.37648600	-0.79318300
C	0.41895100	3.73217700	0.58594600
C	-0.83145700	3.04763000	1.23843200
O	-0.92128900	1.82568900	0.49496900
C	-0.98526900	1.45394600	-2.13763600
H	-0.71272300	1.95257600	-3.07106500
C	-2.24250100	0.66328600	-2.21944500
C	-2.29256000	-0.73288700	-2.10417300
C	-3.50482400	-1.42218400	-2.16488400
C	-4.69960300	-0.72838400	-2.35366700
C	-4.66694700	0.66441800	-2.47515200
C	-3.45579200	1.34818000	-2.40544900
H	-1.36739800	-1.28845700	-1.97300700
H	-3.51179000	-2.50300400	-2.06408200
H	-5.64339200	-1.26384100	-2.41405700
H	-5.59081700	1.21949100	-2.61880400
H	-3.43650500	2.43237700	-2.48388600
H	2.61685000	-3.93657400	-0.16066800
C	-4.79811300	-2.82756000	0.84783800
C	-3.94503200	-3.83218100	0.38334900
H	-4.34662800	-4.62750300	-0.24004600
C	-2.57723500	-3.82197200	0.66722900
C	-2.33309000	-0.58733200	2.71797400
H	-1.55567000	-0.90109700	3.42271400
C	-1.65362000	-4.85658600	0.07332900
H	-1.22383000	-5.52356300	0.82977600
H	4.34822200	1.21009800	2.17161400
C	4.68230700	0.05583500	0.38556900
C	4.26296500	-1.05429100	-0.35082200
H	4.73497000	-1.27149900	-1.30400700
H	-4.90503500	-0.99598900	1.96927300
C	3.20916200	-1.86421300	0.07927500
C	2.22491700	-0.06034000	3.31383700
C	-2.89980500	-1.74927200	1.94423200
H	2.34859500	-0.80905200	4.10593500
C	2.57882600	-1.53055500	1.28454200
C	2.97299000	-0.42971300	2.05833500
C	4.03897100	0.34219100	1.59452500
H	-2.18741600	-5.47717400	-0.65164500
H	-0.81253200	-4.37665600	-0.44023600
H	-3.12215000	-0.07704500	3.27854800
H	-1.88145300	0.14079300	2.03351000

H	3.42261600	-3.22186400	-1.57550200
H	1.74833600	-2.79906300	-1.19428400
H	2.57272800	0.90020600	3.70281100
H	1.15093300	0.02130600	3.11484400
C	-4.25736500	-1.79656200	1.62045900
C	2.72756200	-3.02287600	-0.75608200
C	-2.08256300	-2.78582000	1.47102200
C	-6.26073300	-2.81785300	0.48121200
H	-6.89262500	-2.61762900	1.35384600
H	-6.46165900	-2.03030900	-0.25515100
H	-6.57296800	-3.77218200	0.04592200
C	5.76921100	0.96299900	-0.13267200
H	6.36098700	0.47426200	-0.91223600
H	5.33030600	1.86604100	-0.57341200
H	6.44570100	1.28001300	0.66871000
C	-0.68110700	2.73345600	2.72435800
H	-0.47651200	3.64546500	3.29754900
H	-1.60585900	2.29445700	3.11278400
H	0.13058900	2.02432500	2.89781100
C	-2.12217200	3.84434500	0.99918900
H	-2.21202100	4.12010100	-0.05532500
H	-2.97681000	3.21188300	1.25968000
H	-2.16401000	4.75527400	1.60708800
C	0.44777900	5.25391100	0.69600000
H	0.46715600	5.57453200	1.74453200
H	1.34626200	5.64252100	0.20469400
H	-0.42145300	5.69938300	0.20721400
C	1.73545800	3.13914900	1.11395600
H	2.56678800	3.51201700	0.50658700
H	1.92440600	3.42161100	2.15602900
H	1.72937400	2.04848000	1.04213200
N	0.23223400	0.80928300	-1.49381300
C	1.41683900	0.67372900	-2.27022400
C	2.43232200	1.64025100	-2.23986100
C	1.59720600	-0.47056700	-3.06427100
C	3.60408500	1.45133200	-2.97422400
H	2.27265700	2.53762200	-1.65643100
C	2.77157000	-0.65785800	-3.78964500
H	0.80452200	-1.21301300	-3.09464000
C	3.78729400	0.30160300	-3.74405000
H	4.37910600	2.21340800	-2.94737600
H	2.89430700	-1.55426600	-4.39266800
H	4.70310600	0.15915400	-4.31132800
C	2.48860200	-3.80098000	3.35113400

H	3.21026600	-4.23503500	2.64889900
H	3.01346200	-3.01790100	3.91001900
H	2.19144400	-4.58116000	4.05658700
C	-0.76900500	-4.53466000	3.58356500
H	-1.54555200	-4.01520600	4.15686600
H	-1.26550700	-5.32741300	3.01322500
H	-0.08266500	-5.00667700	4.29132000

TS13

Cu	-0.55492500	-0.39368700	-0.15746300
C	-1.04365400	1.41103700	-0.57093600
N	-2.11800000	1.82049300	-1.29335700
C	-2.10954500	3.20489200	-1.50805100
C	-0.98489200	3.67588800	-0.89533900
N	-0.35514400	2.55715200	-0.32999600
B	0.56823300	-1.84352600	2.23285400
O	1.76415000	-1.45073600	1.64089300
C	2.81453500	-1.95753700	2.49897900
C	2.11173100	-1.92833100	3.90396000
O	0.72680600	-2.18846800	3.56331200
C	-0.64867000	-3.08673700	0.92380700
H	-1.25247700	-3.83337100	1.42944200
C	-0.35634700	-3.17174700	-0.44582500
C	0.41551100	-2.14141800	-1.10872800
C	0.59403900	-2.16636300	-2.50835300
C	0.03882000	-3.16329200	-3.29272700
C	-0.64496300	-4.22053200	-2.64273300
C	-0.81682300	-4.24463500	-1.27536900
H	1.16056800	-1.60400400	-0.51640900
H	1.21660000	-1.39760800	-2.96523000
H	0.16388600	-3.16758600	-4.37134200
H	-1.04921000	-5.03649800	-3.23908600
H	-1.35626100	-5.06685000	-0.80963200
H	-0.66452000	3.27345100	3.52492200
C	-5.19245700	-0.91132900	-2.22901100
C	-5.25598800	-0.12621700	-1.07296100
H	-6.09541600	-0.24293100	-0.39230000
C	-4.25425000	0.79256800	-0.75598400
C	-1.88880800	0.28123100	-3.73534700
H	-1.07595700	-0.36350200	-3.38202500
C	-4.29450800	1.58868300	0.52237300
H	-5.24727600	1.44835700	1.03769100
H	4.16464300	2.17864600	0.34937200
C	3.06577100	2.63954100	2.13973700

C	1.79009700	2.85734600	2.67362600
H	1.68251400	3.04373100	3.73963500
H	-4.04353000	-1.35150000	-3.99438500
C	0.64638000	2.83387500	1.87361600
C	2.19103600	2.00356700	-1.53138100
C	-3.07896400	0.16128800	-2.81970300
H	1.70803800	2.75592400	-2.16550500
C	0.81263200	2.59232800	0.50174800
C	2.06567800	2.34153900	-0.06778400
C	3.18277200	2.37486100	0.77260300
H	-3.50289400	1.26039600	1.20383300
H	-4.15090900	2.66047500	0.34427800
H	-1.50611200	1.30583100	-3.77694300
H	-2.14758800	-0.03647400	-4.74979500
H	-1.31264400	2.09214800	2.37415300
H	-1.29547400	3.80198500	1.95404500
H	3.24126400	1.92756300	-1.82590100
H	1.70220100	1.04582900	-1.74756200
C	-4.10487600	-0.74869700	-3.09158100
C	-0.72872500	3.01503200	2.46416700
C	-3.17837400	0.91898700	-1.64673200
C	-6.25936500	-1.93794000	-2.52196500
H	-6.41156700	-2.06214700	-3.59918700
H	-5.97752300	-2.91891700	-2.11796900
H	-7.21752900	-1.66052000	-2.07056200
C	4.28472900	2.70017900	3.02804800
H	4.54484500	3.73845900	3.27119300
H	4.11160800	2.17897100	3.97599300
H	5.15438200	2.24476800	2.54499000
C	2.58307500	-2.99779400	4.88137400
H	2.41097500	-3.99992400	4.48325400
H	3.65143300	-2.88286100	5.09801500
H	2.03197700	-2.90708600	5.82290200
C	2.15716400	-0.54065800	4.55456000
H	3.16212500	-0.29667400	4.91610500
H	1.84537900	0.23200200	3.84481500
H	1.47050700	-0.52606100	5.40673800
C	4.02967200	-1.04975100	2.36683000
H	4.81186400	-1.33950300	3.07782900
H	4.44107200	-1.13190100	1.35544400
H	3.76061100	-0.00694900	2.53633400
C	3.14071600	-3.37709400	2.02388800
H	2.26029300	-4.02200800	2.09667200
H	3.43682500	-3.33570000	0.97146400

H	3.95982400	-3.81875100	2.60088100
N	-0.70025000	-1.73630700	1.52620800
C	-1.91396900	-1.34146200	2.15338500
C	-1.90012900	-0.45249600	3.24077900
C	-3.14604400	-1.79814900	1.66206100
C	-3.09627700	-0.04501200	3.82940600
H	-0.94952600	-0.10916300	3.63470100
C	-4.33481500	-1.38615700	2.25973900
H	-3.15140700	-2.47115200	0.81164500
C	-4.32232900	-0.51241500	3.34979500
H	-3.06662000	0.63417600	4.67773900
H	-5.27973800	-1.74886700	1.86360200
H	-5.25152000	-0.19959600	3.81718600
C	-0.41120100	5.04654100	-0.78396700
H	-1.05534400	5.77109600	-1.28884200
H	-0.30572400	5.35585300	0.26257300
H	0.58532000	5.10227800	-1.23839100
C	-3.17761000	3.88857600	-2.29022800
H	-4.16481100	3.73764400	-1.83819400
H	-2.98617900	4.96365100	-2.33968600
H	-3.23002000	3.50331600	-3.31535800

IM18

Cu	-0.85389600	-0.11679400	-0.14716000
C	-1.63358800	1.61528600	-0.53252500
N	-2.72934600	2.01352200	-1.22782500
C	-2.73267500	3.39938500	-1.45253100
C	-1.60436300	3.88142600	-0.85438200
N	-0.95508600	2.77031100	-0.30416100
B	0.88919200	-2.82078800	2.78546200
O	1.91361100	-3.65876000	2.39622400
C	2.96825100	-3.53361600	3.37455800
C	2.68585600	-2.11791700	3.98960000
O	1.24723400	-2.01578700	3.85991700
C	-0.41065100	-3.44152100	0.81751500
H	-0.92433200	-4.39678900	0.77451300
C	0.04643900	-2.78891800	-0.29209000
C	0.68141000	-1.46420900	-0.22107800
C	1.32613900	-0.93099600	-1.38953300
C	1.17246300	-1.49602500	-2.63305500
C	0.40559600	-2.70309200	-2.73268700
C	-0.12424700	-3.31979500	-1.63430900
H	1.11499700	-1.17515800	0.73744000
H	1.94077300	-0.04247200	-1.26114600

H	1.62636100	-1.05736900	-3.51658000
H	0.26443300	-3.15746400	-3.71202900
H	-0.65420100	-4.26401300	-1.74366900
H	-0.54758000	2.85500800	3.61230400
C	-5.60950600	-0.77433800	-2.55219300
C	-5.88062900	0.07499400	-1.47425900
H	-6.83571500	-0.00287300	-0.96010300
C	-4.94619900	1.01001900	-1.02328000
C	-2.06536200	0.32072600	-3.47341300
H	-1.30377900	-0.25487000	-2.93282300
C	-5.23649600	1.87555100	0.17812100
H	-6.09904400	1.48814900	0.72776100
H	3.61262200	2.59579700	-0.54435100
C	2.86475400	2.57108500	1.47576000
C	1.71386300	2.61030300	2.26590600
H	1.80702700	2.55982800	3.34786100
H	-4.14779200	-1.31946100	-4.03216500
C	0.43573400	2.70177200	1.70352800
C	1.32592100	2.69806500	-2.02503500
C	-3.40363700	0.25455100	-2.78093100
H	0.73305400	3.54064200	-2.39713600
C	0.34300900	2.76004700	0.30899000
C	1.47232500	2.71898200	-0.52436400
C	2.72528100	2.63301200	0.08332800
H	-4.38056900	1.90081700	0.85914200
H	-5.46426000	2.91078000	-0.10241000
H	-1.69735100	1.34920100	-3.54738900
H	-2.13626600	-0.09531800	-4.48282800
H	-1.30592200	1.71137400	2.49683800
H	-1.52523200	3.44248000	2.24992000
H	2.30558100	2.73068100	-2.50983200
H	0.81972800	1.78001000	-2.34577200
C	-4.37205700	-0.66662400	-3.19216200
C	-0.80125000	2.68174000	2.56266500
C	-3.71753200	1.08620600	-1.69579800
C	-6.61780300	-1.80842800	-2.99022000
H	-6.51516000	-2.04120200	-4.05496600
H	-6.48156700	-2.74612300	-2.43612500
H	-7.64347200	-1.46959100	-2.81100600
C	4.23261200	2.43955500	2.09936600
H	4.93665800	3.16474600	1.67554000
H	4.19479500	2.59396300	3.18185800
H	4.64804000	1.44003600	1.92230800
C	3.05888300	-1.96191600	5.45872000

H	2.51497800	-2.67127000	6.08594300
H	4.13396600	-2.11788200	5.60281300
H	2.81303000	-0.95015500	5.79764700
C	3.28690700	-0.97416700	3.16283400
H	4.37481400	-0.92105600	3.27758500
H	3.05253700	-1.08966500	2.10027300
H	2.85208200	-0.02888400	3.50057200
C	4.30985100	-3.66665700	2.66206800
H	5.13961300	-3.48870400	3.35599000
H	4.41258700	-4.67885800	2.25884200
H	4.38840700	-2.96496100	1.82903500
C	2.78546500	-4.66975700	4.38692300
H	1.83203700	-4.57234500	4.91551300
H	2.77959100	-5.62225400	3.84906200
H	3.59456500	-4.69075400	5.12458900
N	-0.35827100	-2.77134800	2.09634800
C	-1.39473100	-1.85435200	2.37501400
C	-1.47972500	-1.14329200	3.58985700
C	-2.41283800	-1.64286000	1.41751100
C	-2.54461800	-0.27808800	3.83124400
H	-0.71737200	-1.28129700	4.34376700
C	-3.47952600	-0.77992200	1.67979200
H	-2.38860500	-2.22795000	0.50465100
C	-3.55562500	-0.08383500	2.88515600
H	-2.58803600	0.24430000	4.78417800
H	-4.24999500	-0.66556700	0.92440600
H	-4.38821700	0.58244200	3.09203800
C	-1.06744200	5.26431500	-0.71348000
H	-1.71757000	5.98015900	-1.22298300
H	-1.00072700	5.55760900	0.34115700
H	-0.06072300	5.35479600	-1.13718700
C	-3.78734800	4.08042200	-2.25592700
H	-4.75965900	4.08972000	-1.75068800
H	-3.50171900	5.11739700	-2.45119400
H	-3.92814200	3.57845400	-3.21981000

TS14

Cu	-0.95267000	-0.89882900	-0.41147000
C	-2.49848800	0.16955200	-0.73762800
N	-3.00450100	0.38653900	-1.98131600
C	-3.87411200	1.48263600	-2.01072400
C	-3.91635800	1.96724900	-0.73532700
N	-3.07511000	1.14023600	0.02335500
B	-1.12165000	-2.93691300	2.98952200

O	-2.08139300	-3.84865700	2.58513200
C	-3.08394000	-3.90670900	3.62350200
C	-2.29746400	-3.38384200	4.88026500
O	-1.32722000	-2.48898400	4.28576700
C	0.04505400	-3.21012200	0.86436300
H	-0.41760500	-4.18672600	0.80567400
C	0.52397900	-2.60683800	-0.28364700
C	1.08276600	-1.24644700	-0.37680700
C	1.64193100	-0.79130600	-1.61027500
C	1.55983700	-1.51415000	-2.77523400
C	0.90772500	-2.78751000	-2.72713600
C	0.41748300	-3.30564200	-1.56363400
H	1.40720100	-0.74720400	0.52885300
H	2.14325600	0.17570800	-1.60358900
H	1.96615800	-1.13703800	-3.70802400
H	0.80041500	-3.36303800	-3.64450900
H	-0.05127500	-4.28753300	-1.55966800
H	-5.69006400	-0.34031900	2.56430200
C	-1.75635800	-2.01701500	-5.21417600
C	-2.85991400	-2.38344100	-4.43740400
H	-3.38179300	-3.31215100	-4.65512600
C	-3.29928500	-1.59522200	-3.37198600
C	-0.72251200	1.23821500	-3.49926400
H	-0.15399800	1.06664200	-2.57821800
C	-4.45344700	-2.02138300	-2.50019700
H	-4.93209200	-2.91974400	-2.89974200
H	-0.48662100	2.15284800	3.66658300
C	-2.34808100	1.20553300	4.17881300
C	-3.55383200	0.71108500	3.67008700
H	-4.29113400	0.29772700	4.35358000
H	-0.22741000	-0.53217100	-5.50560900
C	-3.82324900	0.70077600	2.30002500
C	-0.61670700	2.33610500	0.96537700
C	-1.49464100	-0.00317800	-3.86092600
H	-1.07214300	2.92162900	0.15952700
C	-2.85283500	1.23081100	1.43696600
C	-1.65281500	1.78007700	1.90792700
C	-1.42468800	1.75650900	3.28674400
H	-4.10661400	-2.24121600	-1.48338800
H	-5.21428100	-1.23640000	-2.41534200
H	-1.37899800	2.09824400	-3.32717100
H	-0.01249100	1.49698800	-4.28931600
H	-4.85997800	-0.71156300	1.04366500
H	-5.71174400	0.81814600	1.22787100

H	0.09202000	2.97221000	1.50281500
H	-0.05183100	1.52421500	0.48985500
C	-1.09391400	-0.82278500	-4.91752400
C	-5.09030100	0.08749900	1.75716100
C	-2.60426400	-0.40821400	-3.10784000
C	-1.25766800	-2.91441500	-6.31967400
H	-0.85390000	-2.33471100	-7.15650300
H	-0.45137700	-3.56469100	-5.95554500
H	-2.05310500	-3.56134600	-6.70310400
C	-2.01762900	1.07792500	5.64408700
H	-1.36824100	1.89109900	5.98418500
H	-2.91990500	1.07408900	6.26427600
H	-1.48935900	0.13245000	5.82212200
C	-3.13633000	-2.60055700	5.88330600
H	-3.58590500	-1.71945500	5.42218900
H	-3.93383000	-3.22816000	6.29685300
H	-2.50401700	-2.26506700	6.71161700
C	-1.50725500	-4.48589200	5.59425400
H	-2.16535400	-5.17070500	6.13919300
H	-0.91279600	-5.06541800	4.88126200
H	-0.82034800	-4.02027200	6.30703500
C	-3.59199100	-5.33976200	3.73373200
H	-4.30166000	-5.43770700	4.56317200
H	-4.10724500	-5.61911300	2.80925900
H	-2.77166200	-6.04358000	3.88883800
C	-4.21339500	-2.96662100	3.19872900
H	-3.84111600	-1.94350600	3.11938600
H	-4.57930700	-3.27505400	2.21472900
H	-5.05173900	-2.98592900	3.90358900
N	-0.02008800	-2.59059000	2.15791700
C	1.10549000	-1.90580600	2.68928400
C	0.92867900	-0.81234900	3.55146900
C	2.40861300	-2.28731400	2.33737800
C	2.03132400	-0.13202900	4.06143600
H	-0.07511700	-0.49701300	3.80146000
C	3.50572500	-1.59624800	2.84706500
H	2.53966500	-3.11679100	1.65079000
C	3.32927700	-0.51503800	3.71339600
H	1.87254000	0.71213600	4.72891300
H	4.50755500	-1.90571000	2.56027200
H	4.18746300	0.02492200	4.10336600
C	-4.60479400	3.15352100	-0.15199800
H	-5.15707200	3.68955100	-0.92817500
H	-5.31252300	2.87728600	0.63763000

H	-3.88245300	3.84834800	0.29255700
C	-4.54385000	1.92357500	-3.26653000
H	-5.16938600	1.12657600	-3.68576300
H	-5.18099400	2.79117800	-3.07648600
H	-3.81277300	2.19730900	-4.03626100

IM19

Cu	-0.14995500	0.09906300	-0.43983800
C	-1.89534700	0.91677700	-0.28450000
N	-3.11645000	0.45409600	-0.67174600
C	-4.09664200	1.45703800	-0.63790900
C	-3.46593600	2.58346500	-0.19789000
N	-2.13004900	2.22210600	0.01496200
B	1.69888200	-1.91803200	0.80551000
O	2.13441400	-2.93753300	1.63891300
C	1.37759800	-2.84413100	2.86759600
C	0.05914600	-2.15059500	2.38608300
O	0.55815000	-1.29679300	1.32687600
C	1.68818700	-0.33438000	-1.10108800
H	1.64536700	-0.56308700	-2.17169000
C	2.43947300	0.93637700	-0.89312100
C	3.08883800	1.24423400	0.31851900
C	3.78412100	2.43973200	0.48643700
C	3.85492900	3.37764300	-0.54656500
C	3.20893800	3.09475600	-1.75381000
C	2.51655900	1.89931200	-1.92151000
H	3.06233800	0.51845500	1.12631900
H	4.28616400	2.63583600	1.43164900
H	4.40942300	4.30327000	-0.41870400
H	3.26035600	3.80417000	-2.57739700
H	2.03684100	1.68321900	-2.87456900
H	-0.32614200	2.52534200	-2.22172800
C	-3.75712800	-3.57952000	-1.74166500
C	-3.20004100	-2.67776900	-2.65515400
H	-2.92051600	-3.02740700	-3.64615800
C	-2.98268300	-1.33762300	-2.32874400
C	-4.25897000	-1.30180400	1.28783100
H	-4.42707600	-2.14959600	1.95764100
C	-2.34777200	-0.38739500	-3.31123800
H	-2.29438000	-0.83644400	-4.30694100
H	0.32875700	4.21301100	3.32856000
C	0.94105300	4.78714600	1.34749300
C	0.68902300	4.62604000	-0.01819700
H	1.31500200	5.14199900	-0.73890200

H	-4.53573600	-3.80297000	0.25096300
C	-0.31999600	3.78292600	-0.48316800
C	-1.71977000	2.47603200	2.83425500
C	-3.90913300	-1.78033700	-0.09935300
H	-1.42979200	2.71755500	3.86071700
C	-1.09690000	3.10950400	0.46845300
C	-0.88537000	3.24875400	1.84491800
C	0.14174400	4.09794400	2.26353200
H	-1.32952500	-0.13267200	-2.99096500
H	-2.90452800	0.55373700	-3.38315500
H	-3.45600300	-0.68627000	1.70533100
H	-5.16776000	-0.68757400	1.29431100
H	-1.58945800	3.75923700	-2.24150800
H	0.10161000	4.21266800	-2.54873400
H	-1.59161300	1.39853700	2.68725000
H	-2.79024300	2.68799600	2.72486200
C	-4.10914300	-3.11263300	-0.47270300
C	-0.54840200	3.56487700	-1.95573600
C	-3.34736200	-0.91057900	-1.04325500
C	-3.94270600	-5.03052400	-2.11336900
H	-4.32161700	-5.13593000	-3.13582900
H	-4.64269700	-5.53104700	-1.43717600
H	-2.98970700	-5.57255000	-2.06391800
C	2.08498100	5.65141100	1.81331200
H	2.16444400	6.56740500	1.21765700
H	3.03232000	5.11000400	1.70439700
H	1.97561500	5.93438500	2.86509400
C	-0.63544100	-1.28690100	3.42919900
H	0.00530600	-0.46607300	3.75806400
H	-0.92008700	-1.88536500	4.30203000
H	-1.54685000	-0.85725800	3.00259500
C	-0.93111600	-3.12667000	1.74362400
H	-0.42448500	-3.78194000	1.02860700
H	-1.68558200	-2.55772900	1.19614600
H	-1.43437800	-3.74797500	2.49227000
C	1.19539100	-4.24619800	3.43602000
H	0.55988000	-4.22322100	4.32857900
H	2.16874800	-4.65734900	3.72123100
H	0.74591000	-4.91834700	2.70192300
C	2.18570800	-1.97194300	3.83441100
H	1.71314800	-1.91456400	4.82060300
H	2.29972100	-0.95653100	3.44201600
H	3.18315300	-2.40539400	3.95120300
N	2.27623100	-1.50707100	-0.41252800

C	3.40324300	-2.13830000	-1.00050300
C	4.22038400	-1.44930200	-1.91431200
C	3.70868600	-3.48543300	-0.72609400
C	5.30878600	-2.08191300	-2.51374900
H	4.01811400	-0.41194500	-2.14313000
C	4.80170700	-4.10439000	-1.32665200
H	3.08693400	-4.04427100	-0.03940700
C	5.61357000	-3.41179800	-2.22668300
H	5.92555200	-1.51911900	-3.21018000
H	5.01117300	-5.14595000	-1.09453500
H	6.46287600	-3.90028100	-2.69609500
C	-3.95453900	3.97188200	0.03438500
H	-3.82112500	4.27591700	1.07924500
H	-5.01741100	4.04909700	-0.20903000
H	-3.40836700	4.69509800	-0.58241300
C	-5.50086400	1.21687200	-1.07606400
H	-5.53646700	0.84532000	-2.10694000
H	-6.07489500	2.14598200	-1.03036000
H	-6.00857000	0.47493900	-0.44916000

TS1a

C	6.74933300	2.42612000	2.74385000
C	5.86429400	1.51817700	3.32544500
C	5.76858200	0.21521100	2.83021600
C	6.55695500	-0.17820200	1.74304300
C	7.44113100	0.73942500	1.15384200
C	7.54047200	2.03253700	1.66036700
H	5.24567900	1.82116600	4.16559400
H	5.07695000	-0.48872800	3.28173500
H	8.03538600	0.44621400	0.29241900
H	8.22711200	2.73726400	1.20007900
C	10.35196300	-3.99199600	2.18184400
C	9.77012200	-3.09514300	3.08244900
C	8.58997500	-2.43489200	2.74516800
C	7.98089400	-2.67900400	1.50528300
C	8.57617800	-3.56636400	0.59883300
C	9.75740000	-4.22426300	0.94101500
H	10.24097300	-2.90490900	4.04276900
H	8.14836900	-1.72016700	3.43364100
H	8.12319400	-3.71682700	-0.37701300
H	10.22025100	-4.90355100	0.23138900
C	2.84428400	-3.80693000	3.10644400
C	4.12166100	-3.97973300	3.64356500
C	5.22900900	-3.40830800	3.01582500

C	5.06006800	-2.66204000	1.84231300
C	3.77636800	-2.49966900	1.29589100
C	2.67405100	-3.06713300	1.93413400
H	4.25726300	-4.56205900	4.55055600
H	6.22182200	-3.54754400	3.43168500
H	3.64459600	-1.93404200	0.37736200
H	1.68294300	-2.93771900	1.50863500
P	6.44679800	-1.84089700	0.98692000
Cu	6.18946300	-1.66676300	-1.17841800
B	4.82927400	-0.24258700	-1.92993400
O	4.97122200	1.10241900	-2.16718200
C	3.82649500	1.78298800	-1.57119700
C	2.74446500	0.64322500	-1.51636100
O	3.56848800	-0.56289300	-1.47247200
C	1.88650500	0.54363100	-2.77838900
H	1.31788200	-0.39018400	-2.74736600
H	1.18390900	1.38057700	-2.85128500
H	2.50437700	0.52049500	-3.67869700
C	1.86249300	0.65629000	-0.27277700
H	1.28184400	1.58393200	-0.21670500
H	1.15903900	-0.18163000	-0.31436500
H	2.45423900	0.55827600	0.64001400
C	3.46313300	2.96983800	-2.45516700
H	2.56707500	3.47435600	-2.07643900
H	4.28587500	3.69139900	-2.45547800
H	3.28098300	2.66126100	-3.48655600
C	4.27468400	2.26657000	-0.18924800
H	5.16504500	2.89048400	-0.30388600
H	3.49538600	2.86094200	0.29896100
H	4.53963300	1.43228700	0.46408300
C	5.97058100	-1.34211700	-3.26813300
H	6.16116100	-0.39192500	-3.78061300
C	4.84173600	-2.10258200	-3.88957000
C	4.55260500	-3.41851000	-3.50406400
C	3.47079000	-4.09412100	-4.06221100
C	2.66457600	-3.46996400	-5.01967900
C	2.95653700	-2.16637300	-5.42079900
C	4.03928800	-1.48938200	-4.85756000
H	5.19337700	-3.90199700	-2.77345300
H	3.25608600	-5.11413500	-3.75435500
H	1.82166200	-4.00036300	-5.45402500
H	2.34550100	-1.67651900	-6.17427800
H	4.26896500	-0.47304000	-5.17003700
N	7.10809400	-2.11862000	-2.97132300

C	8.26559200	-1.41414500	-2.63731500
C	8.34163200	-0.01301000	-2.41024900
C	9.45318100	-2.16634900	-2.44205700
C	9.53886400	0.57714900	-1.98875100
H	7.46936000	0.61616900	-2.54822600
C	10.62834500	-1.56721900	-2.02007800
H	9.40394000	-3.23576400	-2.62716500
C	10.68549300	-0.18457300	-1.78075100
H	9.56346200	1.65239100	-1.82165000
H	11.51595500	-2.17815800	-1.87326700
H	11.60934000	0.28130400	-1.45080700
H	6.82005400	3.43922800	3.12946800
H	1.98450000	-4.25407300	3.59742000
H	11.27658100	-4.49843800	2.44408800

TS1a'

Cu	-0.19472100	-0.37263100	-0.29905900
B	-0.68955600	-2.12922000	0.69509200
O	-1.86291100	-2.60723200	1.25324400
C	-1.58386600	-3.94407500	1.75341800
C	-0.05880000	-3.84830700	2.09738800
O	0.41499200	-2.87714500	1.12331400
C	-0.17806600	-1.49908800	-2.25999800
H	-0.71540300	-0.91355700	-3.00331500
C	1.21663300	-1.78608900	-2.49096800
C	1.84002900	-1.26828500	-3.65279600
C	3.19542300	-1.45997000	-3.88528900
C	3.98170600	-2.16074100	-2.96111500
C	3.37682500	-2.68475900	-1.81636200
C	2.01359700	-2.51928000	-1.58096100
H	1.24015100	-0.70635800	-4.36539200
H	3.64536100	-1.06202300	-4.79187500
H	5.04368600	-2.30265800	-3.13879500
H	3.97315300	-3.23974700	-1.09624600
H	1.55900700	-2.94127400	-0.69316000
C	0.73075000	-5.13887400	1.91112200
H	0.35867900	-5.92428900	2.57957000
H	1.78533200	-4.96322100	2.14760400
H	0.67098700	-5.49835300	0.88173300
C	0.20737000	-3.25817300	3.48581600
H	1.27702300	-3.04299800	3.57793400
H	-0.07252300	-3.95519300	4.28274400
H	-0.34321300	-2.32355000	3.62470200
C	-2.50133400	-4.21377800	2.93880900

H	-2.41293100	-3.43289100	3.69740400
H	-2.27022500	-5.18147100	3.39943000
H	-3.54126800	-4.23833100	2.59816000
C	-1.87530500	-4.92597200	0.61374900
H	-2.90907300	-4.78937200	0.28465100
H	-1.74094300	-5.96566300	0.93089200
H	-1.22260300	-4.73167600	-0.24211200
N	-0.91573300	-2.03099300	-1.22512100
C	-2.32907900	-1.96934600	-1.47489300
C	-2.89497200	-3.00374300	-2.22882900
C	-3.14191600	-0.93666700	-1.00083700
C	-4.26365600	-3.01244000	-2.48624600
H	-2.25114300	-3.79747400	-2.59407900
C	-4.51518600	-0.95430000	-1.25239200
H	-2.69686900	-0.13687200	-0.41391700
C	-5.08113400	-1.99012600	-1.99395000
H	-4.69418600	-3.82229500	-3.06876400
H	-5.13929300	-0.15155700	-0.86946600
H	-6.14889800	-2.00066200	-2.19291100
C	1.51824800	1.37132600	4.94457800
C	1.20720000	2.59082600	4.33998400
C	0.96122400	2.64751500	2.96775400
C	1.02469300	1.48060500	2.19388400
C	1.32163600	0.25489100	2.80652200
C	1.57469400	0.20588000	4.17708700
H	1.15036000	3.49692700	4.93670400
H	0.70362700	3.59381800	2.50121100
H	1.32808800	-0.65675700	2.21566900
H	1.80050600	-0.74680500	4.64689800
C	4.82811400	2.58344800	-1.49604400
C	4.43756500	3.21625900	-0.31171700
C	3.21449200	2.90353900	0.27813300
C	2.36662300	1.96199700	-0.32559600
C	2.76411700	1.32806000	-1.50923500
C	3.99349000	1.63787000	-2.09159200
H	5.09145300	3.94638300	0.15697200
H	2.92486400	3.37925700	1.20980500
H	2.12301800	0.58273100	-1.96588700
H	4.29492300	1.12272700	-2.99785500
C	-2.20682900	4.98695900	-0.30663800
C	-0.91118500	5.08728000	-0.81374700
C	0.00925100	4.05822900	-0.60270200
C	-0.36710000	2.91994900	0.11895100
C	-1.67417400	2.82092500	0.62553600

C	-2.58654200	3.85161800	0.41530100
H	-0.61242400	5.96816400	-1.37494000
H	1.01694500	4.13981900	-0.99677700
H	-1.96789900	1.93833100	1.18884900
H	-3.59434600	3.76910200	0.81214000
P	0.74981900	1.49851300	0.38421700
H	1.70594500	1.32800500	6.01377700
H	-2.92020900	5.78890300	-0.47326900
H	5.78780700	2.82278000	-1.94570500

TS10'

Cu	-0.19901000	0.11329400	-0.24306400
C	0.47692300	1.77680900	0.33182600
N	-0.25686300	2.88195700	0.63030000
C	0.53736900	3.89814800	1.18088600
C	1.80787000	3.40264700	1.22399200
N	1.74081100	2.10473600	0.69713000
B	-0.67588700	-1.64388100	0.74561200
O	-1.85614300	-2.16396900	1.25581000
C	-1.56851500	-3.52609000	1.67716500
C	-0.05552900	-3.42613500	2.06880100
O	0.42776900	-2.39224100	1.16874200
C	-0.03554000	-0.96778600	-2.18243000
H	-0.51165700	-0.33121500	-2.92633000
C	1.33100600	-1.37969500	-2.40207200
C	2.06349900	-0.81589000	-3.47335300
C	3.36093500	-1.22517600	-3.75073600
C	3.97970300	-2.20327200	-2.96207900
C	3.27620300	-2.75024200	-1.88580200
C	1.97343500	-2.35236500	-1.60232500
H	1.58808400	-0.05989500	-4.09495200
H	3.89369000	-0.78688700	-4.59152800
H	4.99066700	-2.53220800	-3.18724800
H	3.74709000	-3.50306300	-1.25809700
H	1.43999100	-2.77853300	-0.76260500
H	3.15847100	3.13891300	-1.45846800
C	-4.41795700	2.92613200	-0.05804000
C	-3.52698600	3.39307500	-1.03217000
H	-3.91428400	3.74396400	-1.98575600
C	-2.14878900	3.40076400	-0.81842000
C	-1.97527900	1.83610100	2.67565900
H	-1.19016400	2.45896200	3.11748600
C	-1.18549600	3.84642200	-1.88915700
H	-0.53224800	4.65528900	-1.54116600

H	4.36377600	-1.30352700	2.26811600
C	4.93303600	-0.61901900	0.31064400
C	4.62916400	0.27378700	-0.72326400
H	5.19729700	0.23342400	-1.64747400
H	-4.58050400	2.06414700	1.90571700
C	3.57746000	1.18162500	-0.61760400
C	2.20778400	0.26991700	2.84147300
C	-2.52646300	2.43637600	1.40843600
H	2.03631500	1.27170400	3.25141700
C	2.83897200	1.18950200	0.57387800
C	3.09262200	0.29969600	1.62300800
C	4.15388600	-0.59708400	1.46879200
H	-1.72234200	4.19751400	-2.77459400
H	-0.53316300	3.01672800	-2.18637000
H	-2.76701000	1.69496900	3.41668900
H	-1.52858000	0.85777200	2.45559400
H	3.90540800	1.98577900	-2.58654400
H	2.20168400	1.81774300	-2.13571100
H	2.64636000	-0.35345800	3.62581700
H	1.23061600	-0.15059400	2.57843100
C	-3.90169100	2.45115300	1.14997300
C	3.19632900	2.08549500	-1.76112700
C	-1.67273100	2.93108100	0.41480100
C	-5.90416200	2.93132700	-0.32108900
H	-6.45027200	2.39906900	0.46361000
H	-6.13643000	2.45326200	-1.27960100
H	-6.29664400	3.95505000	-0.36602200
C	6.07546000	-1.59183700	0.15947800
H	6.07178100	-2.34022700	0.95798700
H	7.04458700	-1.07732400	0.18804600
H	6.01207300	-2.11528800	-0.80034600
C	0.76225400	-4.69032300	1.82912900
H	0.39017600	-5.51979800	2.44223500
H	1.80744100	-4.50852000	2.10040900
H	0.73323300	-4.99134800	0.77972500
C	0.16103300	-2.91782000	3.49777300
H	1.21936600	-2.67373400	3.63018000
H	-0.11704800	-3.67056800	4.24332700
H	-0.42362600	-2.01114300	3.67979000
C	-2.51311000	-3.88659200	2.81630500
H	-2.45814500	-3.15587900	3.62644100
H	-2.27800700	-4.87841600	3.22017200
H	-3.54288100	-3.90527700	2.44554700
C	-1.81276000	-4.43563500	0.46796100

H	-2.84027900	-4.29410400	0.12121300
H	-1.66809400	-5.49171300	0.72013100
H	-1.14433400	-4.17329800	-0.35682800
N	-0.84163700	-1.50592200	-1.19922500
C	-2.23779300	-1.44955100	-1.51699100
C	-2.72349600	-2.38429700	-2.44185000
C	-3.12171100	-0.53136300	-0.94144300
C	-4.07713100	-2.41220500	-2.76676200
H	-2.02767200	-3.09073800	-2.88387200
C	-4.47964700	-0.57128100	-1.26264400
H	-2.75020400	0.19468900	-0.22645400
C	-4.96482100	-1.50852600	-2.17337200
H	-4.44140900	-3.14629200	-3.48055000
H	-5.15390900	0.13922800	-0.79415400
H	-6.02148500	-1.53433300	-2.42486900
C	3.09129700	3.99033000	1.70025200
H	2.92986100	5.00169500	2.08226700
H	3.83142400	4.04343500	0.89301600
H	3.53293400	3.38735000	2.50217700
C	-0.03668300	5.20827700	1.59750600
H	-0.81293000	5.08128300	2.36152700
H	-0.49871900	5.73357900	0.75287200
H	0.74426500	5.85205400	2.01043300

TS2'

Cu	-0.21171500	-0.46019800	0.47331900
B	-1.66582500	1.23678500	-1.52616700
O	-0.80109200	0.19318900	-1.74679700
C	-1.12705700	-0.38857700	-3.05277700
C	-1.84391300	0.82096300	-3.75673200
O	-2.39965400	1.56780000	-2.62738300
C	-1.73293100	1.99181000	-0.13978100
H	-2.75858100	2.37047100	-0.01368700
C	-0.79490600	3.20556000	-0.21598500
C	0.27339200	3.36546700	0.67271900
C	1.10551800	4.48101400	0.58616600
C	0.89068600	5.44586400	-0.39681100
C	-0.16488300	5.28702400	-1.29703000
C	-1.00096200	4.17443600	-1.20825100
H	0.45582100	2.61316800	1.43023600
H	1.93570600	4.58289300	1.27833800
H	1.54392300	6.31102900	-0.46679300
H	-0.34192700	6.03230800	-2.06809100
H	-1.82194200	4.05330200	-1.90970400

C	-0.87617700	1.77315500	-4.46430800
H	-1.42158800	2.67038100	-4.77114600
H	-0.06555400	2.08516400	-3.79872700
H	-0.43876100	1.31062200	-5.35426400
C	-2.98662100	0.42984400	-4.68352500
H	-3.76180600	-0.12266900	-4.14966300
H	-3.44007300	1.32951900	-5.11054300
H	-2.61607800	-0.19033200	-5.50699200
C	-2.04455900	-1.57962800	-2.78363500
H	-2.27172600	-2.11727900	-3.70966600
H	-1.54906400	-2.26101400	-2.08758600
H	-2.98299200	-1.26443800	-2.32225100
C	0.16653600	-0.85308600	-3.70931300
H	0.60223200	-1.67023500	-3.12862300
H	-0.03506900	-1.22211900	-4.72100500
H	0.90685400	-0.05338300	-3.77167200
N	-1.39695900	1.06567800	0.93633700
C	-1.77808100	1.37782000	2.20647500
C	-2.42619400	2.58947700	2.58070400
C	-1.50558200	0.43003700	3.23663500
C	-2.76530000	2.82865900	3.90548800
H	-2.62701200	3.34931000	1.83566000
C	-1.85183400	0.68567200	4.55312600
H	-1.05396900	-0.51622200	2.95452300
C	-2.48337700	1.88755600	4.90267200
H	-3.24974600	3.76512100	4.16857300
H	-1.64075700	-0.06041600	5.31427100
H	-2.75412700	2.08597300	5.93527000
I	-1.13494500	-2.87311100	1.02520000
C	-5.16085600	-0.02632000	-1.00585300
H	-6.19814600	0.21332000	-0.74107200
H	-5.19251200	-0.85960200	-1.72013100
H	-4.73356200	0.83805200	-1.52485600
C	-4.34515900	-0.40029300	0.23358900
H	-3.29307200	-0.56293400	-0.02555900
H	-4.35398900	0.43315400	0.94899300
C	-4.86474000	-1.66476100	0.92876400
H	-4.83345600	-2.51044300	0.22488600
H	-5.94077000	-1.52313800	1.15516000
C	-4.12871000	-2.02040300	2.17003600
H	-4.24032600	-3.00055600	2.61993000
H	-3.58995600	-1.26692400	2.73262800
C	3.58051600	-3.44735800	-2.94664900
C	4.12519300	-2.16242600	-2.93621100

C	3.69459100	-1.22461000	-1.99627200
C	2.70786500	-1.56599000	-1.06061800
C	2.16462000	-2.86025900	-1.07370500
C	2.60404500	-3.79501800	-2.01014600
H	4.88632600	-1.88651300	-3.66092300
H	4.11914600	-0.22653700	-1.99822200
H	1.38516200	-3.12579300	-0.36566400
H	2.17244400	-4.79188400	-2.01293400
C	4.30451900	-1.13077200	4.12931300
C	3.03398700	-0.55158300	4.12549800
C	2.36515400	-0.34600800	2.91953800
C	2.96979700	-0.70734600	1.70691800
C	4.24344300	-1.29134100	1.71629000
C	4.90664600	-1.50247000	2.92509100
H	2.55788500	-0.27113800	5.06067400
H	1.36716100	0.08420500	2.91788100
H	4.70904800	-1.58304500	0.77974300
H	5.89207300	-1.95985000	2.92746800
C	3.74727900	3.61276700	-1.49828000
C	4.34650500	3.03902700	-0.37743600
C	3.84967700	1.84615000	0.15447100
C	2.74142000	1.22465700	-0.43084100
C	2.13020000	1.82067500	-1.54558200
C	2.63594400	2.99988500	-2.08228400
H	5.20701600	3.51543500	0.08435900
H	4.32944200	1.39662000	1.01740000
H	1.25052200	1.35714100	-1.97463600
H	2.14599600	3.45772900	-2.93629100
P	2.05202500	-0.36708600	0.16442200
H	3.91370900	-4.17402800	-3.68246300
H	4.13457500	4.54121900	-1.90805700
H	4.82183400	-1.29984800	5.06949100

TS8'

C	1.55865900	5.53920800	-1.82489300
C	1.56570900	4.27376900	-2.41308900
C	0.95409600	3.19557900	-1.77013600
C	0.31085200	3.38198300	-0.53970500
C	0.30377300	4.65652700	0.04560600
C	0.92965900	5.72717200	-0.59121800
H	2.05455900	4.11859100	-3.37092200
H	0.95573100	2.21220700	-2.22843000
H	-0.19337700	4.80920600	0.99797900
H	0.92245500	6.70954100	-0.12715900

C	-0.43722400	2.91006800	4.76041600
C	-1.64294600	3.09762200	4.08427200
C	-1.72404800	2.86759400	2.70816500
C	-0.59936300	2.43391200	1.99438100
C	0.61859800	2.26948600	2.67918500
C	0.69653900	2.50688000	4.04976800
H	-2.52548700	3.43023500	4.62414600
H	-2.66633600	3.02215700	2.19512900
H	1.50868200	1.97052700	2.13487100
H	1.64311600	2.36750900	4.56460200
C	-4.94607600	2.61973000	-1.33300200
C	-4.70314200	1.79901600	-0.23142100
C	-3.40419600	1.62760600	0.23919100
C	-2.32554700	2.29692300	-0.36258400
C	-2.58029200	3.11789700	-1.47027900
C	-3.88060400	3.27187500	-1.95322900
H	-5.51660300	1.25772900	0.24064700
H	-3.23671500	0.95855100	1.07389500
H	-1.76392300	3.63445800	-1.96198100
H	-4.05749400	3.90771700	-2.81636100
P	-0.60636300	1.97518400	0.21005200
C	-0.37729700	-6.00658400	-0.90259400
C	-0.06581200	-5.49480100	0.35823900
C	-0.53907200	-4.24256800	0.74521500
C	-1.33591800	-3.48827000	-0.12936600
C	-1.63707100	-3.99980800	-1.39907000
C	-1.16153100	-5.25466700	-1.77994900
H	0.55680700	-6.06019100	1.04513700
H	-0.28183000	-3.85535200	1.72297000
H	-2.24122600	-3.42039700	-2.08878700
H	-1.40385100	-5.64258700	-2.76544300
C	-5.81634800	-1.14009900	-1.96076100
C	-5.82966200	-1.70507200	-0.68385100
C	-4.63602100	-1.90225300	0.01057400
C	-3.41111100	-1.52911900	-0.56234000
C	-3.40962200	-0.94846400	-1.83720400
C	-4.60217200	-0.76535000	-2.53537700
H	-6.77107700	-1.99679500	-0.22577800
H	-4.66418200	-2.33768100	1.00300900
H	-2.47451000	-0.62479100	-2.27858200
H	-4.57805200	-0.30896900	-3.52057400
C	-3.19148100	-1.90134400	4.74673100
C	-3.26958000	-3.06371700	3.97623300
C	-2.85030500	-3.05644800	2.64535200

C	-2.33817000	-1.88546300	2.06959900
C	-2.25545100	-0.72861400	2.85599000
C	-2.68356700	-0.72974200	4.18216900
H	-3.65715300	-3.98038300	4.41205800
H	-2.90748200	-3.96628700	2.05716300
H	-1.81672500	0.17264100	2.44564400
H	-2.59773900	0.17947500	4.77014800
P	-1.80202700	-1.77262100	0.31527900
Cu	0.02527700	-0.33029700	-0.17654300
B	3.73411300	0.40065400	0.06600900
O	3.31051300	1.51582200	0.76827900
C	4.41754800	2.45388800	0.78967200
C	5.22927300	2.03498500	-0.48959500
O	4.91601400	0.62056300	-0.60686800
C	6.74124800	2.18124700	-0.36769300
H	7.13777600	1.58372900	0.45578900
H	7.21810300	1.84366500	-1.29304300
H	7.01552200	3.22968000	-0.20590900
C	4.72755400	2.70604300	-1.76873800
H	3.64547500	2.60168200	-1.86458100
H	4.97296100	3.77260800	-1.78779300
H	5.19754400	2.22304200	-2.63028600
C	5.17827600	2.20192600	2.09535100
H	4.48862300	2.32617700	2.93594200
H	5.57535800	1.18259800	2.13111600
H	6.00760800	2.90491400	2.22181800
C	3.85634100	3.86884200	0.76171400
H	3.20737900	4.02853600	-0.09819900
H	3.26593600	4.04892100	1.66554800
H	4.66893900	4.60369300	0.73376500
C	1.84538500	-0.83896500	0.94896300
H	1.73711300	0.13499400	1.40891500
C	1.69596900	-1.89629300	1.95377800
C	0.79821200	-1.64651900	3.01645300
C	0.55867700	-2.58325600	4.01174800
C	1.23305000	-3.81034100	3.99909400
C	2.16405400	-4.05682900	2.98786200
C	2.39564500	-3.12265500	1.97872600
H	0.28444100	-0.69239200	3.04279700
H	-0.16128300	-2.35800500	4.79314500
H	1.04506600	-4.55163400	4.77053400
H	2.71775000	-4.99259700	2.97691400
H	3.12191200	-3.35080000	1.21130300
N	2.99324500	-0.82343300	0.08349600

C	3.26882600	-1.92359700	-0.77108600
C	2.24207900	-2.80852300	-1.13770200
C	4.56521900	-2.15463100	-1.26380600
C	2.49787500	-3.87531400	-1.99246000
H	1.24354600	-2.65606400	-0.75695500
C	4.80953100	-3.22479900	-2.12291300
H	5.37449500	-1.49727300	-0.97842600
C	3.78125300	-4.09044500	-2.49838100
H	1.67842500	-4.53267800	-2.26348700
H	5.81888700	-3.38193700	-2.49429800
H	3.97795100	-4.92286100	-3.16813500
H	-0.00442500	-6.98170300	-1.20353200
H	-3.51756900	-1.91230900	5.78302700
H	-5.95691300	2.73927400	-1.71222300
H	-0.37830000	3.08347900	5.83116200
H	2.04056800	6.37563900	-2.32345400
H	-6.74767700	-0.98660900	-2.49914400
I	0.19758400	-0.41708800	-2.88416200
C	2.50586100	1.54728800	-7.00432500
H	3.54986400	1.82031000	-7.20456500
H	1.98298700	2.45576000	-6.67932400
H	2.05681100	1.22654600	-7.95092500
C	2.41208200	0.45232600	-5.94003900
H	1.36386000	0.18297600	-5.76844400
H	2.91360000	-0.45837700	-6.29491200
C	3.03362500	0.87438500	-4.60434000
H	2.54715200	1.79336200	-4.24384500
H	4.08940600	1.16274400	-4.78098300
C	2.99392200	-0.16680200	-3.54067000
H	3.29878100	0.09479200	-2.53850400
H	3.07196400	-1.21715000	-3.79827700

TS2-OA

Cu	-0.54000700	-1.78420200	-1.45048300
B	-4.06808800	0.46935300	-1.93317300
O	-4.66347200	0.12903000	-0.74312500
C	-6.02443200	0.63622100	-0.79095700
C	-5.90544600	1.80173300	-1.83628300
O	-4.81123200	1.34349100	-2.68228900
C	-2.67577200	-0.13471800	-2.38174500
H	-2.25619200	0.49394500	-3.19091400
C	-2.88712600	-1.52663600	-2.95714600
C	-3.35194700	-2.56626500	-2.13255300
C	-3.49497700	-3.86025200	-2.63343300

C	-3.17519000	-4.13895600	-3.96437800
C	-2.72511700	-3.11098700	-4.79357000
C	-2.58502100	-1.81625400	-4.29229300
H	-3.60820800	-2.34916100	-1.10268400
H	-3.85784900	-4.65036100	-1.98105400
H	-3.27811800	-5.14851600	-4.35248500
H	-2.46788500	-3.31857600	-5.82829100
H	-2.21537700	-1.02313700	-4.93705000
C	-7.13731900	2.01663200	-2.70650800
H	-8.00257500	2.28937600	-2.09170500
H	-6.95126900	2.83200100	-3.41234100
H	-7.38422000	1.12110300	-3.28083200
C	-5.44769100	3.12275100	-1.20972000
H	-4.55660600	2.97730900	-0.59193900
H	-5.19211000	3.82332900	-2.01051800
H	-6.23582900	3.57171100	-0.59662200
C	-6.43504100	1.07374100	0.60953200
H	-7.41303600	1.56769700	0.59005100
H	-6.51345700	0.19852500	1.26237100
H	-5.70344000	1.75921600	1.04239300
C	-6.90144200	-0.52329600	-1.27214900
H	-6.75976700	-1.37342900	-0.59803200
H	-7.96265300	-0.25431400	-1.27681700
H	-6.61454900	-0.84052500	-2.27933900
N	-1.77733900	-0.24495900	-1.22896900
C	-1.37867700	0.91856300	-0.63045100
C	-1.67506900	2.22312800	-1.11316900
C	-0.61199000	0.84399800	0.56799200
C	-1.23164600	3.35992500	-0.43284300
H	-2.25236800	2.34927800	-2.02237700
C	-0.17692200	1.98034900	1.22817100
H	-0.37674700	-0.13448800	0.96955500
C	-0.47674700	3.25955700	0.73510500
H	-1.47734500	4.34033300	-0.83531800
H	0.40378600	1.86922000	2.14119700
H	-0.13182900	4.14931500	1.25286400
C	3.15128500	1.65332700	-0.19072100
H	2.65651900	1.33292400	0.73186900
H	3.37290900	2.72252800	-0.10234000
H	4.10179700	1.11215100	-0.27116300
C	2.25269900	1.38533400	-1.40074500
H	1.33229900	1.97059100	-1.31424900
H	2.75618000	1.69788600	-2.32507400
C	1.88969200	-0.11696100	-1.48522600

H	1.38477600	-0.38089700	-0.55129000
H	2.79965200	-0.72244100	-1.54636400
C	1.01862200	-0.37363100	-2.67342700
H	1.51442300	-0.40111300	-3.63519700
H	0.06000000	0.13272900	-2.71044600
I	1.02871900	-3.05078200	-3.14265100
C	3.06234300	-1.35003100	2.81863900
C	3.27240600	-2.06597200	1.63603300
C	2.19729200	-2.65051300	0.97191100
C	0.89663600	-2.53938900	1.49282700
C	0.69408700	-1.83480000	2.68589500
C	1.77392000	-1.23830000	3.34147400
H	4.27369600	-2.15713000	1.22454200
H	2.35820900	-3.18233700	0.03791300
H	-0.30724900	-1.74141900	3.09317900
H	1.60480200	-0.68726300	4.26238200
C	0.18712800	-7.68628000	-0.08888000
C	0.76332700	-7.04695900	1.01101400
C	0.58298500	-5.67624800	1.19697800
C	-0.17882100	-4.93627300	0.28196500
C	-0.74296400	-5.58046100	-0.82910400
C	-0.56484800	-6.95168600	-1.00784400
H	1.35466800	-7.61520100	1.72365300
H	1.03920700	-5.17782500	2.04682400
H	-1.30802400	-5.00415400	-1.55484700
H	-1.00264700	-7.44327400	-1.87200800
C	-4.21697100	-2.73550800	3.18005500
C	-3.93994100	-1.78773300	2.19440100
C	-2.81699400	-1.93007700	1.37794500
C	-1.96211000	-3.02999800	1.55031200
C	-2.24738700	-3.98553300	2.53733100
C	-3.37104300	-3.83603200	3.34863400
H	-4.59344300	-0.93467700	2.04351000
H	-2.61515500	-1.20536100	0.59309400
H	-1.59835100	-4.84658000	2.66383800
H	-3.58910100	-4.57938100	4.11059900
P	-0.49367400	-3.14757000	0.46556300
H	-5.09323800	-2.62461800	3.81329200
H	0.33143400	-8.75334900	-0.23330800
H	3.90011000	-0.88251200	3.32796500

TS8-OA

C	5.58424900	5.49033000	-0.58079300
C	5.77695100	5.18750700	-1.93069700

C	6.47055100	4.03534400	-2.29389900
C	6.99231000	3.18241200	-1.31040300
C	6.79073000	3.48727400	0.04114600
C	6.08819900	4.63804900	0.40272000
H	5.37439000	5.84040900	-2.69975700
H	6.59733300	3.78434900	-3.34311500
H	7.17892600	2.82535900	0.80872300
H	5.93315400	4.86665500	1.45349200
C	12.30833000	3.11454500	-2.28358800
C	11.42899200	3.86407700	-1.49954200
C	10.09648900	3.47045000	-1.36957600
C	9.63877800	2.31868600	-2.02519500
C	10.52090100	1.57686900	-2.82167200
C	11.85121300	1.97351100	-2.94535100
H	11.77848200	4.75842900	-0.99096800
H	9.41378000	4.05790200	-0.76409900
H	10.15426300	0.70719000	-3.35244200
H	12.52115300	1.40437300	-3.58189700
C	8.01763900	-1.17216400	1.75506200
C	6.98430000	-1.23601800	0.81707100
C	6.96398300	-0.35326200	-0.26205400
C	7.97487600	0.60829000	-0.41206900
C	9.00332900	0.67181000	0.53679300
C	9.02345800	-0.21456500	1.61470000
H	6.19515000	-1.97527100	0.92301300
H	6.15695500	-0.39906000	-0.98632000
H	9.79537100	1.40483100	0.42298300
H	9.82893100	-0.16004800	2.34175200
P	7.91896400	1.71286500	-1.87971600
Cu	6.93858500	0.58025700	-3.67516600
B	8.71595700	-2.08902300	-4.58496700
O	9.04652500	-3.43033600	-4.58792800
C	9.63426900	-3.72443100	-3.29390900
C	10.17148500	-2.32180600	-2.84911000
O	9.20612400	-1.42666500	-3.46885400
C	11.54453200	-2.00101600	-3.44906400
H	11.78315600	-0.95192800	-3.26122700
H	12.32727500	-2.61718800	-2.99556900
H	11.55412600	-2.16645600	-4.53030800
C	10.18075200	-2.07143400	-1.34820100
H	10.83887600	-2.78826400	-0.84407400
H	10.55556500	-1.06480600	-1.14675400
H	9.18193700	-2.14544900	-0.91651600
C	10.69864900	-4.79802200	-3.48170500

H	11.23196100	-4.98258400	-2.54255800
H	10.22669600	-5.73413500	-3.79615000
H	11.42179200	-4.51056200	-4.24738400
C	8.51444400	-4.23754400	-2.38304000
H	8.02020100	-5.08523000	-2.86715000
H	8.90592300	-4.56987600	-1.41643600
H	7.76659900	-3.46065500	-2.19806700
C	7.75196400	0.01514800	-5.47935600
H	6.88335500	0.29277900	-6.08590200
C	8.90306400	0.89726300	-5.77368600
C	8.73348600	2.29794800	-5.72011600
C	9.79332600	3.16593900	-5.95070100
C	11.06583800	2.66590000	-6.24741000
C	11.24842600	1.28478900	-6.32311100
C	10.18482000	0.41282900	-6.09108600
H	7.74866800	2.69648300	-5.48153000
H	9.63116000	4.23915000	-5.89240000
H	11.89709200	3.34352600	-6.41809300
H	12.22650900	0.87904800	-6.57148200
H	10.33663100	-0.65784500	-6.17956500
N	7.97086500	-1.41897200	-5.59565100
C	7.50059000	-2.07502000	-6.76492400
C	7.46770900	-1.38796800	-7.98888100
C	7.03336400	-3.39941800	-6.72158700
C	6.97513700	-2.00944900	-9.13561300
H	7.84947100	-0.37462900	-8.04049700
C	6.55138500	-4.01365400	-7.87457400
H	7.05645700	-3.94090800	-5.78515100
C	6.51217500	-3.32457300	-9.08889500
H	6.96202900	-1.45922400	-10.07264900
H	6.19303700	-5.03833800	-7.81863500
H	6.12692200	-3.80558900	-9.98312700
H	8.03819400	-1.86530600	2.59126700
H	13.34359300	3.42725100	-2.38844600
H	5.03490100	6.38350400	-0.29698500
C	3.78173200	-4.69981600	-3.04479100
H	3.83845300	-4.68505000	-1.94978500
H	3.97485000	-5.72550500	-3.37805800
H	2.75514000	-4.44117100	-3.32879800
C	4.78721800	-3.72333200	-3.66228000
H	5.80707700	-4.01596700	-3.38649100
H	4.73704800	-3.77350000	-4.75675600
C	4.52315800	-2.26841400	-3.20907400
H	4.56926300	-2.21277200	-2.11500000

H	3.51190700	-1.97760100	-3.50632800
C	5.55325400	-1.37090700	-3.83551400
H	5.50425000	-1.26853300	-4.91216000
H	6.55939300	-1.55502100	-3.46123600
I	4.33168300	0.95409200	-3.06546600

TS11-OA

Cu	0.07042000	-0.81956400	-0.54291900
C	0.36107900	-1.99544700	1.00193000
N	-0.64674500	-2.68584400	1.59210500
C	-0.22246100	-3.35469600	2.74669600
C	1.10791100	-3.07735800	2.87587800
N	1.43387100	-2.24470900	1.79466700
B	-1.67811800	1.26646200	-3.21996700
O	-0.40105400	1.39216600	-3.70438100
C	-0.48368800	1.87621200	-5.06872000
C	-1.94420000	1.46188400	-5.47368700
O	-2.63113500	1.45799100	-4.18802700
C	-1.98072900	0.81067000	-1.73146600
H	-2.15404400	-0.27018800	-1.86571300
C	-3.29053900	1.33036700	-1.14436300
C	-3.33787700	2.00485600	0.07940100
C	-4.55804900	2.40718800	0.62872800
C	-5.75408000	2.14499800	-0.03844400
C	-5.71604600	1.48195500	-1.26856700
C	-4.49841600	1.07748200	-1.81260000
H	-2.41621700	2.20452300	0.61061100
H	-4.56902600	2.92868100	1.58265900
H	-6.70331700	2.45791600	0.38787800
H	-6.63887600	1.27771300	-1.80601400
H	-4.47722100	0.56394200	-2.76830600
H	2.89611500	-4.32950000	0.71687300
C	-4.51145400	-2.41751000	-0.07268400
C	-3.69456300	-3.51872300	-0.34569500
H	-4.04729900	-4.28926600	-1.02672900
C	-2.42012900	-3.64612900	0.21302800
C	-2.25015200	-0.41429500	2.27049900
H	-1.74986100	-0.81486800	3.15948300
C	-1.51712700	-4.79732500	-0.14756100
H	-1.11424500	-5.30098700	0.73856400
H	4.47965300	1.13819400	2.29690800
C	5.14981300	-0.42398400	0.97869900
C	4.81312400	-1.65388100	0.39950500
H	5.51278300	-2.13091000	-0.28259600

H	-4.65112300	-0.54895800	0.98827800
C	3.59277800	-2.27970700	0.66054900
C	2.02862100	0.23880000	3.09346100
C	-2.77561400	-1.51212000	1.38153900
H	1.94100400	-0.31826100	4.03469300
C	2.71030400	-1.64527900	1.54648200
C	3.00779600	-0.41831700	2.15266000
C	4.23583500	0.17884000	1.84732700
H	-2.05565000	-5.53780800	-0.74543100
H	-0.66653900	-4.43958400	-0.73936100
H	-3.06132600	0.24404300	2.59045100
H	-1.52169000	0.19219900	1.71959900
H	4.04331100	-3.97483800	-0.58979400
H	2.35990400	-3.42099900	-0.69286200
H	2.34487700	1.25739000	3.33354700
H	1.02666100	0.28711200	2.65615500
C	-4.03772700	-1.42329600	0.79084600
C	3.20652900	-3.57227800	-0.01215400
C	-1.98686300	-2.63147600	1.07443400
C	-5.88419400	-2.29879900	-0.68709400
H	-6.66700300	-2.54343200	0.04303600
H	-6.06662100	-1.27612900	-1.03056400
H	-6.00129100	-2.97747300	-1.53794300
C	6.47353600	0.22998200	0.66536200
H	6.62716200	0.31530000	-0.41626300
H	6.53359400	1.23405300	1.09550600
H	7.30999300	-0.35656500	1.06533400
C	-2.65833300	2.43782400	-6.39995500
H	-2.12825900	2.52091400	-7.35553600
H	-3.67119400	2.07653000	-6.60318500
H	-2.73581900	3.43162800	-5.95406400
C	-2.03390400	0.03413300	-6.01952900
H	-1.52944200	-0.67520700	-5.35634100
H	-3.08801500	-0.25201300	-6.08723500
H	-1.59119700	-0.04112400	-7.01814000
C	0.62435700	1.21091900	-5.87758500
H	0.54669800	1.47706800	-6.93773800
H	1.59855100	1.55412700	-5.51339100
H	0.58871800	0.12393800	-5.78008900
C	-0.27365800	3.39171000	-5.00926500
H	0.67403700	3.59811900	-4.50381500
H	-0.24303200	3.83298800	-6.01088700
H	-1.06720600	3.87770400	-4.43470000
N	-0.82698500	0.90385200	-0.83549900

C	-0.20105900	2.10147600	-0.68802600
C	-0.64414200	3.33110100	-1.26115600
C	0.98567000	2.16870000	0.10293800
C	0.06692800	4.50768500	-1.07825100
H	-1.57144200	3.35762900	-1.82215300
C	1.68562200	3.35678400	0.27722100
H	1.31364700	1.26941900	0.61303000
C	1.24466100	4.54011700	-0.31892400
H	-0.30700500	5.42348000	-1.53056100
H	2.58503200	3.35460400	0.88952300
H	1.79197900	5.46838400	-0.18584000
C	2.12150900	-3.50324800	3.88140600
H	2.93797200	-4.06806200	3.41521400
H	2.57348300	-2.64349500	4.39016600
H	1.66040000	-4.14106600	4.64001700
C	-1.15647400	-4.15807500	3.58481300
H	-2.00346000	-3.55073300	3.92442400
H	-1.57068900	-5.00768300	3.02959500
H	-0.64027100	-4.54734300	4.46628700
C	5.42780400	-0.21757300	-3.12515100
H	5.74867300	-1.11083600	-2.57643300
H	6.23199300	0.52481800	-3.06487200
H	5.30923200	-0.49972300	-4.17764800
C	4.12138700	0.33546700	-2.54894200
H	4.26554100	0.62239100	-1.50116100
H	3.82864100	1.24584600	-3.08653300
C	2.97645100	-0.70638900	-2.63832700
H	3.28400100	-1.60774100	-2.10046300
H	2.80386200	-0.98256000	-3.68162100
C	1.75636600	-0.10360200	-2.03025200
H	1.14627600	0.56379400	-2.62584900
H	1.88719900	0.19879500	-0.99202100
I	0.03476100	-2.30356300	-2.91129900

TS17-OA

Cu	0.76156300	-0.42982400	-1.63032900
C	0.45543400	-1.77934300	-0.16336000
N	-0.45100200	-2.77714100	-0.02922900
C	-0.32100200	-3.45086200	1.19631300
C	0.69978100	-2.83669900	1.85828000
N	1.15888500	-1.82551400	1.00266300
H	3.99576400	-3.24152900	1.51792700
C	-3.54274400	-3.73491600	-2.73187100
C	-2.24386000	-4.20065100	-2.94456600

H	-2.03435700	-4.82106500	-3.81135900
C	-1.19612400	-3.87353000	-2.08114300
C	-3.05583900	-1.59478100	0.39286700
H	-2.40499500	-1.76859400	1.25392000
C	0.20677000	-4.36105100	-2.33284700
H	0.85955600	-3.53039900	-2.62452500
H	2.39799300	2.33701000	2.43683400
C	4.07491700	1.09390300	1.90165900
C	4.45490700	-0.17034600	1.44719100
H	5.50989900	-0.39024500	1.30374300
H	-4.79214800	-2.52692600	-1.46599200
C	3.51545900	-1.16687300	1.15555800
C	0.27373700	0.67814600	2.03099700
C	-2.77154400	-2.54231800	-0.74709700
H	-0.15762700	-0.01657900	2.76213600
C	2.16277200	-0.85641900	1.33176900
C	1.73797500	0.39620400	1.80724200
C	2.71055400	1.35958600	2.07655100
H	0.64741000	-4.81287800	-1.43638200
H	0.22011700	-5.10276500	-3.13620600
H	-4.09499200	-1.69094700	0.72448500
H	-2.91032400	-0.55564300	0.07560200
H	4.95377200	-2.47730400	0.24089500
H	3.27643300	-2.92704200	-0.07209600
H	0.12506900	1.69622600	2.40125000
H	-0.29932100	0.56020200	1.10771200
C	-3.78756100	-2.90728700	-1.63285800
C	3.95575900	-2.52824900	0.68349400
C	-1.48869100	-3.05842300	-0.98018800
C	-4.65592100	-4.07298400	-3.69103500
H	-5.56864400	-4.36761100	-3.16064200
H	-4.90724400	-3.20483300	-4.31339200
H	-4.37274800	-4.88905700	-4.36269800
C	5.10503300	2.15007500	2.21915400
H	4.85056200	3.10776600	1.75244700
H	5.17283100	2.32330900	3.30070100
H	6.09843400	1.85722800	1.86669000
C	1.29305600	-3.07063200	3.20483400
H	2.34053500	-3.38696200	3.13968100
H	1.26772600	-2.15921000	3.81371800
H	0.73781200	-3.84857300	3.73529200
C	-1.18865500	-4.60536500	1.56359000
H	-2.24482500	-4.31793200	1.61831500
H	-1.11209700	-5.41000000	0.82311600

H	-0.89282000	-5.00793200	2.53596200
C	5.45830700	3.57931600	-1.27025600
H	6.04180400	2.94404800	-0.59346900
H	5.53233800	4.61223400	-0.91079700
H	5.93214600	3.53330500	-2.25782900
C	3.99949800	3.11934000	-1.33896700
H	3.52610000	3.21251800	-0.35382600
H	3.42998900	3.76879000	-2.01374600
C	3.89310600	1.65010200	-1.80954500
H	4.39762800	1.00942500	-1.08062500
H	4.40931000	1.53411400	-2.76751400
C	2.44540800	1.27417300	-1.93169900
H	1.90521400	1.67551800	-2.78113600
H	1.90769500	1.33868300	-0.98883800
I	3.05046100	-1.29501400	-2.79584600
B	-3.19378200	0.96248000	-2.31333000
O	-4.32717300	0.90598600	-3.10580000
C	-5.42445300	1.43975600	-2.32539400
C	-4.67817800	2.32798700	-1.26741100
O	-3.42388500	1.62630900	-1.11677800
C	-0.82201800	0.95296600	-1.76758500
H	-1.15372700	0.87184000	-0.73267100
C	-0.39344600	2.32100600	-2.05415700
C	-0.48937100	2.89924700	-3.34120700
C	-0.02272300	4.18664400	-3.58941900
C	0.55736800	4.95052300	-2.56957100
C	0.66405000	4.39823200	-1.29296700
C	0.20600700	3.10558000	-1.04101700
H	-0.95005800	2.32849500	-4.14088400
H	-0.11980600	4.60443300	-4.58862700
H	0.91408200	5.95697000	-2.76834800
H	1.10555800	4.97603000	-0.48446400
H	0.27035000	2.70050500	-0.03427800
C	-5.35639700	2.41684800	0.09443800
H	-5.46562600	1.43102600	0.55212200
H	-6.34782700	2.87530300	0.00635600
H	-4.75304900	3.03716100	0.76463700
C	-4.33868000	3.72838900	-1.79058600
H	-3.84875200	3.67478700	-2.76756800
H	-3.63855600	4.20158600	-1.09609000
H	-5.23007900	4.35843600	-1.87663100
C	-6.35993800	2.19825800	-3.25925400
H	-7.15813300	2.68959700	-2.69143100
H	-6.82263600	1.50160700	-3.96560800

H	-5.82145400	2.95406600	-3.83463500
C	-6.15070600	0.24734900	-1.69438500
H	-7.04807800	0.56079800	-1.15122100
H	-5.49252900	-0.28648300	-1.00319400
H	-6.44879200	-0.44583100	-2.48704300
N	-1.90652400	0.45329600	-2.63350600
C	-1.62768000	-0.34469100	-3.76311000
C	-0.32407300	-0.43124500	-4.27902000
C	-2.63767800	-1.08459500	-4.40602300
C	-0.02299400	-1.28098900	-5.34338000
H	0.46052100	0.18664400	-3.86173500
C	-2.33496700	-1.90265200	-5.48912600
H	-3.65437100	-1.02122100	-4.04571200
C	-1.02475800	-2.02761900	-5.95858600
H	1.00569800	-1.34222200	-5.68602200
H	-3.13554700	-2.46685200	-5.96140500
H	-0.79532200	-2.68258300	-6.79422800

IM1-ⁿBu

Cu	-0.09519900	-1.66567500	-1.56050900
B	-3.86177000	0.31565200	-1.59991000
O	-4.39588300	0.16238100	-0.35037200
C	-5.76472000	0.65471800	-0.41175700
C	-5.70414500	1.64685400	-1.62839700
O	-4.63575400	1.07428600	-2.43795800
C	-2.50445800	-0.34256900	-2.08796700
H	-2.17115000	0.24308500	-2.96329400
C	-2.75707800	-1.76476600	-2.56707100
C	-3.53398200	-2.65524600	-1.81136400
C	-3.70356400	-3.97387400	-2.22842600
C	-3.09518700	-4.42483400	-3.40308800
C	-2.31397900	-3.54963100	-4.15790300
C	-2.15153000	-2.22639500	-3.74240700
H	-3.98706000	-2.31557700	-0.88812800
H	-4.30043600	-4.65193700	-1.62550400
H	-3.22374100	-5.45517100	-3.72333800
H	-1.82204700	-3.89406300	-5.06234300
H	-1.53701000	-1.54793900	-4.32722300
C	-6.97090300	1.71110100	-2.47127300
H	-7.81387200	2.07764300	-1.87475800
H	-6.82112300	2.40031200	-3.30798900
H	-7.22972500	0.73234200	-2.88008900
C	-5.24615300	3.05378100	-1.23297500
H	-4.33657600	3.01615300	-0.62640900

H	-5.02750000	3.62242700	-2.14202300
H	-6.02126800	3.58540100	-0.67204300
C	-6.11392200	1.30038300	0.92331300
H	-7.09896300	1.77786400	0.87528400
H	-6.14795800	0.53644100	1.70573300
H	-5.37338100	2.04991600	1.21001400
C	-6.65350200	-0.56669300	-0.66540000
H	-6.47143500	-1.30258700	0.12331400
H	-7.71523700	-0.30025100	-0.65861600
H	-6.41628200	-1.03641600	-1.62478800
N	-1.48705900	-0.37619900	-1.03172000
C	-1.10702700	0.83410900	-0.48535300
C	-1.54209000	2.09587800	-0.95948000
C	-0.23145200	0.82264200	0.63022400
C	-1.14157000	3.27248800	-0.32672300
H	-2.19059500	2.16170200	-1.82536900
C	0.17341100	2.00181900	1.24074600
H	0.12336400	-0.13073200	1.00445400
C	-0.27967500	3.23997000	0.77040000
H	-1.49672700	4.22584500	-0.70980600
H	0.84558600	1.95254300	2.09317000
H	0.03508400	4.16110400	1.25120800
C	3.28045100	2.39184900	-1.42384300
H	3.02696300	2.33832300	-0.35837800
H	3.49256000	3.43938400	-1.66657500
H	4.20080900	1.81664100	-1.58180800
C	2.13070900	1.84637800	-2.27378400
H	1.22592800	2.43744800	-2.08934500
H	2.36738100	1.94472700	-3.34165800
C	1.82848100	0.36976000	-1.94692000
H	1.62801500	0.32794300	-0.86659300
H	2.70530300	-0.26059400	-2.13009200
C	0.65180000	-0.15965600	-2.72749300
H	0.89450100	-0.65135700	-3.66599100
H	-0.16540400	0.54961800	-2.83486200
I	1.67622800	-3.29542700	-2.61986300
C	2.43731100	-1.54677900	3.49431600
C	2.81355900	-1.71132200	2.15931400
C	1.90670600	-2.22526900	1.23413200
C	0.60939800	-2.58631100	1.63594900
C	0.24318000	-2.43028700	2.98020400
C	1.15300500	-1.91069900	3.90222400
H	3.81197800	-1.43351800	1.83386400
H	2.20132000	-2.34493800	0.19574000

H	-0.75670500	-2.69938800	3.30229000
H	0.85555000	-1.78910800	4.94010600
C	0.05979700	-7.74687900	0.00150600
C	0.45893700	-7.09400200	1.16949200
C	0.30200900	-5.71286600	1.28730600
C	-0.24961400	-4.97754600	0.23115000
C	-0.63538800	-5.63391000	-0.94588700
C	-0.48956400	-7.01588300	-1.05391200
H	0.89262300	-7.65958300	1.98949700
H	0.60910900	-5.20644200	2.19697100
H	-1.03806700	-5.06043900	-1.77314000
H	-0.78906400	-7.51838500	-1.96924400
C	-4.76764600	-2.83743100	2.23960500
C	-3.94422600	-1.71624000	2.12957400
C	-2.67131500	-1.82852300	1.57382800
C	-2.19473100	-3.07689000	1.14445600
C	-3.02392000	-4.20228200	1.26408400
C	-4.30514400	-4.08030800	1.80069700
H	-4.29482100	-0.74317200	2.45634000
H	-2.05969800	-0.94271300	1.46378300
H	-2.66997600	-5.17120100	0.93124400
H	-4.93799200	-4.95950400	1.88553000
P	-0.55225400	-3.18072300	0.34225300
H	-5.76270000	-2.74539700	2.66677200
H	0.18368400	-8.82254200	-0.08845300
H	3.14150400	-1.13708800	4.21299600

IM2-"Bu

C	5.79519100	6.03759100	-1.55203700
C	5.73402500	5.37837400	-2.77953900
C	6.21565300	4.07355000	-2.90008800
C	6.76577100	3.42150900	-1.79106200
C	6.80270900	4.08152000	-0.55192400
C	6.32634700	5.38559300	-0.43542700
H	5.29501900	5.86953400	-3.64309500
H	6.12055900	3.54313500	-3.83864600
H	7.19928700	3.56867000	0.31943800
H	6.36057100	5.88983100	0.52631500
C	12.01696300	2.01565300	-1.42309600
C	11.24230900	3.16489700	-1.26570000
C	9.85505000	3.10092400	-1.40353000
C	9.22816200	1.88702900	-1.71317500
C	10.01607900	0.74117900	-1.90558300
C	11.39873800	0.80516400	-1.74184700

H	11.71558700	4.11441900	-1.03116100
H	9.26186600	3.99942100	-1.27789000
H	9.55158400	-0.18970500	-2.21539800
H	12.00061900	-0.08711500	-1.88320200
C	5.68534400	-0.44060600	1.74623200
C	4.85415600	0.17921300	0.80810400
C	5.40485800	0.85886800	-0.27442700
C	6.80010500	0.93151700	-0.42590500
C	7.62964100	0.31777100	0.51836200
C	7.07077800	-0.36828800	1.59983800
H	3.77464400	0.12094100	0.91280900
H	4.75781100	1.31001400	-1.02214400
H	8.70804200	0.36876300	0.40909400
H	7.72153900	-0.84326500	2.32906800
P	7.41875300	1.71936100	-1.96268300
Cu	6.81727400	0.31834400	-3.82499600
B	9.35692600	-2.28218200	-5.21557200
O	9.79654400	-3.50894500	-5.65057800
C	10.47721600	-4.12668100	-4.52685900
C	10.94710600	-2.87671300	-3.69860600
O	9.92315400	-1.89265400	-4.02018900
C	12.28100900	-2.30383800	-4.18396100
H	12.43559400	-1.32227100	-3.72711100
H	13.12031400	-2.95030000	-3.90995000
H	12.28149000	-2.17686200	-5.27099400
C	10.96100800	-3.08428300	-2.18925600
H	11.64781800	-3.89396100	-1.91960000
H	11.29750600	-2.17413900	-1.68515800
H	9.96572500	-3.32873300	-1.81253200
C	11.60229000	-5.00367300	-5.06141100
H	12.18959500	-5.42283800	-4.23694500
H	11.17924900	-5.83370900	-5.63512700
H	12.26943900	-4.44316500	-5.71917600
C	9.43678900	-4.97947200	-3.79291000
H	9.00872100	-5.69581500	-4.50026100
H	9.88318100	-5.53715400	-2.96383300
H	8.62174500	-4.36440800	-3.39857400
C	7.88953300	-0.24988600	-5.61831700
H	6.95535200	-0.04757500	-6.13650400
C	8.72385600	0.93394400	-5.41981600
C	8.06686500	2.19186800	-5.41511100
C	8.77408100	3.36359900	-5.14358600
C	10.14476100	3.31466700	-4.90072300
C	10.81271500	2.08509800	-4.95277500

C	10.11845400	0.91059800	-5.20044800
H	7.00514000	2.23555900	-5.64224400
H	8.24711200	4.31207900	-5.12372300
H	10.69529400	4.22414700	-4.68145400
H	11.88265400	2.04390400	-4.77442900
H	10.64800000	-0.03013800	-5.20957100
N	8.38287300	-1.52240400	-5.94604700
C	7.69614000	-2.16084100	-7.03792000
C	7.62072500	-1.50230400	-8.26922800
C	7.08314300	-3.40679300	-6.87620200
C	6.93118800	-2.08503700	-9.33193100
H	8.10905600	-0.53961100	-8.38757400
C	6.40663800	-3.98992800	-7.94528100
H	7.12972300	-3.90454800	-5.91486100
C	6.32503100	-3.33182900	-9.17442000
H	6.87360500	-1.56484200	-10.28352300
H	5.92732300	-4.95537300	-7.81157200
H	5.78709600	-3.78564100	-10.00139300
H	5.25332700	-0.97728000	2.58616500
H	13.09631600	2.06384000	-1.30834700
H	5.41628300	7.05160200	-1.45878600
C	4.81543100	-3.53930300	-0.71047700
H	5.37230900	-3.13015700	0.14073100
H	4.61816400	-4.59966900	-0.51358500
H	3.85189600	-3.01800400	-0.75211800
C	5.59354400	-3.34553600	-2.01532600
H	6.54173100	-3.90068400	-1.96837400
H	5.02830300	-3.76510300	-2.85793800
C	5.88916500	-1.85487900	-2.29022700
H	6.42899000	-1.45113400	-1.42810200
H	4.93947200	-1.31201900	-2.35570000
C	6.69492400	-1.66495000	-3.55348300
H	6.19587700	-2.02317200	-4.45356700
H	7.71595800	-2.02684300	-3.47541500
I	4.33065600	1.16971400	-4.51325700

IM3-ⁿBu

Cu	-0.09881600	-0.58014100	-0.47026000
C	0.51000300	-1.78426700	1.00590800
N	-0.45314900	-2.36981800	1.76758600
C	0.08934100	-3.11627100	2.81835300
C	1.44241200	-3.00250100	2.70236400
N	1.66961200	-2.18007000	1.58710400
B	-1.47906700	1.19563200	-3.34748500

O	-0.13147400	1.42104200	-3.47436500
C	0.09960200	1.94213900	-4.81082500
C	-1.17485800	1.44802300	-5.58440700
O	-2.16655600	1.37060600	-4.51942200
C	-2.12315400	0.67292500	-1.99836300
H	-2.11694400	-0.41528200	-2.16302300
C	-3.59274500	1.01068800	-1.75899500
C	-4.06357000	1.54268500	-0.55373400
C	-5.42341400	1.80124500	-0.36683500
C	-6.34132600	1.52509900	-1.37869700
C	-5.88400100	0.97708300	-2.57982400
C	-4.52686300	0.71945800	-2.76609300
H	-3.36802200	1.75166900	0.24839000
H	-5.76216100	2.22006200	0.57763400
H	-7.39896100	1.72758400	-1.23371300
H	-6.58627700	0.74775600	-3.37707300
H	-4.18054200	0.30207000	-3.70494800
H	2.42589600	-4.51371700	0.41420800
C	-4.52343100	-2.05937100	0.68809000
C	-3.76890400	-3.18286400	0.33383200
H	-4.22488500	-3.96322700	-0.26955500
C	-2.43399200	-3.32347800	0.71270000
C	-1.97678200	-0.05246600	2.68976200
H	-1.02039700	-0.34117000	3.13391200
C	-1.63836100	-4.54124900	0.32349000
H	-1.30278800	-5.10774300	1.20114800
H	5.42546500	0.44568000	1.55037600
C	5.54792900	-1.24390100	0.22167000
C	4.87642500	-2.37482000	-0.25270500
H	5.36222800	-3.01577700	-0.98417400
H	-4.50716600	-0.21228100	1.78233300
C	3.58512800	-2.69937600	0.17445400
C	2.94484700	0.15315400	2.65532800
C	-2.58759700	-1.16261800	1.87359400
H	3.58248300	0.99685100	2.93260000
C	2.98228900	-1.85216600	1.11351000
C	3.62643700	-0.72221000	1.63321900
C	4.91156000	-0.43299100	1.16823000
H	-2.24075400	-5.20689600	-0.29942400
H	-0.75762200	-4.25636600	-0.25947000
H	-2.65329000	0.24955700	3.49679500
H	-1.80012700	0.82719900	2.06263200
H	3.51056900	-4.50690400	-0.99075400
H	2.00534700	-3.56741500	-1.01225400

H	1.99857300	0.55249400	2.27281900
H	2.70201200	-0.40439200	3.56778400
C	-3.92641100	-1.07984900	1.48307100
C	2.84601700	-3.88818500	-0.38167700
C	-1.85569500	-2.28148700	1.45684000
C	-5.93551400	-1.88646000	0.19049900
H	-6.56626400	-1.38949900	0.93515500
H	-5.94459200	-1.25922900	-0.70854900
H	-6.39183300	-2.84867500	-0.06341200
C	6.91275600	-0.88123300	-0.30899100
H	6.82399300	-0.26063200	-1.21002500
H	7.49205600	-0.31319700	0.42593200
H	7.48584400	-1.77274100	-0.58334700
C	-1.68682200	2.40276800	-6.65500800
H	-0.93292000	2.54412200	-7.43768100
H	-2.58519300	1.98525600	-7.11989400
H	-1.94349800	3.37804800	-6.23562700
C	-1.02871000	0.02977200	-6.14321600
H	-0.68247500	-0.66790700	-5.37371200
H	-2.00777600	-0.31320000	-6.49129300
H	-0.33372600	0.00211400	-6.98888700
C	1.41586500	1.38072500	-5.33474400
H	1.57664800	1.68410600	-6.37543400
H	2.24762000	1.76625000	-4.73738900
H	1.43096200	0.29063700	-5.27969800
C	0.18024000	3.46529100	-4.67562200
H	0.95723700	3.71451800	-3.94683200
H	0.42871300	3.94206300	-5.62927000
H	-0.76438800	3.87973300	-4.31173900
N	-1.26155400	0.88333800	-0.82478700
C	-0.98850600	2.19119600	-0.46751400
C	-1.47446900	3.32319900	-1.16791400
C	-0.21065400	2.44125300	0.69315600
C	-1.20232600	4.61352600	-0.72353400
H	-2.10180800	3.19464400	-2.04077100
C	0.05848600	3.73111600	1.12645600
H	0.17091200	1.58913400	1.24589500
C	-0.43471400	4.83456700	0.42123200
H	-1.60090400	5.45726300	-1.28064800
H	0.65641900	3.87880700	2.02211500
H	-0.22606700	5.84481100	0.75996200
C	2.56097900	-3.57609000	3.50267400
H	3.19624900	-4.22912300	2.89287400
H	3.20720200	-2.79376500	3.91738800

H	2.16608300	-4.16701300	4.33293700
C	-0.76534900	-3.81037600	3.82269100
H	-1.44999300	-3.10621800	4.30903000
H	-1.37896700	-4.59310000	3.36391400
H	-0.14471300	-4.27278300	4.59453100
C	4.56385300	-0.09910600	-3.31987500
H	4.86373000	-1.08353200	-2.94345100
H	5.47264800	0.47534100	-3.53660300
H	4.02826500	-0.25336100	-4.26335400
C	3.68011500	0.62179100	-2.29864000
H	4.23559400	0.77350800	-1.36577300
H	3.40784400	1.61764800	-2.67148600
C	2.38932300	-0.18644600	-2.00619000
H	2.67011000	-1.17990700	-1.65448600
H	1.81945300	-0.31222600	-2.92804700
C	1.56192500	0.54228600	-1.00262300
H	1.10275200	1.45156300	-1.36879700
H	1.97678600	0.63000700	-0.00092500
I	-0.40077200	-2.53069500	-2.60064700

IM4-"Bu

Cu	1.11108000	-0.25007400	-1.66187300
C	0.29278700	-1.65788200	-0.34440700
N	-0.49686500	-2.76183800	-0.26569100
C	-0.30249800	-3.46177600	0.94061400
C	0.62564800	-2.76069200	1.64641400
N	0.96831800	-1.66854300	0.84349500
H	4.39674700	-2.42613900	1.55172600
C	-3.82345700	-3.92174900	-2.60525600
C	-2.54941300	-4.39984900	-2.90727400
H	-2.42254100	-5.09816200	-3.73076000
C	-1.41643300	-4.01152300	-2.18198800
C	-3.05139900	-1.67975900	0.38992300
H	-2.46914400	-1.99250800	1.26263300
C	-0.06518000	-4.55370000	-2.54954800
H	0.45204400	-3.86096200	-3.22188100
H	1.55951400	2.57045800	2.46083100
C	3.40848000	1.62289800	1.88735300
C	3.98120200	0.43445500	1.44019200
H	5.05978400	0.37638000	1.31612000
H	-4.95525000	-2.68308600	-1.25941300
C	3.20893800	-0.69195500	1.12166000
C	-0.27098700	0.61238600	2.06975200
C	-2.86657200	-2.61777000	-0.77724700

H	-0.49011900	0.09030700	3.01094900
C	1.81966600	-0.58547800	1.25065400
C	1.20786300	0.57159900	1.77437300
C	2.01914700	1.66466500	2.07136400
H	0.58577800	-4.67069900	-1.67919900
H	-0.16105000	-5.52012100	-3.05413900
H	-4.10452100	-1.63710100	0.68378900
H	-2.74088100	-0.66116700	0.13714400
H	4.63490400	-1.77113600	-0.07740400
H	3.18202700	-2.68622600	0.27570200
H	-0.62234000	1.64269500	2.17347200
H	-0.86404500	0.12679400	1.29384900
C	-3.96492700	-3.04032800	-1.52730600
C	3.88578200	-1.96755900	0.69412300
C	-1.59538700	-3.10456900	-1.13158900
C	-5.02029500	-4.31929900	-3.43341900
H	-5.92100400	-4.41698000	-2.81765600
H	-5.23182500	-3.56281100	-4.20070100
H	-4.85310700	-5.27042100	-3.94874100
C	4.25365600	2.83801900	2.17937600
H	3.96149800	3.68089100	1.54154100
H	4.13885600	3.16409400	3.22028900
H	5.31415300	2.63791400	2.00144200
C	1.23868500	-2.98521000	2.98549000
H	2.31641700	-3.16983700	2.90964300
H	1.10276400	-2.11322700	3.63617100
H	0.78078700	-3.84888200	3.47443600
C	-1.03572100	-4.72057900	1.25487300
H	-2.11980000	-4.56211500	1.28194300
H	-0.84128200	-5.49350600	0.50260700
H	-0.72097000	-5.10612800	2.22816600
C	6.09430000	2.20280100	-1.78791000
H	6.39068600	1.48764900	-1.01018100
H	6.63592300	3.13920200	-1.60879800
H	6.42883400	1.79800800	-2.75024300
C	4.57824700	2.41743500	-1.77762600
H	4.27139900	2.82792900	-0.80653700
H	4.29867700	3.16594000	-2.53126200
C	3.80724100	1.10645600	-2.03647500
H	4.13772800	0.36380500	-1.30525300
H	4.06723500	0.70722700	-3.02079300
C	2.31883200	1.35273700	-1.92849900
H	1.92285300	1.94339300	-2.75281500
H	2.06394700	1.83202300	-0.98131300

I	2.73580000	-2.06296700	-2.81614100
B	-2.82871700	0.90785200	-2.11792500
O	-3.90253600	0.86197200	-2.97873900
C	-5.05109600	1.38300200	-2.26227100
C	-4.38222400	2.20847000	-1.10009800
O	-3.13094900	1.50518700	-0.90640300
C	-0.47730700	1.12031800	-1.59471900
H	-0.69323200	0.94301200	-0.54690700
C	-0.29051100	2.56241900	-1.83662200
C	-0.60289400	3.16710800	-3.06830200
C	-0.44799200	4.53963500	-3.24891700
C	0.02191900	5.34384100	-2.20715300
C	0.33337500	4.75856500	-0.97822200
C	0.17926400	3.38653500	-0.79719300
H	-0.98801100	2.55689900	-3.87773200
H	-0.70154200	4.98536300	-4.20706600
H	0.13839800	6.41425400	-2.35055700
H	0.69075100	5.37371400	-0.15644900
H	0.41093400	2.93840900	0.16414200
C	-5.14868400	2.20757300	0.21682500
H	-5.28465400	1.19433000	0.60123200
H	-6.13326400	2.67238500	0.09413300
H	-4.59231000	2.78233400	0.96391400
C	-4.01909900	3.64074300	-1.50751500
H	-3.46830500	3.65564700	-2.45205800
H	-3.36542300	4.06886600	-0.74208300
H	-4.90814700	4.27205000	-1.60616300
C	-5.88614800	2.20947900	-3.23373000
H	-6.72135300	2.69179500	-2.71351800
H	-6.29748500	1.55886700	-4.01173400
H	-5.28347200	2.97936800	-3.71945800
C	-5.85482200	0.18151100	-1.75973900
H	-6.79258000	0.49256200	-1.28797100
H	-5.27700200	-0.40028400	-1.03833800
H	-6.08923100	-0.46750100	-2.60882600
N	-1.50133600	0.48740800	-2.41954900
C	-1.18626200	-0.21270700	-3.61537000
C	-0.03676000	0.07266900	-4.36437600
C	-2.03949300	-1.23630000	-4.05240900
C	0.26438100	-0.66968900	-5.50678400
H	0.63632100	0.85948400	-4.05355400
C	-1.74384000	-1.95550200	-5.20502800
H	-2.92196300	-1.47346500	-3.47383400
C	-0.58568000	-1.68421600	-5.93818800

H	1.18023500	-0.45335600	-6.04781400
H	-2.41460300	-2.75168400	-5.51617800
H	-0.34656300	-2.26264000	-6.82569500

TS1-insertion

Cu	5.16578300	-2.33864900	-0.78308400
I	3.51608400	-3.95561500	0.78527400
C	7.44530000	-2.15204500	-1.41514600
C	8.47510900	-1.63294600	-0.45007100
H	6.90461400	-1.37706000	-1.95445600
H	7.73443800	-2.97271400	-2.06448300
C	9.45348700	-0.67836200	-1.16675700
H	8.00222200	-1.08059500	0.36916800
H	9.02894700	-2.46406600	-0.00015900
C	10.51362800	-0.13578200	-0.20538200
H	9.93610800	-1.20695300	-1.99900000
H	8.88718500	0.15233300	-1.60020300
H	11.19792600	0.54624900	-0.72193900
H	10.04492700	0.41726300	0.61618900
H	11.10919700	-0.94692000	0.22971000
C	6.48038300	-3.47944900	-0.07754100
O	7.16879200	-4.27641800	0.39469000
B	4.04188800	-2.23180700	-4.95778500
O	2.90341900	-2.98313700	-4.98358800
C	2.28856400	-2.78296700	-6.28562500
C	3.50890200	-2.31246200	-7.16045800
O	4.38069100	-1.68881600	-6.17061200
C	4.96996000	-2.12122300	-3.67486000
H	5.72466400	-1.33144400	-3.86644800
C	5.69298800	-3.45964200	-3.66688400
C	5.19190400	-4.54298300	-2.93264200
C	5.87473200	-5.76068500	-2.91813600
C	7.04618300	-5.92283300	-3.65988900
C	7.52515200	-4.86032900	-4.43225200
C	6.85061700	-3.63939300	-4.43589100
H	4.27712700	-4.41969400	-2.36460200
H	5.48464400	-6.58157000	-2.32305900
H	7.57762600	-6.87020900	-3.64501500
H	8.42888600	-4.97990700	-5.02393100
H	7.23154400	-2.80745600	-5.02389900
C	4.30563700	-3.47485400	-7.75956900
H	4.56969800	-4.20667100	-6.99006500
H	3.74503300	-3.98363600	-8.55019300
H	5.23404000	-3.08507600	-8.18801200

C	3.17389500	-1.28095300	-8.22997700
H	4.08508600	-0.99371800	-8.76417400
H	2.46790200	-1.69524500	-8.95850900
H	2.73657600	-0.38064700	-7.79324500
C	1.21579300	-1.70567400	-6.10525300
H	0.65333600	-1.54118500	-7.03021900
H	0.52031600	-2.03002000	-5.32593500
H	1.65379100	-0.75859200	-5.78063300
C	1.65460400	-4.09798400	-6.72325300
H	1.24031400	-4.01130100	-7.73420800
H	2.37799800	-4.91577300	-6.70764300
H	0.83881900	-4.35440600	-6.04068800
N	4.21270700	-1.91490800	-2.44934500
C	3.23034000	-0.94688800	-2.49467300
C	2.18128500	-1.00371800	-1.54384800
C	3.18594600	0.09496700	-3.45794200
C	1.13738600	-0.09393100	-1.57644700
H	2.20464100	-1.80033900	-0.80944000
C	2.13581300	1.01219500	-3.47037600
H	3.97741700	0.19118500	-4.19398200
C	1.10307200	0.92561400	-2.53656300
H	0.34490100	-0.17114900	-0.83910500
H	2.13001700	1.80268000	-4.21716600
H	0.28586900	1.64064300	-2.55099000
C	1.09319900	1.80456000	1.37385000
C	1.38001200	0.54884500	1.91695200
C	2.60966400	-0.05547700	1.67149400
C	3.57113500	0.59971000	0.88443800
C	3.28079700	1.85470100	0.34108200
C	2.04244900	2.45096600	0.58333100
H	0.64218900	0.03540200	2.52688700
H	2.82277100	-1.04010400	2.07688000
H	4.01088500	2.36460700	-0.27697400
H	1.82229800	3.42265900	0.15057200
C	6.79424700	-0.47993000	4.96504200
C	6.15904500	0.68312100	4.51927000
C	5.65947900	0.75144200	3.22097000
C	5.80259400	-0.33906500	2.34672800
C	6.42363600	-1.50550500	2.80792500
C	6.92067000	-1.57458200	4.11090200
H	6.04609700	1.53266900	5.18687200
H	5.14812200	1.64708700	2.88150000
H	6.49539300	-2.37138800	2.16207200
H	7.39302600	-2.48880300	4.45798700

C	7.80073700	2.81098300	-1.64881600
C	6.80109800	2.08256600	-2.29853900
C	6.02347100	1.17205600	-1.58458200
C	6.22032400	0.99259800	-0.20447900
C	7.22595000	1.72515500	0.43899600
C	8.01209000	2.62674800	-0.28165500
H	6.62780600	2.21708800	-3.36249900
H	5.24756700	0.61076800	-2.09359900
H	7.39977100	1.58904500	1.50067000
H	8.79155600	3.18544700	0.22869100
P	5.16750400	-0.26382000	0.62779600
H	8.41351300	3.51422800	-2.20535100
H	7.17687000	-0.53453600	5.98026700
H	0.13089300	2.27238900	1.56211500

TS2-insertion

C	2.57391600	3.08077500	1.62410200
C	2.39173600	1.70826800	1.45590700
C	3.35936500	0.94848200	0.79577000
C	4.51394800	1.56289900	0.29671900
C	4.70730800	2.93995100	0.49544900
C	3.73637200	3.69567500	1.14854300
H	1.50273100	1.22041300	1.84479300
H	3.23020300	-0.12310600	0.68962300
H	5.62085500	3.41353000	0.14820000
H	3.88925800	4.76106000	1.29597000
C	6.46785700	2.19639300	-4.80787100
C	5.56583700	2.84340500	-3.96487200
C	5.32386900	2.35699000	-2.67941400
C	5.99392400	1.22039500	-2.21582800
C	6.89510000	0.56734900	-3.07636800
C	7.13153100	1.05153500	-4.36115300
H	5.03554200	3.72646300	-4.30984300
H	4.60081200	2.85494800	-2.04554700
H	7.42985800	-0.31442800	-2.73440200
H	7.83406200	0.53689500	-5.01053400
C	9.64898900	1.63672400	1.77568700
C	8.47031700	1.30752300	2.45042300
C	7.31201000	1.01598500	1.73462000
C	7.31270100	1.05157900	0.33038800
C	8.49364000	1.39572300	-0.33846900
C	9.65483900	1.68443900	0.38187700
H	8.45392200	1.26965800	3.53560300
H	6.40307800	0.75600900	2.26807100

H	8.51383800	1.44711100	-1.42054800
H	10.56393500	1.94754200	-0.15149300
P	5.76923000	0.52763200	-0.53406600
Cu	5.52602600	-1.88316500	-0.35317300
B	2.91235100	-3.52133200	-2.78384400
O	1.61123900	-3.27829600	-3.16006700
C	0.87500900	-4.51107500	-2.94986500
C	2.01596400	-5.59789600	-2.98991600
O	3.18516500	-4.84638500	-2.57530500
C	2.31270000	-6.11620300	-4.40002500
H	3.23754100	-6.70000700	-4.37268700
H	1.50666800	-6.75527100	-4.77471100
H	2.45552100	-5.28727600	-5.10026800
C	1.83230200	-6.75762400	-2.01831300
H	0.91533400	-7.31356700	-2.24400800
H	2.67873800	-7.44634400	-2.10552200
H	1.78844100	-6.40344700	-0.98655200
C	-0.16870800	-4.64141600	-4.05349800
H	-0.70404500	-5.59374000	-3.96829600
H	-0.89860100	-3.83100400	-3.96338100
H	0.28402200	-4.58054100	-5.04534100
C	0.19300200	-4.39461000	-1.58425000
H	-0.45361700	-3.51173200	-1.58985700
H	-0.42280300	-5.27340400	-1.36716700
H	0.92716400	-4.26887200	-0.78397300
C	5.23362000	-2.46495700	-2.39903700
H	5.71681200	-1.60107000	-2.84870100
C	6.08460700	-3.66649600	-2.49151400
C	7.27623700	-3.55043800	-3.23596800
C	8.17764900	-4.61158500	-3.33662500
C	7.91624200	-5.81047600	-2.67787400
C	6.75540700	-5.92813400	-1.90295500
C	5.85477400	-4.87482600	-1.80064700
H	7.48004500	-2.62327100	-3.76600300
H	9.08102000	-4.49519500	-3.92898000
H	8.61391300	-6.63997900	-2.74953700
H	6.55629600	-6.84928200	-1.36216100
H	4.98183000	-4.96746600	-1.17140200
N	3.86229100	-2.44231300	-2.72584100
C	3.33771100	-1.13626900	-3.02069300
C	3.67142400	-0.51275600	-4.22642900
C	2.47564900	-0.50748100	-2.12164100
C	3.12460800	0.72908800	-4.53966800
H	4.34093700	-1.01626400	-4.91699900

C	1.94480000	0.74527600	-2.43157000
H	2.22427000	-1.01586100	-1.19869600
C	2.26049500	1.36146900	-3.64248600
H	3.37985600	1.20650500	-5.48041900
H	1.28585500	1.23659500	-1.72180400
H	1.83958600	2.33313800	-3.88580600
H	10.55439100	1.85657800	2.33385000
H	6.65058000	2.57688100	-5.80867800
H	1.82062700	3.67113100	2.13829100
I	3.42478300	-3.07665400	0.76868600
C	7.91139500	-2.50077200	-0.25343300
C	9.15081700	-2.09970400	0.50997400
H	7.80218800	-1.96152600	-1.19220500
H	7.75038000	-3.56878000	-0.38750700
C	10.40030800	-2.12848300	-0.39074700
H	9.05172300	-1.08868800	0.91750600
H	9.29532300	-2.76762700	1.36732300
C	11.67203100	-1.75557900	0.37609700
H	10.50687200	-3.12235900	-0.84457800
H	10.24953900	-1.42347100	-1.22027700
H	12.55071900	-1.75511400	-0.27924000
H	11.57722200	-0.75695400	0.81860900
H	11.86150000	-2.46372500	1.19150600
C	6.50820300	-2.02227200	1.31899400
O	6.91959900	-2.21899000	2.38473900

TS3-insertion

Cu	5.28353100	-1.89743600	-0.04741500
I	4.04970800	-2.78596700	2.69384100
C	6.49241800	-3.76893800	-0.51831300
C	7.86875500	-3.43735500	-1.02168300
H	5.71777600	-3.89042800	-1.26856800
H	6.43586800	-4.51459700	0.27428000
C	8.55094800	-4.68241800	-1.63060500
H	7.80914600	-2.66396800	-1.79254600
H	8.50640600	-3.05478600	-0.21672400
C	9.93824300	-4.34670400	-2.18355600
H	8.62878200	-5.46490600	-0.86453200
H	7.91845200	-5.08342600	-2.43118100
H	10.42273900	-5.23223800	-2.61053900
H	9.86555900	-3.58632900	-2.96918000
H	10.59073600	-3.95392400	-1.39411200
C	6.48713600	-2.44709700	1.37179400
O	7.37709300	-2.76676800	2.03450500

C	5.20939300	0.21380700	0.13627300
N	4.33092300	1.20885600	-0.19879400
C	4.81009900	2.48040600	0.15727400
C	6.03614500	2.28565800	0.70789900
N	6.24946600	0.90341500	0.69496200
H	5.81510900	1.56066600	3.31371600
C	0.44382500	1.16209500	-1.86428400
C	0.65607500	0.82070000	-0.52587500
H	-0.19224800	0.55735500	0.09983800
C	1.93510800	0.77866700	0.03249400
C	3.98076600	1.96294900	-3.01259300
H	3.84311200	3.01214800	-3.30326900
C	2.13342900	0.39178800	1.47018600
H	2.83961000	1.05735900	1.97916300
H	10.51781200	-0.76688500	0.56037700
C	9.71299200	-0.62647700	2.55219500
C	8.60265000	-0.24214200	3.31053700
H	8.63309200	-0.34863600	4.39185200
H	1.40537000	1.77786000	-3.68813400
C	7.43537600	0.23946800	2.71652100
C	8.47138300	0.18350800	-0.97128900
C	2.84615200	1.50709100	-2.12673500
H	9.40158300	-0.15322400	-1.43653100
C	7.41595300	0.34482500	1.31713400
C	8.52026600	0.01223800	0.52264800
C	9.65725100	-0.48534600	1.16235800
H	1.18359400	0.41434600	2.01124700
H	2.54187100	-0.62087500	1.55200500
H	3.99954100	1.36677400	-3.92946500
H	4.95143900	1.87875900	-2.52013600
H	6.46354200	0.53933800	4.61090700
H	5.42249900	-0.15980400	3.36295700
H	7.65322500	-0.38988300	-1.41138700
H	8.30840400	1.23250100	-1.25042800
C	1.54797500	1.50478200	-2.64601500
C	6.22101800	0.57001800	3.54541000
C	3.02306300	1.10376900	-0.79369900
C	-0.93872900	1.11590900	-2.46641300
H	-1.71390600	1.23424300	-1.70276700
H	-1.07655800	1.89808100	-3.22065800
H	-1.11406100	0.15180300	-2.96283800
C	10.93036200	-1.21514300	3.21977900
H	11.12067300	-0.74805100	4.19184800
H	10.78984000	-2.28923700	3.39649900

H	11.82542800	-1.09700900	2.60069200
C	7.05055600	3.24844100	1.22474500
H	7.27062600	3.08271300	2.28453900
H	7.99782000	3.15373700	0.68110600
H	6.69179900	4.27376300	1.10523700
C	4.01851200	3.72890600	-0.03760000
H	3.88984200	3.98094500	-1.09534000
H	3.01804800	3.63052500	0.39702100
H	4.52251400	4.56666000	0.45126200
B	3.31392400	-1.75126200	-3.96586700
O	2.92368900	-2.96164000	-4.46787300
C	1.99438600	-2.70300700	-5.55555100
C	2.37005000	-1.23402000	-5.97035300
O	2.88793500	-0.68537300	-4.72643700
C	4.32902600	-1.54661900	-2.76562300
H	4.28464700	-0.49049400	-2.48671100
C	5.67582800	-1.78481000	-3.44029900
C	6.01458300	-3.06731800	-3.90103700
C	7.20584000	-3.28569600	-4.58790200
C	8.08668000	-2.22514000	-4.82819900
C	7.75576400	-0.94532200	-4.38511700
C	6.55435200	-0.72960600	-3.70374200
H	5.32368900	-3.88371000	-3.72007500
H	7.45098900	-4.28406900	-4.93988400
H	9.01607400	-2.39696400	-5.36397400
H	8.42956700	-0.11234700	-4.56748700
H	6.29617400	0.27020000	-3.36976300
C	3.51990500	-1.16679600	-6.97978800
H	4.36971500	-1.77018500	-6.64603600
H	3.20939300	-1.51294200	-7.97069400
H	3.85608500	-0.12887600	-7.06481700
C	1.19994000	-0.37127700	-6.42656400
H	1.55768700	0.63393000	-6.67215700
H	0.73075800	-0.79319000	-7.32227500
H	0.44286800	-0.28159700	-5.64444300
C	0.58188100	-2.82600500	-4.97874200
H	-0.17785100	-2.73584200	-5.76223200
H	0.47918600	-3.80301300	-4.49885500
H	0.39747100	-2.06733400	-4.21495600
C	2.22100400	-3.75376900	-6.63606600
H	1.59230000	-3.55376500	-7.51113300
H	3.26586300	-3.78325700	-6.95238300
H	1.95641600	-4.74093800	-6.24507100
N	4.15163700	-2.43129200	-1.61689800

C	2.84874000	-2.72895700	-1.23402400
C	2.64081700	-3.86942300	-0.41891800
C	1.70431600	-2.01343500	-1.64624900
C	1.36497300	-4.28390000	-0.06954800
H	3.50672000	-4.42190100	-0.07327000
C	0.42435000	-2.44428700	-1.30412300
H	1.81516200	-1.10252900	-2.22024200
C	0.23969100	-3.58020100	-0.51685800
H	1.24499600	-5.16216600	0.55853500
H	-0.43602300	-1.87287100	-1.64368000
H	-0.75968600	-3.90860400	-0.24625700

TS4-insertion

Cu	4.73590100	-1.62643400	-0.04111000
B	3.10484800	-4.04988800	-1.85263100
O	4.28830000	-4.54940700	-1.35379600
C	4.21396900	-5.99406400	-1.39917300
C	2.66123000	-6.25806800	-1.50800400
O	2.17049700	-5.02952200	-2.10338600
C	1.97612900	-6.40936900	-0.14804800
H	0.89224000	-6.41006800	-0.30006900
H	2.25741800	-7.34941700	0.33816400
H	2.22422200	-5.57658400	0.51435900
C	2.27404400	-7.41600200	-2.42309300
H	2.67944500	-8.36153700	-2.04559600
H	1.18371600	-7.50260700	-2.45586500
H	2.63101800	-7.26286300	-3.44387900
C	4.87449400	-6.53768000	-0.13672300
H	4.78605400	-7.62873800	-0.08733800
H	5.93974300	-6.28272900	-0.14381300
H	4.42858900	-6.10237900	0.75922600
C	4.99382800	-6.43666900	-2.64181100
H	6.01326900	-6.04253200	-2.58011500
H	5.04824700	-7.52728800	-2.71758300
H	4.53371400	-6.04945800	-3.55625300
C	3.91587800	-1.65358500	-1.99808500
H	3.43016500	-0.69118600	-1.87896800
C	5.02131400	-1.60212000	-2.96397400
C	5.73437500	-0.39709700	-3.14622100
C	6.76098600	-0.29629400	-4.07755800
C	7.14174900	-1.40700600	-4.83924400
C	6.47184300	-2.61468400	-4.65038100
C	5.42926500	-2.71359600	-3.72880300
H	5.46294200	0.46429300	-2.54646400

H	7.26876300	0.65521500	-4.21350300
H	7.94570200	-1.32787000	-5.56517400
H	6.75407100	-3.49030200	-5.22924400
H	4.90403200	-3.65236900	-3.61937000
N	2.91417000	-2.67383800	-2.16359200
C	1.65520000	-2.21677100	-2.64295800
C	1.60597700	-1.39737300	-3.77998100
C	0.46247000	-2.57119100	-1.99951600
C	0.38272600	-0.94007900	-4.26729600
H	2.53142900	-1.14621900	-4.28893900
C	-0.75696700	-2.12246400	-2.50104700
H	0.50696200	-3.18724400	-1.11010000
C	-0.80632100	-1.30320700	-3.63184900
H	0.35929400	-0.31228500	-5.15440100
H	-1.67659000	-2.40456000	-1.99563900
H	-1.76153900	-0.95430900	-4.01443200
I	2.67464700	-2.69341500	1.40295500
C	6.74848800	-2.80868800	-0.77232900
C	7.99696300	-3.42462600	-0.20742300
H	6.89441900	-1.83922000	-1.24076200
H	6.08768200	-3.47552900	-1.31071300
C	9.03564700	-3.63536100	-1.33017200
H	8.44625100	-2.78530800	0.55796300
H	7.77237200	-4.38745900	0.26745000
C	10.35087200	-4.20596100	-0.79206400
H	8.61761000	-4.29952300	-2.09726500
H	9.22347500	-2.67497900	-1.82805200
H	11.07901000	-4.36041500	-1.59649000
H	10.79899000	-3.52540300	-0.05799000
H	10.18929700	-5.17000700	-0.29503300
C	5.84986100	-2.47358400	1.26818200
O	6.34871700	-3.03035900	2.14846000
C	5.06323800	0.43939200	0.20620300
N	4.19069100	1.47040400	0.02377600
C	4.78492600	2.71817500	0.26263100
C	6.08060300	2.46426500	0.59317600
N	6.22521600	1.06846900	0.54573100
H	5.96406800	1.25953600	3.24371600
C	0.02281200	0.94195600	-0.44253700
C	0.63323700	0.83711300	0.81311200
H	0.02997000	0.59111300	1.68303900
C	2.00147900	1.02954700	0.98127200
C	2.99009300	1.87543600	-2.64235000
H	2.49281700	2.69317100	-3.17582600

C	2.63403600	0.95644600	2.34578600
H	3.28645900	1.81740300	2.53469100
H	10.51370100	-0.49678200	-0.02892200
C	9.73641600	-0.82868100	1.94750300
C	8.63634600	-0.62575200	2.78904800
H	8.68422600	-0.96454200	3.82069200
H	0.35054000	1.38508900	-2.51671200
C	7.47228300	-0.00303600	2.33971300
C	8.48554400	0.73400200	-1.29520200
C	2.19249100	1.48359200	-1.42247900
H	9.42322800	1.24076000	-1.54840700
C	7.41813900	0.40649400	0.99523400
C	8.51103200	0.25695700	0.13337200
C	9.66065100	-0.36669400	0.63308000
H	1.86527800	0.92866800	3.12255600
H	3.23364400	0.04737500	2.44305700
H	3.07537000	1.03839800	-3.34324800
H	4.00177400	2.20030400	-2.38992800
H	6.57851500	-0.03148500	4.29580800
H	5.44879300	-0.40211600	2.98491900
H	8.36818300	-0.10619900	-1.98661900
H	7.65771600	1.41938400	-1.48659800
C	0.81105200	1.28576100	-1.53882200
C	6.30495800	0.21832600	3.26738000
C	2.77178300	1.31032600	-0.16089300
C	-1.46088500	0.71230800	-0.58652100
H	-2.03436300	1.43732500	0.00475100
H	-1.77695200	0.79209300	-1.62980800
H	-1.73364200	-0.28801400	-0.23284800
C	10.96077400	-1.55626200	2.44465300
H	11.16953000	-1.32142100	3.49366800
H	10.81979200	-2.64284600	2.37665000
H	11.84625200	-1.30244200	1.85327400
C	7.20562600	3.36862800	0.96464800
H	7.62279500	3.10318700	1.94271200
H	8.02599200	3.31755500	0.23905500
H	6.85894400	4.40417600	1.01084600
C	4.01989300	3.99314000	0.16265000
H	3.66616300	4.17564900	-0.85847100
H	3.13683000	3.97501800	0.81109600
H	4.64791800	4.83694000	0.46009900

IM20

Cu	0.58944500	0.53248300	-2.94903500
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I	0.50834000	-0.20941200	-5.59269200
C	-5.50057000	-1.44836600	-1.53236300
H	-5.04723800	-1.40366000	-0.53521500
H	-6.17726800	-2.30995500	-1.56064400
H	-6.10374900	-0.54119500	-1.65885100
C	-4.41987500	-1.55007900	-2.61218200
H	-3.83861700	-2.46882400	-2.46598900
H	-4.88603800	-1.62620000	-3.60432500
C	-3.46788700	-0.35224600	-2.57634700
H	-3.04415600	-0.25489900	-1.57552300
H	-4.01093700	0.57904100	-2.77589000
C	-2.32702700	-0.51204000	-3.59139300
H	-2.69440300	-0.47799300	-4.62418700
H	-1.79630800	-1.45407700	-3.46090100
O	-1.54447300	1.80617200	-3.52996800
C	-1.36373400	0.63246500	-3.47587700
B	0.28679300	-0.88937400	1.10325000
O	1.53412500	-1.46059900	1.12078900
C	1.52181900	-2.53303200	2.09900600
C	0.32577800	-2.11787200	3.03370500
O	-0.49586700	-1.30411000	2.15089800
C	-0.11632700	0.15017700	-0.03427200
H	0.66587700	0.92308800	0.02302400
C	-1.42923000	0.91622000	0.12512300
C	-1.54633400	2.14032400	-0.54659800
C	-2.72656900	2.87867800	-0.51574800
C	-3.82232100	2.40978100	0.21131600
C	-3.71140600	1.21079500	0.91611100
C	-2.52535500	0.47304700	0.87892300
H	-0.70665500	2.51022100	-1.12340500
H	-2.78344900	3.81582700	-1.06216200
H	-4.74871900	2.97719600	0.23741600
H	-4.55083700	0.84450400	1.50150500
H	-2.44774600	-0.44011200	1.45601500
C	-0.52395700	-3.27636400	3.54171400
H	0.07388600	-3.95476900	4.16044000
H	-1.34428700	-2.89003000	4.15481400
H	-0.95360800	-3.84367300	2.71394000
C	0.74228900	-1.20778700	4.19227300
H	1.34011800	-0.36436300	3.83362500
H	-0.15752400	-0.80661100	4.66793200
H	1.32078900	-1.75145700	4.94590400
C	2.88248200	-2.57715700	2.78705500
H	2.88722100	-3.32359300	3.58909500

H	3.65240200	-2.85930700	2.06204300
H	3.15428500	-1.60757800	3.20976500
C	1.27978900	-3.83379100	1.32705400
H	2.05521700	-3.93938700	0.56334300
H	1.32287000	-4.70456300	1.98968600
H	0.31697900	-3.82306700	0.81249400
N	0.11003300	-0.49494500	-1.34541200
C	-0.31319500	-1.79871000	-1.52321500
C	-1.35798900	-2.42029300	-0.79667300
C	0.36000800	-2.58887000	-2.49035300
C	-1.69649000	-3.75520900	-1.02265000
H	-1.92427400	-1.85007200	-0.07406900
C	0.00095200	-3.90965500	-2.72144300
H	1.17887100	-2.14263000	-3.04233100
C	-1.02823500	-4.51251800	-1.98588900
H	-2.50547400	-4.19899100	-0.44669600
H	0.53725900	-4.47824600	-3.47702300
H	-1.30239000	-5.54808500	-2.16375300
C	2.29304900	1.65365600	-2.92198400
N	2.47144700	2.99704200	-3.00090600
C	3.82604000	3.34291900	-3.11078400
C	4.51635900	2.16612000	-3.09931800
N	3.55535700	1.15503800	-2.98890200
H	4.39129700	1.02088900	-0.40889900
C	-0.77561300	5.67373600	-2.67975400
C	-0.06691500	5.26975300	-1.54428200
H	-0.37628800	5.62544400	-0.56474700
C	1.02037700	4.39679400	-1.63344400
C	1.13827100	3.81214600	-5.41850200
H	0.62339500	4.35217000	-6.21796600
C	1.75665000	3.93999500	-0.39958600
H	2.81567400	4.22306400	-0.42812700
H	4.16723500	-3.12881500	-4.53580500
C	3.95172400	-2.99668100	-2.39996000
C	3.84786400	-2.12028600	-1.31429100
H	3.79102800	-2.51618500	-0.30571600
H	-0.89742000	5.51872600	-4.82200200
C	3.77564900	-0.74155200	-1.49717700
C	4.16638100	-0.53043600	-5.31107700
C	0.72064300	4.33205400	-4.06903400
H	5.23161900	-0.37512700	-5.53337200
C	3.80746900	-0.24849800	-2.81103200
C	3.99621500	-1.08108900	-3.91918400
C	4.05661000	-2.46052700	-3.68523100

H	1.31105800	4.37205300	0.50024200
H	1.72577500	2.84937400	-0.30515600
H	0.89973900	2.74731200	-5.51874800
H	2.21847400	3.91152400	-5.57549300
H	3.81599200	-0.32070100	0.61193400
H	2.66863400	0.65224400	-0.29941000
H	3.76854600	-1.22497200	-6.05479800
H	3.64703500	0.42046500	-5.43863900
C	-0.35975600	5.20664200	-3.93004100
C	3.66413800	0.20403100	-0.33127200
C	1.38837200	3.93386900	-2.90387900
C	-1.98444100	6.56903500	-2.55677400
H	-1.94795500	7.17005900	-1.64254300
H	-2.06835500	7.24905200	-3.41101900
H	-2.90776200	5.97568200	-2.52343600
C	3.89885700	-4.48770500	-2.18039400
H	4.43824600	-4.78135500	-1.27288500
H	2.85699400	-4.81340600	-2.06202000
H	4.32553400	-5.03711300	-3.02560300
C	5.97420300	1.86862300	-3.17483200
H	6.29104800	1.23121100	-2.34137100
H	6.23173100	1.34369200	-4.10213300
H	6.55531700	2.79385400	-3.13798400
C	4.27507400	4.75940500	-3.22133100
H	3.87856000	5.23792700	-4.12484700
H	3.93761000	5.35658700	-2.36611200
H	5.36623600	4.81015500	-3.26313500

TS15

Cu	0.62412700	0.54208200	-2.97831200
I	0.46713400	-0.13690200	-5.60454000
C	-5.60849700	-1.56304000	-1.69899400
H	-5.22639300	-1.51847600	-0.67210700
H	-6.25929400	-2.44085200	-1.78141700
H	-6.22477600	-0.67005500	-1.85853500
C	-4.45458100	-1.62483900	-2.70362700
H	-3.86486700	-2.53445700	-2.53389100
H	-4.85078300	-1.69219300	-3.72622700
C	-3.53211100	-0.41021700	-2.58088300
H	-3.16259900	-0.33822700	-1.55657300
H	-4.08412500	0.51725500	-2.77532900
C	-2.33936100	-0.50730600	-3.54416100
H	-2.64880400	-0.38507000	-4.58837200
H	-1.82432100	-1.46296300	-3.46405600

O	-1.54008500	1.78618400	-3.23873500
C	-1.37771600	0.61038500	-3.28279800
B	0.21583300	-0.81011900	1.04867100
O	1.47779900	-1.34677800	1.05153300
C	1.51186200	-2.40668200	2.04384400
C	0.31268200	-2.02021300	2.98720900
O	-0.54236400	-1.23958500	2.10754000
C	-0.24067000	0.21949100	-0.07844200
H	0.53075900	1.00430700	-0.05357200
C	-1.55821300	0.95840500	0.15410700
C	-1.68588800	2.24996800	-0.37429000
C	-2.87474100	2.96781000	-0.26479700
C	-3.96795900	2.41008100	0.39983900
C	-3.84673000	1.14023700	0.96562400
C	-2.65340200	0.42440500	0.84948900
H	-0.84968000	2.69189200	-0.90286900
H	-2.94139700	3.96107100	-0.70086900
H	-4.89972300	2.96246400	0.48679100
H	-4.68243300	0.70312300	1.50602800
H	-2.56791300	-0.54204200	1.33032000
C	-0.49570900	-3.19993000	3.51373700
H	0.12879100	-3.85488400	4.13140900
H	-1.32088800	-2.83336900	4.13239400
H	-0.91664800	-3.78682100	2.69521400
C	0.71157800	-1.08773900	4.13440100
H	1.27931200	-0.22897200	3.76346000
H	-0.19608800	-0.71060900	4.61466900
H	1.31358200	-1.60609600	4.88748100
C	2.87912300	-2.39650500	2.72045500
H	2.91103900	-3.12395700	3.53918000
H	3.65195300	-2.67356900	1.99686100
H	3.12611700	-1.41023100	3.11909700
C	1.30698600	-3.72521600	1.29202200
H	2.07216200	-3.80977100	0.51592200
H	1.39517500	-4.58494600	1.96461300
H	0.33631900	-3.75919100	0.79417800
N	-0.06118900	-0.42792300	-1.39821700
C	-0.37600000	-1.76946600	-1.54247800
C	-1.39345700	-2.43649500	-0.81958300
C	0.36508200	-2.53933200	-2.47206000
C	-1.64481700	-3.79500000	-1.01549700
H	-2.00805400	-1.88261900	-0.12455600
C	0.09276500	-3.88593600	-2.67657300
H	1.16445700	-2.05843900	-3.02364600

C	-0.91139100	-4.53310100	-1.94587500
H	-2.43643900	-4.27324700	-0.44311300
H	0.67917000	-4.43753500	-3.40694700
H	-1.11823900	-5.58753800	-2.10262300
C	2.33226100	1.62078400	-2.93451900
N	2.52097800	2.96306100	-3.01059700
C	3.87760900	3.29672100	-3.13339800
C	4.55745100	2.11366600	-3.13502100
N	3.58814900	1.11084400	-3.01762700
H	4.39560200	1.02402600	-0.46947600
C	-0.71291400	5.64630000	-2.61850000
C	0.00272600	5.21925000	-1.49591100
H	-0.29918800	5.55704900	-0.50759000
C	1.08685600	4.34524000	-1.60943600
C	1.18614700	3.84674300	-5.40844300
H	0.67948900	4.41767900	-6.19158800
C	1.83381500	3.86630300	-0.39045600
H	2.88994100	4.16067800	-0.41873500
H	4.14708000	-3.18807900	-4.54364800
C	3.97697400	-3.03880400	-2.40503400
C	3.89280600	-2.15345200	-1.32472500
H	3.86392300	-2.54306900	-0.31237700
H	-0.84394200	5.54027900	-4.76294100
C	3.81453400	-0.77608800	-1.51627500
C	4.13945700	-0.59487700	-5.33864000
C	0.77496400	4.33322600	-4.04440700
H	5.20029900	-0.43380600	-5.57746200
C	3.82833300	-0.29358200	-2.83464200
C	3.99343800	-1.13510600	-3.93998100
C	4.05394000	-2.51296000	-3.69642000
H	1.39023200	4.27357600	0.52192900
H	1.81528200	2.77371300	-0.32186100
H	0.93247400	2.78867200	-5.54054200
H	2.26756500	3.93541000	-5.56247500
H	3.92349600	-0.32976300	0.58575900
H	2.69550300	0.57955500	-0.28373300
H	3.73565600	-1.29828000	-6.07072900
H	3.61044000	0.35038900	-5.46706200
C	-0.30333300	5.20668000	-3.88057200
C	3.70891200	0.17747300	-0.35548800
C	1.44563300	3.90651500	-2.89109600
C	-1.92220500	6.53671300	-2.46924100
H	-1.87760300	7.12401100	-1.54639300
H	-2.01727400	7.22945100	-3.31201400

H	-2.84272300	5.93920300	-2.43528400
C	3.93919900	-4.52806800	-2.17063400
H	4.52373800	-4.81241700	-1.28841600
H	2.90603300	-4.85686200	-1.99843000
H	4.32623800	-5.08285500	-3.03117300
C	6.01124300	1.80222300	-3.22928900
H	6.33351300	1.16315800	-2.39914700
H	6.25066100	1.27326400	-4.15916600
H	6.60157700	2.72191000	-3.20218100
C	4.33855200	4.70976800	-3.23838900
H	3.94011100	5.19809200	-4.13573700
H	4.01221300	5.30367600	-2.37655400
H	5.42980600	4.75121200	-3.28733900

IM21

Cu	2.04060200	-0.63212400	-1.49472400
I	1.99284200	-3.19674500	-1.82383500
C	-4.56335100	-2.68321200	-5.74664500
H	-5.35411400	-2.51108500	-5.00618400
H	-4.86933500	-3.52918400	-6.37233400
H	-4.51104100	-1.79440400	-6.38743100
C	-3.21976900	-2.94878900	-5.06325000
H	-3.28909700	-3.85839900	-4.45123700
H	-2.44974700	-3.14680700	-5.82135400
C	-2.76782100	-1.78461700	-4.17763500
H	-3.53175400	-1.59209300	-3.41272700
H	-2.68640100	-0.86962900	-4.77997900
C	-1.41593300	-2.05803500	-3.49490200
H	-0.63259700	-2.21815700	-4.23955900
H	-1.47920900	-2.96020300	-2.88559800
O	-0.26651400	0.01676400	-3.18359000
C	-0.98541900	-0.85630400	-2.68087500
B	-0.41546500	0.03509300	0.70691400
O	0.84627000	-0.49990500	0.62781000
C	1.18782900	-1.05108400	1.94369300
C	0.20445200	-0.26116000	2.88649900
O	-0.89034300	0.08997900	1.98473000
C	-1.13014000	0.49751100	-0.62829900
H	-0.33250600	0.95759600	-1.21986800
C	-2.27231600	1.49774700	-0.57770800
C	-2.82281400	1.93593800	-1.79271400
C	-3.83375300	2.89363300	-1.81630400
C	-4.31908000	3.43052600	-0.61981600
C	-3.78752100	2.99152800	0.59192600

C	-2.77107100	2.03166200	0.61452300
H	-2.43991700	1.52763800	-2.72267000
H	-4.24238700	3.22393400	-2.76761700
H	-5.10852700	4.17683400	-0.63481100
H	-4.16768300	3.39040900	1.52897400
H	-2.36649800	1.69460300	1.56066600
C	-0.37465600	-1.07308300	4.03842200
H	0.42314600	-1.41554500	4.70637800
H	-1.05952000	-0.44651400	4.61821000
H	-0.92874600	-1.94163500	3.67882100
C	0.78163300	1.05773400	3.39893300
H	1.17113700	1.65754500	2.57437100
H	-0.01184900	1.63007800	3.88971000
H	1.58452200	0.88706700	4.12327700
C	2.67088700	-0.79818900	2.17775100
H	2.97285100	-1.16321800	3.16555000
H	3.24532900	-1.34100400	1.42030700
H	2.91845200	0.26185100	2.10455000
C	0.90812600	-2.55118000	1.90686200
H	1.46274200	-2.99906500	1.07928300
H	1.21968700	-3.02251200	2.84478100
H	-0.15330700	-2.75345400	1.74941800
N	-1.48959500	-0.71277500	-1.41286000
C	-2.29712000	-1.70197200	-0.76028100
C	-3.63771200	-1.42572000	-0.47047100
C	-1.72973800	-2.91955700	-0.37081000
C	-4.40601400	-2.36904000	0.21240600
H	-4.06690000	-0.47984300	-0.77891900
C	-2.51010300	-3.86349600	0.29683600
H	-0.68911500	-3.11968400	-0.60883200
C	-3.84605100	-3.58898400	0.59594500
H	-5.44606700	-2.15092500	0.43767700
H	-2.06650000	-4.81166900	0.58715200
H	-4.44933300	-4.32336300	1.12219800
C	2.87962000	0.96983100	-2.22680300
N	2.79583200	2.31498400	-2.03568000
C	3.64002500	3.02569700	-2.90221800
C	4.26765200	2.08863400	-3.66804000
N	3.78424800	0.85038700	-3.23539000
H	6.20950200	0.46653200	-2.07178100
C	0.30533100	4.17560500	0.81556200
C	1.58164700	3.72350100	1.16644400
H	1.93364700	3.85890200	2.18624500
C	2.41810700	3.09563600	0.23937600

C	0.21662500	3.24407100	-2.89472700
H	-0.75886700	3.71707600	-3.03177200
C	3.78711500	2.59329900	0.62270300
H	4.57558000	3.10408000	0.05626000
H	3.28731800	-2.59404700	-6.21169600
C	4.87103500	-2.91225600	-4.79257300
C	5.55909100	-2.36670900	-3.70556600
H	6.35636900	-2.93843500	-3.23691200
H	-1.11642900	4.35189900	-0.78908700
C	5.21997300	-1.12046600	-3.17898000
C	2.28300200	-0.17596500	-5.45250000
C	0.68635200	3.41197600	-1.47267200
H	2.52279500	0.87376100	-5.65984600
C	4.17350400	-0.41777200	-3.78714800
C	3.45954200	-0.92334800	-4.87986200
C	3.83712700	-2.17340900	-5.37323100
H	3.97746800	2.75384100	1.68783100
H	3.88750100	1.52458400	0.40702100
H	0.12517800	2.18404600	-3.15248000
H	0.91994800	3.69227500	-3.60600700
H	6.78019100	-1.17247400	-1.69330100
H	5.20875700	-0.60826300	-1.09505000
H	1.95172200	-0.63953500	-6.38657800
H	1.44190200	-0.18070100	-4.74794600
C	-0.12314900	4.01559300	-0.50603900
C	5.89872600	-0.57733300	-1.94810500
C	1.94501000	2.94266700	-1.06911100
C	-0.58972000	4.83665500	1.83411600
H	-0.31316900	4.54958300	2.85389100
H	-0.52472400	5.93080000	1.77027300
H	-1.63530300	4.55921500	1.66917000
C	5.19393900	-4.29980900	-5.28649500
H	6.24550300	-4.55439400	-5.11662200
H	4.58457200	-5.04053300	-4.75297700
H	4.98245600	-4.40757000	-6.35567200
C	5.27458000	2.20632700	-4.76014700
H	6.19628500	1.66666400	-4.51346200
H	4.89650300	1.78448700	-5.69853800
H	5.52816900	3.25526300	-4.93490600
C	3.74886200	4.51174300	-2.86593200
H	2.79009800	4.99607800	-3.08405700
H	4.07184400	4.86711400	-1.88003400
H	4.47717600	4.85506100	-3.60526500

IM22

Cu	-0.66213100	-0.57030200	0.43406900
C	-0.70446400	-2.08930200	1.60712500
N	-1.63289300	-3.07732500	1.66182100
C	-1.33878200	-4.01645800	2.65819400
C	-0.17991000	-3.59502500	3.24376600
N	0.18265800	-2.41632600	2.58010500
H	2.23200200	-3.90750400	1.48821100
C	-4.99164000	-3.21512200	-0.88689700
C	-3.80292800	-3.86286800	-1.23776900
H	-3.74625700	-4.39953500	-2.18151200
C	-2.67667700	-3.82715900	-0.41253000
C	-3.98877000	-1.66523800	2.46564400
H	-3.66131100	-2.25982300	3.32632600
C	-1.38108300	-4.48222600	-0.81891900
H	-1.01155400	-5.17275500	-0.05184900
H	2.29757400	0.93714000	4.87346600
C	3.57913900	-0.08108200	3.47656100
C	3.64515600	-1.09658200	2.51682200
H	4.58138400	-1.27716800	1.99448100
H	-5.95998500	-2.00644900	0.60787000
C	2.53290900	-1.87892400	2.19901500
C	-0.09548000	-0.33152000	4.51758800
C	-3.94416000	-2.45739700	1.18372200
H	-0.51861400	-1.22968400	4.98236700
C	1.33947800	-1.62316500	2.88547300
C	1.22551500	-0.61162400	3.84724600
C	2.36435600	0.14506000	4.13182000
H	-1.50262400	-5.03993600	-1.75125300
H	-0.59977400	-3.72807700	-0.97202500
H	-5.00036300	-1.30149600	2.66415100
H	-3.32051300	-0.79778600	2.40418400
H	3.61607400	-3.06585000	0.76362400
H	1.96076400	-2.65795500	0.27617200
H	0.01386500	0.43457600	5.28971300
H	-0.83011700	0.02424400	3.78533600
C	-5.04438000	-2.52064100	0.32632200
C	2.59321500	-2.93746300	1.12737600
C	-2.77662400	-3.12670600	0.79573300
C	-6.18189900	-3.23260300	-1.81423100
H	-6.17784300	-4.12028900	-2.45476500
H	-7.12419700	-3.21654300	-1.25676900
H	-6.17596600	-2.35354800	-2.47127500
C	4.78450300	0.77773900	3.77078100

H	5.71624600	0.21616100	3.64689100
H	4.82669900	1.63593100	3.08792700
H	4.75549700	1.17273600	4.79130800
C	0.63919500	-4.15924800	4.35325700
H	1.65468400	-4.40144100	4.01845900
H	0.73455600	-3.44830400	5.18220000
H	0.18061400	-5.07312300	4.73917200
C	-2.21478800	-5.19388800	2.91689200
H	-3.22970600	-4.88448600	3.19254600
H	-2.30240600	-5.83146500	2.02950500
H	-1.80973400	-5.79887500	3.73201700
I	-0.61731500	1.39739900	-1.07622800

IM23

Cu	-0.80672800	-0.83356600	0.11312300
C	-0.92406600	-2.23621700	1.37336200
N	-1.86098700	-3.19345000	1.60024600
C	-1.49109400	-4.05242000	2.64505000
C	-0.27792400	-3.61109400	3.08673800
N	0.04174400	-2.50278400	2.29394300
H	1.94771800	-4.14462800	1.15922600
C	-5.43627200	-3.51562100	-0.61462300
C	-4.27054100	-4.15917900	-1.04358800
H	-4.29040200	-4.74465800	-1.95964600
C	-3.07362000	-4.06057000	-0.33082800
C	-4.15545400	-1.77144400	2.54249800
H	-3.77254800	-2.32473300	3.40785500
C	-1.80618100	-4.71364200	-0.81976100
H	-1.34995000	-5.34768200	-0.05047900
H	2.40582000	1.06238000	3.93153600
C	3.51823500	-0.12391100	2.52221700
C	3.47764100	-1.25004400	1.69420100
H	4.34234100	-1.49447800	1.08233700
H	-6.28774600	-2.24682800	0.90088700
C	2.34183000	-2.05819500	1.61034600
C	-0.00746300	-0.21276800	4.00407500
C	-4.21608200	-2.63080700	1.30534300
H	-0.39924500	-1.04666800	4.59757200
C	1.23601200	-1.71384600	2.39751500
C	1.23336900	-0.59477600	3.23939000
C	2.39186700	0.18324600	3.29208900
H	-1.99931200	-5.32917100	-1.70248100
H	-1.06330600	-3.95241600	-1.08665100
H	-5.14496700	-1.38138000	2.79565400

H	-3.48078200	-0.92135000	2.38534700
H	3.24987400	-3.41133200	0.20084200
H	1.55341200	-3.02059500	-0.14040700
H	0.19082400	0.62604200	4.67652300
H	-0.80121000	0.08508400	3.30810000
C	-5.39086500	-2.75858500	0.56042500
C	2.27519600	-3.22554700	0.65984000
C	-3.07569400	-3.30018600	0.84544200
C	-6.70695700	-3.60631100	-1.42401100
H	-6.78957100	-4.57209900	-1.93338300
H	-7.59288100	-3.47448200	-0.79455500
H	-6.73450300	-2.82663700	-2.19607700
C	4.73239000	0.77112700	2.54378200
H	5.64842800	0.21060800	2.33092600
H	4.64400200	1.55695600	1.78262300
H	4.84998300	1.26598800	3.51329200
C	0.62880900	-4.10102000	4.16282000
H	1.60973500	-4.38275800	3.76222700
H	0.80122400	-3.33153800	4.92462800
H	0.19783500	-4.97644900	4.65535100
C	-2.35366300	-5.18766400	3.07804400
H	-3.33446500	-4.83994900	3.42334200
H	-2.53316800	-5.89130400	2.25667800
H	-1.87910300	-5.73415500	3.89708900
O	-0.61740900	0.51057300	-1.07566300
C	0.50315700	1.34462700	-1.13437100
C	1.77280100	0.53315700	-1.47190100
H	1.98119100	-0.18450500	-0.66880900
H	1.61389500	-0.02750300	-2.40021700
H	2.65765700	1.17254200	-1.59657100
C	0.25133700	2.38347500	-2.24401000
H	-0.65349000	2.95650600	-2.01308900
H	1.09018600	3.08284800	-2.35712400
H	0.09167300	1.87086200	-3.19904300
C	0.71874000	2.07359500	0.20973900
H	-0.19085900	2.62252000	0.47968900
H	0.92581600	1.34331200	1.00156000
H	1.55667000	2.78350900	0.17161000

TS16

B	-4.37667000	-4.22961000	-2.04177700
C	-4.97211600	-5.89934400	-0.56227300
C	-4.34293700	-7.20497000	-1.05682900
H	-5.00859900	-8.05885900	-0.89191600

H	-3.41532200	-7.38535200	-0.50740500
H	-4.09813300	-7.13774900	-2.12041200
C	-6.21562800	-5.46930900	-1.40598400
C	-7.12992900	-4.48425500	-0.66504000
H	-7.70231400	-4.97726700	0.12872500
H	-7.83451600	-4.05158000	-1.38239500
H	-6.54588200	-3.67086800	-0.22482900
C	-7.03321600	-6.61258400	-1.99567000
H	-7.86730400	-6.20640600	-2.57715800
H	-7.44714900	-7.24752500	-1.20346300
H	-6.42727800	-7.23154400	-2.66051100
C	-5.20603000	-5.96000100	0.94294100
H	-5.52540500	-4.99270600	1.33373200
H	-4.27389200	-6.23709700	1.44639500
H	-5.96364600	-6.71257800	1.19194000
O	-5.60127400	-4.72971700	-2.48921100
O	-4.03410000	-4.82530200	-0.83655100
B	-2.69972800	-3.89840900	-3.60415700
C	-0.99561400	-5.38672000	-3.06029500
C	-1.05798900	-5.83715000	-1.59818600
H	-0.05339000	-5.96704600	-1.18039900
H	-1.57173100	-6.79992800	-1.54962100
H	-1.62218100	-5.12833500	-0.99004100
C	-0.42713200	-3.93016100	-3.21780100
C	0.13828700	-3.65746100	-4.62021100
H	1.07054100	-4.20416500	-4.80039000
H	0.34252900	-2.58627900	-4.71478000
H	-0.58804000	-3.92816500	-5.39065800
C	0.59248800	-3.52005800	-2.15977700
H	0.90820600	-2.48568600	-2.33487200
H	1.48243800	-4.15863400	-2.20415700
H	0.16784400	-3.58088700	-1.15576800
C	-0.26565800	-6.44126900	-3.89138100
H	-0.31302400	-6.21103100	-4.95789700
H	-0.73555800	-7.41786800	-3.73559800
H	0.78685100	-6.51864000	-3.59306900
O	-1.60764200	-3.12503500	-3.05663800
O	-2.33550600	-5.27033100	-3.58152000
C	-3.71260000	-3.37217000	-7.07070300
C	-4.23222900	-3.76875300	-5.68305900
H	-3.51279800	-2.29740900	-7.09666400
H	-2.77995200	-3.90241300	-7.29319700
H	-4.44587200	-3.61706000	-7.84845400
C	-4.44292000	-5.28546500	-5.61273200

C	-5.54441700	-3.03074800	-5.38035300
H	-4.84040400	-5.57653600	-4.63901400
H	-5.16123600	-5.58554100	-6.38553400
H	-3.50322000	-5.81747700	-5.77735200
H	-6.31162500	-3.28685600	-6.12174000
H	-5.91390400	-3.31167800	-4.39078000
H	-5.37851800	-1.94942300	-5.41394000
O	-3.23118900	-3.29451400	-4.76768400
Cu	-3.96844900	-2.31406700	-2.56900500
C	-4.06492700	-0.41698300	-2.19800900
N	-4.07334100	0.07132600	-0.93149700
C	-3.96205600	1.46625400	-0.90532300
C	-3.89003000	1.86108400	-2.21078800
N	-3.96103000	0.68829500	-2.97526500
H	-1.34451000	0.75362300	-3.35469900
C	-4.31030300	-2.52611700	2.38628500
C	-3.08318000	-2.26867800	1.76755100
H	-2.18766800	-2.76600000	2.13202200
C	-2.97493300	-1.40638900	0.67528300
C	-6.65222100	-0.45078400	0.18788500
H	-6.59844200	0.64056800	0.10362800
C	-1.65907300	-1.20332400	-0.03026100
H	-1.49185400	-0.15287100	-0.29291300
H	-5.91161500	0.89324700	-7.11422300
C	-3.79721700	0.49483900	-7.18628700
C	-2.64595300	0.29911800	-6.41792300
H	-1.70363000	0.08163500	-6.91466600
H	-6.42294800	-2.11805500	2.33629500
C	-2.67134800	0.35321400	-5.02163700
C	-6.39610900	1.02899400	-4.43134100
C	-5.40068100	-1.04121400	0.78620100
H	-6.37817700	1.90324000	-3.77012900
C	-3.89930000	0.63050100	-4.40802000
C	-5.08021000	0.82037100	-5.13748900
C	-5.00493700	0.75509700	-6.53034500
H	-0.82825300	-1.53872100	0.59740200
H	-1.63376000	-1.78006900	-0.96321200
H	-7.52899500	-0.70419800	0.79018800
H	-6.80907200	-0.84087200	-0.82536400
H	-0.53826000	0.16857500	-4.82523700
H	-1.46906900	-0.95149000	-3.81202200
H	-7.20679900	1.16430000	-5.15236900
H	-6.63613000	0.16164500	-3.80464300
C	-5.45814900	-1.90878300	1.88055800

C	-1.43625800	0.07172200	-4.20741300
C	-4.14773000	-0.79090300	0.21487000
C	-4.38563300	-3.45042700	3.57684300
H	-3.97817500	-2.97174000	4.47670400
H	-5.41846600	-3.73972500	3.79402300
H	-3.80814900	-4.36463900	3.40354200
C	-3.74652600	0.37371800	-8.68937600
H	-2.79851600	0.74762100	-9.09024900
H	-3.83806200	-0.67672700	-8.99483000
H	-4.56227200	0.92755600	-9.16492100
C	-3.73330800	3.20500200	-2.83505000
H	-2.81345500	3.26234200	-3.42879000
H	-4.56607200	3.43909600	-3.50828700
H	-3.69099800	3.97975400	-2.06506700
C	-3.91800100	2.23400800	0.37102800
H	-4.82767900	2.08350600	0.96408100
H	-3.07176800	1.92146300	0.99412700
H	-3.81640900	3.30361100	0.16994400

TS13'

Cu	0.10248400	0.02049300	0.66958300
B	-1.59028600	-2.27239500	0.05899800
O	-2.42131500	-1.32771600	-0.53069200
C	-3.65243500	-2.00923100	-0.87744400
C	-3.22889500	-3.52797400	-0.84101000
O	-2.15898700	-3.52142400	0.14008400
C	-2.61553300	-4.01513800	-2.15848400
H	-2.15562300	-4.99249100	-1.99155400
H	-3.37164300	-4.10685400	-2.94554100
H	-1.82295500	-3.34304300	-2.49859600
C	-4.31421100	-4.48676900	-0.36840600
H	-5.17502000	-4.46387600	-1.04641900
H	-3.91768400	-5.50648300	-0.35544600
H	-4.65505100	-4.24285200	0.64052900
C	-4.11734600	-1.51190000	-2.24162700
H	-5.01034300	-2.05515000	-2.57096600
H	-4.36382600	-0.44799300	-2.17851300
H	-3.33448400	-1.63431300	-2.99276400
C	-4.67608100	-1.64381100	0.20193700
H	-4.76967200	-0.55420400	0.24570900
H	-5.66263400	-2.06834800	-0.01112100
H	-4.34881000	-1.99827600	1.18430400
C	0.46217500	-2.07857200	-0.73667100
H	0.26113200	-1.27548800	-1.43748100

C	0.87302100	-3.34860300	-1.24679800
C	1.40262100	-3.42348500	-2.56762000
C	1.80977700	-4.62410800	-3.12783100
C	1.72055700	-5.82409700	-2.40785400
C	1.20458800	-5.77551600	-1.11136500
C	0.79155600	-4.57703500	-0.53446700
H	1.48507100	-2.50380000	-3.14510300
H	2.20323700	-4.62894000	-4.14288400
H	2.04353700	-6.76357400	-2.84716500
H	1.11547600	-6.69193300	-0.53052200
H	0.36739800	-4.59312000	0.46140900
N	-0.26724900	-1.91349400	0.55291800
C	0.29191800	-2.39064900	1.77901400
C	1.66491100	-2.65003900	1.89379200
C	-0.54063400	-2.56490200	2.89546500
C	2.18972400	-3.06457700	3.11671700
H	2.28787600	-2.54057200	1.01411300
C	-0.00367000	-2.97909400	4.11098300
H	-1.60780500	-2.38404300	2.79685400
C	1.36671300	-3.23408300	4.23122400
H	3.25382400	-3.27416400	3.18947000
H	-0.66102500	-3.11276300	4.96640400
H	1.78038400	-3.57568300	5.17600900
C	0.20570700	1.84951300	1.10047200
N	0.88581100	2.39389900	2.13998600
C	0.62691100	3.76381600	2.26828200
C	-0.24315400	4.08058900	1.26396400
N	-0.47966400	2.88974800	0.56428700
H	0.82819800	4.25536200	-1.53520500
C	3.29194400	0.00159400	4.64684500
C	3.85606300	0.70809800	3.58174500
H	4.92211400	0.62033200	3.38767000
C	3.08073700	1.51245900	2.74210300
C	-0.39026800	0.95461200	4.27216900
H	-0.77699100	1.97831500	4.21929700
C	3.68366800	2.22018400	1.55498400
H	3.48772800	3.29866700	1.57301600
H	-4.57384900	1.87832600	-1.22434700
C	-3.10387900	2.40334900	-2.70492800
C	-1.77548000	2.79245800	-2.90757200
H	-1.41663000	2.95933100	-3.92018100
H	1.46040700	-0.45588600	5.67798700
C	-0.89059700	2.96278000	-1.84074100
C	-3.15751200	1.99385700	1.09445700

C	1.10121000	0.90147500	4.06152000
H	-2.78694500	2.70728000	1.83779000
C	-1.37602300	2.73589100	-0.54630400
C	-2.69283800	2.32745800	-0.29925800
C	-3.54460100	2.18358600	-1.39674600
H	4.76636200	2.07210700	1.52308500
H	3.25958400	1.83479300	0.61976400
H	-0.65917800	0.53050100	5.24312000
H	-0.90483800	0.37198600	3.49882800
H	0.75191200	3.48903400	-3.13165300
H	1.21901000	2.54636900	-1.70385200
H	-4.24982800	1.97406600	1.14699700
H	-2.78820600	1.00128700	1.37971700
C	1.91590700	0.11183700	4.87211000
C	0.55232600	3.33739000	-2.06757900
C	1.71049200	1.60258300	3.01035500
C	4.13397300	-0.89623600	5.51729800
H	3.94145000	-0.71829900	6.58145900
H	3.90031500	-1.94852400	5.31673000
H	5.20244800	-0.74750900	5.33450800
C	-4.02974300	2.18170700	-3.87527000
H	-4.01053300	1.13030100	-4.18986300
H	-5.06594500	2.42578000	-3.61876400
H	-3.73850000	2.78817900	-4.73868900
C	-0.90036900	5.36275500	0.88446300
H	-0.63099500	5.66954200	-0.13296900
H	-1.99264900	5.27502000	0.91618400
H	-0.60209400	6.16051200	1.56936500
C	1.23861200	4.58412700	3.35130700
H	0.99174200	4.18206600	4.34067000
H	2.33205400	4.60310400	3.27483700
H	0.87682000	5.61421800	3.30090700

TS17^{OSS}

Cu	0.22108800	0.02335400	-0.22767200
C	0.18880100	-1.94284600	0.22094100
N	-0.89381600	-2.73630500	0.45916400
C	-0.52793300	-4.04623000	0.80134600
C	0.83331000	-4.06769800	0.79644100
N	1.24289400	-2.77513300	0.44094500
B	-2.38565500	1.37987700	-0.89784400
O	-1.27073400	0.99377000	-1.63017600
C	-1.33329800	1.71605400	-2.90221300
C	-2.88355900	1.89844900	-3.06479300

O	-3.33562000	1.98990100	-1.68513000
C	-1.17062600	0.85890000	1.16903800
H	-1.27751000	0.01450000	1.84489300
C	-0.41201300	1.96713400	1.72907600
C	0.50662100	1.73376400	2.78176000
C	1.21843000	2.77356800	3.36293400
C	1.05360400	4.08757100	2.90607400
C	0.14152900	4.33901600	1.87414500
C	-0.57523100	3.30248200	1.29133100
H	0.62597000	0.71905200	3.15217900
H	1.90751200	2.56377900	4.17650500
H	1.61391300	4.90078100	3.35633800
H	-0.00613300	5.35595400	1.52052400
H	-1.29669300	3.51503600	0.50989800
H	2.08475100	-0.67930700	2.52852500
C	-4.94445600	-1.69269300	-0.11254700
C	-4.40353300	-1.74276700	1.17076000
H	-5.02894300	-1.49056300	2.02258800
C	-3.06162300	-2.07297700	1.39219300
C	-1.87059200	-2.58055100	-2.21366900
H	-2.45726300	-2.65545800	-3.13382800
C	-2.52958600	-2.13269800	2.80259500
H	-1.43802200	-2.09124900	2.83250200
H	5.03272700	-2.58077900	-2.11363100
C	5.32986100	-1.87892500	-0.10141000
C	4.71083300	-1.64965500	1.12961100
H	5.29117300	-1.23619300	1.94938800
H	-4.52168000	-1.94021000	-2.20761700
C	3.35507700	-1.91776400	1.32997300
C	2.37226700	-3.17072200	-2.14712900
C	-2.76307400	-2.29093200	-1.03331500
H	1.68028300	-2.37546300	-2.45070600
C	2.62848000	-2.44176700	0.25752900
C	3.21070100	-2.69239800	-0.99101400
C	4.56801300	-2.41087500	-1.14557900
H	-2.84027500	-3.05846200	3.30459200
H	-2.92410500	-1.29561100	3.38599900
H	-1.12599100	-1.78797200	-2.34156000
H	-1.31832900	-3.51805100	-2.08239600
H	2.00929500	-2.38663500	2.96972800
H	3.42411100	-1.41182300	3.42325300
H	1.76925600	-4.04957500	-1.89094400
H	3.00009500	-3.42159900	-3.00647100
C	-4.10949100	-1.97049500	-1.20224900

C	2.68423100	-1.59003800	2.63768200
C	-2.25923600	-2.33765100	0.27715700
C	-6.39567400	-1.34747800	-0.33435000
H	-6.86171600	-0.98880700	0.58662400
H	-6.96081000	-2.21918300	-0.68851700
H	-6.50136100	-0.56171200	-1.09104100
C	6.77593200	-1.50779100	-0.31554100
H	7.26289800	-2.17726700	-1.03254700
H	7.34176700	-1.53607800	0.62124500
H	6.85232700	-0.48826800	-0.71519900
C	-3.57069400	0.68014800	-3.68385700
H	-4.65368500	0.78381100	-3.56369100
H	-3.25845400	-0.23754800	-3.18259300
H	-3.34663500	0.59253400	-4.75156300
C	-3.30384300	3.17129900	-3.78899400
H	-2.91162500	3.17908000	-4.81190700
H	-2.94765600	4.06286700	-3.26980100
H	-4.39597100	3.22089000	-3.84186900
C	-0.59405400	3.04086800	-2.70503500
H	-1.08161600	3.65648700	-1.94263100
H	-0.55578900	3.61122100	-3.63861100
H	0.42600300	2.83024900	-2.37716600
C	-0.65856500	0.87790100	-3.97723800
H	-1.09229500	-0.12234700	-4.03849300
H	0.40545800	0.78048600	-3.74540200
H	-0.76065500	1.36370000	-4.95421800
N	-2.42247500	1.19122500	0.50887100
C	-3.56296800	1.38883900	1.32546400
C	-3.44506800	1.41552400	2.72626600
C	-4.84718100	1.53041500	0.76659800
C	-4.57557400	1.54055600	3.53479000
H	-2.46934600	1.35255200	3.18877200
C	-5.96448000	1.66853000	1.58319600
H	-4.96370800	1.52338800	-0.30780500
C	-5.84632600	1.66088000	2.97542300
H	-4.45038600	1.55523500	4.61442600
H	-6.94267100	1.77472100	1.12092100
H	-6.72367700	1.76287100	3.60724500
C	1.80814100	-5.15609300	1.09024600
H	2.45857000	-4.89301600	1.93247900
H	2.45996900	-5.35418700	0.23205400
H	1.28060100	-6.07981800	1.34191900
C	-1.53212500	-5.11493900	1.06719700
H	-1.03124200	-6.07629700	1.20796200

H	-2.23484900	-5.21440500	0.23215900
H	-2.12431300	-4.90725500	1.96545400
I	2.44552400	0.88852300	-1.37021700
C	5.97851200	1.58547800	2.25152400
H	6.53161500	1.18980500	1.39081200
H	6.53379600	2.45241800	2.63170600
H	5.98856600	0.81797400	3.03499000
C	4.55141500	1.96645100	1.85549700
H	3.99424500	2.30150800	2.73960500
H	4.02401300	1.08907800	1.46561000
C	4.50411100	3.06717900	0.79037700
H	5.02361200	3.96634300	1.17365500
H	5.09505400	2.75252200	-0.08500900
C	3.12273700	3.42039100	0.36269300
H	2.25880400	3.04423800	0.88402600
H	2.95812000	4.14057000	-0.43164300

IM24

Cu	0.26775000	-0.22810800	-0.81315900
C	0.04274800	-1.97780200	0.07007900
N	-1.02706400	-2.82026900	0.03906000
C	-0.72424100	-4.09193500	0.54854900
C	0.58164300	-4.03942700	0.93065900
N	1.02090100	-2.74355700	0.63464200
B	-2.32783800	1.73045200	-0.36031700
O	-1.54281400	1.22054700	-1.36724800
C	-1.95336000	1.88645700	-2.61228900
C	-3.41552900	2.35427200	-2.25598800
O	-3.36403700	2.50330800	-0.80626000
C	-0.71854800	1.14476300	1.38612600
H	-0.59541000	0.31206200	2.06991300
C	0.40450900	1.93964200	1.02915000
C	1.71633300	1.45647800	1.29213200
C	2.83495700	2.18076600	0.91846200
C	2.69635100	3.41605000	0.27539500
C	1.41395800	3.92416500	0.03253400
C	0.28606800	3.21110200	0.40592700
H	1.83592800	0.48783700	1.75740400
H	3.82107900	1.76552600	1.10373200
H	3.57361400	3.97335800	-0.03754400
H	1.29823700	4.88992500	-0.45185500
H	-0.70007300	3.63373900	0.24483100
H	0.71121500	-1.37493700	2.88929400
C	-4.90761000	-1.97117500	-1.36549700

C	-4.60511000	-1.87263200	-0.00396900
H	-5.38305500	-1.59165400	0.70035200
C	-3.31838100	-2.12411600	0.47993500
C	-1.47033000	-2.87115000	-2.79508200
H	-1.86519100	-3.00237800	-3.80625100
C	-3.00433700	-2.03499500	1.95170500
H	-2.11366000	-1.42498400	2.12443700
H	5.30032800	-1.93307200	-0.76611900
C	4.93437400	-1.30413600	1.25933500
C	3.99268800	-1.27092100	2.29193100
H	4.26642900	-0.84147300	3.25271200
H	-4.09991600	-2.35191400	-3.32401700
C	2.69590300	-1.76213200	2.11449300
C	2.91249100	-3.02742600	-1.49421800
C	-2.57726600	-2.54620100	-1.82492100
H	2.22358100	-2.37839400	-2.04437100
C	2.36167400	-2.28641500	0.86031100
C	3.29138300	-2.39221700	-0.18314700
C	4.57242600	-1.88514600	0.03945400
H	-2.80217200	-3.02413200	2.38097600
H	-3.83221100	-1.58432900	2.50238400
H	-0.72271700	-2.06937500	-2.82017300
H	-0.93990300	-3.78673600	-2.50918500
H	1.53279400	-2.71737400	3.67513700
H	2.02512700	-1.05808100	4.03819200
H	2.42340400	-3.99748000	-1.34529600
H	3.79627300	-3.17701400	-2.11974000
C	-3.88179000	-2.29643200	-2.26015400
C	1.68859300	-1.72279900	3.23765400
C	-2.32696600	-2.47023200	-0.44832200
C	-6.31370300	-1.73145300	-1.85878400
H	-6.82855500	-0.98518400	-1.24486600
H	-6.90840300	-2.65341700	-1.82029100
H	-6.31894300	-1.38061500	-2.89552600
C	6.30810600	-0.70760100	1.44466200
H	7.08296600	-1.33845400	0.99550600
H	6.54826900	-0.57271900	2.50401900
H	6.37282000	0.27566900	0.96123100
C	-4.47876600	1.29675000	-2.54614300
H	-5.42926000	1.61616800	-2.10700500
H	-4.20085100	0.33765100	-2.10798600
H	-4.62455400	1.15796900	-3.62200400
C	-3.82288300	3.69340300	-2.85788600
H	-3.80272500	3.64277700	-3.95191700

H	-3.16258500	4.49932700	-2.53337500
H	-4.84250500	3.93978500	-2.54564900
C	-0.99383800	3.05114700	-2.85006900
H	-1.07508900	3.80434800	-2.06243700
H	-1.20523300	3.53044900	-3.81153000
H	0.03114500	2.67501700	-2.85998200
C	-1.86061600	0.87124400	-3.74196400
H	-2.42864000	-0.03250800	-3.51133500
H	-0.81290700	0.59757800	-3.89211300
H	-2.24586200	1.30393300	-4.67227800
N	-2.04113000	1.45999500	1.02651300
C	-3.04512600	1.36780800	2.02101200
C	-2.69912100	1.44219400	3.37921800
C	-4.38990500	1.14775500	1.67608100
C	-3.66870000	1.26921200	4.36594700
H	-1.67127500	1.65137300	3.65560600
C	-5.35162500	0.99263600	2.66928700
H	-4.67296300	1.09171300	0.63362700
C	-5.00056800	1.03879400	4.02169000
H	-3.37772600	1.32817300	5.41119700
H	-6.38626400	0.82418400	2.38168400
H	-5.75486000	0.90814800	4.79174900
C	1.48434300	-5.06754000	1.52144400
H	1.83942100	-4.77317200	2.51586100
H	2.37065600	-5.22476600	0.89652600
H	0.96086000	-6.02211600	1.61857800
C	-1.71655900	-5.20393600	0.56431200
H	-1.25337000	-6.11739500	0.94630600
H	-2.09727300	-5.41050000	-0.44274600
H	-2.58301600	-4.97447400	1.19499100
I	1.99509100	0.49593500	-2.63719500

IM25

Cu	5.65633700	-2.11020200	-0.83138400
B	3.68853300	-4.50390800	-2.16008900
O	2.52947900	-5.07829900	-2.63154800
C	1.52719300	-4.87757000	-1.59168200
C	2.40746500	-4.69988600	-0.29760900
O	3.63531000	-4.16206200	-0.83966100
C	2.77395300	-6.01945000	0.38703000
H	3.56941600	-5.81684600	1.10953500
H	1.91642900	-6.45496700	0.91059300
H	3.14577500	-6.75158200	-0.33751300
C	1.86640100	-3.70680700	0.72185700

H	0.90322300	-4.04442600	1.12218300
H	2.58406500	-3.61868700	1.54170900
H	1.74220800	-2.71903300	0.27553800
C	0.60171300	-6.08720100	-1.57776300
H	-0.13047100	-6.00123100	-0.76698800
H	0.05648800	-6.14646600	-2.52518300
H	1.15935700	-7.01690800	-1.44787200
C	0.74950500	-3.61026100	-1.96544600
H	0.31213200	-3.74540700	-2.96027900
H	-0.06282400	-3.42023100	-1.25617300
H	1.40803300	-2.73887200	-1.99146200
C	6.02056400	-3.70475200	-2.23687500
H	6.63938200	-3.16309200	-2.94637900
C	6.87771700	-4.60411800	-1.43129100
C	8.20602700	-4.21137200	-1.18878300
C	9.06313300	-5.00696400	-0.43965400
C	8.61373300	-6.22600900	0.07334500
C	7.30275500	-6.63542400	-0.17731200
C	6.44045400	-5.83424500	-0.91959500
H	8.55700300	-3.25933600	-1.57532500
H	10.08121400	-4.67584800	-0.25826600
H	9.27886000	-6.85167200	0.66187400
H	6.94517400	-7.58263600	0.21710600
H	5.42341300	-6.15802900	-1.09758600
N	4.88436100	-4.27456100	-2.91806400
C	4.93875100	-4.30201100	-4.33168000
C	6.16849700	-4.49719800	-4.98590300
C	3.79031400	-4.08112600	-5.11298800
C	6.25139900	-4.43265900	-6.37560600
H	7.05442000	-4.72245900	-4.40155000
C	3.88274400	-4.03689600	-6.50259100
H	2.83569500	-3.94025100	-4.62429600
C	5.11204600	-4.19509200	-7.14601400
H	7.21370800	-4.58530500	-6.85701100
H	2.98277900	-3.85944900	-7.08570000
H	5.17820000	-4.14807000	-8.22892500
I	5.84239600	-3.19975900	1.66578400
C	4.43924700	0.28586400	-7.22859100
H	4.02468900	-0.66823200	-7.57451900
H	5.00025900	0.73095700	-8.05795000
H	3.59800600	0.95084800	-6.99685100
C	5.32738700	0.06920600	-6.00097700
H	6.16114800	-0.59403000	-6.26982200
H	5.77805700	1.02354000	-5.69091400

C	4.55706100	-0.54773000	-4.83183400
H	4.09135100	-1.48239900	-5.15825800
H	3.73991100	0.11108500	-4.51563200
C	5.46153500	-0.84709800	-3.63598800
H	5.91000100	0.06079500	-3.21941800
H	6.29767800	-1.48311300	-3.94324800
O	3.54167200	-1.68908100	-2.46988700
C	4.73146100	-1.54053700	-2.49999400
C	5.95556600	-0.19125100	-0.13293500
N	5.09369400	0.85761900	-0.02876100
C	5.68872500	1.97115600	0.57969400
C	6.97681300	1.61550400	0.83943300
N	7.11228100	0.28777500	0.40473900
H	8.49776600	0.12305200	3.69276900
C	1.18996100	0.63407200	-1.61395300
C	1.48728000	0.08687300	-0.36063100
H	0.70877200	-0.43330100	0.19185500
C	2.75948500	0.18398400	0.20364600
C	4.51267500	2.27945600	-2.50612800
H	4.36652200	3.35358100	-2.33317400
C	3.05806600	-0.38064900	1.56592400
H	3.53307100	0.37014500	2.20897300
H	10.89897000	-1.61747500	-1.34602700
C	10.71757800	-1.89567500	0.77905500
C	9.93207800	-1.61385400	1.89863600
H	10.24574600	-1.97640800	2.87484400
H	1.96073900	1.80639500	-3.24235100
C	8.73975800	-0.89296000	1.80869800
C	8.66660600	-0.23590600	-1.97297300
C	3.47760300	1.47068800	-1.76090100
H	8.19991300	0.75396000	-1.93919000
C	8.33236200	-0.45985200	0.53689800
C	9.10340200	-0.70363600	-0.60860800
C	10.29404300	-1.42098100	-0.46387900
H	2.13897400	-0.71669900	2.05331500
H	3.74805100	-1.23004300	1.51695000
H	4.43493100	2.11724900	-3.58517200
H	5.53138600	2.03796200	-2.19457200
H	7.82744100	-1.51842000	3.64344200
H	6.96393500	-0.21089400	2.85426400
H	9.51808600	-0.19385100	-2.65871100
H	7.92808500	-0.92157200	-2.40032200
C	2.18559900	1.34715200	-2.28242100
C	7.95945300	-0.60091900	3.06567100

C	3.75213000	0.84293700	-0.53864900
C	-0.17110900	0.43354100	-2.23173300
H	-0.96672000	0.50138900	-1.48179200
H	-0.37235100	1.17313700	-3.01309300
H	-0.24066900	-0.56132000	-2.69035200
C	11.98977300	-2.69538300	0.91796400
H	12.68935100	-2.21703900	1.61401000
H	11.78049800	-3.69790300	1.31021000
H	12.49783200	-2.81048500	-0.04444800
C	8.10817000	2.39338500	1.41969800
H	8.37929700	2.04557600	2.42183900
H	9.00236400	2.30937400	0.79247000
H	7.83897300	3.45057900	1.49016100
C	4.93499800	3.22566700	0.86119600
H	4.61957300	3.73563400	-0.05561700
H	4.03080700	3.01796000	1.44472400
H	5.55640800	3.91703800	1.43603700

TS18

Cu	5.66304400	-2.13975800	-0.80507200
B	3.59163800	-4.53911000	-2.15793300
O	2.41259700	-5.14566500	-2.52476500
C	1.49196500	-4.91584500	-1.41914900
C	2.46708300	-4.72321300	-0.20161700
O	3.63466700	-4.15503800	-0.84864100
C	2.92186300	-6.03680400	0.43942000
H	3.77864500	-5.81798900	1.08300900
H	2.12571300	-6.48944400	1.03982000
H	3.23516000	-6.75989300	-0.32130500
C	1.97635900	-3.75317800	0.86288200
H	1.04246800	-4.11437700	1.30973100
H	2.73504300	-3.66276400	1.64409300
H	1.80780100	-2.76309700	0.43805500
C	0.55746500	-6.11249100	-1.30963600
H	-0.10383700	-6.00410800	-0.44270600
H	-0.06436700	-6.18160500	-2.20789800
H	1.11491900	-7.04600900	-1.20877300
C	0.70917700	-3.64165200	-1.75831300
H	0.20594200	-3.78235200	-2.72066600
H	-0.05134600	-3.42602300	-1.00081900
H	1.37960300	-2.78114800	-1.83871800
C	5.88596700	-3.70317200	-2.50847300
H	6.43557500	-3.23041100	-3.31553500
C	6.82919100	-4.48281700	-1.67031200

C	8.13648500	-3.98791700	-1.50609400
C	9.07244000	-4.68367200	-0.75144800
C	8.72671500	-5.89893500	-0.15686200
C	7.43839000	-6.40696800	-0.32892400
C	6.49527100	-5.70769000	-1.07542600
H	8.40977900	-3.04076300	-1.96371200
H	10.07066000	-4.27613400	-0.62908600
H	9.45477000	-6.44439700	0.43673700
H	7.15994900	-7.34982300	0.13319400
H	5.49651300	-6.10660300	-1.19407600
N	4.71607000	-4.33881900	-3.02695000
C	4.58721100	-4.32993400	-4.44130900
C	5.70245000	-4.63464300	-5.23888000
C	3.38795800	-3.95585000	-5.06745100
C	5.62749700	-4.53989300	-6.62718600
H	6.62236400	-4.95993900	-4.76270900
C	3.31687400	-3.88262800	-6.45709700
H	2.52670900	-3.70969200	-4.46190800
C	4.43505500	-4.16016500	-7.24642500
H	6.50239800	-4.77799500	-7.22596800
H	2.38242300	-3.58400500	-6.92448300
H	4.37535900	-4.09099400	-8.32867400
I	5.87783900	-3.31210600	1.64746700
C	5.12066200	0.21786600	-7.29309000
H	4.93871500	-0.78796300	-7.68971200
H	5.72675700	0.76739100	-8.02204100
H	4.15015000	0.72295300	-7.21381400
C	5.81188800	0.13904300	-5.92924900
H	6.79159800	-0.34587100	-6.04427300
H	6.01431500	1.15173900	-5.55096000
C	4.98080600	-0.64277500	-4.91031500
H	4.74996500	-1.63324800	-5.31533400
H	4.01484000	-0.15156100	-4.74359400
C	5.69552400	-0.80629700	-3.56653800
H	5.87441500	0.16107700	-3.08889400
H	6.67985500	-1.26098500	-3.70626000
O	3.69493000	-1.75846400	-2.65041300
C	4.89148300	-1.64734800	-2.58354900
C	5.98519300	-0.20618100	-0.18409700
N	5.10935800	0.83828000	-0.13984700
C	5.67053100	1.97217300	0.46398600
C	6.95041200	1.63462500	0.78251100
N	7.11441400	0.29922800	0.38658400
H	8.12224700	0.25125600	3.66251500

C	1.17993900	0.44851200	-1.63320100
C	1.52720300	-0.06107300	-0.37673000
H	0.77964100	-0.59113100	0.20796200
C	2.80856900	0.09246500	0.15275200
C	4.39783300	2.22764800	-2.62971900
H	4.11022500	3.28519700	-2.56991300
C	3.15481800	-0.42088600	1.52483800
H	3.64867300	0.35453200	2.12277000
H	11.05782700	-1.53863600	-1.05868700
C	10.67917000	-1.88110500	1.03317800
C	9.80124700	-1.62033800	2.08597800
H	10.02840500	-2.00470100	3.07725400
H	1.86519800	1.62421800	-3.29634900
C	8.61863100	-0.89731700	1.90712000
C	8.89458800	-0.09769600	-1.83108900
C	3.42872500	1.37266600	-1.84801700
H	8.60524100	0.95898200	-1.79177100
C	8.32609300	-0.44044700	0.61432800
C	9.20114800	-0.64647900	-0.46181100
C	10.37248000	-1.36956700	-0.23126400
H	2.25272400	-0.73813800	2.05473300
H	3.84244300	-1.27306300	1.48758200
H	4.39458500	1.95705200	-3.69014800
H	5.42128100	2.14594600	-2.25730100
H	7.71140700	-1.46982300	3.76298800
H	6.70684400	-0.40066000	2.80136500
H	9.76278800	-0.19082000	-2.48979900
H	8.06106300	-0.63336800	-2.29143300
C	2.13097500	1.18744000	-2.33631500
C	7.73614700	-0.60697500	3.09436100
C	3.76020300	0.77104100	-0.62731500
C	-0.18754200	0.18896300	-2.21364900
H	-0.96379700	0.21592500	-1.44126400
H	-0.44443100	0.92302400	-2.98391900
H	-0.22487200	-0.80530200	-2.67713900
C	11.91368500	-2.72003300	1.25144700
H	12.36354400	-2.52600800	2.23093100
H	11.66548700	-3.78892200	1.21574400
H	12.67056200	-2.53111000	0.48321900
C	8.05329100	2.43200600	1.39021000
H	8.31480300	2.07711500	2.39239200
H	8.96089900	2.37618100	0.77888600
H	7.75909900	3.48190200	1.46827600
C	4.89538100	3.22551800	0.68725800

H	4.63240700	3.72447700	-0.25203600
H	3.95958100	3.01817900	1.21848200
H	5.47888700	3.92600800	1.29012100

IM26

Cu	5.49171000	-2.34673600	0.69866300
B	3.68540200	-3.92689200	-2.69912600
O	2.45064300	-4.42668600	-3.05755900
C	1.58585700	-4.26122300	-1.91025400
C	2.60898300	-4.20826300	-0.72311500
O	3.78338400	-3.60030500	-1.36289700
C	3.04643800	-5.59062200	-0.23658100
H	3.90844500	-5.47331800	0.42445400
H	2.24682500	-6.08466800	0.32450600
H	3.33271900	-6.23255100	-1.07631000
C	2.15763200	-3.33878000	0.43726900
H	1.20424600	-3.70904500	0.83318100
H	2.89008500	-3.37199800	1.24586200
H	2.02622000	-2.30454500	0.12608100
C	0.61267400	-5.43250300	-1.85672600
H	0.00158900	-5.38362000	-0.94863200
H	-0.05678800	-5.39730200	-2.72224100
H	1.13924500	-6.38879600	-1.87225600
C	0.83041400	-2.94537200	-2.11818200
H	0.30314100	-2.99076600	-3.07629200
H	0.10064200	-2.76159300	-1.32389500
H	1.52462200	-2.10208300	-2.14406300
C	6.11353300	-3.53573700	-3.47993800
H	6.66304900	-4.05714600	-4.27451600
C	6.66627700	-4.06370200	-2.16661600
C	7.37863800	-3.25661700	-1.27389600
C	7.94893100	-3.80720300	-0.12158600
C	7.79580100	-5.16513400	0.15291000
C	7.07790200	-5.97277700	-0.72977600
C	6.52304400	-5.42652800	-1.88463100
H	7.50251100	-2.20027600	-1.47016200
H	8.49105200	-3.16910300	0.56613400
H	8.20395900	-5.58176800	1.06718100
H	6.94230200	-7.02842000	-0.51324900
H	5.96048400	-6.05414500	-2.57040400
N	4.70175800	-3.83902600	-3.69355900
C	4.31693000	-3.81955900	-5.07122700
C	4.77467300	-4.81173200	-5.94508400
C	3.54362900	-2.76670600	-5.57144900

C	4.47920500	-4.74165800	-7.30646300
H	5.36090300	-5.63615600	-5.54853300
C	3.23649200	-2.70572600	-6.93040700
H	3.20481900	-1.99628700	-4.88639800
C	3.71142500	-3.68616900	-7.80378300
H	4.83993600	-5.51680000	-7.97688600
H	2.63659700	-1.88320900	-7.30999900
H	3.48056200	-3.63180500	-8.86371100
I	5.37973700	-3.97462800	2.71548100
C	7.63511600	-1.57670000	-8.54060100
H	7.21781800	-2.56995200	-8.74484000
H	8.43524000	-1.38908800	-9.26514800
H	6.83944200	-0.84392100	-8.72017600
C	8.14875300	-1.48572900	-7.10102800
H	8.97525800	-2.19544500	-6.95652100
H	8.56495600	-0.48591400	-6.91538800
C	7.04571800	-1.78148600	-6.08200800
H	6.63557100	-2.77886100	-6.27744200
H	6.21263200	-1.08116000	-6.21862600
C	7.53195600	-1.68705200	-4.61930600
H	7.87062500	-0.66971600	-4.40671900
H	8.36899100	-2.38028400	-4.46121700
O	5.68371900	-1.17829500	-3.18527300
C	6.39175300	-2.03327900	-3.68576700
C	5.63147700	-0.40907000	0.46840400
N	4.63785000	0.52011800	0.47939700
C	5.13301700	1.82659300	0.60674900
C	6.48816000	1.71319900	0.67021700
N	6.76569000	0.34281800	0.57454200
H	7.03777900	0.36228600	3.19543900
C	0.47205600	-0.10939300	0.67592100
C	1.26260700	-0.19262300	1.82546300
H	0.79255500	-0.39860600	2.78387400
C	2.64905100	-0.02099200	1.77917300
C	3.14945800	0.52397000	-1.98219300
H	3.76211300	1.43310300	-1.99467500
C	3.48775900	-0.13289500	3.02609700
H	4.22241300	0.67695100	3.09659900
H	10.85409500	-0.87009000	-1.11312500
C	10.62094900	-1.33302000	0.97578800
C	9.76283000	-1.23927600	2.07523100
H	10.08967200	-1.61515600	3.04151800
H	0.49353300	0.20765300	-1.45160500
C	8.48579100	-0.67881500	1.96990200

C	8.50043400	0.33418300	-1.73164200
C	2.48011400	0.31079100	-0.64995100
H	8.60143200	1.42716400	-1.73912000
C	8.08054000	-0.21277800	0.70993900
C	8.92799600	-0.24441500	-0.40639300
C	10.19170400	-0.81915800	-0.25214100
H	2.85723600	-0.10620900	3.91921300
H	4.04533000	-1.07788200	3.03485800
H	2.40376400	0.60796700	-2.77860800
H	3.82251300	-0.30608700	-2.21921400
H	8.15552700	-0.68729700	4.09355100
H	6.83352700	-1.39247000	3.15301100
H	9.13059700	-0.05334700	-2.53692800
H	7.45694000	0.10775900	-1.96666800
C	1.09593800	0.14748200	-0.54879200
C	7.57940400	-0.58926200	3.16909200
C	3.23239500	0.23369200	0.52944000
C	-1.01678000	-0.34325900	0.74496300
H	-1.42593600	-0.04555000	1.71582900
H	-1.54700500	0.21130300	-0.03618600
H	-1.25030300	-1.40727600	0.60553400
C	11.96876800	-1.99939700	1.10189200
H	12.33843500	-1.96325800	2.13147600
H	11.90826600	-3.05642800	0.81189500
H	12.71327400	-1.52588000	0.45315700
C	7.55699100	2.73549900	0.85383300
H	8.18828700	2.49571900	1.71698000
H	8.21533100	2.80594500	-0.01937000
H	7.11286900	3.72043900	1.01957700
C	4.23505600	3.01396700	0.67422800
H	3.64652700	3.12930600	-0.24331900
H	3.52447000	2.92960200	1.50431400
H	4.82235000	3.92475200	0.81691300