

Supporting Information

**Computational Insights into Synergistic Interplay of
Ligand and Fluorine Effects in Palladium-Catalyzed
Regiodivergent Decarboxylative Allylic Alkylation**

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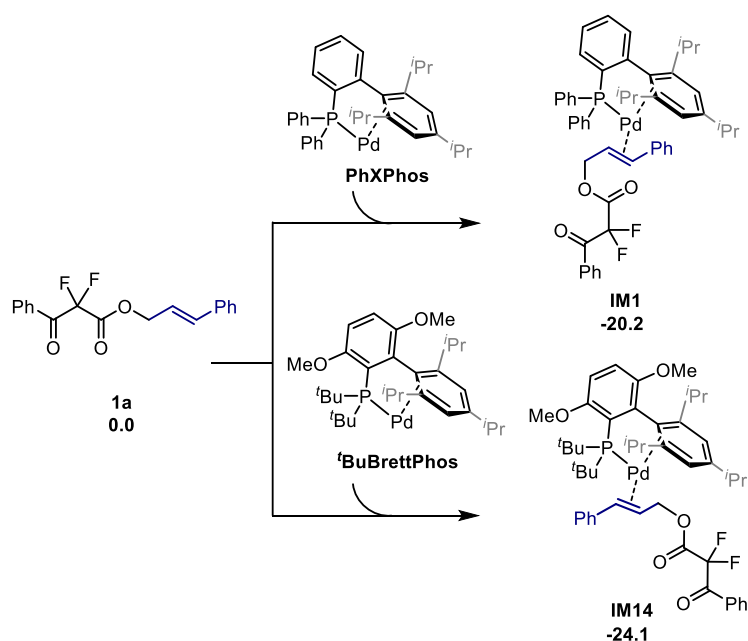
Web: <https://www.x-mol.com/groups/gphuang>

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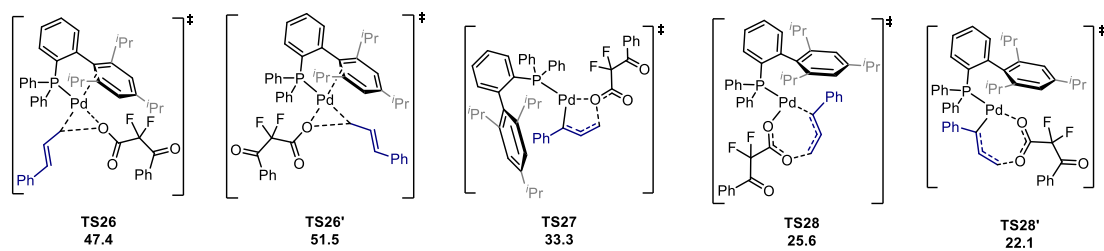
1. Formation of intermediates IM1 and IM14.

As shown in Scheme S1, the computations show that the coordination of the C-C double bond of **1a** to the Pd(0) center of Pd/PhXPhos and Pd/^tBuBrettPhos to forge intermediates **IM1** and **IM14** is highly exergonic by 20.2 and 24.1 kcal/mol, respectively. Therefore, with more electron-deficient and small ligand PhXPhos, we set the free energy of **IM1** to be zero on the relative free energy scale. On the other hand, with electron-rich and bulky ligand ^tBuBrettPhos, we set the free energy of **IM14** to be zero on the relative free energy scale.

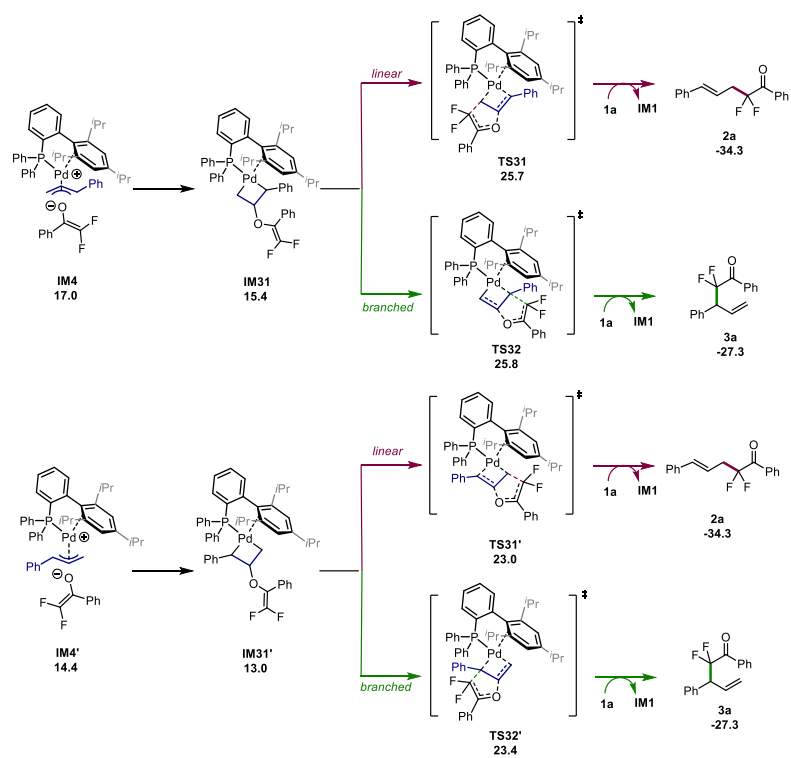


Scheme S1. Formation of the **IM1** and **IM14**. Energies are given in kcal/mol.

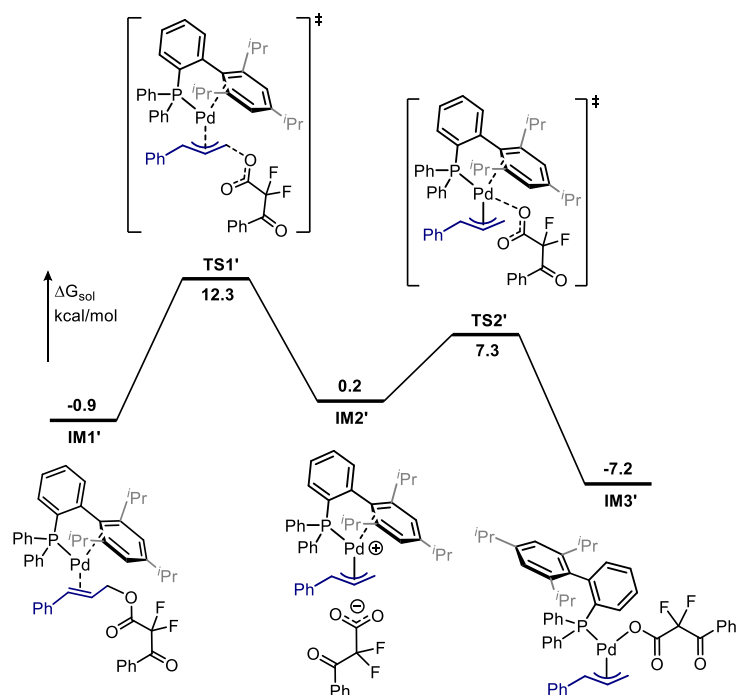
2. Other possible mechanism of Pd/PhXPhos-catalyzed decarboxylative allylic alkylation.



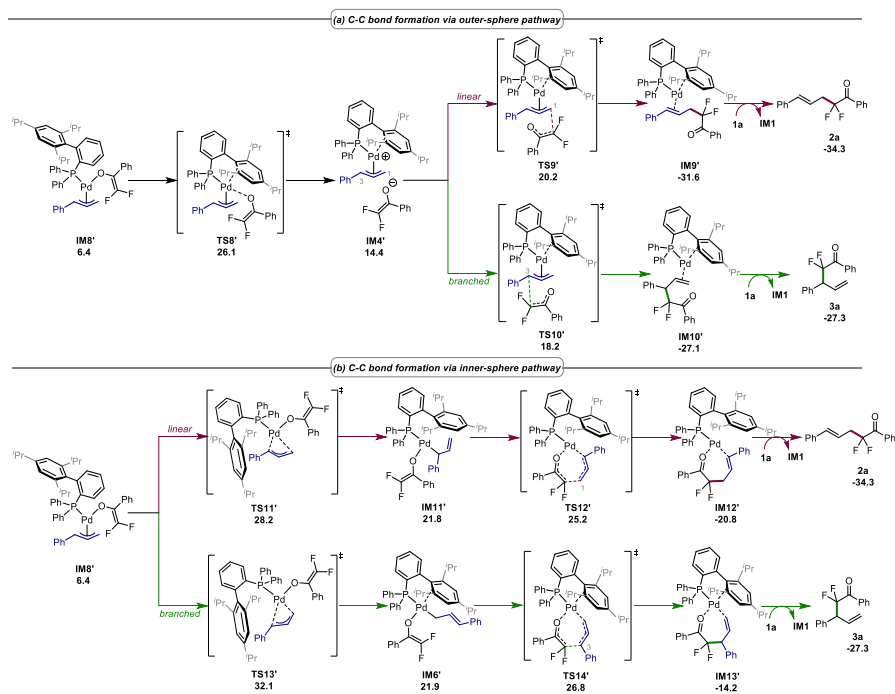
Scheme S2. C-O oxidative addition via the three-, five- and seven-membered transition states. Energies are given in kcal/mol.



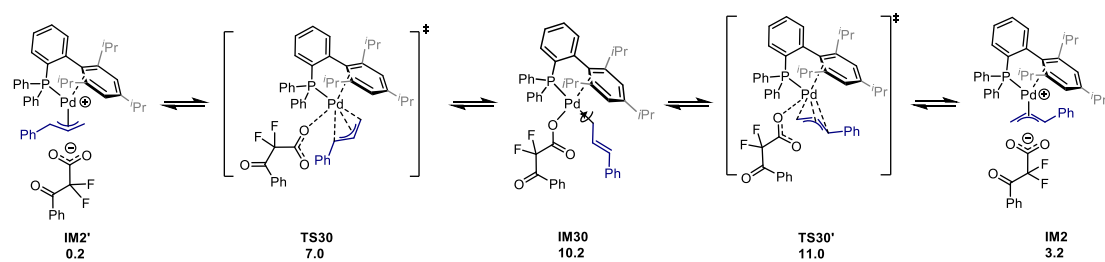
Scheme S3. Nucleophilic attack via the five-membered rearrangement transition states. Energies are given in kcal/mol.



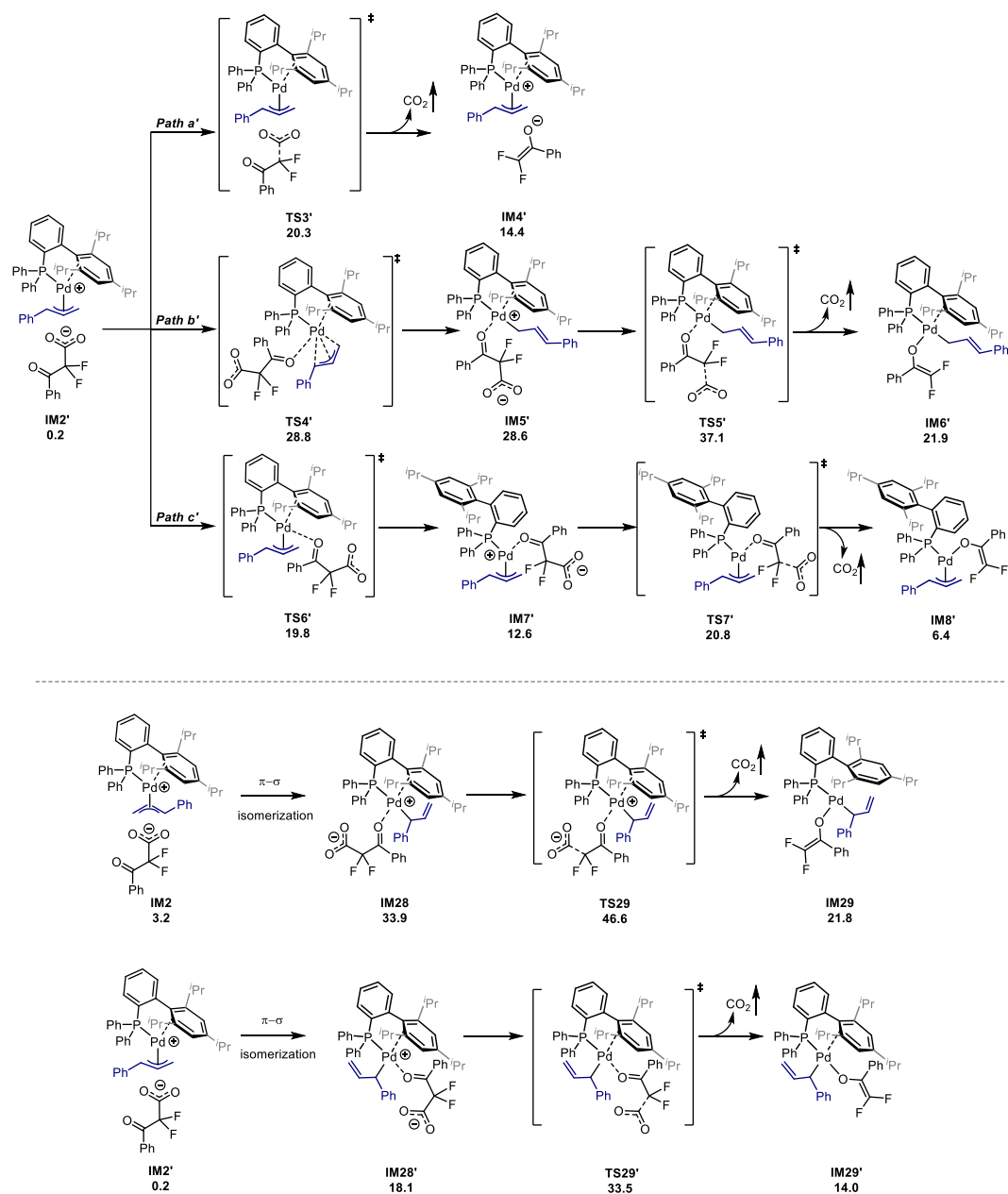
Scheme S4. C-O oxidative addition starting from **IM1'** via S_N2 back-side attack pathway.



Scheme S5. Nucleophilic attack starting from **IM8'**. Energies are given in kcal/mol.

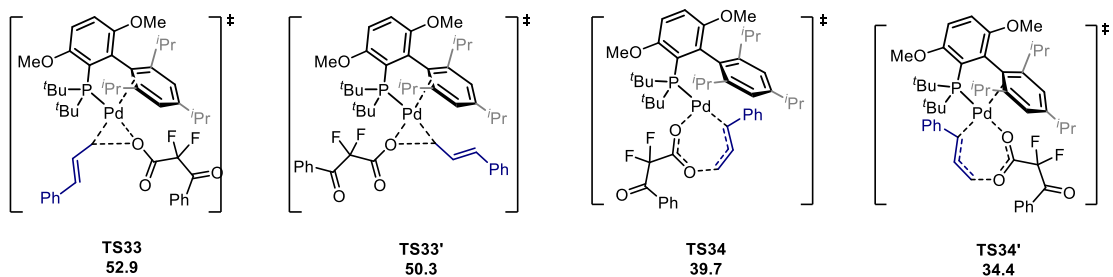


Scheme S6. The interconversion of **IM2** and **IM2'** through the π - σ - π isomerization. Energies are given in kcal/mol.

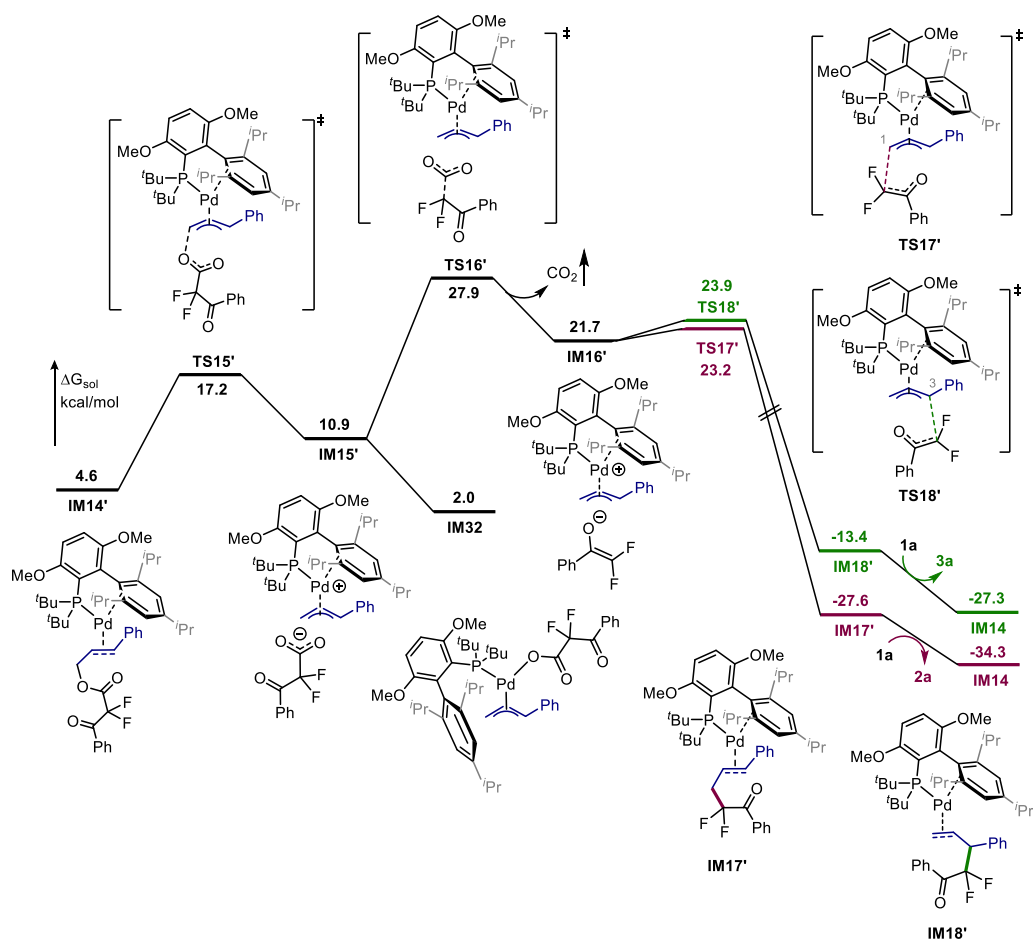


Scheme S7. CO₂ extrusion starting from **IM2** and **IM2'**. Energies are given in kcal/mol.

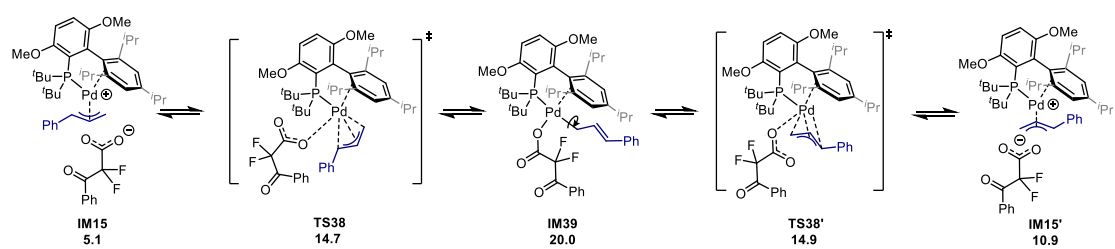
3. Other possible mechanism of Pd/*t*BuBrettPhos-catalyzed decarboxylative allylic alkylation.



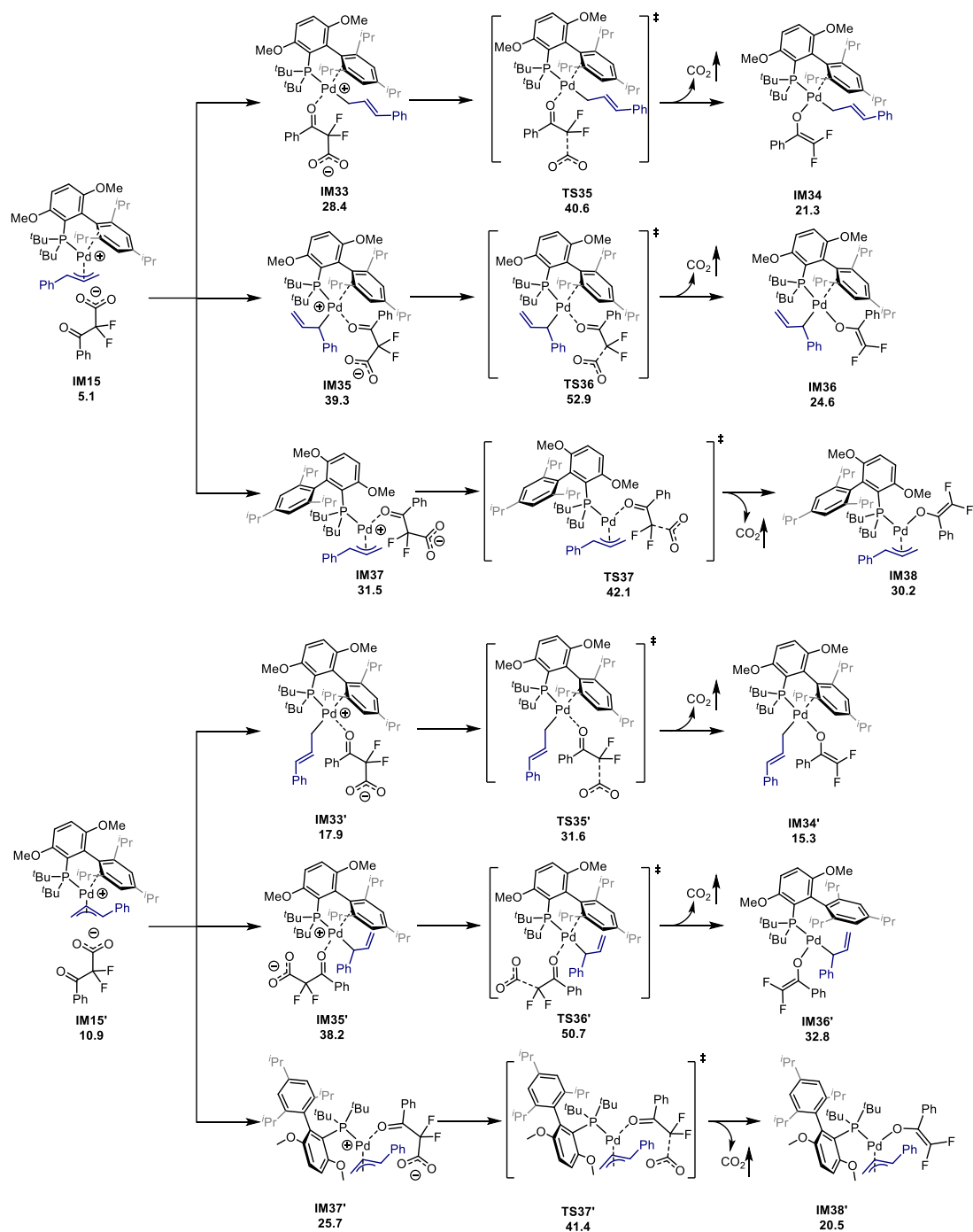
Scheme S8. C-O oxidative addition via the three-, five- and seven-membered transition states. Energies are given in kcal/mol.



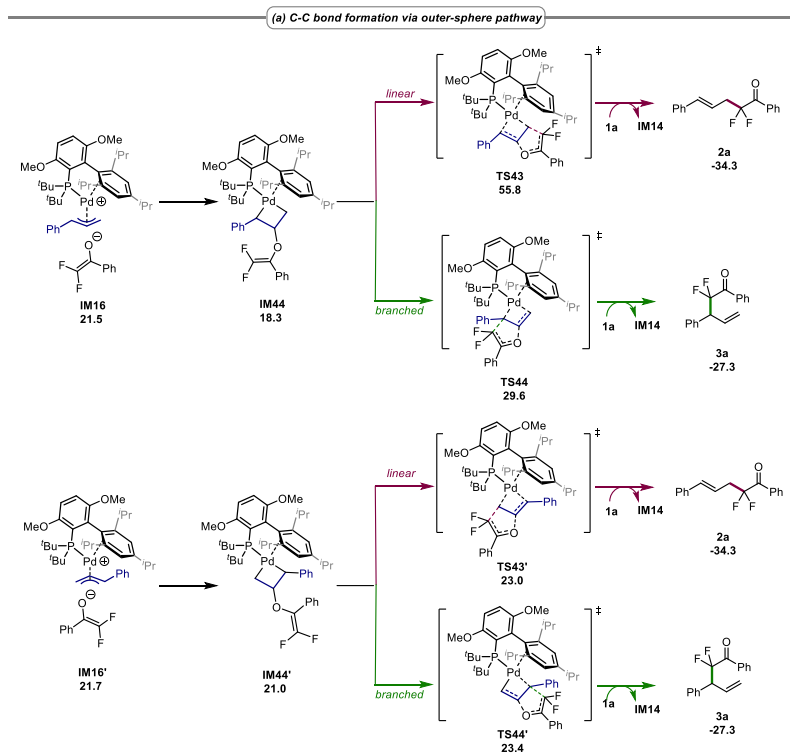
Scheme S9. Calculated energy profile starting from **IM14'** of Pd/BuBrettPhos-catalyzed decarboxylative allylic alkylation of allyl difluoro- β -ketoester **1a**. Note that the CO₂ extrusion should be considered to be irreversible to provide the driving force of the reaction.



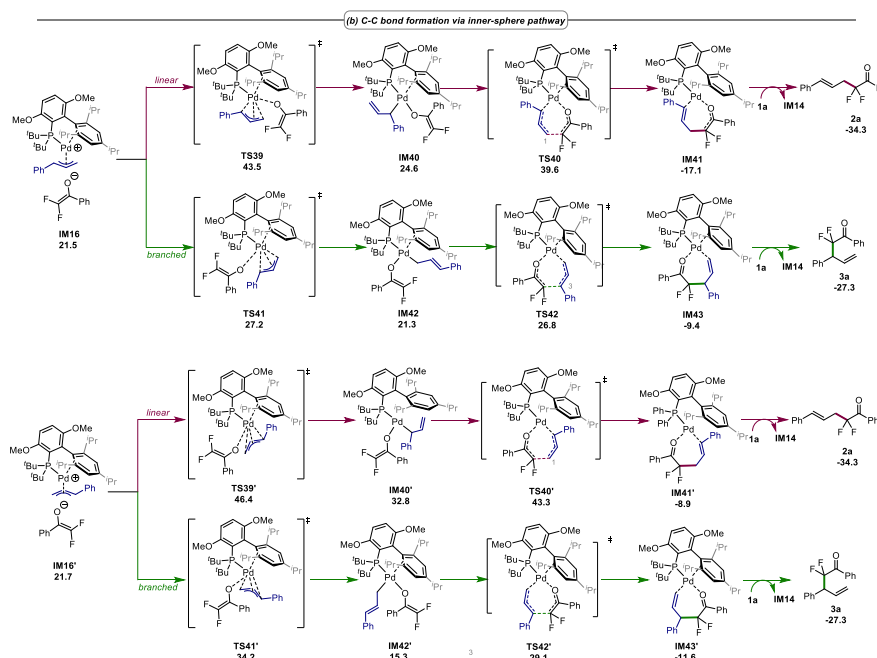
Scheme S10. The interconversion of **IM15** and **IM15'** through the π - σ - π isomerization. Energies are given in kcal/mol.



Scheme S11. CO₂ extrusion starting from **IM15** and **IM15'**. Energies are given in kcal/mol.

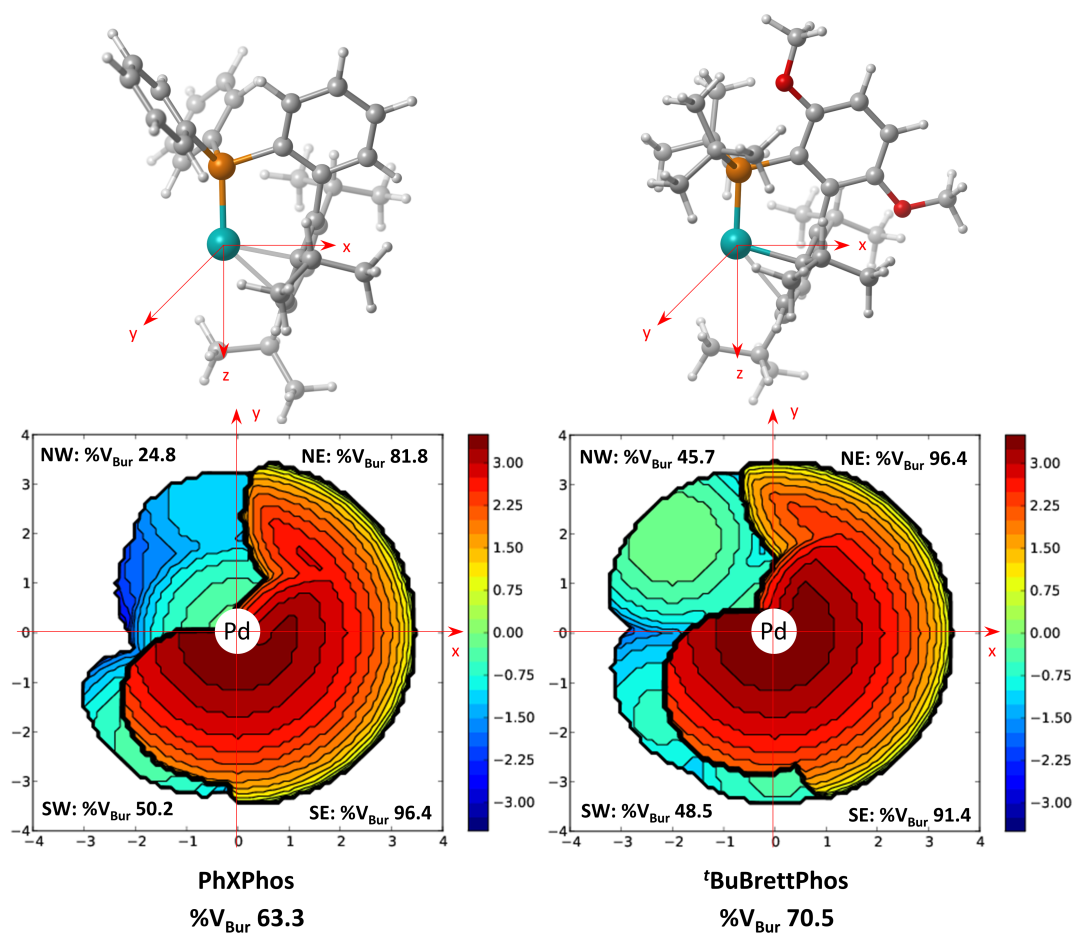


Scheme S12. Nucleophilic attack via the five-membered rearrangement transition states. Energies are given in kcal/mol.



Scheme S13. Nucleophilic attack via the inner-sphere pathway starting from **IM16** and **IM6'**. Energies are given in kcal/mol.

4. Ligand buried volume.



Scheme S14. Ligand buried volume ($V_{\text{Bur}}\%$) was calculated based on the B97D-optimized geometries. The red and blue zones indicate the more- and less-hindered zones in the catalytic pocket, respectively.

5. Conformation search.

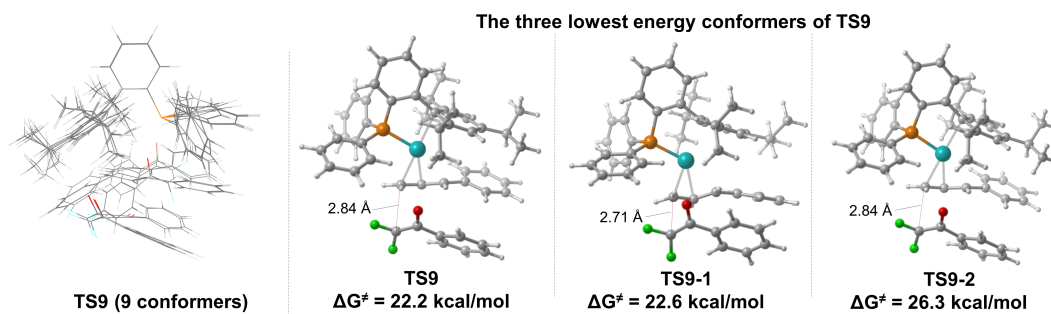


Figure S1. Conformation search for TS9.

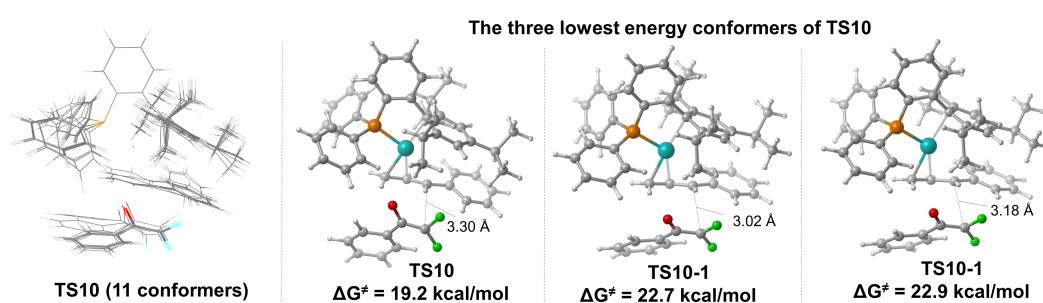


Figure S2. Conformation search for TS10.

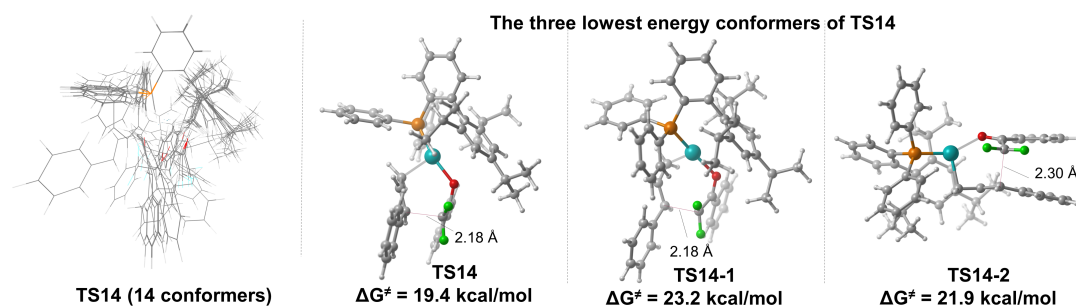


Figure S3. Conformation search for TS14.

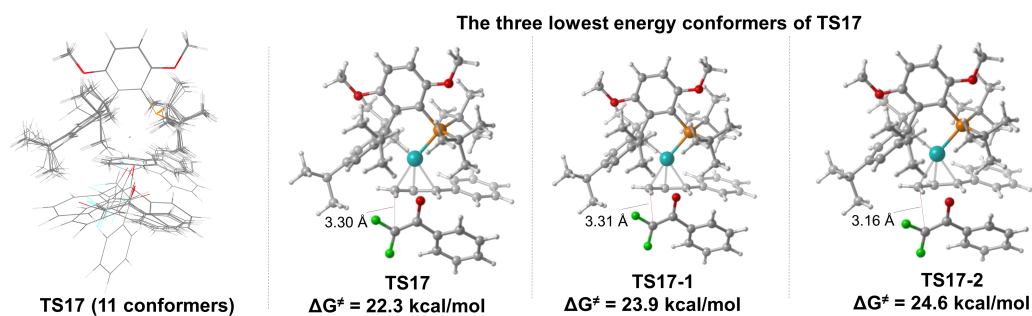


Figure S4. Conformation search for TS17.

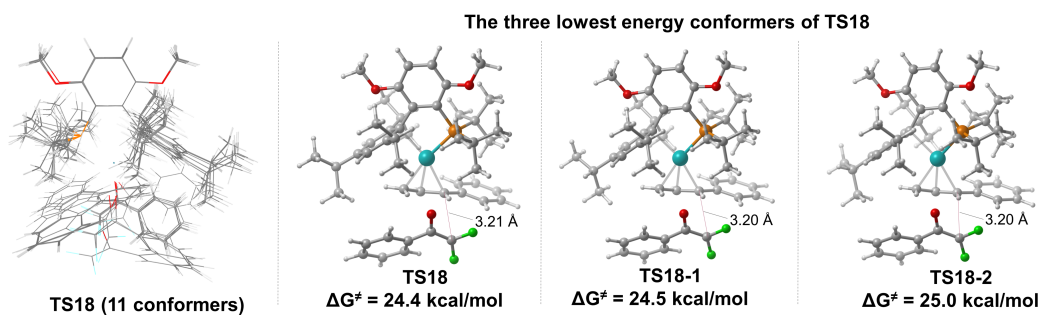


Figure S5. Conformation search for TS18.

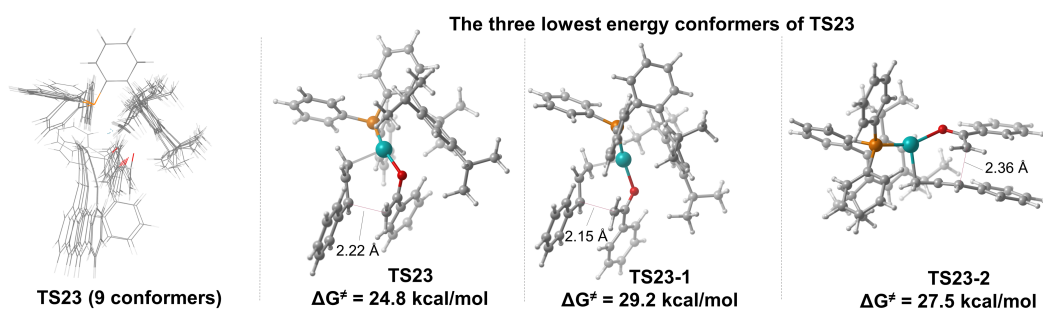


Figure S6. Conformation search for TS23.

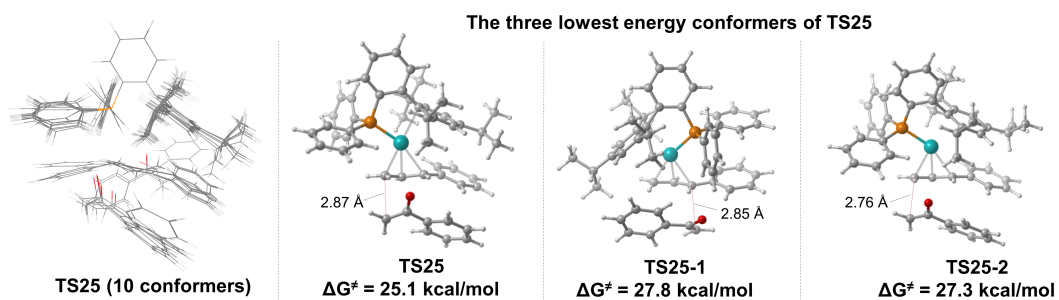


Figure S7. Conformation search for TS25.

6. IRC calculations.

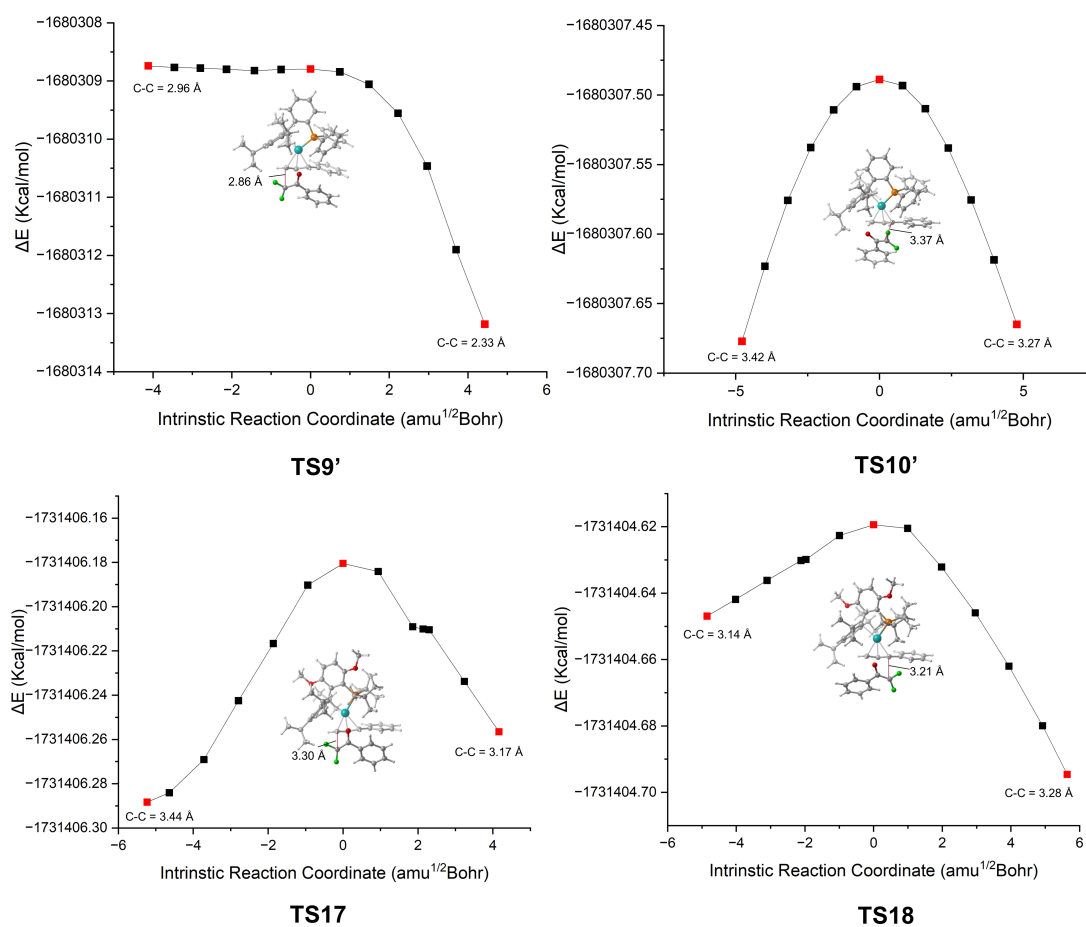


Figure S8. IRC calculations of TS9, TS10, TS17 and TS18.

7. Table of calculated energies and energy corrections

Stationary point	Single-point energy ω B97M-V-SMD/ def2-TZVPP (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
1a	-1119.772820726657	0.219526
1b	-921.250779487413	0.236583
2a	-931.186385729525	0.210576
2b	-732.647612799185	0.227911
3a	-931.176677892675	0.211956
3b	-732.640686305295	0.229288
CO ₂	-188.622674369139	-0.009467
IM1	-2868.809073754874	0.770905
TS1	-2868.792179195103	0.772242
IM2	-2868.811333674295	0.778285
TS2	-2868.806314612438	0.778730
IM3	-2868.833529975891	0.779686
TS3	-2868.772141941144	0.769588
IM4	-2680.141612262454	0.762550
TS4	-2868.786537597276	0.775533
IM5	-2868.796372367190	0.772079
TS5	-2868.773529110653	0.771999
IM6	-2680.154194599878	0.765520
TS6	-2868.789334633459	0.780217
IM7	-2868.806839825293	0.780438
TS7	-2868.784895359817	0.777140
IM8	-2680.170695813902	0.768951
TS8	-2680.141423415342	0.768932
TS9	-2680.133268279035	0.762510
TS9'	-2680.136808262709	0.762898
IM9	-2680.224776428954	0.764987
TS10	-2680.140428871553	0.765011
TS10'	-2680.140246359803	0.763152
IM10	-2680.205576179976	0.765308
TS11	-2680.110625132458	0.764952
IM11	-2680.147773647515	0.763924

TS12	-2680.137553881471	0.764612
IM12	-2680.210080508491	0.765204
TS13	-2680.143311598879	0.765590
TS14	-2680.137977011502	0.762874
IM13	-2680.199647450003	0.764545
IM14	-2950.212772774038	0.905168
TS15	-2950.186049008973	0.901083
IM15	-2950.203679751494	0.904241
TS16	-2950.160757891455	0.896474
IM16	-2761.531771296415	0.890614
TS17	-2761.530838018789	0.890931
IM17	-2761.618783144649	0.895711
TS18	-2761.526709928845	0.890156
IM18	-2761.606439842453	0.891122
IM19	-2670.291916429266	0.793512
TS19	-2670.259554869787	0.791260
IM20	-2670.277338795890	0.796502
IM21	-2670.303486560814	0.796571
TS20	-2670.249743314355	0.797619
IM22	-2670.281893412040	0.796930
TS21	-2670.264317708458	0.795531
IM23	-2481.648127335709	0.784188
TS22	-2481.610993559326	0.780287
IM24	-2481.633888177945	0.780387
TS23	-2481.607226371941	0.780584
TS24	-2481.613607545453	0.785212
IM25	-2481.616086610641	0.780018
TS25	-2481.606771450957	0.780628
IM26	-2481.642698917187	0.779497
IM27	-2481.683870853040	0.784091

8. Cartesian coordinates

1a

C	-6.35265700	4.58796300	-1.92808500
C	-4.98534000	4.69273000	-1.65256800
C	-4.42304500	4.04847600	-0.52338900
C	-5.28314700	3.30457500	0.31824300
C	-6.65332800	3.19969500	0.04249700
C	-7.19402300	3.84106400	-1.08296700
H	-6.76702400	5.09263700	-2.80355000
H	-4.34755500	5.28170200	-2.31364400
H	-4.86325400	2.80431000	1.19461300
H	-7.29752900	2.61854300	0.70573600
H	-8.26122400	3.76346600	-1.30071900
C	-2.99373800	4.11682600	-0.18925200
C	-2.01562900	4.72351300	-0.89668000
H	-2.71126200	3.61514000	0.74377200
H	-2.22652500	5.22882900	-1.84277100
C	-0.60050200	4.77113600	-0.42493200
H	-0.46329400	4.25827300	0.53828200
H	-0.22152600	5.80177700	-0.33526600
O	0.23583200	4.08914500	-1.43761600
C	1.55878800	4.19788000	-1.25624900
O	2.13510200	4.73690000	-0.33271800
C	2.30779300	3.53550200	-2.45291600
C	2.35445600	4.48346800	-3.69885700
O	1.86436400	5.60346800	-3.57642400
F	3.59194300	3.25040500	-2.05917500
F	1.70297200	2.34286000	-2.79068900
C	2.99143400	3.99242000	-4.95062300
C	2.96517500	4.85099400	-6.07627100
C	3.62061200	2.72898900	-5.05819800
C	3.54931900	4.45518400	-7.28196300
H	2.48128100	5.82334400	-5.98178800
C	4.20690200	2.33993500	-6.26894800
H	3.65803800	2.05369200	-4.20707100
C	4.17217200	3.19755000	-7.38077900
H	3.52257600	5.12310800	-8.14489200
H	4.69200000	1.36522300	-6.34439700
H	4.63007800	2.88796700	-8.32247400

1b

C	-6.42783700	4.54434200	-1.84621000
C	-5.05364100	4.65291500	-1.60823200
C	-4.46488200	4.04580300	-0.47188200

C	-5.30712300	3.33589700	0.41603000
C	-6.68422000	3.22737400	0.17818800
C	-7.25089700	3.83098400	-0.95537800
H	-6.86192900	5.02054800	-2.72813300
H	-4.43083600	5.21670400	-2.30465400
H	-4.86742400	2.86506100	1.29904600
H	-7.31372400	2.67292000	0.87759900
H	-8.32348400	3.75048700	-1.14386600
C	-3.02658900	4.11822400	-0.17676900
C	-2.06371900	4.68950300	-0.93236600
H	-2.72284100	3.65111100	0.76762200
H	-2.29810600	5.15886300	-1.89170200
C	-0.63275800	4.74835700	-0.50472300
H	-0.46866200	4.24649100	0.46104800
H	-0.26684200	5.78519000	-0.42334900
O	0.17112000	4.07634300	-1.53479600
C	1.51333000	4.17471200	-1.37901100
O	2.07022000	4.70302100	-0.43154700
C	2.22977700	3.54330700	-2.56359000
C	2.32696500	4.52195800	-3.75492300
O	1.85005200	5.65248600	-3.68779000
C	3.03208400	4.03175200	-4.98486300
C	3.16135800	4.91354100	-6.08234100
C	3.56872200	2.72864400	-5.08462100
C	3.81185800	4.50248800	-7.25006600
H	2.74427000	5.91724200	-5.99556900
C	4.21983900	2.31789200	-6.25593000
H	3.47996800	2.03073100	-4.25162700
C	4.34298700	3.20313300	-7.33943000
H	3.90713400	5.19162400	-8.09153800
H	4.63060000	1.30868800	-6.32327100
H	4.85147100	2.88208700	-8.25095400
H	3.24524300	3.25591200	-2.25163500
H	1.70691700	2.63268700	-2.89643000
2a			
C	-6.61066100	0.15309400	1.42638800
C	-5.22842300	0.32833800	1.27216800
C	-4.70430400	1.17589700	0.26781000
C	-5.61930800	1.84246200	-0.58389000
C	-6.99885300	1.66775300	-0.43063600
C	-7.50336200	0.82311400	0.57529500
H	-6.98965000	-0.50655700	2.21015400
H	-4.53542200	-0.19491500	1.93617300

H	-5.24618300	2.49791500	-1.37267500
H	-7.68610200	2.19101400	-1.09934800
H	-8.58094300	0.68927900	0.69116400
C	-3.24490600	1.32081700	0.15603800
C	-2.56705900	2.11700000	-0.69679000
H	-2.66462200	0.71066000	0.85816300
H	-3.09723200	2.74394700	-1.41787500
C	-1.06472400	2.20658600	-0.72617500
H	-0.60817700	1.52882200	0.00908000
H	-0.71952800	3.22735200	-0.49096300
C	-0.49395500	1.86405500	-2.10287400
F	-0.86886300	0.57830200	-2.46229200
F	-1.04291200	2.71982100	-3.05517100
C	1.06456500	1.96610500	-2.20988400
O	1.69240800	2.30002300	-1.20757300
C	1.72419000	1.65841000	-3.51379900
C	1.01476300	1.27368000	-4.67674300
C	3.13484100	1.76458300	-3.57106300
C	1.70730500	1.00412700	-5.86396900
H	-0.06796700	1.18379900	-4.65998800
C	3.82013600	1.49436400	-4.75839700
H	3.67324400	2.06109400	-2.67056500
C	3.10674500	1.11326800	-5.90932700
H	1.15222900	0.70828400	-6.75605100
H	4.90796500	1.57978300	-4.79076000
H	3.64097400	0.90193700	-6.83802200

2b

C	-6.56616400	-0.04749100	1.15818400
C	-5.18466700	0.16272100	1.04722500
C	-4.66113600	1.19334300	0.23070100
C	-5.57968000	2.01494400	-0.46859700
C	-6.95882000	1.80610800	-0.35810900
C	-7.46147000	0.77340400	0.45460600
H	-6.94271700	-0.85121100	1.79501400
H	-4.49061300	-0.47800700	1.59752400
H	-5.20978900	2.82679500	-1.09743200
H	-7.64754000	2.45367400	-0.90573400
H	-8.53860200	0.61471400	0.53927900
C	-3.20167100	1.36011700	0.14982100
C	-2.51515600	2.22638800	-0.62681100
H	-2.62396700	0.69191700	0.79997500
H	-3.05325700	2.90052300	-1.30296800
C	-1.01449900	2.32004100	-0.66453100

H	-0.56824100	1.67731900	0.11024500
H	-0.68603100	3.35205800	-0.45058700
C	-0.46178200	1.91573000	-2.04673700
C	1.05571800	2.08864400	-2.17407700
O	1.72596000	2.54553000	-1.24729900
C	1.70045200	1.68498300	-3.47311400
C	0.95966200	1.15350600	-4.55245500
C	3.09719000	1.84629100	-3.61548100
C	1.60196400	0.79199200	-5.74501100
H	-0.11887700	1.01939700	-4.46483400
C	3.73756400	1.48571200	-4.80574100
H	3.66023400	2.25762400	-2.77697700
C	2.99085400	0.95712800	-5.87401400
H	1.01985400	0.38136300	-6.57248100
H	4.81734500	1.61503800	-4.90463600
H	3.49040300	0.67493400	-6.80330300
H	-0.71960800	0.86497900	-2.26606000
H	-0.94378300	2.50919300	-2.84506900

3a

C	-3.02053400	2.74943600	-0.09336800
C	-2.03253500	2.67846000	-0.99594500
H	-3.76889500	3.54395700	-0.14939200
H	-3.12211300	2.02421400	0.71706700
H	-1.97887800	3.42319100	-1.79403200
C	-0.97111800	1.59318800	-1.07234400
H	-1.23296800	0.91611000	-1.90419100
C	-0.76722400	0.75466500	0.18297800
C	-0.63671500	-0.64208400	0.07591300
C	-0.60895800	1.35916200	1.44655800
C	-0.35250000	-1.42401200	1.20630400
H	-0.74672000	-1.11512600	-0.90223400
C	-0.32995700	0.57921800	2.57818400
H	-0.70258900	2.44129600	1.53524900
C	-0.19675500	-0.81455400	2.46067900
H	-0.25061600	-2.50640400	1.10463300
H	-0.21125200	1.06076200	3.55131100
H	0.02493200	-1.42064400	3.34161600
C	0.38915800	2.18701000	-1.52622500
F	0.21406200	2.87276600	-2.71574100
F	0.83877600	3.12800500	-0.61840000
C	1.44713300	1.06279200	-1.82441100
O	1.22064500	0.39394100	-2.83023400
C	2.63757200	0.82255000	-0.95891400

C	3.70194300	0.08418900	-1.53288100
C	2.73381600	1.22653700	0.39287400
C	4.84000000	-0.22362800	-0.78330300
H	3.61739900	-0.23472900	-2.57201200
C	3.86714900	0.89376500	1.14633000
H	1.92000400	1.76350300	0.86891700
C	4.92436000	0.17880200	0.56196600
H	5.65947100	-0.78032600	-1.24198000
H	3.92198100	1.19473500	2.19420200
H	5.80975500	-0.06815000	1.15165000

3b

C	3.77439300	1.10043800	1.06383500
C	2.75398200	0.30743200	1.42484500
H	4.70225300	1.12020400	1.64113700
H	3.72528100	1.75505800	0.19026100
H	2.86594900	-0.33820500	2.30305700
C	1.41594000	0.16844200	0.72420100
H	0.63282600	0.42338900	1.45828500
C	1.16501400	-1.27916400	0.29651300
C	-0.06695600	-1.89950100	0.57434900
C	2.14059700	-1.99311000	-0.42511900
C	-0.32191500	-3.20993600	0.13976000
H	-0.83043100	-1.34749500	1.12764500
C	1.88953500	-3.30243100	-0.85977600
H	3.10020200	-1.51637900	-0.63738500
C	0.65662400	-3.91516400	-0.57830500
H	-1.28334200	-3.67822800	0.36263000
H	2.65583200	-3.84551900	-1.41763000
H	0.46113600	-4.93515900	-0.91642400
C	1.26373700	1.13465100	-0.48775500
C	-0.10588300	1.01894400	-1.15841200
O	-0.21113800	0.57317500	-2.30070300
C	-1.32158500	1.43100100	-0.37346700
C	-1.23952900	2.20188700	0.80768000
C	-2.59288000	1.02786200	-0.83986000
C	-2.40205800	2.56111800	1.50458100
H	-0.27005100	2.53559900	1.17897800
C	-3.75187500	1.37690700	-0.13831700
H	-2.64567000	0.43494200	-1.75356700
C	-3.65915600	2.14540300	1.03613500
H	-2.32701300	3.16439900	2.41153100
H	-4.72844100	1.05230400	-0.50354600
H	-4.56378300	2.42004600	1.58285800

H	1.43136200	2.16726200	-0.13829400
H	2.02300400	0.89913500	-1.24575100
CO₂			
C	-4.48465300	-0.45629700	-0.47183800
O	-5.66224400	-0.45629700	-0.47183800
O	-3.30706300	-0.45629700	-0.47183800
IMI			
Pd	-0.39694600	0.92450200	0.74277800
P	0.45200100	-1.17573700	0.54620700
C	2.08116600	-1.04105200	-0.29846400
C	2.75341200	-2.13620800	-0.87608700
C	4.00438100	-1.96053000	-1.48337100
H	4.51995500	-2.81244200	-1.93161800
C	4.58866300	-0.68315800	-1.51125500
H	5.56453700	-0.53703600	-1.97915700
C	3.91462200	0.41145300	-0.95079000
C	2.64852400	0.25373600	-0.34966600
C	1.97694000	1.49692800	0.18454500
C	2.33008200	1.98754700	1.48521900
C	2.94011000	1.06453100	2.53418900
H	3.11286600	0.08072500	2.07469600
C	4.29836600	1.58569800	3.04575600
H	4.18645500	2.56775400	3.53388500
H	4.72329000	0.88542700	3.78447700
H	5.01716900	1.69647300	2.21719600
C	1.94685500	0.86016900	3.69794000
H	0.99297900	0.46455400	3.31758000
H	2.35551500	0.14858400	4.43442800
H	1.74460300	1.81675500	4.20609900
C	2.05835900	3.32045500	1.80280400
H	2.31866100	3.68871000	2.79758000
C	1.46723300	4.21532300	0.88556400
C	1.34919400	5.68565700	1.27214200
H	0.87311700	5.72090200	2.26581800
C	2.76048100	6.30816700	1.40306800
H	2.69076600	7.35644400	1.74045300
H	3.37935800	5.75264200	2.12551900
H	3.27826300	6.29201900	0.42873700
C	0.49759100	6.52699600	0.30867400
H	-0.50589300	6.09603000	0.17890400
H	0.38680000	7.55051800	0.70191300
H	0.97612300	6.59734200	-0.68318800

C	1.04745900	3.70415000	-0.34646300
H	0.55071800	4.35732600	-1.06331100
C	1.27412200	2.35746500	-0.71849900
C	0.92412400	1.90505300	-2.13699100
H	1.05554100	0.81425200	-2.18826400
C	1.89002000	2.54627400	-3.15710400
H	1.80254900	3.64525800	-3.13426300
H	2.93500600	2.28009300	-2.93241900
H	1.65615100	2.20251700	-4.17887200
C	-0.54134300	2.20985600	-2.50543700
H	-0.74376800	3.29318200	-2.50319500
H	-0.76435100	1.82713200	-3.51558300
H	-1.22747500	1.73747500	-1.78497600
C	-2.04344400	2.38021300	1.12937100
C	-2.43302900	1.03298000	1.36046000
H	-2.53598800	0.69196100	2.39721900
C	-3.29279800	0.29832400	0.37035200
O	-4.74358600	0.57597000	0.62352800
C	-5.27205100	1.62211100	-0.01560900
O	-4.73877000	2.37427800	-0.80965900
C	-6.77861800	1.76070600	0.36546300
C	-7.68218200	0.79094400	-0.46821600
O	-7.13804300	0.09833500	-1.32441700
F	-7.17349400	3.05499800	0.12160000
F	-6.95893000	1.52209400	1.71203600
C	-9.14583300	0.75902700	-0.19273900
C	-9.92356900	-0.18244500	-0.90894300
C	-9.78203000	1.62266500	0.73058200
C	-11.30327800	-0.26319800	-0.70436600
H	-9.42368900	-0.84059500	-1.62009500
C	-11.16602700	1.53903100	0.92808000
H	-9.20729700	2.35778800	1.28806800
C	-11.92800000	0.59858200	0.21552800
H	-11.89413000	-0.99450600	-1.25910700
H	-11.65033500	2.20993100	1.63982100
H	-13.00642500	0.53671700	0.37558500
H	-2.33248000	2.82622500	0.17472600
C	-1.71425800	3.33746600	2.19924400
C	-1.13232100	2.93165700	3.42522300
C	-1.97799600	4.71360400	2.01344100
C	-0.83395600	3.86489400	4.42343400
H	-0.88476300	1.87866700	3.56574600
C	-1.68634100	5.64911700	3.01607200
H	-2.43126800	5.04088100	1.07496800

C	-1.10942200	5.23197500	4.22649800
H	-0.37783600	3.52859500	5.35787600
H	-1.90036000	6.70682200	2.84585600
H	-0.87438900	5.95988500	5.00615800
H	-3.07270000	0.58421300	-0.66446600
H	-3.22778200	-0.78935400	0.48438500
H	4.36265100	1.40627700	-0.98213900
H	2.28873100	-3.12398200	-0.85131900
C	0.81065800	-2.06826400	2.11736600
C	-0.25289000	-2.19667000	3.03848000
C	2.08800400	-2.54357100	2.47341700
C	-0.04354400	-2.79718300	4.28632100
H	-1.24126100	-1.81029600	2.77861800
C	2.29843900	-3.13241500	3.73170800
H	2.92013300	-2.44724600	1.77521100
C	1.23606500	-3.26171400	4.63918000
H	-0.87451900	-2.89168500	4.98870700
H	3.29512700	-3.49011700	3.99976900
H	1.40262900	-3.71761200	5.61737400
C	-0.47808500	-2.40278300	-0.46436300
C	-1.26040000	-1.90213900	-1.52657800
C	-0.43833400	-3.79183900	-0.22744600
C	-1.97844800	-2.77921800	-2.35171600
H	-1.31279200	-0.82276600	-1.68675100
C	-1.16606800	-4.66714400	-1.04958600
H	0.15205500	-4.18462600	0.60244900
C	-1.93293800	-4.16348800	-2.11313100
H	-2.58393300	-2.38261800	-3.16952400
H	-1.13501700	-5.74203000	-0.85776300
H	-2.50118400	-4.84620500	-2.74838900
TS1			
C	1.74217700	0.16926300	0.09246400
C	1.81223700	-1.17726600	-0.34490400
H	2.14428100	-1.41181000	-1.35935900
C	1.51030800	-2.24532900	0.54698000
O	3.42552500	-2.82596800	1.25686600
C	3.77824100	-1.97717100	2.14936600
O	3.09530700	-1.17297700	2.81118100
C	5.32184200	-1.90952000	2.43762900
C	5.87047300	-0.45401200	2.26414600
O	6.33103300	0.13391700	3.23589000
F	6.06745400	-2.74681700	1.61941700
F	5.53949400	-2.31992900	3.72847300

C	5.80460400	0.16164500	0.90071100
C	5.32101700	-0.52248800	-0.23884000
C	6.25747500	1.49457500	0.76146200
C	5.28814800	0.12262800	-1.48288000
H	4.96848400	-1.54782100	-0.15896900
C	6.22831300	2.12916200	-0.48273700
H	6.62707200	2.01274300	1.64696500
C	5.74270900	1.44346800	-1.61025600
H	4.90664800	-0.40947300	-2.35619100
H	6.57528600	3.16015500	-0.57760500
H	5.70500400	1.94334100	-2.57937000
H	1.75236600	0.33285000	1.17228800
C	2.12163000	1.31368100	-0.73730900
C	2.00134700	1.30031400	-2.14751000
C	2.64255500	2.47151600	-0.11881300
C	2.40322500	2.40173500	-2.90960700
H	1.56222700	0.42980800	-2.63502100
C	3.05933800	3.56884900	-0.88223300
H	2.75125500	2.48529100	0.96695000
C	2.93781400	3.54267800	-2.28071400
H	2.29600100	2.37632900	-3.99665100
H	3.47016500	4.44860100	-0.38333700
H	3.25262300	4.40187800	-2.87686400
H	1.23262100	-2.04527400	1.57729100
H	1.35759500	-3.25220700	0.16702200
Pd	-0.31502700	-0.78195900	-0.23656500
P	-1.82445900	-2.46568600	-0.56470700
C	-3.48621400	-1.73262100	-0.33210300
C	-4.66456200	-2.49586800	-0.21578900
C	-5.90256200	-1.85884000	-0.05791100
H	-6.81506800	-2.45104600	0.03394200
C	-5.96098500	-0.45524900	-0.01629800
H	-6.92189500	0.04860900	0.10577300
C	-4.78625800	0.30394900	-0.11722600
C	-3.53175500	-0.32275000	-0.26532600
C	-2.31486800	0.57427200	-0.32957400
C	-1.96734600	1.18917900	-1.58278700
C	-2.37484400	0.54884900	-2.90440900
H	-2.95307100	-0.35979900	-2.68632500
C	-3.27144500	1.48287000	-3.74198300
H	-2.73477500	2.40632800	-4.01501400
H	-3.58147700	0.98049900	-4.67348400
H	-4.17683500	1.76655200	-3.18106400
C	-1.12726800	0.10972800	-3.69899500

H	-0.51248100	-0.57515000	-3.09342200
H	-1.42544200	-0.41123000	-4.62360200
H	-0.50900200	0.98060100	-3.97066200
C	-1.24203800	2.38260000	-1.57248900
H	-0.98938000	2.85388000	-2.52425500
C	-0.84910100	3.01985200	-0.37616600
C	-0.24044700	4.41468600	-0.45753600
H	0.56754300	4.37379000	-1.20550100
C	-1.30594000	5.41347100	-0.97300000
H	-0.86492100	6.41750200	-1.09186600
H	-1.71589200	5.09751900	-1.94546700
H	-2.14274200	5.48612600	-0.25752800
C	0.35464000	4.92625400	0.86380200
H	1.09575400	4.22414700	1.27270700
H	0.85072500	5.89627500	0.69980000
H	-0.43411800	5.07646000	1.62046200
C	-1.08782100	2.35298600	0.83161700
H	-0.74385100	2.79024900	1.76843300
C	-1.80958600	1.14137800	0.88768200
C	-2.15259700	0.52965800	2.24444900
H	-2.64392600	-0.43805100	2.06655500
C	-3.14856200	1.42821700	3.00869600
H	-2.70631000	2.41795600	3.20928100
H	-4.07241700	1.57420800	2.42638100
H	-3.41539800	0.96837000	3.97471100
C	-0.88965300	0.26031200	3.08650700
H	-0.33695800	1.19042300	3.29394100
H	-1.16669300	-0.19153000	4.05344700
H	-0.20637000	-0.42533600	2.56135500
H	-4.83126500	1.39352300	-0.07279500
H	-4.60529300	-3.58576400	-0.24294900
C	-1.80681700	-3.15440900	-2.26727900
C	-0.58598000	-3.68696200	-2.73845400
C	-2.91527100	-3.09458900	-3.13408000
C	-0.48198700	-4.16123300	-4.05221000
H	0.28269500	-3.72277700	-2.07704400
C	-2.80232200	-3.55727300	-4.45559100
H	-3.86130300	-2.68264800	-2.78131000
C	-1.58924400	-4.09124800	-4.91648300
H	0.46433900	-4.57629500	-4.40493000
H	-3.66536600	-3.50112000	-5.12234100
H	-1.50388000	-4.44979600	-5.94418400
C	-1.76787100	-3.91998600	0.55180000
C	-1.39278200	-3.69346600	1.89358000

C	-2.07417000	-5.22725800	0.12352300
C	-1.33852100	-4.76130200	2.79933800
H	-1.13087200	-2.68421800	2.21860100
C	-2.00982900	-6.29503800	1.03303100
H	-2.34903100	-5.41000600	-0.91675500
C	-1.64509100	-6.06385800	2.36925000
H	-1.04183600	-4.57962200	3.83414400
H	-2.24127900	-7.30758200	0.69573700
H	-1.58973300	-6.89743700	3.07217900

IM2

Pd	0.13344700	0.19436800	-1.15973800
P	-0.13839400	-2.03816500	-1.44575500
C	-1.38749700	-2.49203900	-0.18941100
C	-1.65834000	-3.83590300	0.13656000
C	-2.71100300	-4.15458600	1.00406000
H	-2.91121300	-5.19621300	1.26141100
C	-3.50952000	-3.12572200	1.52753700
H	-4.34852000	-3.36237100	2.18474600
C	-3.22506700	-1.78757900	1.22071100
C	-2.13927300	-1.44053300	0.39084700
C	-1.89050000	0.03692800	0.15897300
C	-1.49028000	0.86496900	1.27996900
C	-0.84391000	0.28267600	2.53582100
H	-0.40303400	-0.68978000	2.27858900
C	-1.87492100	0.08402700	3.67289500
H	-2.64572800	-0.65605100	3.41934100
H	-2.37305100	1.03987900	3.91066900
H	-1.35429300	-0.26618400	4.57942200
C	0.29397200	1.17776900	3.07402800
H	0.84758200	0.62715400	3.84595700
H	-0.10015900	2.09918600	3.53524200
H	0.99858800	1.44701400	2.27994900
C	-1.72499300	2.24116500	1.20879600
H	-1.43597200	2.86598000	2.05372300
C	-2.33152800	2.86613400	0.09984600
C	-2.67094300	4.34847200	0.18466300
H	-1.75538100	4.87288100	0.49863000
C	-3.73923900	4.57771300	1.28187500
H	-3.40797300	4.18458500	2.25569300
H	-4.68200700	4.07221900	1.01178200
H	-3.94450700	5.65538900	1.39545800
C	-3.14554400	4.96658600	-1.13989800
H	-3.27752700	6.05359100	-1.01903100

H	-4.11570800	4.54119500	-1.44888200
H	-2.41935500	4.79591700	-1.94862000
C	-2.64182000	2.07329100	-1.00779600
H	-3.10144300	2.52512400	-1.88524300
C	-2.46284900	0.67276000	-0.99899400
C	-3.08474000	-0.12959400	-2.13742800
H	-2.76408300	-1.17253100	-2.05296800
C	-4.62381700	-0.12683000	-2.00205400
H	-5.02175300	0.89830000	-2.07881700
H	-4.93311900	-0.54510300	-1.03069000
H	-5.07552800	-0.73612200	-2.80278000
C	-2.64866900	0.38217900	-3.52292200
H	-2.99019100	-0.31253100	-4.30570000
H	-1.55155200	0.45927200	-3.57544100
H	-3.07712700	1.37532600	-3.73661200
C	0.16204300	5.72858000	-1.27251700
C	0.48822700	4.39230900	-1.52053600
C	1.05393800	3.58689400	-0.50057900
C	1.23205300	4.15200400	0.78734100
C	0.89116200	5.48650200	1.03614300
C	0.36336300	6.28344500	0.00512500
H	-0.26273900	6.33961800	-2.07099500
H	0.31212300	3.96822600	-2.51029000
H	1.67340100	3.53898500	1.57392600
H	1.04679300	5.90834400	2.03101700
H	0.10344300	7.32675000	0.19514000
C	1.52015300	2.22542600	-0.72098000
C	1.68609000	1.60464200	-1.96659200
H	1.94209100	1.71523000	0.14848300
H	1.38947400	2.12297900	-2.88209500
C	2.07857100	0.23102100	-2.02917800
H	2.19181600	-0.23449200	-3.01063200
H	2.68878600	-0.19486000	-1.23045100
O	1.91420100	-0.53832300	1.07485800
C	2.35131400	-1.00274000	2.17377900
O	1.91291000	-1.92231400	2.89324200
C	3.64666500	-0.25538900	2.67171000
C	4.12362000	0.78142600	1.61808700
O	3.94772900	1.98171600	1.83157000
F	3.38432700	0.39452800	3.85686600
F	4.67119900	-1.16057800	2.94332700
C	4.73385600	0.28563200	0.33990500
C	4.83015400	-1.08394100	0.00212000
C	5.15081000	1.25237600	-0.60098500

C	5.31797600	-1.46859100	-1.25274600
H	4.50325600	-1.85052600	0.69879900
C	5.64588800	0.86568700	-1.85163400
H	5.06166300	2.30652900	-0.33714200
C	5.72581500	-0.49793600	-2.18336800
H	5.36120600	-2.52882100	-1.50612300
H	5.96282200	1.62489000	-2.57015200
H	6.10365700	-0.80250800	-3.16225700
H	-1.03645200	-4.62604700	-0.28716800
H	-3.84386600	-0.99112300	1.63445400
C	1.29117100	-3.15746500	-1.19804400
C	2.00624700	-3.68353500	-2.29447600
C	1.71891400	-3.43284700	0.11671600
C	3.14088300	-4.47858300	-2.07380700
H	1.67455200	-3.48793100	-3.31508500
C	2.85542500	-4.22640000	0.32729700
H	1.20095800	-3.01028400	0.97540700
C	3.56895000	-4.75049700	-0.76338100
H	3.68531500	-4.88911500	-2.92708100
H	3.18149800	-4.41894700	1.35070400
H	4.45345400	-5.36867000	-0.59420100
C	-0.82525500	-2.52559600	-3.08522100
C	-1.87253600	-3.45704300	-3.22862700
C	-0.27901800	-1.91855300	-4.23531600
C	-2.36298400	-3.77548100	-4.50409400
H	-2.31730600	-3.91863700	-2.34697900
C	-0.75506500	-2.25646500	-5.51031800
H	0.50657900	-1.16913800	-4.12795300
C	-1.80239500	-3.18197500	-5.64682300
H	-3.18283100	-4.48986100	-4.60330500
H	-0.32139000	-1.78284900	-6.39342000
H	-2.18489500	-3.43376900	-6.63798000

TS2

Pd	-1.90659300	0.05213500	1.14006900
C	-2.09188100	1.61278900	2.59686400
P	-1.71867300	1.41122600	-0.67493300
C	-2.77968100	0.48616600	3.13917100
C	-2.03302000	-0.68007800	3.40711300
H	-0.95067500	-0.57508500	3.52155000
H	-1.04519100	1.79589900	2.86587800
H	-3.87099600	0.47333500	3.15827000
C	-1.35057000	0.60793600	-2.29206200
C	-2.09250200	-0.54505100	-2.66710400

C	1.84003300	4.18471000	0.44612700
C	0.54399500	4.72022900	0.39019300
C	-0.53631400	3.91558000	-0.00683800
C	-0.32151500	2.56485200	-0.35043900
C	0.98385500	2.02812100	-0.28962100
C	2.05727600	2.83968200	0.10174700
H	2.67885900	4.81017800	0.75969200
H	0.36795800	5.76556300	0.65401600
H	-1.53906600	4.34174900	-0.04591000
H	1.14986200	0.98129300	-0.54279600
H	3.06027100	2.41552800	0.14766800
C	-5.17915900	4.46526900	-1.20521500
C	-4.16735100	4.38634500	-2.17766300
C	-3.15301700	3.42494800	-2.06072300
C	-3.14852900	2.53150400	-0.97061100
C	-4.18930700	2.58397600	-0.02488500
C	-5.19571400	3.55666500	-0.13463000
H	-5.96122800	5.22221000	-1.29226300
H	-4.16347400	5.07933300	-3.02145400
H	-2.35411700	3.37746700	-2.80329800
H	-4.20301900	1.85355200	0.78463800
H	-5.99657800	3.59561900	0.60678700
C	-0.34112300	1.10466600	-3.13987900
H	0.22979900	1.98540800	-2.84582100
C	-1.77850900	-1.17740100	-3.88283800
H	-2.33932900	-2.06337200	-4.17820600
C	-0.04865900	0.46082900	-4.35017100
H	0.73890400	0.85313200	-4.99651800
C	-0.76339100	-0.68747000	-4.71768800
H	-0.53502400	-1.20306500	-5.65264500
C	-3.21073900	-1.01972100	-1.78597900
C	-4.50126900	-0.44537100	-1.93608100
C	-2.95985800	-1.97949600	-0.75967900
C	-5.48754600	-0.75090900	-0.98359500
C	-3.97612000	-2.22124300	0.18963300
C	-5.23188900	-1.59815600	0.10553300
H	-6.47780400	-0.30482400	-1.07829600
H	-3.79449000	-2.92465400	1.00245000
C	-1.70208900	-2.84601400	-0.79417300
C	-1.93568200	-4.01891900	-1.77833000
C	-1.27898900	-3.42378800	0.56629600
H	-0.87021500	-2.23904600	-1.17339100
H	-2.19442000	-3.66736300	-2.78734900
H	-1.02321700	-4.63412600	-1.85026700

H	-2.75873700	-4.66047700	-1.41865800
H	-1.16890100	-2.64301800	1.32590300
H	-2.00297100	-4.16907300	0.93400800
H	-0.30543300	-3.92582600	0.46048700
C	-4.83906700	0.41058300	-3.15848900
C	-6.01932600	1.37743500	-2.95608000
C	-5.15025100	-0.50993700	-4.36366900
H	-3.95156300	1.01148000	-3.40908300
H	-5.90238200	1.97888800	-2.04702300
H	-6.08845300	2.05825700	-3.81923600
H	-6.97433300	0.82912500	-2.89129000
H	-4.30609700	-1.17006800	-4.60574500
H	-6.02635200	-1.14114600	-4.13829500
H	-5.38255700	0.09607600	-5.25608800
C	-6.30830700	-1.86291800	1.14885400
C	-7.54996200	-2.53194700	0.52082600
C	-6.70858700	-0.56103200	1.87634400
H	-5.88622500	-2.55499900	1.89426700
H	-7.27878000	-3.47525900	0.01989400
H	-8.30480200	-2.75162900	1.29482300
H	-8.01331500	-1.86891300	-0.22852100
H	-5.83097500	-0.07993900	2.33735600
H	-7.15381900	0.15904100	1.16995100
H	-7.44950300	-0.76672300	2.66728400
O	0.33215600	-0.71079000	1.46252700
C	1.14046400	-1.31158100	0.68590500
O	1.20992400	-1.33856800	-0.55664800
C	2.22834800	-2.09824600	1.51898000
C	3.11169300	-1.11699400	2.34381400
O	3.02406300	-1.10781700	3.56785600
C	3.99648100	-0.16789500	1.59040000
C	4.68423700	0.81563300	2.33885000
C	4.17026000	-0.20953900	0.18662300
C	5.52886900	1.73261700	1.70624700
H	4.53796400	0.84298200	3.41906500
C	5.02337600	0.70899100	-0.44208600
H	3.63517200	-0.93920800	-0.41548400
C	5.70563800	1.67790500	0.31146100
H	6.05129500	2.48895800	2.29578000
H	5.15003200	0.66872000	-1.52571200
H	6.36824600	2.39074000	-0.18447800
F	1.59427400	-2.97075100	2.37895600
F	3.03758500	-2.88015000	0.71008800
H	-2.65948800	2.49859600	2.30719200

C	-2.56876200	-1.99744700	3.73527300
C	-3.95539700	-2.26803000	3.83668600
C	-1.65349800	-3.06079700	3.93588800
C	-4.40832300	-3.55869900	4.12910400
H	-4.67789300	-1.46640200	3.68620100
C	-2.11065800	-4.35239400	4.22093800
H	-0.58564500	-2.86420700	3.82993600
C	-3.48935100	-4.60763100	4.31914400
H	-5.48059500	-3.75041800	4.20869300
H	-1.39100800	-5.16118600	4.36130600
H	-3.84708400	-5.61487700	4.54230400

IM3

Pd	-0.13524400	0.30034900	1.02163300
P	-0.46073100	-1.95035800	0.69684300
C	0.09397500	-2.70530900	-0.89444200
C	-0.66675900	-3.75523800	-1.45666100
C	-0.23468900	-4.42632100	-2.60773600
H	-0.84075800	-5.23324400	-3.02409100
C	0.97727300	-4.05995000	-3.20993200
H	1.33042100	-4.57796300	-4.10393100
C	1.73474700	-3.01688100	-2.66143500
C	1.31272000	-2.31818800	-1.51016600
C	2.20452500	-1.20490000	-1.03811100
C	1.99400400	0.11223800	-1.52847900
C	0.80884500	0.44502700	-2.43165100
H	-0.01076100	-0.24461200	-2.18119500
C	1.18316000	0.21974700	-3.91526800
H	2.01836600	0.88186500	-4.20135100
H	0.32025900	0.45474300	-4.56119900
H	1.48633400	-0.82048300	-4.10686900
C	0.26991600	1.87472100	-2.25180700
H	-0.64664800	1.98712700	-2.84352700
H	0.98983400	2.62903100	-2.61066700
H	0.02348400	2.08724400	-1.20371100
C	2.94203900	1.10286300	-1.21893600
C	4.06793700	0.83866700	-0.42401500
C	5.07422300	1.93545500	-0.09837200
H	4.70001300	2.87582500	-0.53975900
C	6.44993000	1.62838300	-0.72944900
H	6.36587600	1.50561600	-1.82141200
H	6.86678600	0.69610900	-0.31336800
H	7.16283000	2.44414600	-0.52213000
C	5.21492200	2.14547500	1.42518200

H	4.24810100	2.39951200	1.88783200
H	5.92660600	2.96094400	1.63667700
H	5.59202500	1.23084100	1.91133400
C	4.24216400	-0.46518000	0.06290700
C	3.33327400	-1.49626700	-0.23209500
C	3.61923300	-2.90212800	0.29205400
H	2.73378100	-3.52636600	0.11123000
C	4.79916000	-3.53156000	-0.48033500
H	5.71724300	-2.93689800	-0.33974900
H	4.58572800	-3.57821900	-1.56037200
H	4.99392400	-4.55594700	-0.11974600
C	3.89060400	-2.92055100	1.81058700
H	4.79591900	-2.34476200	2.06396200
H	4.04459300	-3.95642700	2.15161800
H	-1.60338700	-4.05365600	-0.98611300
H	2.67447000	-2.72031700	-3.12966100
H	2.79964500	2.11588200	-1.59947900
H	5.11292300	-0.68863400	0.68176200
C	0.28558100	-3.04053200	1.98150400
C	0.78339000	-4.32439900	1.68635000
C	0.27362200	-2.59466000	3.31902600
C	1.29506600	-5.13476200	2.71124600
H	0.77421300	-4.69032200	0.65938200
C	0.77613800	-3.41034300	4.34316600
H	-0.14806100	-1.61655200	3.55332300
C	1.29826700	-4.67847000	4.03868900
H	1.69013200	-6.12385300	2.47032400
H	0.76046800	-3.05535400	5.37557900
H	1.70002600	-5.31004600	4.83363500
C	-2.25677800	-2.36038000	0.79248400
C	-2.79550200	-3.12590100	1.84668100
C	-3.11961400	-1.83914200	-0.19585700
C	-4.17850600	-3.35700100	1.91316700
H	-2.14518800	-3.54259000	2.61554800
C	-4.49923600	-2.06884200	-0.12122700
H	-2.72381300	-1.23612200	-1.01028600
C	-5.03199000	-2.82712700	0.93393800
H	-4.58478600	-3.94994200	2.73560700
H	-5.14775600	-1.62227800	-0.87339400
H	-6.10897800	-2.99721500	0.99576600
H	3.04236800	-2.50116900	2.37088900
C	0.25671800	2.35842200	2.05810600
C	1.43093700	1.62475700	1.80626200
H	-0.35572400	2.08267500	2.92275700

H	2.12654600	1.95950000	1.03744100
C	1.56172500	0.29278600	2.31023100
H	1.17044200	0.05636700	3.30538600
O	-2.94452900	1.28383300	1.94909200
C	-2.88504500	1.26203300	0.71468000
O	-1.90268200	0.92312800	-0.05255300
C	-4.15759400	1.69633200	-0.09610200
C	-4.02080100	1.51929200	-1.64267900
O	-4.51934800	0.51633100	-2.15158900
C	-3.28582800	2.53335800	-2.46061000
C	-3.24585800	2.31885800	-3.85912500
C	-2.61312900	3.65306700	-1.92197500
C	-2.56056200	3.20115000	-4.69925900
H	-3.75788100	1.44724800	-4.26725300
C	-1.93215300	4.53735100	-2.76851000
H	-2.59379000	3.83338400	-0.85161200
C	-1.90314700	4.31816000	-4.15418500
H	-2.53727000	3.02053900	-5.77599100
H	-1.41155300	5.39120000	-2.33497400
H	-1.36550500	5.00939900	-4.80719800
H	2.42384300	-0.29292400	1.99164200
C	-0.12119300	3.61731500	1.40753300
C	0.70996700	4.28536800	0.47622500
C	-1.37295400	4.19383700	1.73102700
C	0.31371600	5.50414100	-0.08407700
H	1.67323900	3.85594900	0.19983500
C	-1.77048100	5.41048800	1.16279100
H	-2.03923600	3.65866300	2.40795600
C	-0.92422800	6.07658600	0.26059400
H	0.97191400	6.01125400	-0.79288800
H	-2.74352900	5.83374900	1.41915400
H	-1.22910400	7.02907800	-0.17775700
F	-5.22271300	0.94820800	0.33574100
F	-4.45592500	3.01698900	0.22012400
TS3			
Pd	-0.08423100	0.72225500	0.72126200
P	1.54335600	-0.60904200	-0.10688800
C	2.78868000	0.49733000	-0.88263600
C	3.98371800	0.01440300	-1.45322600
C	4.91339700	0.90216300	-2.00789700
H	5.83683100	0.52052500	-2.44737400
C	4.65297200	2.28274600	-1.98898400
H	5.37305300	2.98298300	-2.41681400

C	3.46802000	2.76517500	-1.41882400
C	2.51911400	1.88306800	-0.85909600
C	1.27622800	2.50186500	-0.27033500
C	0.11383900	2.66848100	-1.09295100
C	0.01568600	1.98955800	-2.45731300
H	0.67710500	1.11115400	-2.45166900
C	0.52957100	2.95728200	-3.54754800
H	1.56897400	3.26762600	-3.35511400
H	-0.10208400	3.86064100	-3.58256800
H	0.48924300	2.46901300	-4.53553600
C	-1.40294800	1.49361600	-2.78689500
H	-1.37354200	0.88597600	-3.70587100
H	-2.09535500	2.33210600	-2.96195100
H	-1.80033400	0.88489200	-1.96701700
C	-0.85559300	3.62569900	-0.71428900
H	-1.72789800	3.75374800	-1.34932500
C	-0.70250500	4.42680200	0.42237600
C	-1.65943800	5.55866300	0.77526400
H	-1.94316300	5.42278400	1.82938200
C	-2.94586200	5.59109100	-0.06485800
H	-3.62322700	6.36733600	0.32547100
H	-3.47161800	4.62693700	-0.04322200
H	-2.72312600	5.83775700	-1.11711300
C	-0.92455000	6.91726600	0.66718800
H	-0.02386000	6.94210800	1.30149300
H	-1.59217300	7.73694500	0.98199500
H	-0.61382700	7.10618300	-0.37449000
C	0.40951600	4.19246000	1.26053700
H	0.50434400	4.77133600	2.18062100
C	1.39699200	3.25610800	0.94682300
C	2.57656100	3.03895000	1.88855700
H	3.21833700	2.25633300	1.45886600
C	3.42693100	4.31743300	2.03420200
H	3.81984800	4.64353100	1.05789200
H	4.27996700	4.13733900	2.70979300
H	2.82656700	5.14151900	2.45352500
C	2.09587500	2.53363700	3.26451300
H	1.48696600	3.30021500	3.77043800
H	2.95826400	2.30021900	3.91123700
H	1.48428000	1.62519800	3.14551800
C	-2.14036300	1.31160300	2.17050300
C	-1.20933000	0.39868600	2.67475900
H	-2.76559500	0.96476000	1.34207100
H	-0.61810600	0.64706900	3.55989600

C	-0.91128900	-0.80131700	1.95107700
H	-0.17986600	-1.49240700	2.37869700
H	-1.68868200	-1.22990500	1.30782700
O	-7.14282600	0.76236100	0.31530200
C	-6.23535500	0.41776300	0.99019500
O	-5.45467700	0.05732400	1.80080700
C	-4.39878200	1.14269700	-1.11838800
C	-3.92140900	-0.15612600	-1.02798900
O	-2.86461800	-0.41338900	-0.31560100
F	-5.30212500	1.64061300	-2.00836200
F	-3.67451600	2.18760600	-0.60507100
C	-4.66088600	-1.29727100	-1.67550000
C	-4.08497600	-2.58363500	-1.53499300
C	-5.86806800	-1.19714900	-2.41136600
C	-4.67169600	-3.71565100	-2.11703500
H	-3.16713100	-2.67026800	-0.95474800
C	-6.45526400	-2.33149600	-2.98894400
H	-6.36263600	-0.23642900	-2.52683400
C	-5.86219500	-3.59848900	-2.85223100
H	-4.19869700	-4.69348600	-1.99055300
H	-7.38841900	-2.22261100	-3.54789000
H	-6.32448600	-4.47842700	-3.30614700
C	-2.46345200	2.59330300	2.78271300
C	-3.68941800	3.21809200	2.44259500
C	-1.63532600	3.21812100	3.74929800
C	-4.09335600	4.39817400	3.07747800
H	-4.32085500	2.75767300	1.68483200
C	-2.03448400	4.40396200	4.37292600
H	-0.67607700	2.76886800	4.00393800
C	-3.26948300	4.99623700	4.04601800
H	-5.04634400	4.85790400	2.80877500
H	-1.38390300	4.87223500	5.11505200
H	-3.58020100	5.92085300	4.53685500
H	4.19344600	-1.05521900	-1.45147700
H	3.26364000	3.83683600	-1.40171500
C	2.49244900	-1.56251600	1.13878600
C	2.08095600	-2.86477000	1.49479800
C	3.55982100	-0.95646300	1.83461100
C	2.73451800	-3.55068600	2.52958900
H	1.25825800	-3.34078800	0.95877300
C	4.20848400	-1.64700800	2.86835000
H	3.88696200	0.04800100	1.56236100
C	3.79738700	-2.94396700	3.21892700
H	2.41353800	-4.56015900	2.79430300

H	5.03777300	-1.17262900	3.39727900
H	4.30422400	-3.47965800	4.02396700
C	1.00271800	-1.83578800	-1.35510700
C	1.89539100	-2.78725600	-1.89655100
C	-0.34029200	-1.80302400	-1.78195400
C	1.45278000	-3.67564900	-2.88529400
H	2.92206200	-2.84850100	-1.53293700
C	-0.77424600	-2.69747800	-2.77521800
H	-1.05675400	-1.11426000	-1.32377300
C	0.11971100	-3.62439800	-3.33181400
H	2.14458800	-4.41034900	-3.30285600
H	-1.81774500	-2.67248100	-3.09279800
H	-0.22212900	-4.31819500	-4.10301100

IM4

C	1.69300200	-0.29781200	1.14358000
C	2.18625700	0.24822200	-0.08340600
H	1.64047400	0.35696800	2.02548900
H	2.55000600	-0.42233200	-0.86643400
C	2.05870000	1.61877500	-0.34295600
H	1.82216900	2.26867900	0.49782200
C	1.74404500	4.28183200	1.87267000
C	1.87625900	3.18840900	2.70155800
O	0.94450300	2.27773700	2.75736700
F	0.66796500	4.44626400	1.04895600
F	2.61034300	5.31918400	1.66533200
C	3.11068600	3.00950900	3.54673500
C	4.33664100	3.70160000	3.38606900
C	3.04399800	2.02177900	4.55979300
C	5.43696500	3.41968300	4.20825900
H	4.44369200	4.45642200	2.61005000
C	4.14213700	1.74687300	5.38547800
H	2.10646700	1.47753600	4.67725400
C	5.34948800	2.44439400	5.21642900
H	6.37236000	3.96473600	4.05501500
H	4.05560200	0.98361400	6.16398600
H	6.20973800	2.22967200	5.85527100
Pd	-0.06602200	0.30072500	0.09024400
P	-1.38640700	-1.23203000	1.10033600
C	-3.03178200	-1.11755600	0.30151100
C	-4.07244500	-2.03038900	0.56328600
C	-5.30956600	-1.88953900	-0.07718800
H	-6.11397100	-2.59891200	0.12610700
C	-5.50627400	-0.83409900	-0.98417900

H	-6.46657900	-0.71919900	-1.49068700
C	-4.47008900	0.07289400	-1.24509600
C	-3.21926800	-0.05281900	-0.60526200
C	-2.14852500	0.94832800	-0.97115900
C	-1.42926200	0.75391100	-2.20157700
C	-1.43474200	-0.59999100	-2.90771000
H	-1.89675300	-1.33384300	-2.23244800
C	-2.29093100	-0.53645400	-4.19030900
H	-1.87487700	0.19798000	-4.89935500
H	-2.31334800	-1.52085600	-4.68714900
H	-3.32639000	-0.24088300	-3.95798000
C	-0.01137300	-1.09932500	-3.21609600
H	0.57978100	-1.16068300	-2.28817900
H	-0.05103700	-2.10096700	-3.67602800
H	0.50446000	-0.42344100	-3.91634100
C	-0.80973000	1.86051200	-2.80500300
H	-0.27809500	1.72137100	-3.74761600
C	-0.86867000	3.14741600	-2.24421000
C	-0.27897100	4.31475100	-3.02525600
H	0.68012000	3.97194000	-3.44220400
C	-1.20709500	4.65758300	-4.21618200
H	-0.76481400	5.46288300	-4.82683700
H	-1.36966700	3.78017100	-4.86313900
H	-2.19028400	5.00087900	-3.85184600
C	-0.01377500	5.57330200	-2.18219500
H	-0.96007400	6.03793200	-1.85681800
H	0.57963200	5.34446800	-1.28662900
H	0.53160000	6.31595000	-2.78641100
C	-1.51042900	3.30827500	-1.00292000
H	-1.51939900	4.28632000	-0.52723100
C	-2.15920400	2.24624800	-0.35415500
C	-2.93526800	2.48116400	0.93764400
H	-3.10403200	1.50267700	1.41287900
C	-4.31936600	3.09104600	0.61414600
H	-4.91012600	2.43437000	-0.04337500
H	-4.88793500	3.25140000	1.54548600
H	-4.19765300	4.06587600	0.11286900
C	-2.18302300	3.36708500	1.95033300
H	-2.10788900	4.40605500	1.59074700
H	-2.74866500	3.38411800	2.89720600
H	-1.16541300	3.00069000	2.14794600
H	1.80090300	-1.37331800	1.31084900
C	2.44674800	2.27513500	-1.58501700
C	2.53698600	1.58896000	-2.82089300

C	2.79212000	3.64848600	-1.54703200
C	2.96290300	2.25195000	-3.97574800
H	2.25325600	0.53822300	-2.86926100
C	3.23468600	4.30569000	-2.70106800
H	2.73649700	4.18507200	-0.60078600
C	3.31686500	3.61387700	-3.92096500
H	3.01909900	1.71041600	-4.92280800
H	3.50519700	5.36197600	-2.64996800
H	3.65126800	4.12942300	-4.82366800
H	-4.62028200	0.88888100	-1.95341000
H	-3.90777200	-2.85307300	1.26067700
C	-0.85989100	-2.97322300	0.88934400
C	0.00389600	-3.56491000	1.83588800
C	-1.20571700	-3.68654300	-0.27784800
C	0.50989400	-4.85454400	1.61617900
H	0.27037800	-3.02165200	2.74393700
C	-0.69655500	-4.97560800	-0.49157200
H	-1.87641700	-3.23694000	-1.01154900
C	0.16288200	-5.56158700	0.45284900
H	1.17342900	-5.30664900	2.35605400
H	-0.97426700	-5.52327300	-1.39458600
H	0.55840400	-6.56512700	0.28433300
C	-1.64377400	-0.99707700	2.89550800
C	-2.32323800	-1.95351700	3.68155400
C	-1.17549800	0.19724000	3.47601500
C	-2.54493900	-1.70227200	5.04196000
H	-2.66086700	-2.89172300	3.23767100
C	-1.40434800	0.44008900	4.84042100
H	-0.61240400	0.92543800	2.89043000
C	-2.09013600	-0.50267000	5.62086300
H	-3.06800400	-2.44209100	5.65181800
H	-1.03102700	1.36608100	5.28084000
H	-2.26426200	-0.31281800	6.68230500
TS4			
Pd	3.84333400	0.23030800	17.60454300
C	3.64012600	-1.53693400	18.71795300
H	3.82440900	-2.34980900	18.00268300
H	4.30747300	-1.56722000	19.58422900
C	2.27845800	-1.13543700	18.96161700
C	1.25097400	-1.34306800	18.05874100
H	1.48128100	-1.90143900	17.14610000
C	-0.12878500	-0.91596200	18.21298400
C	-0.60276000	-0.23262600	19.36491900

C	-1.04640100	-1.18871100	17.16626200
C	-1.93555100	0.17531400	19.44914800
H	0.06928500	-0.01942300	20.19341800
C	-2.38261400	-0.78464600	17.25715000
H	-0.69279100	-1.71740700	16.27743100
C	-2.83057200	-0.09606400	18.39710700
H	-2.27482500	0.71513900	20.33390900
H	-3.07320900	-0.99987500	16.43923000
H	-3.87079500	0.22823000	18.46751600
O	2.92143500	4.04687400	21.69321300
C	2.95845600	2.89588700	22.20881200
O	3.37153500	2.48003500	23.31265000
C	2.38708300	1.81797000	21.21280300
C	1.33741900	2.38775900	20.23668200
O	1.53108300	2.33798500	19.01980000
F	3.44572100	1.30242000	20.47497400
F	1.81414400	0.69519400	21.84794100
C	0.06615900	2.92367800	20.81371500
C	-0.88682200	3.46691500	19.92354000
C	-0.24022800	2.85773300	22.19200700
C	-2.11849800	3.93290900	20.39451200
H	-0.64293900	3.50885200	18.86296200
C	-1.47750200	3.32026000	22.65978900
H	0.47795500	2.44539400	22.89848400
C	-2.41958200	3.85735600	21.76604100
H	-2.84569700	4.35202900	19.69537000
H	-1.70393900	3.26506800	23.72644900
H	-3.38151100	4.21836800	22.13707100
H	2.08370000	-0.59376400	19.88283500
P	6.08252600	0.18949800	17.69280300
C	6.70083900	0.96893500	16.15774100
C	8.01923800	0.76637000	15.70367800
C	8.47763000	1.43521900	14.56089400
H	9.49922200	1.27838200	14.20993500
C	7.61762700	2.30938700	13.87556800
H	7.96880700	2.83782800	12.98714500
C	6.30203700	2.50023100	14.32257900
C	5.81925800	1.82701600	15.46272900
C	4.37990700	2.04261300	15.84998100
C	3.36318300	1.24420000	15.22388900
C	3.72718700	0.07718900	14.30483500
H	4.77705400	-0.19042100	14.49237700
C	3.61011900	0.52260400	12.83039000
H	2.57155800	0.80824500	12.59524100

H	3.90614800	-0.29818100	12.15579100
H	4.25922400	1.38906000	12.62893800
C	2.88063800	-1.18278400	14.56449300
H	3.01694900	-1.52860900	15.60095400
H	3.18761000	-1.99085200	13.87970700
H	1.80722600	-0.99385700	14.40317300
C	2.01985600	1.66446400	15.32309600
C	1.66072500	2.84466700	15.99156300
C	0.22038300	3.33236700	16.01944100
H	0.15881600	4.12328900	16.78478100
C	-0.77741200	2.22155700	16.39785200
H	-1.79296100	2.63994200	16.49276500
H	-0.49704100	1.75218300	17.34907900
H	-0.81267500	1.44178700	15.62098400
C	-0.15147900	3.95736200	14.65492600
H	0.53149000	4.78205600	14.39290300
H	-1.18171000	4.35126300	14.67821000
H	-0.09251600	3.19805300	13.85645300
C	2.66988800	3.59153400	16.62024500
C	4.01696000	3.21488200	16.58264200
C	5.05594700	4.04522900	17.32462700
H	6.02021000	3.52160400	17.26525200
C	5.23372500	5.42631700	16.65759400
H	4.28825600	5.99279200	16.67971800
H	5.55091600	5.32742800	15.60580200
H	5.99531600	6.01342900	17.19750500
C	4.69259000	4.19167500	18.81714600
H	3.77641000	4.78431200	18.95092600
H	5.50809100	4.70240400	19.35267700
H	8.67998500	0.08986600	16.24895800
H	5.63135400	3.17058300	13.78295300
H	1.24676800	1.06694200	14.83946600
H	2.38759500	4.48008300	17.18552300
C	6.77211000	1.17136000	19.07449200
C	7.69301700	2.21793800	18.86197100
C	6.27874800	0.92731100	20.37314200
C	8.09121200	3.02392500	19.93879000
H	8.08113100	2.41483900	17.86245100
C	6.66473100	1.74659400	21.44091600
H	5.55916700	0.12865200	20.54126600
C	7.56748100	2.80009700	21.22217400
H	8.79587800	3.84030400	19.76804100
H	6.22018300	1.59326400	22.42476800
H	7.84909900	3.45438100	22.04908500

C	6.87032300	-1.46182700	17.75614300
C	6.41210500	-2.44714200	16.85476300
C	7.90528500	-1.76777500	18.66093400
C	6.99443400	-3.72087300	16.85141400
H	5.59918600	-2.21342100	16.16353700
C	8.47850400	-3.05018300	18.65958700
H	8.25871200	-1.00970800	19.36129100
C	8.02689700	-4.02494200	17.75662500
H	6.63860100	-4.47856200	16.15036800
H	9.27810900	-3.28417300	19.36506700
H	8.47352800	-5.02113800	17.75968800
H	4.52098300	3.21882300	19.29174700

IM5

Pd	0.23562300	-0.17650700	0.03769100
P	0.53106500	0.26213200	2.17863200
C	2.18744100	-0.33807900	2.69042300
C	2.50237500	-0.53023600	4.05181100
C	3.76833200	-0.99594600	4.42833700
H	4.00333700	-1.14513100	5.48381400
C	4.72367000	-1.27980700	3.43921600
H	5.71177700	-1.64913500	3.72056900
C	4.40663600	-1.10448800	2.08521700
C	3.13722300	-0.63666200	1.68399500
C	2.87833800	-0.53214900	0.20333000
C	2.74333500	-1.73413400	-0.55567200
C	2.45750300	-3.07795600	0.10963200
H	2.39384900	-2.92077300	1.19647600
C	3.59358500	-4.08969500	-0.14874400
H	3.70563700	-4.28698500	-1.22741200
H	3.37380000	-5.04746200	0.35179600
H	4.55649800	-3.71199700	0.23164200
C	1.09873900	-3.64407000	-0.36174100
H	0.28601000	-2.92578500	-0.17402300
H	0.87478200	-4.58588600	0.16723200
H	1.11277300	-3.85638200	-1.44252700
C	2.83743800	-1.67148000	-1.95610000
C	3.01707300	-0.45928900	-2.63731600
C	3.13996600	-0.36364400	-4.15691200
H	2.35448700	0.33223300	-4.49366900
C	2.94805000	-1.69703100	-4.89687200
H	2.98202400	-1.52573300	-5.98417100
H	1.98246600	-2.16355600	-4.65694600
H	3.75222100	-2.40786400	-4.63960500

C	4.50503400	0.25508000	-4.54493000
H	4.65458300	1.23945600	-4.07484300
H	4.56782300	0.38300500	-5.63827000
H	5.32893500	-0.40585700	-4.22594100
C	3.07162200	0.72474000	-1.87708900
C	3.03978600	0.72036700	-0.47539200
C	3.27266900	2.00590700	0.31191800
H	2.79263800	1.89807300	1.29363300
C	4.78798500	2.19229100	0.55799500
H	5.32137200	2.28963100	-0.40236000
H	5.21271400	1.33611300	1.10508500
H	4.96780400	3.10603700	1.14914200
C	2.67805500	3.26054300	-0.35361900
H	3.24377600	3.54215000	-1.25699700
H	2.72943100	4.10627600	0.34981700
H	1.74454300	-0.33592900	4.81280200
H	5.14272200	-1.34288500	1.31596300
H	2.73594600	-2.59804700	-2.51978500
H	3.15506600	1.67709000	-2.40016500
C	0.45554400	2.05791400	2.54540500
C	1.05849900	2.61653000	3.69101300
C	-0.21617800	2.89227700	1.62790100
C	0.98520800	3.99858100	3.91632700
H	1.59661400	1.97913600	4.39374200
C	-0.29356300	4.27302200	1.86346200
H	-0.65027400	2.46168800	0.72452400
C	0.30715500	4.82676600	3.00514400
H	1.46023700	4.42898600	4.80025000
H	-0.80926000	4.91355800	1.14582800
H	0.25529400	5.90294500	3.18197200
C	-0.63782500	-0.55523100	3.32739700
C	-0.69619400	-1.96658100	3.30309200
C	-1.52595400	0.16722000	4.14625400
C	-1.62573300	-2.64428900	4.10170100
H	-0.02034500	-2.52779100	2.65408000
C	-2.46213400	-0.51840800	4.93868000
H	-1.48754400	1.25731300	4.16377400
C	-2.51321600	-1.92020000	4.91852200
H	-1.66497300	-3.73534900	4.08133700
H	-3.15155100	0.04653500	5.56915600
H	-3.24438800	-2.44922800	5.53281400
H	1.63059500	3.10499700	-0.64214900
C	-2.82695700	-5.78127700	-0.72538100
C	-2.61297600	-4.43683700	-0.40633800

C	-2.83869500	-3.41603600	-1.36721700
C	-3.28095800	-3.80418800	-2.65819900
C	-3.49277700	-5.15134200	-2.97618100
C	-3.26766900	-6.14778900	-2.01129900
H	-2.64437500	-6.55139200	0.02778200
H	-2.25500900	-4.16957000	0.58931000
H	-3.44880400	-3.02989700	-3.40919300
H	-3.83416900	-5.42419700	-3.97737300
H	-3.42952300	-7.19950100	-2.25702000
C	-2.59095200	-2.00335800	-1.10665200
C	-2.25926300	-1.44022400	0.09613700
H	-2.66434700	-1.33126300	-1.96613900
H	-2.21533900	-2.05072000	1.00257500
C	-1.88443700	-0.03934100	0.21875600
H	-2.13185100	0.58410800	-0.65214700
H	-2.13098400	0.42709200	1.17974500
O	-2.04422700	2.64002000	-4.44243400
C	-1.90728500	1.76944200	-3.56544200
O	-2.73721600	1.07989200	-2.90779000
C	-0.41742700	1.40068500	-3.14768600
C	-0.27928000	-0.12477400	-3.10202500
O	-0.05425900	-0.73890900	-2.04004000
F	0.56281000	1.92687600	-3.98392500
F	-0.16487100	1.94899800	-1.89621700
C	-0.49307200	-0.89719400	-4.34681200
C	-0.57102200	-0.28858000	-5.62207200
C	-0.61250400	-2.30450500	-4.23981500
C	-0.74381300	-1.08236600	-6.76279100
H	-0.51111500	0.79249700	-5.72258400
C	-0.79660600	-3.08730200	-5.38221000
H	-0.57536900	-2.76303700	-3.25333100
C	-0.85275000	-2.47810400	-6.64896400
H	-0.80049300	-0.60678800	-7.74341500
H	-0.90208100	-4.16936800	-5.28496000
H	-0.99008800	-3.08917800	-7.54362000
TS5			
Pd	0.01142200	-0.12702600	-0.01925600
P	0.43286600	0.24715300	2.12228300
C	2.07285600	-0.43410500	2.57935900
C	2.40993200	-0.68909900	3.92533700
C	3.66046300	-1.22657000	4.25527900
H	3.91187200	-1.42296700	5.29924900
C	4.57844700	-1.52079400	3.23431500

H	5.55357100	-1.94697100	3.47841500
C	4.24072300	-1.27846300	1.89588300
C	2.98688100	-0.73573200	1.54243000
C	2.71614100	-0.53546400	0.07506100
C	2.49813600	-1.67990700	-0.74848900
C	2.16363300	-3.04656400	-0.15585900
H	2.07063900	-2.93814400	0.93531800
C	3.29543100	-4.06030200	-0.42991400
H	3.43451600	-4.20447100	-1.51391600
H	3.04866000	-5.03854600	0.01579200
H	4.25229900	-3.71619900	-0.00493400
C	0.81481100	-3.57539600	-0.68753200
H	0.00162500	-2.86927800	-0.46824100
H	0.57811600	-4.54644800	-0.22187300
H	0.84779600	-3.72148700	-1.77841600
C	2.61140600	-1.54707200	-2.14296500
C	2.92065400	-0.32255400	-2.75305800
C	3.16679100	-0.18075200	-4.25615300
H	2.41610900	0.52468100	-4.64420700
C	3.04182800	-1.49374700	-5.04703800
H	3.19540700	-1.29421500	-6.11914100
H	2.05388100	-1.95759500	-4.92858400
H	3.80978300	-2.21738500	-4.72238000
C	4.56301000	0.43730400	-4.51469700
H	4.67987200	1.41555500	-4.02337300
H	4.71828900	0.57751600	-5.59725400
H	5.35429700	-0.23206300	-4.13625800
C	3.03741000	0.81371500	-1.92662500
C	2.96924700	0.73765200	-0.52948700
C	3.29649500	1.95477000	0.33223800
H	2.84820800	1.80446900	1.32341700
C	4.82819800	2.04564300	0.52554000
H	5.32754800	2.18921500	-0.44726200
H	5.22798100	1.12903000	0.98682000
H	5.08098500	2.90053000	1.17541000
C	2.74827900	3.28515100	-0.21465800
H	3.23392800	3.56286100	-1.16424400
H	2.95286200	4.08708400	0.51265500
H	1.67989500	-0.48675800	4.71047500
H	4.94836300	-1.51863300	1.10109200
H	2.45578300	-2.43146700	-2.75881800
H	3.22121900	1.78172700	-2.39182800
C	0.45226800	2.04097200	2.51757900
C	1.15532200	2.56514100	3.62167900

C	-0.26011300	2.90966100	1.66478500
C	1.14417500	3.94566400	3.86758200
H	1.72334800	1.90243300	4.27595700
C	-0.27758900	4.28878000	1.92275300
H	-0.77576500	2.50364800	0.79225600
C	0.42580200	4.80782100	3.02112200
H	1.69821000	4.34838800	4.71802500
H	-0.82681900	4.95520700	1.25509900
H	0.42183900	5.88247900	3.21432100
C	-0.71898600	-0.52047900	3.32514600
C	-0.71980200	-1.92859100	3.43978100
C	-1.66736000	0.23621700	4.03964100
C	-1.65282000	-2.56641800	4.26741100
H	0.00936800	-2.52066900	2.88285100
C	-2.60655700	-0.40955400	4.86122600
H	-1.67127600	1.32422100	3.95700500
C	-2.60131500	-1.80773300	4.97683500
H	-1.64296800	-3.65476100	4.35623900
H	-3.34033000	0.18357600	5.41062600
H	-3.33255200	-2.30665900	5.61579700
H	1.66549300	3.23573300	-0.38072600
C	-2.78201400	-5.93640200	-0.15511700
C	-2.69986000	-4.55754500	0.06074600
C	-2.81278700	-3.64369100	-1.02039200
C	-3.01516700	-4.17568600	-2.32025400
C	-3.09248600	-5.55742000	-2.53463800
C	-2.97614400	-6.44643500	-1.45317800
H	-2.69236400	-6.62183100	0.69110300
H	-2.54171400	-4.18016300	1.07267200
H	-3.09563200	-3.48558100	-3.16311600
H	-3.24357100	-5.94113600	-3.54630500
H	-3.03572300	-7.52456200	-1.61663200
C	-2.67931400	-2.19960900	-0.87193300
C	-2.37949400	-1.51526000	0.27435200
H	-2.75668100	-1.61974700	-1.79376600
H	-2.26779400	-2.04939600	1.22172400
C	-2.09300400	-0.08783200	0.29241400
H	-2.43057500	0.47793100	-0.58408600
H	-2.30661000	0.41817800	1.24109200
O	-2.11505100	2.39122200	-4.77557900
C	-2.17490700	2.06039000	-3.62178400
O	-2.74436600	1.92467000	-2.57074100
C	-0.04491800	1.46899500	-3.17367800
C	-0.20720900	0.06123400	-3.14416000

O	-0.48352200	-0.55073200	-2.04409300
F	0.67623000	2.08895400	-4.15339800
F	0.19400100	2.11746100	-1.99601500
C	-0.31145900	-0.74912800	-4.39320400
C	-0.22845300	-0.22244800	-5.70295100
C	-0.48450700	-2.14672300	-4.23679400
C	-0.29435100	-1.07424500	-6.81402200
H	-0.13677100	0.84807900	-5.85879100
C	-0.55518000	-2.99105300	-5.35109400
H	-0.56101200	-2.55517200	-3.23112100
C	-0.45234200	-2.45982300	-6.64769000
H	-0.22937200	-0.64786600	-7.81743300
H	-0.68806400	-4.06545200	-5.20367100
H	-0.50113200	-3.11662800	-7.51903700

IM6

Pd	-0.08517200	-0.10272300	-0.05864700
P	0.43042800	0.22402000	2.08442300
C	2.06887800	-0.46880800	2.53298000
C	2.40516900	-0.75325500	3.87352200
C	3.65728200	-1.29208800	4.19460000
H	3.90671300	-1.51124800	5.23460600
C	4.58013800	-1.55655800	3.16987100
H	5.55724500	-1.98256800	3.40650900
C	4.24378800	-1.28475900	1.83687300
C	2.98689000	-0.74158400	1.49339500
C	2.71797400	-0.51611600	0.03116500
C	2.45316100	-1.64135200	-0.80068700
C	2.07976100	-3.00032000	-0.21403400
H	1.93245700	-2.87812300	0.86983600
C	3.22040100	-4.02019000	-0.42075100
H	3.41699900	-4.16698300	-1.49567600
H	2.94568800	-4.99635500	0.01357000
H	4.15357700	-3.67806000	0.05531400
C	0.75752100	-3.53239400	-0.80423300
H	-0.05387700	-2.80327500	-0.66888300
H	0.47419200	-4.47537300	-0.30826900
H	0.85585000	-3.73374800	-1.88224800
C	2.58066700	-1.50242900	-2.19417800
C	2.94471800	-0.28665700	-2.79050000
C	3.21370500	-0.14672000	-4.28948700
H	2.46375300	0.55208000	-4.69099600
C	3.10345000	-1.46419900	-5.07487100
H	3.28261200	-1.27290700	-6.14456900

H	2.11120000	-1.92238100	-4.97655000
H	3.86171300	-2.18726700	-4.72658200
C	4.61137400	0.47355300	-4.53342400
H	4.72150000	1.45585500	-4.04865300
H	4.78068500	0.60594900	-5.61498300
H	5.39960700	-0.19100000	-4.14025400
C	3.08926000	0.83926300	-1.95365700
C	3.00262000	0.75419100	-0.55896200
C	3.32369000	1.96377900	0.31511200
H	2.85324500	1.81113700	1.29584900
C	4.84996900	2.05639000	0.54190200
H	5.37082500	2.19334700	-0.42062300
H	5.23925600	1.14283600	1.01786400
H	5.08918500	2.91542200	1.19174200
C	2.78368400	3.29242000	-0.24530300
H	3.32323400	3.59236600	-1.15876900
H	2.92174800	4.08937200	0.50263800
H	1.67289200	-0.57181300	4.66148900
H	4.95516800	-1.50096400	1.03855800
H	2.39722800	-2.37548300	-2.81792500
H	3.30287400	1.80632700	-2.40907700
C	0.48383000	2.01111200	2.52419200
C	1.18024000	2.49354800	3.65146900
C	-0.19200300	2.91721800	1.68148100
C	1.20010800	3.86795900	3.92869700
H	1.71904900	1.80199200	4.30058500
C	-0.17824200	4.29078800	1.96887700
H	-0.70343800	2.54057400	0.79328300
C	0.51929300	4.76740700	3.08979300
H	1.74883400	4.23708900	4.79771300
H	-0.69840100	4.98650400	1.30758300
H	0.53986000	5.83738300	3.30690100
C	-0.70675600	-0.54240700	3.30692600
C	-0.70731900	-1.94999900	3.42718800
C	-1.64908300	0.21532800	4.02847900
C	-1.63325100	-2.58544700	4.26496200
H	0.01617400	-2.54469000	2.86558000
C	-2.58151000	-0.42730000	4.86020700
H	-1.65330500	1.30316300	3.94299200
C	-2.57587500	-1.82515000	4.98019100
H	-1.62225100	-3.67358800	4.35671100
H	-3.31016000	0.16791000	5.41437900
H	-3.30160900	-2.32209500	5.62702200
H	1.71611100	3.21691700	-0.48617900

C	-2.85712800	-5.94756400	-0.05333600
C	-2.80147200	-4.56562900	0.15276800
C	-2.87839300	-3.66274200	-0.94063400
C	-3.02079200	-4.20935000	-2.24255400
C	-3.07107800	-5.59379200	-2.44688100
C	-2.98954400	-6.47209000	-1.35332600
H	-2.79770700	-6.62396100	0.80289300
H	-2.69858400	-4.17606500	1.16738700
H	-3.07021200	-3.52814000	-3.09513800
H	-3.17338900	-5.98813100	-3.46066100
H	-3.02972900	-7.55231500	-1.50892200
C	-2.77261600	-2.21525700	-0.80129700
C	-2.44095800	-1.52636900	0.33358600
H	-2.87590500	-1.63956400	-1.72283200
H	-2.27368200	-2.06297900	1.27087100
C	-2.17411900	-0.09479300	0.35225700
H	-2.56831300	0.46995900	-0.50139000
H	-2.34785100	0.40010900	1.31499700
C	0.09792500	1.49849200	-3.14598600
C	-0.27998200	0.18648000	-3.13174200
O	-0.77252100	-0.37136300	-2.03171300
F	0.74513100	2.15793100	-4.14002300
F	0.06043500	2.28361300	-2.04091300
C	-0.24756900	-0.68233700	-4.34238400
C	-0.08390000	-0.21919700	-5.66965400
C	-0.43500200	-2.07234500	-4.14211200
C	-0.08059700	-1.11650200	-6.74605400
H	0.03042800	0.84432500	-5.86803500
C	-0.43332300	-2.96554100	-5.22190200
H	-0.58323700	-2.43299200	-3.12675100
C	-0.25017400	-2.49510600	-6.53267600
H	0.04964700	-0.73240600	-7.76078000
H	-0.57568400	-4.03300700	-5.03431200
H	-0.24630100	-3.18908000	-7.37626500
TS6			
Pd	-2.03018500	0.51814400	1.04483600
C	-1.03139000	0.82739000	3.28236500
O	-1.02560300	-1.79335100	0.26569900
P	-2.23871900	0.60644600	-1.24016100
C	-1.36385300	1.99094000	2.57291900
C	-0.78930300	2.21315300	1.27603700
H	-1.08790600	3.10245600	0.71693800
H	0.22988800	1.87025100	1.06915600

H	-0.13131800	0.28807600	2.97180200
H	-2.16203500	2.64630600	2.92765000
C	-3.02032400	-0.89754000	-1.95728500
C	-4.09013400	-1.51356900	-1.25313800
C	2.11916100	1.03794200	-2.79730600
C	1.29001700	2.16795800	-2.69292000
C	-0.04653200	2.02956200	-2.28900500
C	-0.56571900	0.75087600	-1.98751100
C	0.26919400	-0.38264500	-2.10067500
C	1.60359800	-0.23493400	-2.50464400
H	3.16019300	1.15087500	-3.10771900
H	1.68023800	3.16038600	-2.92972400
H	-0.68131500	2.91385600	-2.21395000
H	-0.09105200	-1.38420100	-1.88052100
H	2.22172600	-1.13056600	-2.57314400
C	-4.29324400	4.47522500	-2.77473100
C	-4.01175800	3.43479600	-3.67731400
C	-3.43168400	2.24328100	-3.21939700
C	-3.14048700	2.08352300	-1.84960000
C	-3.45510700	3.11387000	-0.94387900
C	-4.01974600	4.31284200	-1.40726300
H	-4.73624200	5.40504800	-3.13678400
H	-4.23701200	3.55492200	-4.73875500
H	-3.19824100	1.44157400	-3.92262700
H	-3.26343600	2.96036900	0.11899400
H	-4.25750400	5.11075400	-0.70071100
C	-2.52237400	-1.48634100	-3.13541000
H	-1.70243300	-1.01606800	-3.67657900
C	-4.59586600	-2.73393500	-1.72994200
H	-5.40617500	-3.21791000	-1.18522800
C	-3.04693200	-2.70097800	-3.59875400
H	-2.63731000	-3.15674500	-4.50153300
C	-4.07297700	-3.33379500	-2.88532700
H	-4.46815400	-4.29307900	-3.22423100
C	-4.67225200	-0.82932500	-0.05287500
C	-5.58148900	0.24712800	-0.24661800
C	-4.26496300	-1.20356300	1.26516900
C	-5.96905600	1.00651100	0.86851300
C	-4.65774800	-0.37861600	2.34544600
C	-5.48571400	0.73939300	2.15997500
H	-6.65317500	1.84375800	0.72983700
H	-4.32989700	-0.63438000	3.35338900
C	-3.62720900	-2.56368900	1.53444700
C	-4.75631400	-3.59403400	1.77937900

C	-2.65243800	-2.58859700	2.72476600
H	-3.07638600	-2.87123600	0.64110800
H	-5.46528800	-3.62946700	0.93835900
H	-4.32162300	-4.59880800	1.90949200
H	-5.32298100	-3.33776600	2.69110100
H	-1.91005500	-1.78379000	2.65195000
H	-3.17821800	-2.48161000	3.68693300
H	-2.11503200	-3.54892200	2.73225600
C	-6.20309300	0.50116300	-1.62184900
C	-6.78414200	1.91316000	-1.81121900
C	-7.31590400	-0.54358600	-1.88023000
H	-5.42163300	0.35575700	-2.38247100
H	-6.05696500	2.69187600	-1.54958800
H	-7.07737200	2.05027600	-2.86387600
H	-7.68800400	2.05680300	-1.19516500
H	-6.92609200	-1.57028700	-1.84015300
H	-8.11108700	-0.44465200	-1.12218700
H	-7.76492200	-0.38241400	-2.87489200
C	-5.88406400	1.62412400	3.33295000
C	-7.41271200	1.62820800	3.54893100
C	-5.36404800	3.06489400	3.13713000
H	-5.41527600	1.20714900	4.23844900
H	-7.79061500	0.60609000	3.71178000
H	-7.67673800	2.24242400	4.42612900
H	-7.93156300	2.04814100	2.67165600
H	-4.27265100	3.07555900	2.98407600
H	-5.83059000	3.52722900	2.25150600
H	-5.60142100	3.68980400	4.01434500
C	-0.13558700	-2.61495700	0.51611100
C	1.11109300	-2.22685300	1.23051400
C	1.44175600	-0.85388000	1.27352300
C	1.95953600	-3.16407800	1.86067000
C	2.58455600	-0.41822400	1.95151000
H	0.79903200	-0.15399400	0.74261800
C	3.09890500	-2.72184800	2.54764700
H	1.73491800	-4.22714800	1.80593300
C	3.41167400	-1.35337300	2.60061400
H	2.84062300	0.64367500	1.96652900
H	3.74849600	-3.45040000	3.03649300
H	4.30359700	-1.01690200	3.13356800
C	-1.65173600	0.34576500	4.51024300
C	-1.09979200	-0.79936900	5.13559900
C	-2.79249300	0.95113600	5.09262000
C	-1.66937900	-1.32498400	6.30068700

H	-0.22795200	-1.27918300	4.68582400
C	-3.35970100	0.42459100	6.25701000
H	-3.24161200	1.82633600	4.62440900
C	-2.80365200	-0.71701300	6.86462300
H	-1.23354700	-2.21149400	6.76487400
H	-4.24051600	0.90099800	6.69241500
H	-3.25326400	-1.12816600	7.77045200
O	1.14160800	-3.47857500	-1.66204000
C	0.88944200	-4.45375300	-0.88964900
O	1.40931400	-5.57807700	-0.77546900
C	-0.30685700	-4.07584600	0.06089600
F	-0.43335300	-4.88355000	1.19787800
F	-1.50115400	-4.20107800	-0.62396000

IM7

Pd	-0.03993300	0.31736300	1.49163500
P	-0.56526500	-1.87028600	0.96580300
C	-0.13815800	-2.41536600	-0.74508900
C	-0.92248500	-3.42880600	-1.34493400
C	-0.60724600	-3.93670200	-2.61054200
H	-1.22672500	-4.72018700	-3.05108100
C	0.50909500	-3.43691600	-3.29694900
H	0.77294200	-3.82581100	-4.28250300
C	1.29089800	-2.43485700	-2.70966400
C	0.98619200	-1.90032700	-1.43776100
C	1.93843900	-0.86140400	-0.91521000
C	1.78283600	0.50114700	-1.29087000
C	0.54442900	0.98855100	-2.04570100
H	-0.29518900	0.34103700	-1.74939300
C	0.73801300	0.86047800	-3.57478900
H	1.60076900	1.46636000	-3.89953500
H	-0.15753200	1.23285400	-4.10148900
H	0.91073100	-0.18022100	-3.88442200
C	0.15349600	2.44048100	-1.70493500
H	-0.84011900	2.66061200	-2.12364600
H	0.86557000	3.15886900	-2.14200200
H	0.11370200	2.60690400	-0.62231600
C	2.82058400	1.40018500	-0.99051600
C	3.97919400	1.00435900	-0.30361900
C	5.09991600	1.99824200	-0.02205500
H	4.75602100	2.99254300	-0.35545400
C	6.36300700	1.63598000	-0.83499500
H	6.14103400	1.59276300	-1.91355500
H	6.74961300	0.65049400	-0.52630600

H	7.15768900	2.38279500	-0.67007200
C	5.43979800	2.08839900	1.48148000
H	4.56815100	2.39869500	2.07920800
H	6.24698500	2.82081500	1.64735800
H	5.78328500	1.11313400	1.86327500
C	4.08459600	-0.33572400	0.10131900
C	3.09231800	-1.28292300	-0.20497000
C	3.33497700	-2.75238400	0.13992200
H	2.39863000	-3.30523900	-0.01175500
C	4.38486500	-3.34583000	-0.82611600
H	5.35071200	-2.82487300	-0.71660900
H	4.05889100	-3.24362600	-1.87364500
H	4.54350700	-4.41673800	-0.61344000
C	3.75804200	-2.97639500	1.60456700
H	4.69377900	-2.44563900	1.84439700
H	3.92701300	-4.05033900	1.78287100
H	-1.78622600	-3.82568700	-0.81183100
H	2.16424300	-2.04789600	-3.23630200
H	2.72030300	2.44455700	-1.28478400
H	4.97732500	-0.66076300	0.63863300
C	0.14697600	-3.16477700	2.06368500
C	0.59228200	-4.41042700	1.57968400
C	0.21036700	-2.89679300	3.44668300
C	1.11713300	-5.36349400	2.46555100
H	0.53773900	-4.63410600	0.51444100
C	0.72298300	-3.85676400	4.33130300
H	-0.14978800	-1.94014900	3.82482700
C	1.18655500	-5.08853400	3.84043700
H	1.47138800	-6.32116100	2.07879000
H	0.76470500	-3.63929500	5.40035600
H	1.59786800	-5.83093900	4.52720500
C	-2.38416600	-2.15225600	1.05150200
C	-2.98632400	-2.79795300	2.14747100
C	-3.20105800	-1.58453400	0.05020900
C	-4.38465000	-2.84857400	2.25171700
H	-2.37110300	-3.24795500	2.92708000
C	-4.59609000	-1.63158700	0.16149500
H	-2.74825100	-1.10011500	-0.81381400
C	-5.19199500	-2.25687600	1.26883200
H	-4.84140500	-3.34500100	3.11026400
H	-5.21265000	-1.16689700	-0.60964200
H	-6.27908900	-2.28096600	1.36449600
H	2.97561800	-2.64168800	2.30052800
C	0.76802000	2.37096000	2.49010300

C	1.71037500	1.33223100	2.38960000
H	-0.01545300	2.32019300	3.25453000
H	2.53320200	1.41283700	1.68159400
C	1.44934000	0.05407500	2.96828800
H	0.88359300	-0.00361800	3.90605700
O	-3.61470800	3.67183000	2.36341800
C	-3.02876900	2.67910800	2.84703400
O	-2.23220200	2.54441000	3.80180500
C	-3.36161100	1.29665000	2.05735000
C	-2.89204900	1.38391100	0.60437500
O	-1.69579900	1.13512300	0.31820100
C	-3.79044900	1.83323100	-0.48300900
C	-3.44184900	1.47716500	-1.81036800
C	-4.96058300	2.59421500	-0.25417900
C	-4.25736700	1.85082800	-2.88161800
H	-2.53341500	0.90071200	-1.98312300
C	-5.76077900	2.98171700	-1.33676400
H	-5.19362700	2.92086700	0.75540700
C	-5.42144700	2.60535800	-2.64660700
H	-3.98687200	1.55964100	-3.89861300
H	-6.65297300	3.58392600	-1.15497700
H	-6.05716500	2.90263800	-3.48346400
H	2.17672600	-0.74243200	2.80985000
C	0.84028900	3.62024700	1.72777400
C	1.98486200	3.99027600	0.97777600
C	-0.28178900	4.48449200	1.72045300
C	1.99439100	5.16719300	0.22386900
H	2.86925000	3.35714000	0.98981600
C	-0.27371700	5.65342200	0.94984100
H	-1.15865600	4.23195400	2.31386900
C	0.85897200	5.99723700	0.19345500
H	2.88757300	5.43947000	-0.34329200
H	-1.15694000	6.29493100	0.94350300
H	0.86372300	6.91012200	-0.40610500
F	-2.75475200	0.22389800	2.67889200
F	-4.72181700	1.04895100	2.12462600

TS7

Pd	0.02242700	0.38693600	1.48550500
P	-0.57239800	-1.76429300	0.93841300
C	-0.14025200	-2.33849600	-0.76565500
C	-0.94115400	-3.33973400	-1.36425700
C	-0.62610900	-3.86785000	-2.62161200
H	-1.26057100	-4.64051900	-3.06004500

C	0.50792500	-3.40210800	-3.30248900
H	0.77154600	-3.80668700	-4.28181700
C	1.30807300	-2.41425100	-2.71627700
C	1.00371800	-1.86022100	-1.45275300
C	1.97614700	-0.84227400	-0.92765300
C	1.85742800	0.52148900	-1.31127200
C	0.66172100	1.02501900	-2.12349500
H	-0.20096900	0.38545200	-1.87865300
C	0.94275600	0.89698700	-3.63936700
H	1.82059800	1.50641300	-3.91369700
H	0.07728000	1.26501700	-4.21665600
H	1.13811100	-0.14290500	-3.93837600
C	0.27137700	2.47995600	-1.80049200
H	-0.66715900	2.73267300	-2.31758100
H	1.03925200	3.18768900	-2.15054200
H	0.11637400	2.62496500	-0.72689700
C	2.90563100	1.40011900	-0.98581500
C	4.04372400	0.97902900	-0.27983300
C	5.17525900	1.95342400	0.02582100
H	4.83830300	2.96038100	-0.27498000
C	6.42970800	1.60353700	-0.80576200
H	6.20222500	1.60183700	-1.88404800
H	6.80271200	0.60193300	-0.53418700
H	7.23615700	2.33250700	-0.61855200
C	5.52599800	1.99426100	1.52862200
H	4.65469000	2.27042100	2.14337900
H	6.32629700	2.72934500	1.71500600
H	5.88372100	1.01038100	1.87333900
C	4.11850800	-0.36477900	0.11981100
C	3.11004500	-1.28944400	-0.20117600
C	3.31690100	-2.76557400	0.14057200
H	2.37120200	-3.29793400	-0.02665900
C	4.36627900	-3.37549300	-0.81592100
H	5.34107100	-2.87456400	-0.69257700
H	4.05484600	-3.26173500	-1.86665700
H	4.50087600	-4.45045400	-0.60681200
C	3.71674600	-3.00776100	1.60887000
H	4.65463100	-2.48934600	1.86667500
H	3.87219600	-4.08520000	1.77899800
H	-1.81906200	-3.71239100	-0.83732800
H	2.19717700	-2.05526200	-3.23620900
H	2.83301200	2.44785000	-1.27600000
H	4.99728300	-0.71016300	0.66744000
C	0.09555700	-3.07531600	2.04906100

C	0.50505000	-4.33780300	1.57754900
C	0.15602700	-2.80158600	3.43092400
C	0.99250500	-5.30143400	2.47358400
H	0.45220800	-4.56706900	0.51343700
C	0.63000100	-3.77147500	4.32620000
H	-0.17633100	-1.83130200	3.79989900
C	1.05866700	-5.02061500	3.84728500
H	1.32000100	-6.27209800	2.09549200
H	0.66905700	-3.54893200	5.39442500
H	1.44032000	-5.77135300	4.54215800
C	-2.39654400	-2.03286900	0.99576300
C	-3.02012000	-2.75014000	2.03470100
C	-3.19020900	-1.45323800	-0.01658000
C	-4.41684200	-2.88402300	2.05700900
H	-2.42179700	-3.20548400	2.82426000
C	-4.58412900	-1.58989300	0.00876300
H	-2.72017400	-0.89678600	-0.82645300
C	-5.20085200	-2.30501000	1.04741500
H	-4.89031400	-3.44124800	2.86800800
H	-5.18313400	-1.11953500	-0.77251200
H	-6.28789100	-2.40361600	1.07358600
H	2.92765500	-2.67214700	2.29651300
C	0.81546700	2.38074300	2.43608500
C	1.79056300	1.36677000	2.35865700
H	0.06015700	2.35450400	3.22811300
H	2.59583000	1.46447500	1.63365300
C	1.56653400	0.08420600	2.93399600
H	1.01474600	0.00280100	3.87750000
O	-4.37756300	3.56620600	2.89005300
C	-3.34891600	3.04092200	3.21897900
O	-2.33971400	2.97461100	3.87185600
C	-3.33010300	1.04427000	2.12913000
C	-2.87237500	1.35048700	0.81876900
O	-1.62107300	1.35562300	0.49593700
C	-3.82917200	1.80166200	-0.23456400
C	-3.39059700	1.71691300	-1.57877300
C	-5.14259300	2.25999100	0.01851500
C	-4.24125600	2.06024300	-2.63558500
H	-2.37720600	1.37211600	-1.77807000
C	-5.98575400	2.61465600	-1.04400900
H	-5.49619800	2.36493200	1.03955300
C	-5.54599400	2.51163500	-2.37370800
H	-3.88434800	1.97751500	-3.66490800
H	-6.99306700	2.97734900	-0.82751800

H	-6.21080700	2.78358200	-3.19663100
H	2.30461200	-0.69638400	2.75152800
C	0.85566400	3.59321400	1.60770900
C	2.04074300	4.03904500	0.97428300
C	-0.33897400	4.31831500	1.38981200
C	2.02399400	5.15982500	0.13674800
H	2.97882800	3.51341600	1.14871900
C	-0.35605100	5.43130500	0.54111200
H	-1.25396500	3.97925200	1.86984600
C	0.82382100	5.85550700	-0.09258600
H	2.94979900	5.49396600	-0.33750700
H	-1.29322600	5.96534600	0.37172600
H	0.81113900	6.72457500	-0.75371600
F	-2.51180800	0.33324500	2.95956500
F	-4.61182200	0.62369600	2.32597700

IM8

Pd	0.07684100	0.31408800	1.50375900
P	-0.53344300	-1.81035400	0.96675700
C	-0.17952500	-2.33203200	-0.76726200
C	-1.01997200	-3.29447100	-1.37220400
C	-0.73252900	-3.81585500	-2.63940300
H	-1.39730500	-4.55815700	-3.08545400
C	0.41785500	-3.38697100	-3.31678400
H	0.66594500	-3.79321000	-4.29951400
C	1.25235700	-2.42957200	-2.72644600
C	0.97071500	-1.87119100	-1.46008800
C	1.95880200	-0.86139800	-0.94063600
C	1.83966100	0.50835400	-1.30899800
C	0.64351100	1.02149400	-2.11297600
H	-0.22946100	0.42869900	-1.80364300
C	0.86683800	0.82743500	-3.63167800
H	1.76332900	1.38341800	-3.95572200
H	0.00082000	1.22318200	-4.18981500
H	0.99769400	-0.22793900	-3.90808900
C	0.31178000	2.50237300	-1.84716200
H	-0.66281500	2.74270400	-2.29770900
H	1.06584100	3.16629300	-2.30271400
H	0.24716900	2.71071900	-0.77560400
C	2.87756000	1.38812700	-0.95399300
C	4.01060900	0.96365300	-0.24256800
C	5.13213400	1.94146600	0.08981200
H	4.79763500	2.94833800	-0.21464400
C	6.40454600	1.59891500	-0.71737100

H	6.19783600	1.59658100	-1.79983500
H	6.77818100	0.59925000	-0.43947300
H	7.20325800	2.33227500	-0.51431700
C	5.45364300	1.98080300	1.59929600
H	4.57602400	2.27755900	2.19497000
H	6.26459000	2.70089000	1.79915700
H	5.78448900	0.99131700	1.95509800
C	4.09253000	-0.38723300	0.12949300
C	3.09187200	-1.31225600	-0.21535900
C	3.30396900	-2.79176100	0.10541900
H	2.35473800	-3.32085600	-0.05093800
C	4.33558600	-3.39120400	-0.87667500
H	5.31193800	-2.89029700	-0.76535300
H	4.00576100	-3.26684400	-1.92054800
H	4.47494700	-4.46826500	-0.68128400
C	3.73149900	-3.05232700	1.56245900
H	4.69308700	-2.56707200	1.79726200
H	3.85510800	-4.13476900	1.72540700
H	-1.90527800	-3.64272200	-0.84017600
H	2.14827800	-2.09374700	-3.25015500
H	2.79802000	2.44094600	-1.22534100
H	4.96960900	-0.73636300	0.67732200
C	0.17776500	-3.16804200	1.99505500
C	0.51560600	-4.42938400	1.46644600
C	0.35341100	-2.93043300	3.37339000
C	1.04461300	-5.42603300	2.30074000
H	0.37604500	-4.63243000	0.40455600
C	0.86698100	-3.93314800	4.20889400
H	0.08228800	-1.95876000	3.78483500
C	1.22332600	-5.18075700	3.67136800
H	1.31599000	-6.39516400	1.87683400
H	0.99595900	-3.73645600	5.27523700
H	1.63739700	-5.95742200	4.31759900
C	-2.35387200	-2.03640600	1.15009800
C	-2.91067500	-2.67077300	2.27889300
C	-3.21275600	-1.46395300	0.18827600
C	-4.30328000	-2.72576800	2.44132600
H	-2.26306500	-3.12276700	3.03084200
C	-4.60287500	-1.52742700	0.35063600
H	-2.79745300	-0.96095900	-0.68343300
C	-5.15206400	-2.15248400	1.48066700
H	-4.72287000	-3.21884400	3.32086200
H	-5.24915700	-1.06189700	-0.39530900
H	-6.23515400	-2.18971600	1.61454300

H	2.97261100	-2.69082200	2.27035900
C	0.71728100	2.31155400	2.52720000
C	1.76592700	1.38007900	2.40819400
H	-0.01534300	2.19681300	3.33400800
H	2.54287900	1.55876100	1.66595300
C	1.64069000	0.06940000	2.95733100
H	1.12410200	-0.06147300	3.91498200
C	-3.19507500	1.23643300	1.90806700
C	-2.69174000	1.42021700	0.64863000
O	-1.42127300	1.23772400	0.32045100
C	-3.58647500	1.86187600	-0.46232500
C	-3.22462200	1.51125200	-1.78508400
C	-4.75862300	2.63115200	-0.27584100
C	-4.01946000	1.88692200	-2.87610800
H	-2.30714400	0.94661800	-1.94217900
C	-5.55034900	3.00846900	-1.36937100
H	-5.04678100	2.94653900	0.72594000
C	-5.19050500	2.63601800	-2.67565700
H	-3.71966600	1.59672600	-3.88628800
H	-6.44891500	3.60664200	-1.19908000
H	-5.80881000	2.93474800	-3.52517800
H	2.42584000	-0.65629500	2.74328700
C	0.61456100	3.52970500	1.71577400
C	1.74135500	4.13342800	1.10957900
C	-0.66727400	4.07002300	1.46052200
C	1.58701200	5.23860100	0.26435700
H	2.73768500	3.73585400	1.30943000
C	-0.81927200	5.16700800	0.60465000
H	-1.54294700	3.58765600	1.89871200
C	0.30567400	5.75356400	0.00027500
H	2.46654200	5.69759800	-0.19311000
H	-1.81900400	5.55251400	0.39419100
H	0.18577300	6.60627500	-0.67137500
F	-2.47058600	0.74683300	2.94976800
F	-4.51002900	1.20260700	2.23149500
TS8			
Pd	-0.93641300	-0.03982900	0.22929400
C	-1.05067900	-0.41871800	2.59998300
O	1.07528300	1.27590500	0.85861200
P	-1.07445100	1.09009700	-1.74522600
C	-2.22061000	0.14987300	2.04856200
C	-2.11950900	1.38724700	1.35239900
H	-3.00328500	1.79517900	0.85725300

H	-1.34641800	2.11166500	1.62771200
H	-0.19456600	0.24339200	2.74502300
H	-3.15230100	-0.41782500	2.01037400
C	0.14566700	0.58412100	-3.03551100
C	0.38077800	-0.80589000	-3.22771600
C	-0.44449800	5.64502200	-0.99619700
C	-1.72311600	5.16532800	-1.32036600
C	-1.91939600	3.80057800	-1.58460900
C	-0.83389900	2.90147000	-1.52199300
C	0.44834800	3.38540100	-1.17858300
C	0.63742800	4.75161800	-0.92791300
H	-0.29214700	6.70776700	-0.79514200
H	-2.57102700	5.85175500	-1.37483500
H	-2.91583400	3.44226100	-1.84321500
H	1.28027600	2.69336200	-1.08894400
H	1.63425800	5.11454200	-0.66855200
C	-5.35320200	1.10749900	-3.55099300
C	-4.27699600	1.57822200	-4.32342300
C	-2.97021100	1.51852800	-3.81801000
C	-2.73370100	0.98515400	-2.53534800
C	-3.80876200	0.48226400	-1.77937800
C	-5.11732100	0.54936300	-2.28379600
H	-6.37056500	1.16204400	-3.94378300
H	-4.45681100	1.99634300	-5.31596000
H	-2.13468300	1.90038700	-4.40787500
H	-3.60343900	0.04155300	-0.80175500
H	-5.94876000	0.16183700	-1.69109100
C	0.85698000	1.52867900	-3.80048400
H	0.67609300	2.59320300	-3.65503900
C	1.34390000	-1.20322600	-4.17065900
H	1.53036800	-2.26544200	-4.32536900
C	1.81387200	1.11082800	-4.73665300
H	2.36285800	1.85390600	-5.31838500
C	2.06339000	-0.25649300	-4.91565600
H	2.81311300	-0.59020600	-5.63584100
C	-0.45195800	-1.77840000	-2.44783400
C	-1.70759500	-2.18306600	-2.95760000
C	-0.03892000	-2.16879300	-1.13045800
C	-2.58480500	-2.88900300	-2.11231600
C	-0.98482800	-2.82328700	-0.30604600
C	-2.26612400	-3.16943400	-0.77855500
H	-3.55967500	-3.19245600	-2.49377900
H	-0.70258900	-3.11811600	0.70415000
C	1.44211100	-2.12819200	-0.74992200

C	2.15878800	-3.30930900	-1.45064300
C	1.71896900	-2.21534700	0.75689100
H	1.87043900	-1.19274400	-1.13070800
H	2.02143700	-3.28846600	-2.54048200
H	3.23999600	-3.27397500	-1.23622200
H	1.76150300	-4.26733300	-1.07417000
H	1.20906700	-1.41692200	1.30641100
H	1.39501600	-3.18424100	1.16974100
H	2.79906700	-2.12097800	0.93422900
C	-2.08447100	-1.91387300	-4.41565200
C	-3.60028700	-1.88062100	-4.68271400
C	-1.43445900	-2.98184200	-5.32755100
H	-1.67271900	-0.93159200	-4.69506000
H	-4.12425500	-1.22855000	-3.97355500
H	-3.78650800	-1.50867200	-5.70282000
H	-4.03750400	-2.89130500	-4.61570200
H	-0.33963200	-2.98866600	-5.23261400
H	-1.80841300	-3.98463800	-5.05985600
H	-1.68991100	-2.78963300	-6.38369000
C	-3.27742100	-3.84354700	0.13729000
C	-3.76633700	-5.19271100	-0.42966900
C	-4.47381300	-2.90257700	0.40041600
H	-2.77784400	-4.03851000	1.09854200
H	-2.92094600	-5.87658300	-0.60847400
H	-4.46260600	-5.67586900	0.27635200
H	-4.29846000	-5.04999700	-1.38467300
H	-4.13066300	-1.93748800	0.80456400
H	-5.01845700	-2.70107100	-0.53682100
H	-5.17959900	-3.35508200	1.11767000
C	2.30281600	0.89329300	1.11338500
C	3.22952500	0.75067000	0.11399400
F	2.93125500	0.93397900	-1.20001800
F	4.52649000	0.36880500	0.23519900
C	2.69006900	0.63824300	2.54322500
C	1.96080600	1.32067900	3.54517000
C	3.66069900	-0.30197700	2.96049800
C	2.18386500	1.07358800	4.90621600
H	1.20418500	2.03989700	3.22930400
C	3.87722100	-0.55829600	4.32270400
H	4.23717400	-0.85209200	2.21912900
C	3.14047700	0.12498700	5.30506200
H	1.60510400	1.61734200	5.65713400
H	4.62003500	-1.30430100	4.61673100
H	3.30736700	-0.08143000	6.36465800

C	-0.93534600	-1.73613500	3.21399600
C	0.30114700	-2.09297700	3.81017800
C	-1.99344000	-2.67879400	3.24195100
C	0.47342000	-3.34719100	4.40585400
H	1.12396400	-1.37735800	3.79061100
C	-1.81755000	-3.93161800	3.83998300
H	-2.95352100	-2.43005200	2.78928800
C	-0.58313300	-4.27463900	4.42208600
H	1.43521400	-3.59975300	4.85727600
H	-2.64464300	-4.64525200	3.85148100
H	-0.44901600	-5.25464800	4.88480000

TS9

C	3.91071300	-1.66779300	2.90114900
C	3.00684100	-0.80070900	2.27935700
C	3.24343100	-0.33360600	0.96200300
C	4.39220700	-0.79664000	0.27866300
C	5.30146400	-1.65610100	0.90698900
C	5.06866800	-2.09410400	2.22147600
H	3.71236300	-2.02094900	3.91590800
H	2.09847400	-0.49128600	2.79788500
H	4.58834900	-0.42946100	-0.72886400
H	6.19361100	-1.98336800	0.36906600
H	5.77433800	-2.76924900	2.71015400
C	2.37788800	0.64550900	0.31566200
C	1.67846500	1.63818500	1.02293200
H	2.47736700	0.77403000	-0.76469000
H	1.75578700	1.66719500	2.11365100
C	0.79455700	2.53530000	0.36818200
H	0.23612600	3.26353800	0.95612500
H	0.82450700	2.67659600	-0.70996100
C	2.41264000	4.52317100	-0.86260300
C	2.89836500	3.43101200	-1.60377900
O	2.15422700	2.84167900	-2.46605300
F	1.26492300	5.15106100	-1.22034700
F	3.16688600	5.35579600	-0.09380700
C	4.24125500	2.85095800	-1.26145200
C	4.87750200	2.97172900	-0.00432300
C	4.86731500	2.05888400	-2.25276000
C	6.10351700	2.33767500	0.24249900
H	4.40111900	3.54294000	0.79085300
C	6.10287400	1.44419200	-2.01317800
H	4.35820600	1.94040100	-3.21014700
C	6.72756400	1.57775300	-0.76047900

H	6.56690700	2.42645300	1.22799000
H	6.57657300	0.85212100	-2.80067700
H	7.68323200	1.08616000	-0.56427400
Pd	-0.08353600	0.48125400	0.30027900
P	-2.24750700	1.17219700	0.21526200
C	-3.20431800	-0.24569000	-0.44208600
C	-4.56520700	-0.16001600	-0.79493500
C	-5.24525000	-1.29480500	-1.25555400
H	-6.29936000	-1.22674600	-1.53133400
C	-4.56184900	-2.51852500	-1.36206500
H	-5.08524800	-3.40781600	-1.71910300
C	-3.20409600	-2.60087300	-1.02236300
C	-2.50350400	-1.46562000	-0.56407100
C	-1.02940700	-1.64142500	-0.26853400
C	-0.12345300	-1.71834900	-1.37999600
C	-0.47391100	-1.10022400	-2.72854600
H	-1.41243000	-0.53715200	-2.61591300
C	-0.70576800	-2.19418300	-3.79316900
H	0.20622000	-2.79715800	-3.93650200
H	-0.96964600	-1.73554100	-4.76059600
H	-1.52313200	-2.87045400	-3.49458800
C	0.61440200	-0.10540600	-3.18167600
H	0.78165200	0.68367700	-2.43419300
H	0.31950900	0.37376700	-4.12969700
H	1.57790500	-0.61490900	-3.34702500
C	1.08920600	-2.41502400	-1.23024200
H	1.74933500	-2.48235700	-2.09420400
C	1.44987700	-3.03870500	-0.02701300
C	2.69049000	-3.91200900	0.11902700
H	3.26869500	-3.51596200	0.96863300
C	3.60650500	-3.92124900	-1.11491700
H	4.51412400	-4.50753300	-0.89998300
H	3.91503500	-2.90383100	-1.39609900
H	3.10006200	-4.38476900	-1.97900100
C	2.27743500	-5.36197100	0.47118300
H	1.69731100	-5.80847000	-0.35432900
H	1.65785500	-5.39717600	1.38123300
H	3.17307500	-5.98361500	0.63905100
C	0.60673400	-2.85517300	1.08784100
H	0.90862000	-3.27108800	2.05077200
C	-0.61825300	-2.18408000	0.99935500
C	-1.51062900	-2.05066800	2.22780300
H	-2.40318900	-1.47835100	1.94021600
C	-1.97776000	-3.42955400	2.73734800

H	-1.11710200	-4.04418900	3.04860200
H	-2.52269100	-3.97689700	1.95098200
H	-2.64624300	-3.31117300	3.60657200
C	-0.80140700	-1.25472000	3.34258500
H	0.10268100	-1.78161600	3.68913500
H	-1.47640600	-1.11854100	4.20370400
H	-0.50323400	-0.26074700	2.97049900
H	-5.08384800	0.79709000	-0.71188200
H	-2.67005400	-3.54774900	-1.11862400
C	-3.02476500	1.58302600	1.82562200
C	-2.59492100	2.75276500	2.49266800
C	-3.94230300	0.72330500	2.46345900
C	-3.07821100	3.05463700	3.77211700
H	-1.88834400	3.42858800	2.00625700
C	-4.41584000	1.02565500	3.75032200
H	-4.28930700	-0.17747900	1.95657900
C	-3.98602600	2.18848600	4.40768800
H	-2.74428400	3.96465700	4.27483700
H	-5.12576700	0.35174200	4.23460200
H	-4.35592700	2.42158600	5.40812700
C	-2.58721900	2.60762100	-0.87049300
C	-3.69408000	3.46094500	-0.67737600
C	-1.68351200	2.86129200	-1.92374000
C	-3.89176700	4.55354300	-1.53487500
H	-4.38388100	3.28200500	0.14924900
C	-1.88257800	3.95792900	-2.77388200
H	-0.81301200	2.22086900	-2.06398500
C	-2.98645200	4.80412100	-2.58063500
H	-4.74720400	5.21473400	-1.38030700
H	-1.15932600	4.15811400	-3.56593500
H	-3.13587600	5.66516800	-3.23538300

TS9'

C	-2.90004200	-4.03299000	6.20089400
C	-2.74870700	-2.82699600	5.51011200
C	-2.84216500	-1.59034500	6.19149700
C	-3.05734900	-1.59999600	7.58804200
C	-3.21843600	-2.80967500	8.27703100
C	-3.14368000	-4.03005700	7.58710600
H	-2.81402700	-4.97987000	5.66371300
H	-2.53349400	-2.82924600	4.43960600
H	-3.13526300	-0.64870800	8.11550700
H	-3.40595900	-2.79702700	9.35320400
H	-3.26271800	-4.97412900	8.12315700

C	-2.73345400	-0.30064900	5.49580100
C	-3.21818800	-0.09574000	4.16224800
H	-2.68874300	0.58083200	6.13857600
H	-3.62454600	-0.94633900	3.60885100
C	-3.05509400	1.13036800	3.51314100
H	-3.29853300	1.21469000	2.45563700
H	-2.68175700	2.01618700	4.02219300
C	-4.76543300	3.13632600	4.61762100
C	-4.14057800	2.78239800	5.82404200
O	-2.92278400	3.11250100	6.06613200
F	-6.09751600	3.03508600	4.36136100
F	-4.20927800	4.05574000	3.78884100
C	-4.86004300	1.86673800	6.77110400
C	-4.46772400	1.90446000	8.12968900
C	-5.82355600	0.90910300	6.37945400
C	-5.04326200	1.04271300	9.07141900
H	-3.70036200	2.62128000	8.42390900
C	-6.38150400	0.02977500	7.31897000
H	-6.11921600	0.83647400	5.33372400
C	-6.00087000	0.09456400	8.66921500
H	-4.73713400	1.10086100	10.11917200
H	-7.10799400	-0.71792500	6.99178000
H	-6.43751400	-0.59251700	9.39757000
Pd	-0.98747100	0.07736900	4.18084500
P	0.68103700	-0.49872700	5.61066100
C	2.25812700	-0.23808400	4.70118400
C	3.49958600	-0.71038100	5.17139800
C	4.66537300	-0.50363700	4.42364700
H	5.62407700	-0.87436200	4.79152300
C	4.59082000	0.17540600	3.19576300
H	5.49307600	0.33610300	2.60221500
C	3.35631800	0.64313200	2.72464700
C	2.17301600	0.44551600	3.46732300
C	0.88746600	0.96088500	2.86127600
C	0.55585000	2.35414900	3.00478500
C	1.18703200	3.18625300	4.11679400
H	1.51782900	2.49065500	4.90318700
C	2.43070000	3.94290700	3.59681400
H	2.14285600	4.63452300	2.78685300
H	2.88182000	4.53539100	4.41059600
H	3.19399100	3.25186500	3.20777700
C	0.19517800	4.17931300	4.75873100
H	-0.75354300	3.70432500	5.04770500
H	0.65401800	4.61911600	5.65918100

H	-0.03510700	5.00872400	4.06919200
C	-0.34452500	2.92967500	2.10282000
C	-0.94886800	2.19133800	1.06404000
C	-1.85738900	2.87282200	0.04912500
H	-2.35950400	2.08104700	-0.53373800
C	-2.94493800	3.75039900	0.70504000
H	-3.60465900	4.17159400	-0.07162100
H	-3.56135800	3.18198700	1.41493300
H	-2.49652600	4.59272600	1.25563400
C	-1.00963000	3.71785100	-0.92998900
H	-0.25647900	3.09691400	-1.44224300
H	-1.65305400	4.18921400	-1.69195400
H	-0.48014800	4.51729500	-0.38527900
C	-0.67643100	0.82232400	0.97751300
C	0.22895500	0.17965800	1.85324100
C	0.60315800	-1.28285000	1.61323900
H	1.26815100	-1.60037100	2.42911200
C	1.38444400	-1.42440600	0.28900000
H	0.76100400	-1.11787800	-0.56699400
H	2.28907100	-0.79555800	0.29719100
H	1.69111900	-2.47238500	0.13393300
C	-0.62538200	-2.21367500	1.63712300
H	-1.36138500	-1.93092800	0.86699100
H	-0.31522100	-3.25502200	1.44727100
H	3.54519800	-1.25643600	6.11493600
H	3.29760000	1.16506600	1.76818200
H	-0.59195400	3.98537600	2.21305900
H	-1.15941000	0.23084700	0.19625500
C	0.77043300	-2.22804100	6.19697400
C	0.28179000	-2.59800200	7.46585800
C	1.20327100	-3.23065100	5.30022700
C	0.23942700	-3.95055200	7.83520700
H	-0.07051100	-1.83526100	8.15903300
C	1.16113400	-4.57914700	5.67641500
H	1.57674700	-2.95332100	4.31246100
C	0.67819300	-4.94262700	6.94544500
H	-0.14674100	-4.22604500	8.81781200
H	1.50572000	-5.34617400	4.97934200
H	0.64129200	-5.99457100	7.23606000
C	0.75380300	0.55894800	7.10945100
C	-0.16245900	1.62323500	7.22329000
C	1.71542500	0.35130000	8.12176400
C	-0.11488900	2.47525700	8.33779000
H	-0.91349900	1.80126100	6.45359300

C	1.75809100	1.20437900	9.23290900
H	2.41846900	-0.47985700	8.04529000
C	0.84371400	2.26830400	9.34110200
H	-0.83304900	3.29351700	8.40580500
H	2.50266800	1.03950100	10.01476500
H	0.88075600	2.93021900	10.20915500
H	-1.12071400	-2.16886000	2.62155900

IM9

C	3.51606100	-0.65253000	2.83164500
C	2.70607100	0.04963900	1.93331200
C	2.97634600	0.03270400	0.54308800
C	4.08444500	-0.71673600	0.09240100
C	4.90089800	-1.41560200	0.99132400
C	4.62168700	-1.39080300	2.36725800
H	3.28272000	-0.63071500	3.89916600
H	1.83303000	0.59478200	2.29414400
H	4.31844800	-0.71999000	-0.97338100
H	5.75605300	-1.98177600	0.61478800
H	5.25312000	-1.93956800	3.06961600
C	2.16628400	0.78282300	-0.42923600
C	1.44552900	1.97069700	-0.12926400
H	2.42960600	0.60758800	-1.47695000
H	1.51770600	2.37023900	0.88816900
C	1.23822700	3.02886800	-1.19754500
H	0.35034300	3.64835200	-0.99753500
H	1.10979000	2.55806400	-2.18259600
C	2.43571200	3.97968400	-1.31765600
C	3.74909900	3.23110300	-1.74427800
O	3.85456400	3.00649600	-2.94931800
F	2.16123500	4.92274300	-2.28823800
F	2.59516500	4.69654500	-0.13610800
C	4.76585200	2.75728900	-0.75752700
C	4.60685600	2.80513200	0.64715600
C	5.93173800	2.15091200	-1.28761400
C	5.58204200	2.25818400	1.48958900
H	3.71404600	3.23802800	1.08529600
C	6.90804000	1.61716000	-0.44317700
H	6.04774900	2.10353900	-2.37057700
C	6.73354900	1.66507900	0.95151800
H	5.42900500	2.27744100	2.56942800
H	7.80030300	1.15328600	-0.86872500
H	7.48626500	1.23262700	1.61369000
Pd	-0.00609700	0.41738400	-0.17865900

P	-2.14526700	1.09011500	0.17762200
C	-3.24728000	-0.30333100	-0.30398200
C	-4.63430300	-0.16204500	-0.50644700
C	-5.41720700	-1.27147800	-0.85313300
H	-6.49146600	-1.15595100	-1.01169100
C	-4.81038200	-2.53076200	-0.99511400
H	-5.41220600	-3.40206000	-1.26212300
C	-3.42792200	-2.67148400	-0.80719300
C	-2.62407400	-1.56190700	-0.47189600
C	-1.13847000	-1.79939800	-0.33558200
C	-0.32817800	-1.86196500	-1.51364700
C	-0.85136400	-1.37556600	-2.86528600
H	-1.78056400	-0.81338400	-2.69094800
C	-1.19238200	-2.57653000	-3.77460100
H	-0.29163500	-3.17994800	-3.97603900
H	-1.59670800	-2.22719000	-4.73956900
H	-1.94282400	-3.22850800	-3.29974600
C	0.13985200	-0.42354900	-3.56555700
H	0.35256900	0.45062100	-2.92919900
H	-0.28244200	-0.07409800	-4.52290300
H	1.09677500	-0.92610500	-3.78173900
C	0.92101800	-2.52362500	-1.45462500
H	1.50644400	-2.59574600	-2.37123300
C	1.40183700	-3.09944800	-0.27412300
C	2.68215900	-3.92592500	-0.20035600
H	3.27102900	-3.53727900	0.64710900
C	3.55829700	-3.84866900	-1.46069700
H	4.49797600	-4.40153600	-1.29991800
H	3.80738800	-2.80756600	-1.71381700
H	3.04551700	-4.30194400	-2.32627200
C	2.33384600	-5.40274000	0.10585000
H	1.74758400	-5.83764600	-0.72168800
H	1.73736100	-5.49086900	1.02782300
H	3.25331400	-6.00022400	0.22940500
C	0.63936900	-2.92698900	0.90037400
H	1.03895000	-3.30434400	1.84421200
C	-0.60937700	-2.29911800	0.90073300
C	-1.36040800	-2.10233500	2.21272500
H	-2.32248600	-1.61785400	1.99386900
C	-1.65734700	-3.44081700	2.91796700
H	-0.72280300	-3.96303900	3.18095100
H	-2.25051700	-4.10723500	2.27018900
H	-2.22275000	-3.26606600	3.84884600
C	-0.57084700	-1.14816600	3.13433000

H	0.40707600	-1.58193200	3.39853200
H	-1.13467400	-0.95422200	4.06199400
H	-0.39181900	-0.19036800	2.62219900
H	-5.09425100	0.82179300	-0.39425900
H	-2.95576200	-3.64821000	-0.92769200
C	-2.63207000	1.49308800	1.90776600
C	-1.90375000	2.50978300	2.56533300
C	-3.61833400	0.78516600	2.62241100
C	-2.16459900	2.81618200	3.90701600
H	-1.12715100	3.05537200	2.02409500
C	-3.86695600	1.08399200	3.97248500
H	-4.18865200	-0.00262800	2.12933400
C	-3.14385700	2.09881600	4.61732300
H	-1.59768200	3.60776600	4.40187600
H	-4.62977600	0.52294300	4.51702400
H	-3.33829600	2.32931800	5.66684000
C	-2.76350900	2.51350900	-0.81238900
C	-3.74713700	3.41422100	-0.35760800
C	-2.19871400	2.68948000	-2.09362000
C	-4.16218400	4.47500000	-1.17888600
H	-4.17751000	3.29147200	0.63787300
C	-2.62233900	3.74343500	-2.91521600
H	-1.41759400	2.00237800	-2.42766900
C	-3.60356800	4.63952200	-2.45712300
H	-4.92054900	5.17394800	-0.81906500
H	-2.17697500	3.87485500	-3.90368200
H	-3.92498100	5.46861100	-3.09106600

TS10

C	1.56949500	0.21736200	1.50893200
C	2.09579400	0.81905800	0.33000100
H	1.28170500	0.85888800	2.35157300
H	2.69307600	0.21510500	-0.35838000
C	1.73976900	2.12551300	-0.04905700
H	1.26254700	2.76860100	0.68728200
C	1.99518800	4.48620000	2.24311700
C	1.92378800	3.30868200	2.96648900
O	0.78242500	2.73428500	3.18935500
F	0.89258000	5.06530800	1.69150900
F	3.08492600	5.25289900	1.96470100
C	3.18374400	2.63325800	3.43607400
C	4.47406400	2.84058600	2.89203000
C	3.03901700	1.63798500	4.43192700
C	5.57170800	2.09151600	3.33961700

H	4.62206200	3.57275700	2.10024400
C	4.13826600	0.89665300	4.88537100
H	2.03990500	1.45917900	4.83117500
C	5.41462800	1.11865000	4.34208800
H	6.55541600	2.26368700	2.89480600
H	3.99819300	0.14105600	5.66332000
H	6.27339300	0.53813200	4.68806400
Pd	-0.12114600	0.47615000	0.19095700
P	-1.37719100	-1.12152100	1.19468500
C	-2.99862600	-1.09886800	0.33958900
C	-4.03211100	-2.01383100	0.62086400
C	-5.24132600	-1.94594500	-0.08189200
H	-6.04099400	-2.65649500	0.13563400
C	-5.41671500	-0.96105300	-1.06958700
H	-6.35518600	-0.90395100	-1.62460300
C	-4.38874900	-0.04958500	-1.34716500
C	-3.16646700	-0.10236400	-0.64488200
C	-2.10470900	0.90615300	-1.02489900
C	-1.34942200	0.68363200	-2.22999600
C	-1.21500700	-0.71690500	-2.81996300
H	-1.69623200	-1.42438100	-2.12976700
C	-1.93964400	-0.81540900	-4.17863300
H	-1.49283700	-0.12342400	-4.91126300
H	-1.86329000	-1.83900900	-4.58220800
H	-3.00666000	-0.56118600	-4.07429100
C	0.26342300	-1.13642700	-2.94452400
H	0.75000200	-1.12271200	-1.95497900
H	0.33819200	-2.15587200	-3.35878800
H	0.81359200	-0.45303000	-3.61129600
C	-0.79622500	1.78416100	-2.90079900
H	-0.24142100	1.61296300	-3.82500500
C	-0.95451500	3.10199300	-2.43516700
C	-0.45163100	4.25472800	-3.29476500
H	0.58373500	4.01701900	-3.58335300
C	-1.28901700	4.33869600	-4.59454700
H	-0.89701900	5.13320700	-5.25170100
H	-1.26586500	3.38719700	-5.14950000
H	-2.34146700	4.57224000	-4.36013000
C	-0.45058400	5.61951700	-2.58663100
H	-1.48009000	5.95732300	-2.37810800
H	0.09972500	5.58361200	-1.63499100
H	0.02654400	6.37323700	-3.23300800
C	-1.59817600	3.29603400	-1.20085700
H	-1.67278400	4.29996800	-0.78723700

C	-2.17858800	2.23774800	-0.48331800
C	-2.94650400	2.50961500	0.80624600
H	-3.04600600	1.55525600	1.34639800
C	-4.36915700	3.01969000	0.47902300
H	-4.92993100	2.29484400	-0.13144100
H	-4.93107300	3.19712900	1.41123700
H	-4.31366500	3.97128500	-0.07596800
C	-2.22542400	3.50225300	1.74134100
H	-2.20241700	4.51463500	1.30560500
H	-2.78237800	3.56781200	2.69086000
H	-1.19227100	3.20464800	1.97258200
H	1.86454100	-0.81094800	1.73331700
C	2.19733700	2.74969900	-1.28725500
C	2.51889500	1.99628500	-2.44382900
C	2.38314800	4.15272200	-1.32387400
C	3.02981800	2.62237000	-3.58511900
H	2.34568400	0.91990400	-2.44422500
C	2.91313800	4.77486100	-2.46057300
H	2.13751700	4.74142800	-0.44165600
C	3.23817800	4.01477200	-3.59679500
H	3.26563600	2.02728800	-4.47038500
H	3.06395900	5.85607300	-2.46243100
H	3.64296100	4.50121900	-4.48672300
H	-4.52434500	0.71378400	-2.11495000
H	-3.88259500	-2.77996400	1.38336200
C	-0.76650600	-2.84161500	1.04996900
C	0.14180200	-3.34067700	2.00921500
C	-1.08669800	-3.62739200	-0.07710500
C	0.71487000	-4.60931800	1.84221000
H	0.39052700	-2.74139900	2.88664500
C	-0.50841500	-4.89494800	-0.23927100
H	-1.79102900	-3.25280900	-0.82091800
C	0.39347300	-5.38835800	0.71761300
H	1.41158600	-4.98924900	2.59211000
H	-0.76635400	-5.49786100	-1.11247600
H	0.84217800	-6.37534400	0.58934400
C	-1.70303600	-0.85666500	2.97595800
C	-2.31070100	-1.84570600	3.77976200
C	-1.35363700	0.38891500	3.53361500
C	-2.57458900	-1.57940100	5.13020800
H	-2.55774300	-2.82146300	3.35763700
C	-1.61858700	0.64705900	4.88778500
H	-0.85572100	1.14890100	2.93284000
C	-2.23096500	-0.33248400	5.68425700

H	-3.04187600	-2.34581300	5.75236500
H	-1.32710200	1.61059100	5.30802600
H	-2.43284000	-0.13319800	6.73895200
TS10'			
C	1.98812000	-0.28135300	0.47683800
C	1.85853500	0.72525900	-0.48771000
H	2.04696300	-0.02695500	1.54439500
H	2.06596600	0.50772200	-1.53828800
C	1.22692100	1.96058200	-0.13506800
H	1.27966100	2.26075400	0.91391600
C	2.34864200	3.42511800	2.68182200
C	2.93180800	2.16808200	2.65774500
O	2.35948100	1.15380200	3.22276200
F	1.15425900	3.65801500	3.29881200
F	2.84716800	4.60372900	2.21400800
C	4.20313400	1.95469000	1.87781600
C	4.63507800	2.75742800	0.79574700
C	4.95331600	0.79529700	2.18128000
C	5.77616600	2.41470900	0.05617300
H	4.06682900	3.64100800	0.50979500
C	6.10057800	0.45901300	1.44962300
H	4.61025300	0.16228500	2.99908600
C	6.51965600	1.26599700	0.37902100
H	6.08055300	3.04510900	-0.78361200
H	6.66593000	-0.43919500	1.71271900
H	7.40795000	1.00183900	-0.20005200
Pd	-0.20184700	0.25452100	0.20298800
P	-2.19885900	1.27331300	-0.24429800
C	-3.49120500	0.08794700	0.30370800
C	-4.86229900	0.28420300	0.04485500
C	-5.80132600	-0.67310600	0.44690000
H	-6.86236500	-0.51862200	0.24157400
C	-5.36841300	-1.83495700	1.10917600
H	-6.09254200	-2.59033800	1.42073700
C	-4.00601900	-2.02718300	1.37465200
C	-3.04810200	-1.06850700	0.98147300
C	-1.60312000	-1.35750100	1.32004100
C	-1.10858600	-0.99565100	2.62656100
C	-1.83753500	0.04449600	3.47154600
H	-2.39768500	0.69870500	2.78653800
C	-2.86196000	-0.63948200	4.40673500
H	-2.34281600	-1.32681400	5.09574100
H	-3.38790700	0.11982800	5.00973400

H	-3.61161200	-1.21359000	3.84166600
C	-0.88161900	0.93094600	4.29725300
H	-0.00874700	1.27187300	3.72251100
H	-1.43433100	1.80548500	4.67696700
H	-0.49647400	0.37993300	5.17144200
C	0.02343500	-1.65141400	3.11828300
H	0.41040600	-1.37028700	4.09832200
C	0.69170800	-2.66328600	2.39747700
C	1.91737500	-3.31136400	3.03124700
H	1.68374500	-3.44585400	4.10247600
C	2.27235400	-4.68963700	2.44655700
H	3.09979300	-5.13837100	3.01926700
H	1.41277100	-5.37953500	2.47805100
H	2.60515300	-4.60230500	1.39858800
C	3.13494600	-2.35641700	2.94903400
H	3.48408900	-2.26970200	1.90793500
H	2.88581500	-1.34497900	3.30337300
H	3.96651200	-2.75517400	3.55495200
C	0.23826300	-2.96956800	1.10943800
H	0.75521200	-3.72285400	0.51445600
C	-0.88848400	-2.33267200	0.54462700
C	-1.38220200	-2.75831000	-0.83653600
H	-2.26494200	-2.15157100	-1.08786700
C	-1.81791600	-4.23928000	-0.83263600
H	-2.60829600	-4.41709400	-0.08588200
H	-2.20605500	-4.52571300	-1.82424800
C	-0.32036900	-2.49708000	-1.92471000
H	0.60844900	-3.05359000	-1.71781800
H	-0.69943900	-2.81696000	-2.91002900
H	-0.07530600	-1.42260000	-1.97364300
H	2.32257200	-1.26962600	0.16177100
C	0.94388800	3.05119200	-1.07199500
C	0.93715000	2.88428900	-2.47728900
C	0.67274000	4.33590400	-0.54057600
C	0.69275700	3.97243000	-3.32162200
H	1.11272600	1.89719900	-2.90735700
C	0.40710200	5.41830800	-1.38773700
H	0.69300700	4.47506700	0.54028200
C	0.42297400	5.24287600	-2.78273700
H	0.69369200	3.82556400	-4.40334900
H	0.20093200	6.40127400	-0.95936800
H	0.22637700	6.08884700	-3.44487700
H	-5.18733900	1.18155100	-0.48397000
H	-3.67011800	-2.92501900	1.89603300

C	-2.60718800	1.61035500	-1.99641300
C	-2.33787800	2.87093000	-2.56833900
C	-3.08657300	0.56340500	-2.81578700
C	-2.57240000	3.08541200	-3.93496700
H	-1.94586400	3.68103500	-1.95390200
C	-3.31284600	0.78360000	-4.18070100
H	-3.29192100	-0.41652200	-2.38139200
C	-3.06045200	2.04746000	-4.74333500
H	-2.36314600	4.06677100	-4.36447600
H	-3.69178700	-0.02925300	-4.80390700
H	-3.24178400	2.21897400	-5.80640700
C	-2.51763600	2.84101200	0.65030600
C	-3.61469200	3.67299500	0.34345300
C	-1.64397700	3.19361600	1.69748200
C	-3.83312300	4.84372600	1.08257300
H	-4.28293100	3.41421600	-0.47935100
C	-1.86762100	4.36471600	2.43767400
H	-0.78719100	2.56112600	1.92612200
C	-2.96144100	5.18864000	2.13072300
H	-4.68125900	5.48750400	0.84005200
H	-1.17631500	4.63259500	3.23649200
H	-3.13310000	6.10326400	2.70221700
H	-0.96695100	-4.89788400	-0.59425900

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C	-1.24212600	0.86484100	-1.79283200
C	-2.10136500	0.29191500	-0.84599400
H	-1.18852800	1.94099000	-1.95290900
H	-2.32990100	-0.77236100	-0.94874700
C	-3.13352000	1.00089300	0.02672100
H	-3.04887800	0.59911700	1.04804200
C	-2.89768100	2.51478800	0.20085400
C	-1.56031800	2.83000800	0.96391300
O	-1.56626900	2.44873000	2.13666500
F	-3.90887900	3.03338700	0.99207000
F	-3.02794500	3.15873300	-1.02181200
C	-0.39045500	3.55935300	0.37918500
C	-0.37999600	4.24594700	-0.85871000
C	0.78824300	3.56576700	1.16418200
C	0.78520500	4.88964800	-1.29925700
H	-1.27004200	4.28981600	-1.47687400
C	1.94585600	4.20760500	0.72274100
H	0.78412400	3.03991800	2.11630900
C	1.95202900	4.86720300	-0.51872100

H	0.77648300	5.41317800	-2.25762600
H	2.84607500	4.17305400	1.33583600
H	2.85971800	5.36032900	-0.87317700
Pd	-0.08108700	0.26787800	-0.03396900
P	2.19833000	0.09365000	0.02319700
C	2.86330100	-1.57374700	0.50195700
C	4.25601700	-1.74853900	0.66170500
C	4.79828600	-2.98961100	1.01712900
H	5.87859800	-3.10089000	1.13151600
C	3.94268700	-4.08195200	1.22958400
H	4.34935000	-5.05571000	1.51099100
C	2.55913500	-3.91712400	1.08911500
C	1.99596600	-2.67280200	0.72848300
C	0.49819500	-2.61964500	0.63163500
C	-0.15331300	-3.11795400	-0.52494400
C	0.62452500	-3.44272200	-1.79751100
H	1.69777200	-3.45177400	-1.55792800
C	0.27144400	-4.82432900	-2.38355700
H	-0.78298200	-4.87015400	-2.70137800
H	0.89619700	-5.03120600	-3.26851600
H	0.44008200	-5.62476500	-1.64430200
C	0.39166500	-2.32059600	-2.83470100
H	0.65566400	-1.34223300	-2.40669900
H	1.00202200	-2.49067500	-3.73778600
H	-0.67008100	-2.28992900	-3.13261500
C	-1.55592900	-3.21927200	-0.53114400
H	-2.04775300	-3.59478500	-1.42869000
C	-2.33530300	-2.81140500	0.56214300
C	-3.85598900	-2.93240600	0.58660400
H	-4.24075100	-2.07038400	1.15812600
C	-4.51922500	-2.89822800	-0.80187800
H	-4.22359700	-2.00443900	-1.37074500
H	-4.25624300	-3.79299300	-1.39102700
H	-5.61436400	-2.88037000	-0.69022900
C	-4.26605400	-4.21660900	1.34500300
H	-3.84251300	-4.23025400	2.36250200
H	-5.36437800	-4.28842400	1.42197100
H	-3.89777900	-5.10897700	0.81090700
C	-1.67143800	-2.28113500	1.68103900
H	-2.26714000	-1.94566300	2.53300100
C	-0.27006800	-2.18247700	1.74732800
C	0.39078100	-1.66496300	3.02246000
H	1.45129600	-1.46997800	2.80788100
C	0.33143000	-2.74269600	4.12712100

H	-0.71560700	-2.98304200	4.37710000
H	0.82760100	-3.67074400	3.79963900
C	-0.22751300	-0.34053500	3.50781400
H	-1.28057900	-0.46563400	3.80599200
H	0.32417200	0.03578800	4.38608400
H	-0.19521700	0.42512300	2.71715600
H	-0.85701600	0.25162400	-2.61165400
C	-4.55000100	0.72375300	-0.47038200
C	-5.55666800	0.36796300	0.44511700
C	-4.86626500	0.80425300	-1.83940600
C	-6.85518400	0.07534400	0.00108900
H	-5.31456000	0.31978400	1.50911700
C	-6.16435200	0.51718800	-2.28606500
H	-4.08463100	1.07651100	-2.54989300
C	-7.16122400	0.14670000	-1.36771000
H	-7.62556300	-0.20815100	0.72174200
H	-6.39736600	0.57839100	-3.35155200
H	-8.16999000	-0.08451100	-1.71695100
H	4.92063900	-0.89696600	0.50677200
H	1.88847000	-4.76151700	1.25994100
C	3.29919200	1.18922600	1.03216400
C	4.42292400	1.85641700	0.50775300
C	2.97878600	1.34893700	2.39670900
C	5.21386400	2.67035700	1.33554500
H	4.67549700	1.74538300	-0.54758500
C	3.77078400	2.15761900	3.22290000
H	2.09912600	0.84957200	2.80670300
C	4.89108000	2.82302300	2.69344300
H	6.08196800	3.18530200	0.91756200
H	3.51002100	2.27582500	4.27696900
H	5.50494900	3.45830500	3.33541200
C	2.81488100	0.34716400	-1.70081400
C	3.59213900	-0.58576700	-2.41299600
C	2.39285600	1.53147200	-2.34678500
C	3.94042800	-0.33963700	-3.75242600
H	3.91633600	-1.50884400	-1.93180300
C	2.76087400	1.78305000	-3.67457300
H	1.76463800	2.24386800	-1.80932900
C	3.53092500	0.84388700	-4.38458600
H	4.53317900	-1.07657600	-4.29931800
H	2.43432300	2.70587800	-4.15970100
H	3.80304400	1.03205900	-5.42548300
H	0.83183300	-2.38554000	5.04323200

TS11

Pd	-11.35661200	-7.23487400	4.35156300
C	-9.39263100	-7.56208600	5.15070900
C	-9.44202600	-8.94200200	4.67958200
H	-9.26383700	-9.13051500	3.62068700
C	-9.63171700	-9.99648600	5.51902200
H	-9.77395000	-9.84758500	6.59092200
H	-9.63458100	-11.02154200	5.14991900
H	-9.51584500	-7.44773900	6.23655200
P	-13.24880000	-8.68312600	4.33019100
C	-14.13822100	-9.42348400	2.87931600
C	-15.54325900	-9.56666900	2.91328800
C	-16.24017300	-10.12712800	1.83543300
H	-17.32610700	-10.23133000	1.88425300
C	-15.53392500	-10.55318300	0.69988300
H	-16.06381400	-10.99130200	-0.14856300
C	-14.14101000	-10.41196400	0.65610700
C	-13.42204500	-9.84853000	1.73240200
C	-11.92883300	-9.76623900	1.59963400
C	-11.31658400	-8.56597000	1.14887300
C	-12.14713400	-7.31453500	0.86678700
H	-12.98452600	-7.30553400	1.58245000
C	-12.74473400	-7.38128800	-0.55812600
H	-11.93558400	-7.41170200	-1.30756200
H	-13.36334300	-6.48921800	-0.75513300
H	-13.37335900	-8.27425500	-0.69121100
C	-11.37446600	-5.99292300	1.04516900
H	-12.07743800	-5.14673400	0.97891600
H	-10.61993000	-5.85711000	0.25203900
H	-10.86797900	-5.93907600	2.02002800
C	-9.93583800	-8.57553600	0.89141500
C	-9.14054000	-9.71318500	1.10574700
C	-7.64196700	-9.68283200	0.83207700
H	-7.38287900	-8.66234400	0.50070500
C	-7.26792100	-10.66226500	-0.30196600
H	-7.82878100	-10.43544900	-1.22333300
H	-7.49975900	-11.69989300	-0.00949300
H	-6.18922600	-10.60324100	-0.52476700
C	-6.82429100	-9.99155300	2.10541100
H	-7.02982800	-9.25923600	2.90076500
H	-5.74448700	-9.96646600	1.88220900
H	-7.06974400	-10.99505900	2.49065200
C	-9.76474200	-10.87742000	1.57915300
C	-11.14906500	-10.92993400	1.82050900

C	-11.77789800	-12.25772200	2.24532800
H	-12.82937100	-12.07609500	2.50802400
C	-11.75756500	-13.25441400	1.06515600
H	-10.72080100	-13.47355800	0.75962300
H	-12.28986300	-12.84533000	0.19139500
H	-12.23956000	-14.20421300	1.35331000
C	-11.10133800	-12.87087700	3.48722100
H	-10.03190400	-13.06982600	3.30894300
H	-11.58374600	-13.82932000	3.74248600
H	-16.09406300	-9.23890000	3.79589300
H	-13.58598500	-10.74142600	-0.22378300
H	-9.45682000	-7.66825200	0.52026100
H	-9.16331600	-11.77235600	1.75046000
C	-13.17413600	-10.05013800	5.55622200
C	-13.68788700	-11.33934800	5.31794000
C	-12.55626500	-9.76776400	6.79454100
C	-13.57707900	-12.33559700	6.30183800
H	-14.17193800	-11.56547400	4.36745300
C	-12.46956000	-10.75775600	7.78253400
H	-12.15607200	-8.76865300	6.97878600
C	-12.97215500	-12.04733900	7.53535900
H	-13.96830700	-13.33575000	6.10309200
H	-11.99953900	-10.52466700	8.74064600
H	-12.89168100	-12.82266800	8.30026700
C	-14.54911200	-7.55970600	5.03012600
C	-15.34137800	-7.88832600	6.14747000
C	-14.69889100	-6.29116700	4.42766000
C	-16.25977700	-6.95680700	6.66119900
H	-15.23501500	-8.86525300	6.62014800
C	-15.62508100	-5.36996700	4.93357500
H	-14.06048700	-6.01385900	3.58607600
C	-16.40409000	-5.69837400	6.05706500
H	-16.86248000	-7.21818800	7.53400200
H	-15.72395100	-4.38939500	4.46353500
H	-17.11367900	-4.97405600	6.46219100
H	-11.19715900	-12.20039300	4.35156100
C	-9.84024400	-3.53065300	5.37130200
C	-10.74639200	-4.53935600	5.61868500
O	-11.30588200	-5.12498300	4.58584400
C	-11.05079900	-5.02206700	6.99694300
C	-12.24896200	-5.75298600	7.17910800
C	-10.17522700	-4.88467500	8.09928600
C	-12.55933700	-6.33054700	8.41727100
H	-12.93322900	-5.85900800	6.34082500

C	-10.48324100	-5.47383000	9.33448800
H	-9.24389200	-4.33103800	7.99284100
C	-11.67353900	-6.20228500	9.50031500
H	-13.49496300	-6.88240200	8.52879900
H	-9.78608400	-5.36640600	10.16878800
H	-11.90898800	-6.65901100	10.46439900
F	-9.53307100	-3.10801100	4.14514600
F	-9.31170900	-2.70896400	6.29591900
C	-8.45837800	-6.59253600	4.57008100
C	-7.88205800	-5.59754300	5.40141200
C	-8.08827100	-6.62099100	3.19890700
C	-6.94837800	-4.68239400	4.88457900
H	-8.12545200	-5.59679700	6.46381600
C	-7.18043300	-5.69692300	2.68637500
H	-8.53911300	-7.36521200	2.54723500
C	-6.60624900	-4.71849200	3.52848500
H	-6.51481800	-3.92600900	5.54206700
H	-6.91406600	-5.72869800	1.62734800
H	-5.89583500	-3.99561900	3.12196400

IM11

Pd	0.28077500	-0.43956100	-0.35056800
P	0.58521100	-0.66826900	1.84309400
C	2.36420300	-0.85696400	2.28117700
C	2.73118200	-1.07855300	3.62519800
C	4.07015500	-1.28529200	3.97414800
H	4.34337500	-1.45308800	5.01774300
C	5.05432600	-1.28114600	2.97130100
H	6.10247900	-1.44617000	3.22919800
C	4.69231100	-1.06207500	1.63637000
C	3.34631000	-0.84388300	1.26635500
C	3.08555400	-0.55666100	-0.18651100
C	2.96339800	-1.62805900	-1.11526000
C	2.73862800	-3.06288900	-0.64773200
H	2.43514800	-3.03371800	0.40990300
C	4.04473600	-3.88063300	-0.73624000
H	4.40749900	-3.91421200	-1.77725300
H	3.87678800	-4.91665500	-0.39565500
H	4.83395600	-3.43349600	-0.11064200
C	1.60460100	-3.75080300	-1.43815900
H	0.70861800	-3.11328700	-1.47278500
H	1.35209300	-4.71590200	-0.96779500
H	1.90822100	-3.95401900	-2.47764100
C	3.05638300	-1.34932700	-2.48995900

C	3.24253000	-0.04822500	-2.97548300
C	3.38521600	0.27408800	-4.46293600
H	2.60317000	1.01180700	-4.70906400
C	3.20181000	-0.93700100	-5.39330700
H	3.23700200	-0.60747500	-6.44382600
H	2.23946100	-1.44024000	-5.22746500
H	4.01172900	-1.67158100	-5.24089400
C	4.75647400	0.93788200	-4.73631400
H	4.90084800	1.84167900	-4.12347600
H	4.83762800	1.22402200	-5.79837400
H	5.57482400	0.23492500	-4.50469300
C	3.29238300	1.00321500	-2.04077500
C	3.23466800	0.78244400	-0.66039100
C	3.32918100	1.96378200	0.30138000
H	3.37283600	1.56942800	1.32691900
C	4.61798100	2.78186500	0.07537900
H	4.63421000	3.22223700	-0.93475600
H	5.51458200	2.15033100	0.18724600
H	4.67967900	3.60654000	0.80544800
C	2.08110200	2.86651300	0.20112000
H	2.03357700	3.35498900	-0.78340300
H	2.11784400	3.65194400	0.97483700
H	1.96100000	-1.09084500	4.39807500
H	5.45692300	-1.04556600	0.85777500
H	2.95973400	-2.17365200	-3.19352300
H	3.38217400	2.02792700	-2.40463800
C	-0.02524300	0.67953200	2.93005200
C	0.81589500	1.77166300	3.23057000
C	-1.37284500	0.71519500	3.35151000
C	0.31749800	2.87878000	3.93139500
H	1.85934900	1.75698300	2.91642600
C	-1.86769500	1.82449400	4.05385500
H	-2.03317000	-0.12744300	3.14343200
C	-1.02544400	2.91065900	4.34157800
H	0.98014800	3.71692900	4.15648200
H	-2.91078200	1.83678900	4.37616100
H	-1.41229800	3.77465600	4.88548500
C	-0.15371700	-2.21533100	2.51648700
C	-0.28134400	-3.30125700	1.62762300
C	-0.52139700	-2.37719800	3.86829000
C	-0.75892400	-4.53764400	2.08517900
H	-0.02747400	-3.16260700	0.57723200
C	-1.01352400	-3.61115900	4.31956300
H	-0.43490300	-1.54029900	4.56242800

C	-1.12896100	-4.69357100	3.43019800
H	-0.86117200	-5.36817000	1.38423000
H	-1.30470800	-3.72752200	5.36567500
H	-1.51235300	-5.65241000	3.78540100
H	1.15867500	2.28005900	0.33117900
C	-3.36553100	-2.80861200	-2.41170500
C	-2.73971600	-1.62694300	-1.99927500
C	-2.51845500	-1.36940300	-0.62429900
C	-2.96734800	-2.32784200	0.31482300
C	-3.59316000	-3.51112600	-0.09798600
C	-3.78926400	-3.76062300	-1.46641700
H	-3.51285000	-2.99034600	-3.47851000
H	-2.39866400	-0.91316600	-2.74337000
H	-2.80992100	-2.14117500	1.37808700
H	-3.92393400	-4.23656100	0.64869700
H	-4.27350100	-4.68337200	-1.79430200
C	-1.84304400	-0.14104000	-0.12486700
C	-1.99339900	1.13645100	-0.84667100
H	-2.01513800	-0.00824000	0.94893000
H	-1.99566700	1.09911100	-1.93771300
C	-2.09035400	2.32822400	-0.21641400
H	-2.06427000	2.39601500	0.87518200
H	-2.17530300	3.26165900	-0.77743400
C	0.22080300	1.36513400	-3.41694900
C	0.02090500	0.01594300	-3.47689700
O	0.04406300	-0.74891600	-2.39424200
F	0.32267300	2.22883200	-4.46148100
F	0.51245300	2.02453000	-2.27496500
C	-0.25530300	-0.70593900	-4.75871300
C	-0.31192600	-0.10942000	-6.04330300
C	-0.43760000	-2.11008600	-4.67921100
C	-0.52792500	-0.88667300	-7.18893500
H	-0.18532100	0.96296800	-6.15974400
C	-0.65560800	-2.88156200	-5.82843300
H	-0.40335900	-2.58228400	-3.69991100
C	-0.69874200	-2.27766400	-7.09483600
H	-0.56299900	-0.39585200	-8.16475600
H	-0.78980000	-3.96201600	-5.73063400
H	-0.86417300	-2.87779000	-7.99250600
TS12			
Pd	0.11852600	0.26162000	-0.03861400
P	0.63420100	-0.64275700	1.92914100
C	2.42994500	-0.66652700	2.40076500

C	2.80177300	-0.78940100	3.75885200
C	4.14882300	-0.81645800	4.14109500
H	4.41256000	-0.91255100	5.19637100
C	5.14916200	-0.70895600	3.16284600
H	6.20348300	-0.71909300	3.44718000
C	4.78961300	-0.58029800	1.81540500
C	3.43723100	-0.55955000	1.41054300
C	3.15986800	-0.39671600	-0.05341800
C	2.89208400	-1.53684200	-0.85837900
C	2.85494600	-2.93537300	-0.24329700
H	2.55026100	-2.84188000	0.80830000
C	4.27471600	-3.54686800	-0.25896000
H	4.63669000	-3.64701000	-1.29625200
H	4.26766300	-4.54863500	0.20423800
H	4.98649500	-2.91433900	0.29452700
C	1.85310900	-3.89316800	-0.91382700
H	0.85186700	-3.44754000	-0.96462200
H	1.78938100	-4.82391300	-0.32778700
H	2.16888800	-4.16221000	-1.93551300
C	2.75104100	-1.36786900	-2.24674400
C	2.86660600	-0.11014800	-2.85473200
C	2.67915400	0.11580700	-4.35229000
H	1.96254800	0.94868500	-4.45577800
C	2.10352700	-1.09061100	-5.11323500
H	1.91725600	-0.81382100	-6.16352500
H	1.15661000	-1.43875000	-4.67573100
H	2.81294800	-1.93565900	-5.10939100
C	4.01127400	0.55998200	-5.00051000
H	4.42264600	1.45111900	-4.50010600
H	3.86209800	0.79904300	-6.06718900
H	4.76042300	-0.24696300	-4.92828500
C	3.13986400	0.99864200	-2.03752900
C	3.28378100	0.88894100	-0.64930500
C	3.51687800	2.15323100	0.17754700
H	3.67790200	1.86442400	1.22626400
C	4.77808700	2.91073700	-0.28976600
H	4.66952700	3.25787000	-1.33040900
H	5.67097100	2.26603100	-0.23813400
H	4.95030600	3.79536300	0.34629800
C	2.27850200	3.07590400	0.13929800
H	2.04180600	3.37253300	-0.89512400
H	2.46154400	3.98908000	0.73253000
H	2.02811300	-0.85108500	4.52459900
H	5.56131800	-0.48277500	1.04977300

H	2.52638000	-2.23898400	-2.85959400
H	3.19411800	1.98754000	-2.49707100
C	-0.11436200	0.09151700	3.44420100
C	-1.04732000	-0.58901800	4.24814200
C	0.27973000	1.40076400	3.79426100
C	-1.57108600	0.02922400	5.39694600
H	-1.35423500	-1.60306400	3.98771400
C	-0.23325900	2.00739200	4.94542200
H	0.98770500	1.94217400	3.16387900
C	-1.15915000	1.32192800	5.75189300
H	-2.29333900	-0.50685600	6.01682800
H	0.07634300	3.02108800	5.20598100
H	-1.56186400	1.79851600	6.64821900
C	0.12231800	-2.42036100	1.99489200
C	0.67749400	-3.34198400	2.90614000
C	-0.86707900	-2.85808700	1.09137600
C	0.24824700	-4.67750300	2.91106700
H	1.45470200	-3.02165100	3.60086900
C	-1.30478200	-4.19119000	1.10620800
H	-1.26521900	-2.15582700	0.35854700
C	-0.74659200	-5.10383300	2.01453300
H	0.69208100	-5.38561900	3.61417200
H	-2.06697600	-4.51846400	0.39592700
H	-1.07742600	-6.14452200	2.01949700
H	1.39554000	2.56121500	0.55101400
C	-1.52932400	4.26458500	1.57962800
C	-1.44219800	3.09742200	0.81182900
C	-2.04125900	1.89475600	1.25386700
C	-2.73014200	1.89705600	2.48320500
C	-2.83096800	3.06955800	3.24569500
C	-2.22840300	4.25643000	2.80072500
H	-1.04925500	5.18122200	1.22857500
H	-0.88738800	3.09138000	-0.12794700
H	-3.18435000	0.97202200	2.84141800
H	-3.36767200	3.04978400	4.19619800
H	-2.29716200	5.16687500	3.40044000
C	-1.99097200	0.65764100	0.41941300
C	-2.53140200	0.76789100	-0.91978200
H	-2.30430500	-0.24241100	0.96412200
H	-2.58736700	1.77690500	-1.33693800
C	-2.88281000	-0.28124300	-1.73669700
H	-2.86689700	-1.30985900	-1.36678800
H	-3.41370000	-0.10024100	-2.67172700
C	-0.93080800	-0.82367600	-3.11910600

C	-0.46622200	0.49261400	-3.10648400
O	0.17409400	0.93338700	-2.06972700
F	-0.41828200	-1.76585100	-2.30166500
F	-1.52862500	-1.42566100	-4.17134300
C	-0.92357300	1.47901800	-4.12728400
C	-1.16694800	1.15598200	-5.48312000
C	-1.05499100	2.82827700	-3.72202200
C	-1.54520400	2.15136400	-6.39466900
H	-1.04781000	0.13205100	-5.83204400
C	-1.44459900	3.81741600	-4.63335300
H	-0.84034900	3.08254600	-2.68433300
C	-1.69274800	3.48415700	-5.97564700
H	-1.72091000	1.88388600	-7.43922600
H	-1.55187900	4.85136700	-4.29674000
H	-1.99124700	4.25546400	-6.68904900

IM12

Pd	0.02633800	0.35041900	-0.00186300
P	0.70978100	-0.66025800	1.93025400
C	2.44810900	-0.56621300	2.57635500
C	2.72611700	-0.49852300	3.95870600
C	4.04703700	-0.46441800	4.42786800
H	4.24118500	-0.41452200	5.50153800
C	5.11102900	-0.50096500	3.51419400
H	6.14417400	-0.47827400	3.86753000
C	4.84308800	-0.56304700	2.13951300
C	3.52144100	-0.59105600	1.65020900
C	3.30325600	-0.66688300	0.16866700
C	3.38375200	-1.91910300	-0.48589500
C	3.64614100	-3.21220100	0.28541100
H	3.42419400	-3.03155600	1.34708000
C	5.13644100	-3.60532600	0.17718500
H	5.41191000	-3.78160800	-0.87646900
H	5.33599700	-4.53074400	0.74475400
H	5.78775900	-2.80926600	0.57149900
C	2.74831100	-4.37853700	-0.17378500
H	1.68668000	-4.09524200	-0.14546000
H	2.89450200	-5.24538400	0.49068300
H	2.99629000	-4.69875200	-1.19919500
C	3.26980400	-1.96115800	-1.88842200
C	3.04441100	-0.80646900	-2.64719000
C	2.98651900	-0.82733400	-4.17051000
H	2.36849700	0.02887100	-4.47853200
C	2.35298700	-2.10281200	-4.75764600

H	2.26958000	-2.00738900	-5.85324400
H	1.34699800	-2.27187300	-4.34634200
H	2.96977800	-2.99352500	-4.55073900
C	4.40823100	-0.62229400	-4.74358600
H	4.85489800	0.31322100	-4.36869900
H	4.38214800	-0.57824600	-5.84627100
H	5.06693500	-1.45684100	-4.44723700
C	2.92771200	0.42295000	-1.97213300
C	3.06525400	0.52417900	-0.57868400
C	3.05736700	1.89075300	0.11055000
H	2.62595800	1.75440300	1.11449400
C	4.50664900	2.40453200	0.27630400
H	4.97700000	2.53077900	-0.71364300
H	5.11812600	1.70352600	0.86284600
H	4.51266200	3.38159400	0.78961000
C	2.21641200	2.96140300	-0.61145500
H	2.67928500	3.26349100	-1.56508400
H	2.14275000	3.85896900	0.02453800
H	1.90268700	-0.47201500	4.67340000
H	5.66523200	-0.58819500	1.42249900
H	3.35168200	-2.92452500	-2.39265100
H	2.71650400	1.31390200	-2.56081100
C	-0.25801800	-0.04607500	3.37934100
C	-1.15471600	-0.84957400	4.10890000
C	-0.09693300	1.30923000	3.74175800
C	-1.87301900	-0.30738400	5.18878000
H	-1.28746600	-1.89903700	3.84217400
C	-0.79711500	1.84040400	4.83092900
H	0.57726300	1.94768100	3.16784400
C	-1.68970400	1.03319400	5.55787400
H	-2.56721600	-0.94048500	5.74655800
H	-0.66240500	2.88947000	5.09892600
H	-2.24419500	1.45137700	6.40092800
C	0.37787200	-2.48042000	1.92902000
C	1.00235500	-3.37417200	2.82215900
C	-0.56625100	-2.97539400	1.00645600
C	0.68384700	-4.74036900	2.79367600
H	1.74029400	-3.00163900	3.53461500
C	-0.89150000	-4.34058300	0.98547800
H	-1.02927500	-2.27911200	0.30195200
C	-0.26550800	-5.22516800	1.87852900
H	1.17855700	-5.42671100	3.48459100
H	-1.62173700	-4.71428500	0.26436400
H	-0.50909600	-6.28957300	1.85616800

H	1.19994700	2.59689300	-0.82585800
C	-1.67233400	4.35162100	1.95645300
C	-1.44423400	3.35447300	1.00216800
C	-2.18317800	2.14764800	1.02546100
C	-3.13429900	1.96605800	2.05239000
C	-3.36488000	2.96582300	3.00739700
C	-2.64041600	4.16657300	2.96137000
H	-1.09178500	5.27677700	1.92020300
H	-0.67766600	3.49388800	0.23861500
H	-3.69249600	1.02791100	2.09732700
H	-4.10429900	2.80108300	3.79401200
H	-2.81718000	4.94624500	3.70564000
C	-2.00324900	1.08567000	0.00729400
C	-1.48275600	1.29242300	-1.29355300
H	-2.66504200	0.22184600	0.15101700
H	-1.17326900	2.30579900	-1.57096800
C	-1.96311400	0.42796900	-2.44601600
H	-2.19254000	-0.59231300	-2.10016200
H	-2.87939900	0.84948100	-2.89503100
C	-0.93129600	0.30192200	-3.56330300
C	-0.45479600	1.67834500	-4.14361200
O	0.72540400	1.99734400	-4.04200100
F	0.16106500	-0.39101800	-3.10821500
F	-1.45914300	-0.45788900	-4.61089300
C	-1.47674400	2.60168000	-4.72553700
C	-2.75053200	2.18249000	-5.17604100
C	-1.13087900	3.97102600	-4.81924500
C	-3.65482800	3.11644300	-5.69865200
H	-3.02752200	1.13169700	-5.14314800
C	-2.04150700	4.90067800	-5.32925600
H	-0.14535200	4.28554000	-4.47482700
C	-3.30733600	4.47496900	-5.77046300
H	-4.63165000	2.78122800	-6.05207500
H	-1.76891800	5.95635500	-5.38308900
H	-4.01910200	5.20026100	-6.16995300

TS13

Pd	-12.01651600	-8.70985600	5.18858900
C	-9.12978000	-7.74968200	5.39431200
C	-9.64874600	-8.97476100	5.00391500
H	-9.50013300	-9.31031800	3.97964800
C	-10.40800500	-9.85007100	5.86422400
H	-10.32852300	-9.69267100	6.94833300
H	-10.46127500	-10.89778400	5.56950100

H	-9.23174400	-7.45879300	6.44376200
P	-13.61111800	-10.05609900	5.95527200
C	-14.42268700	-11.28712500	4.83811600
C	-15.77421700	-11.61863700	5.08986200
C	-16.43353500	-12.59670000	4.33597100
H	-17.47651400	-12.83709900	4.55100700
C	-15.74316500	-13.26132300	3.31168000
H	-16.24116600	-14.02884000	2.71568500
C	-14.40726200	-12.93260000	3.05099700
C	-13.72370300	-11.94575700	3.79519300
C	-12.28996900	-11.69914700	3.42620200
C	-11.95563000	-10.66913200	2.50518000
C	-13.02736700	-9.73401300	1.94416900
H	-13.78308900	-9.58793000	2.73252600
C	-13.72171300	-10.39466000	0.72945100
H	-12.98824200	-10.56725800	-0.07654900
H	-14.51332400	-9.73343700	0.33799100
H	-14.17772100	-11.36023800	0.99322400
C	-12.50581100	-8.34090500	1.54321200
H	-13.35922500	-7.70939000	1.24683000
H	-11.82837000	-8.40049600	0.67449800
H	-11.99219800	-7.83697400	2.37296900
C	-10.62666000	-10.58036200	2.05618700
C	-9.62434400	-11.45758800	2.50241500
C	-8.19286800	-11.33607100	1.99303100
H	-8.15589300	-10.47963800	1.29811200
C	-7.77710200	-12.60232300	1.21196400
H	-8.46817600	-12.79804800	0.37601500
H	-7.78332300	-13.48498500	1.87300000
H	-6.75827700	-12.48825900	0.80513800
C	-7.19494800	-11.06249400	3.14004700
H	-7.42788500	-10.12331800	3.66458000
H	-6.16799200	-10.99122700	2.74421100
H	-7.21950800	-11.88067400	3.87862500
C	-9.97748700	-12.45029500	3.42879800
C	-11.29502600	-12.59096000	3.89947000
C	-11.61590300	-13.71545000	4.88546900
H	-12.63884200	-13.56863400	5.25926800
C	-11.57450000	-15.08284500	4.16862200
H	-10.56803200	-15.27782800	3.76216300
H	-12.29131500	-15.11259600	3.33228800
H	-11.82548000	-15.89570400	4.87123700
C	-10.68024200	-13.71841600	6.11282800
H	-9.63139300	-13.88591000	5.81870400

H	-10.97044400	-14.52936200	6.80074500
H	-16.31292100	-11.11014000	5.89007300
H	-13.86704300	-13.44268100	2.25215600
H	-10.35459000	-9.80159700	1.34175200
H	-9.20933700	-13.13542100	3.79191700
C	-13.19570300	-11.00653000	7.47361100
C	-13.56225000	-12.35175800	7.67035600
C	-12.46268100	-10.33140600	8.47453600
C	-13.18569700	-13.01884300	8.84748100
H	-14.13540200	-12.87864200	6.90739500
C	-12.10263100	-10.99673400	9.65412600
H	-12.18219100	-9.28676400	8.32433400
C	-12.45646700	-12.34492500	9.83918000
H	-13.46435500	-14.06545500	8.98720700
H	-11.54009100	-10.46498100	10.42435500
H	-12.16376200	-12.86673000	10.75264500
C	-15.02253500	-8.97737500	6.45620000
C	-15.55732400	-8.95743800	7.75819000
C	-15.53574100	-8.09847700	5.47718600
C	-16.59128200	-8.06131400	8.07845800
H	-15.16694400	-9.63245600	8.52046800
C	-16.57250400	-7.21415500	5.79913400
H	-15.09986100	-8.08667400	4.47659400
C	-17.09924300	-7.18995100	7.10287600
H	-16.99750900	-8.04640300	9.09217200
H	-16.95758900	-6.53290100	5.03797100
H	-17.89837700	-6.49053600	7.35647500
H	-10.73851800	-12.76885200	6.66464600
C	-10.90182800	-4.89094700	4.37571500
C	-11.65531500	-5.78109400	5.08738700
O	-12.33233200	-6.71234600	4.42079400
C	-11.70423200	-5.75003300	6.58068700
C	-12.83304600	-6.32384600	7.21290900
C	-10.65241900	-5.27910100	7.40240300
C	-12.90749600	-6.43253700	8.60854700
H	-13.65021700	-6.68474700	6.59298800
C	-10.72400100	-5.39694900	8.79799600
H	-9.76613400	-4.83833700	6.95063100
C	-11.84828900	-5.97747200	9.41134600
H	-13.79668600	-6.87515700	9.06265300
H	-9.89257300	-5.03722700	9.40965400
H	-11.89931300	-6.06559900	10.49922000
F	-10.77122300	-4.94547300	3.04052300
F	-10.15868700	-3.88255700	4.87785400

C	-8.41570000	-6.82897900	4.52813700
C	-7.66539100	-5.77162000	5.10721300
C	-8.42423200	-6.94954800	3.11197700
C	-6.94605000	-4.87875700	4.30811400
H	-7.65944700	-5.66441900	6.19407200
C	-7.70288400	-6.05501400	2.31837700
H	-9.03243900	-7.72220100	2.64156800
C	-6.95681800	-5.01803500	2.90894200
H	-6.37832700	-4.07029300	4.77368100
H	-7.73322100	-6.15381400	1.23108900
H	-6.40033900	-4.31747000	2.28307800

TS14

Pd	0.59728800	-0.01345800	-0.64604300
P	0.70918800	0.43508000	1.53849300
C	2.15402100	-0.30130000	2.41830200
C	2.18365500	-0.35077600	3.82849300
C	3.28370600	-0.89351400	4.50509400
H	3.29228400	-0.92584500	5.59656200
C	4.36820700	-1.39727600	3.76932000
H	5.23150900	-1.82430000	4.28411500
C	4.33795900	-1.36451900	2.36852700
C	3.23664900	-0.82565900	1.66947000
C	3.27531200	-0.89525500	0.16844700
C	2.91935300	-2.11706200	-0.47687500
C	2.28193100	-3.27919000	0.28090200
H	2.13210900	-2.97656500	1.32756500
C	3.20146500	-4.51841900	0.27599100
H	3.38577000	-4.86138000	-0.75568200
H	2.73615800	-5.34796000	0.83509800
H	4.17579700	-4.29132800	0.73870700
C	0.89369600	-3.62362700	-0.30307800
H	0.25293500	-2.72769800	-0.31654400
H	0.40818500	-4.41061700	0.29982900
H	0.97880400	-3.98693900	-1.33978500
C	3.11563400	-2.22950000	-1.85820400
C	3.63165700	-1.17667100	-2.63137400
C	3.74719300	-1.36437800	-4.13930600
H	2.85066600	-1.92642800	-4.45056400
C	4.98859800	-2.22100100	-4.47857100
H	5.04419000	-2.41511300	-5.56342900
H	4.95921800	-3.18937600	-3.95280400
H	5.91064600	-1.69670500	-4.17403800
C	3.76692200	-0.04600800	-4.93226100

H	2.90892200	0.58872100	-4.66377400
H	3.72382000	-0.25733400	-6.01324900
H	4.69320500	0.52242300	-4.74169200
C	3.98446500	0.01072700	-1.97740400
C	3.80287500	0.18059100	-0.59441900
C	4.12477300	1.53355400	0.03328300
H	3.84391800	1.50338300	1.09596700
C	5.63408600	1.84355400	-0.04378000
H	5.97167600	1.87694400	-1.09287600
H	6.22395600	1.07303100	0.47967900
H	5.85130100	2.82194500	0.41758700
C	3.29373000	2.65384100	-0.62870000
H	3.57937700	2.78512500	-1.68528300
H	3.45176500	3.61110500	-0.10547300
H	1.33344000	0.03377000	4.39511800
H	5.17299200	-1.77042700	1.79440600
H	2.80351500	-3.14584100	-2.36400800
H	4.36061100	0.85341900	-2.55763400
C	0.85445800	2.25239700	1.82553200
C	1.80036500	2.83966500	2.68718700
C	0.00870700	3.08361100	1.05728300
C	1.90151900	4.23831300	2.77626900
H	2.46716400	2.20899300	3.27587800
C	0.10158400	4.47735200	1.15969000
H	-0.69863600	2.63058500	0.35991100
C	1.05356300	5.05860200	2.01623000
H	2.64611300	4.68441100	3.43930200
H	-0.55642800	5.10931500	0.55926900
H	1.13742900	6.14526800	2.08494000
C	-0.71556000	-0.08026500	2.58903600
C	-1.21251200	-1.38875200	2.40159000
C	-1.33183800	0.76497200	3.53220800
C	-2.29820200	-1.84824400	3.15929200
H	-0.75196000	-2.03755500	1.65294900
C	-2.42551600	0.30409700	4.28397100
H	-0.95933400	1.78044300	3.67680100
C	-2.90814100	-1.00139200	4.10129700
H	-2.67550900	-2.86188500	3.00769600
H	-2.89918700	0.96672400	5.01167000
H	-3.76052600	-1.35634600	4.68432300
H	2.22229200	2.40705200	-0.58984700
C	-2.81605000	-4.92200500	-3.67658800
C	-2.30738400	-3.75433100	-3.09551700
C	-2.75034600	-2.48126200	-3.52551400

C	-3.68984500	-2.41859600	-4.57902600
C	-4.19927800	-3.58738600	-5.16071500
C	-3.76664600	-4.84552500	-4.71005600
H	-2.46163900	-5.89603900	-3.33118100
H	-1.54758000	-3.82068700	-2.31552400
H	-4.02361200	-1.44036900	-4.93279000
H	-4.93165500	-3.51652600	-5.96826200
H	-4.15930500	-5.75767100	-5.16466200
C	-2.21386000	-1.23099900	-2.94543100
C	-1.87768600	-1.16374500	-1.57175800
H	-2.61489200	-0.31196500	-3.38491800
H	-1.84622100	-2.09925500	-1.00838000
C	-1.60216800	0.02965600	-0.85620800
C	-0.46703000	-1.06159200	-4.23381300
C	0.11951500	0.10933700	-3.67330500
O	0.95142800	-0.10281800	-2.71688100
F	0.16695100	-2.23706000	-4.04647900
F	-1.04051100	-1.06208100	-5.46357400
C	-0.41987500	1.47220500	-3.90622600
C	-1.48694500	1.78022200	-4.78541000
C	0.15422000	2.52734900	-3.15268900
C	-1.96412300	3.09487300	-4.89266700
H	-1.95415300	0.99926300	-5.38041500
C	-0.32190200	3.83657800	-3.26789700
H	0.97101900	2.29527900	-2.47090600
C	-1.38900100	4.12883800	-4.13679900
H	-2.79319500	3.30921500	-5.57086900
H	0.13781400	4.63035100	-2.67415700
H	-1.76663900	5.14996600	-4.22384600
H	-1.79490700	0.97337400	-1.38368300
H	-1.89682500	0.03316500	0.19753800

IM13

Pd	0.02812400	-0.98727600	-0.40038700
P	0.54797900	0.07245600	1.54784400
C	2.09696300	-0.37110900	2.46652600
C	2.17236600	-0.27924300	3.87278200
C	3.36425900	-0.56716700	4.55279400
H	3.40251700	-0.48909200	5.64154600
C	4.50302800	-0.94669900	3.82656800
H	5.43976900	-1.16672700	4.34327900
C	4.43331200	-1.05144800	2.43021400
C	3.23915800	-0.78025100	1.73068300
C	3.24735500	-0.94941900	0.23858100

C	2.84826600	-2.19405100	-0.33098100
C	2.41898300	-3.35891900	0.56215600
H	1.99179200	-2.93803500	1.48436600
C	3.66047300	-4.19454500	0.95228700
H	4.12466500	-4.63013000	0.05107600
H	3.37508700	-5.01921300	1.62790000
H	4.41436700	-3.57586200	1.46244100
C	1.34484700	-4.27120700	-0.05739100
H	0.46078000	-3.68443900	-0.34775200
H	1.03787000	-5.03236500	0.67948300
H	1.72043900	-4.80370000	-0.94662800
C	2.97313000	-2.36623800	-1.72007100
C	3.49651000	-1.36433200	-2.55321700
C	3.69670500	-1.63394300	-4.04010700
H	3.04940700	-2.48415000	-4.31142000
C	5.16351800	-2.04959400	-4.29923900
H	5.31979900	-2.29520600	-5.36399300
H	5.43959400	-2.92855200	-3.69376400
H	5.84689600	-1.22558600	-4.03209200
C	3.31285600	-0.44556000	-4.94351400
H	2.26847700	-0.14535000	-4.78487900
H	3.43604100	-0.72469900	-6.00335900
H	3.95851700	0.42753900	-4.75363400
C	3.88515500	-0.15339100	-1.96620200
C	3.75102500	0.08286400	-0.58755200
C	4.17461300	1.43684700	-0.02056300
H	3.83924200	1.49688300	1.02492500
C	5.71297000	1.56983700	-0.02766100
H	6.10330300	1.50550400	-1.05729000
H	6.18178100	0.76680600	0.56437000
H	6.02150100	2.54069700	0.39702700
C	3.51752300	2.61290600	-0.77293400
H	3.84256400	2.64577700	-1.82584400
H	3.80106800	3.56787100	-0.30126800
H	1.29059500	0.02566900	4.43855900
H	5.31356900	-1.35277000	1.85979400
H	2.66127400	-3.30938700	-2.17233600
H	4.28743300	0.64084100	-2.59623500
C	0.68953000	1.90923100	1.37433000
C	1.54525200	2.70481200	2.16242900
C	-0.11216200	2.52610000	0.39112300
C	1.59719200	4.09449100	1.96950200
H	2.17578300	2.23833800	2.92060500
C	-0.07225800	3.91647400	0.21154800

H	-0.75011700	1.90411700	-0.23989400
C	0.78672400	4.70277500	0.99738500
H	2.27085400	4.70085500	2.57930200
H	-0.69665100	4.37883700	-0.55462900
H	0.82867700	5.78421300	0.84905900
C	-0.75452600	-0.12536000	2.84781300
C	-1.30640800	-1.41359700	3.01471500
C	-1.21868100	0.93097700	3.65677700
C	-2.29338300	-1.64416200	3.98297800
H	-0.96444500	-2.22681700	2.37040000
C	-2.21879800	0.70128300	4.61660100
H	-0.80131800	1.93189700	3.53466400
C	-2.75511300	-0.58509300	4.78429100
H	-2.71082700	-2.64626700	4.10513600
H	-2.57645500	1.52883200	5.23372600
H	-3.53309200	-0.76150100	5.53032000
H	2.42347600	2.52191900	-0.74793900
C	-2.89634000	-4.09708200	-5.41067600
C	-2.06182700	-3.27934400	-4.63672000
C	-2.59019700	-2.16667400	-3.95112800
C	-3.96533700	-1.89049900	-4.05700300
C	-4.80369000	-2.71189400	-4.82735700
C	-4.27061600	-3.81805800	-5.50736400
H	-2.47327400	-4.95325000	-5.94102500
H	-0.99465400	-3.49212200	-4.57008900
H	-4.37953200	-1.02938900	-3.52582600
H	-5.87013200	-2.48576200	-4.89740300
H	-4.91950800	-4.45778000	-6.10938500
C	-1.70946100	-1.29617800	-3.06180100
C	-1.32025300	-2.05417800	-1.79265300
H	-2.29066700	-0.40761200	-2.76634600
H	-0.88293400	-3.03718100	-1.98405100
C	-1.95163000	-1.81343700	-0.55829600
C	-0.45201600	-0.76752300	-3.80960400
C	0.07216800	0.54456600	-3.16662600
O	0.89048800	0.44132600	-2.24609300
F	0.55262100	-1.71609400	-3.77895300
F	-0.71046600	-0.55514000	-5.15688300
C	-0.49078000	1.86114300	-3.56956600
C	-1.67847900	2.01373100	-4.32642300
C	0.18649300	3.01885900	-3.11494900
C	-2.17321400	3.29349400	-4.60855200
H	-2.22217400	1.14286600	-4.68672300
C	-0.30170600	4.29304600	-3.41824100

H	1.09468800	2.89749600	-2.52629100
C	-1.48632000	4.43509600	-4.16278800
H	-3.09605700	3.39899400	-5.18214000
H	0.23846200	5.17589500	-3.07078200
H	-1.87168100	5.43014100	-4.39497000
H	-2.69781100	-1.01529800	-0.46696700
H	-2.04323000	-2.61249100	0.18451700

IM14

Pd	-0.49762900	0.38991500	0.51727000
P	-2.46050800	1.62022200	0.62162000
C	-2.78375400	2.34028100	2.38580000
C	-3.42554800	1.23692100	3.25178900
H	-4.42902400	0.96503700	2.89481900
H	-2.79924800	0.33589200	3.27738000
H	-3.51737100	1.60973300	4.28758300
C	-1.38454600	2.65612000	2.97174200
H	-1.50739900	3.02600800	4.00606000
H	-0.74885300	1.75771600	2.98785200
H	-0.86181200	3.42957700	2.39054100
C	-3.64470400	3.61715000	2.49346200
H	-4.66268100	3.45717300	2.12447100
H	-3.70379200	3.89951800	3.56044200
H	-3.20393900	4.46793300	1.95684600
C	-2.50455200	3.03380100	-0.66645500
C	-3.84171200	3.76148100	-0.90647200
H	-4.60421400	3.07575200	-1.30144800
H	-4.23782700	4.23398100	0.00044200
H	-3.67015000	4.55226900	-1.65985300
C	-2.05969000	2.38567500	-1.99314200
H	-2.78822600	1.63872900	-2.33938100
H	-1.97789300	3.16826700	-2.76822100
H	-1.07780300	1.90791600	-1.88291300
C	-1.41353100	4.04781100	-0.25573300
H	-1.69526100	4.63949700	0.62588200
H	-0.46110500	3.53964100	-0.05384700
H	-1.25132000	4.74875700	-1.09312600
C	-3.81917600	0.39741700	0.22288500
C	-5.21123100	0.67662300	0.33441000
O	-5.54460000	1.95031600	0.71113000
C	-6.92350800	2.31176700	0.76037900
H	-6.94199300	3.37582400	1.03004400
H	-7.40943500	2.16931800	-0.22084600
H	-7.46471800	1.72738100	1.52568100

C	-6.17057000	-0.31674400	0.09679700
H	-7.23463900	-0.09914000	0.17529100
C	-5.76727900	-1.62064000	-0.21999100
H	-6.52822400	-2.38335300	-0.37735500
C	-4.40490100	-1.92895300	-0.31251100
O	-3.93060000	-3.19429400	-0.56934200
C	-4.88764800	-4.23947200	-0.74708400
H	-5.50792600	-4.37183400	0.15738200
H	-5.54419900	-4.04087200	-1.61300700
H	-4.30045500	-5.14867200	-0.93021300
C	-3.41663600	-0.92047100	-0.12014400
C	-1.98610900	-1.39274900	-0.29274200
C	-1.31078200	-2.02102400	0.80959000
C	-1.94072000	-2.09019200	2.20069900
H	-2.81849500	-1.43096100	2.20622800
C	-2.43676200	-3.52460700	2.49327600
H	-2.96356300	-3.55465000	3.46235400
H	-3.12083900	-3.87089900	1.70523100
H	-1.58718100	-4.22565500	2.54406300
C	-0.98665200	-1.61774300	3.31275900
H	-0.09106300	-2.25674500	3.36757200
H	-0.65915600	-0.58295600	3.12840200
H	-1.49257900	-1.66149000	4.29207900
C	-0.14844300	-2.79103200	0.55706400
H	0.34436600	-3.28405000	1.39764900
C	0.36931000	-2.96545800	-0.72730700
C	1.59399800	-3.83642500	-0.97409400
H	2.03701600	-4.07763700	0.00487600
C	1.18323200	-5.15727300	-1.66337400
H	0.44176000	-5.70537800	-1.05920100
H	0.73383100	-4.95432700	-2.65027900
H	2.06197900	-5.80749900	-1.81333200
C	2.67324900	-3.11011900	-1.80393100
H	3.00459600	-2.19227900	-1.30117300
H	3.55116800	-3.76396600	-1.93933400
H	2.29186400	-2.84215100	-2.80358900
C	-0.31505700	-2.35879900	-1.79964000
H	0.05497300	-2.51475600	-2.81443700
C	-1.48110600	-1.60639800	-1.62381100
C	-2.23656400	-1.12572100	-2.86267800
H	-3.02849700	-0.43795200	-2.53554100
C	-2.91569700	-2.31480700	-3.58291800
H	-3.47911200	-1.95580400	-4.46133000
H	-2.15259600	-3.02950400	-3.93389200

H	-3.60138200	-2.85114700	-2.91451200
C	-1.33394900	-0.37915500	-3.86676700
H	-0.78749700	0.44188800	-3.39047100
H	-0.59888300	-1.06497600	-4.32049300
H	-1.94781400	0.03544600	-4.68388700
C	1.60347000	1.84010300	-3.42768000
C	1.46972300	1.22874000	-2.17732500
C	1.64025500	1.97006400	-0.98329900
C	1.96127300	3.34181200	-1.09484200
C	2.08886300	3.95722000	-2.34874200
C	1.90945800	3.21035500	-3.52439700
H	1.45135500	1.24824500	-4.33325800
H	1.18857700	0.17711600	-2.11297900
H	2.10543000	3.92652600	-0.18281000
H	2.32957300	5.02160300	-2.40621000
H	2.00145700	3.68809900	-4.50229300
C	1.47959900	1.35158800	0.34918600
C	1.60636800	-0.04497200	0.57967600
H	1.64384100	2.03065300	1.19280700
H	1.85964400	-0.70766400	-0.25146000
C	2.01222900	-0.53783600	1.93228700
H	1.60568500	0.07851400	2.74113700
H	1.76909200	-1.59243900	2.09188200
O	3.50000800	-0.38100000	2.12183800
C	4.28373900	-1.37163500	1.69258000
O	3.95479300	-2.47119800	1.28235000
C	5.76198300	-0.88602500	1.77898300
C	5.99264700	0.48787100	1.04605000
O	6.43645400	1.42595500	1.69571700
F	6.58875200	-1.83999800	1.23050600
F	6.09638400	-0.75704700	3.09919600
C	5.60732500	0.58061800	-0.38864800
C	5.31227600	-0.55050500	-1.18603400
C	5.51399600	1.87205500	-0.95906100
C	4.93282300	-0.38384400	-2.52381300
H	5.38514200	-1.55588200	-0.77830000
C	5.12708900	2.03152900	-2.29113500
H	5.73351600	2.73684500	-0.33274200
C	4.83497700	0.90270700	-3.07658600
H	4.70619000	-1.26188700	-3.13036900
H	5.02986000	3.03090800	-2.71538100
H	4.52184500	1.02992100	-4.11378900

TS15

Pd	-0.34417800	0.15553300	0.36803300
P	-1.40119100	-1.67358300	-0.64784700
C	-0.59843300	-1.90461200	-2.37550300
C	-1.36404200	-2.77454900	-3.39359100
H	-2.33402300	-2.32699800	-3.65040700
H	-0.75726000	-2.82123000	-4.31585800
H	-1.53512300	-3.79921100	-3.04483000
C	-0.46179200	-0.49015100	-2.97623200
H	0.14488100	0.16110800	-2.33279900
H	0.04424600	-0.56541100	-3.95411800
H	-1.44451000	-0.02544100	-3.13652300
C	0.82647800	-2.46542200	-2.16436800
H	0.83005800	-3.50288400	-1.80357500
H	1.35177900	-2.44189400	-3.13424000
H	1.39426200	-1.84782700	-1.45847800
C	-1.46080900	-3.36406100	0.28371400
C	-2.65599200	-3.35688200	1.25804800
H	-2.64386100	-4.30347900	1.82652800
H	-2.57545200	-2.53834000	1.98389600
H	-3.61938900	-3.28372900	0.73473800
C	-0.15997500	-3.42483300	1.11258500
H	0.73301200	-3.42854300	0.47512000
H	-0.07708100	-2.57787500	1.80474300
H	-0.15859500	-4.35796300	1.70300200
C	-1.53346200	-4.64314900	-0.57791000
H	-1.51492000	-5.50715000	0.11011300
H	-2.45282800	-4.69339800	-1.16835500
H	-0.67136000	-4.74501500	-1.24952100
C	-3.14959400	-1.06140500	-0.89890900
C	-4.19674500	-1.85097200	-1.45596500
O	-3.86070000	-3.11533500	-1.85574300
C	-4.82936000	-3.89626100	-2.55614300
H	-5.17593900	-3.37715900	-3.46661600
H	-4.31516100	-4.82576200	-2.83296200
H	-5.69635500	-4.13119000	-1.91392100
C	-5.50235700	-1.35033600	-1.55453400
H	-6.29666000	-1.94996700	-1.99586400
C	-5.81000800	-0.07873200	-1.05510700
H	-6.83651800	0.27901600	-1.11660600
C	-4.80653200	0.70445200	-0.47201500
O	-5.03630100	1.93290200	0.09926800
C	-6.37528800	2.43288700	0.08449000
H	-7.05899200	1.75766000	0.62908700
H	-6.33146900	3.40535500	0.59141700

H	-6.74179600	2.56838000	-0.94845100
C	-3.46100500	0.23932700	-0.42567700
C	-2.48136500	1.21952500	0.18457400
C	-2.12881300	2.40133600	-0.56764500
C	-2.35727000	2.49693800	-2.07290600
H	-2.66145000	1.50621100	-2.43738600
C	-3.50294900	3.48485500	-2.39510900
H	-3.66907900	3.52527800	-3.48471600
H	-4.43924400	3.18836600	-1.90379400
H	-3.24201400	4.49940800	-2.05142400
C	-1.08221900	2.92423800	-2.83089800
H	-0.79223500	3.95364400	-2.56517700
H	-0.23347500	2.26593500	-2.61018600
H	-1.26711400	2.89926200	-3.91735400
C	-1.63920400	3.52371100	0.10987100
H	-1.39123100	4.41392800	-0.46964300
C	-1.47102000	3.55184200	1.50672500
C	-0.96281200	4.80432300	2.20659600
H	-0.97566300	4.60798300	3.29245900
C	0.49104300	5.13296500	1.80021800
H	0.84214100	6.03374700	2.33038900
H	1.17487200	4.30390500	2.04072100
H	0.56028300	5.32934800	0.71776300
C	-1.88548200	6.01123300	1.92788100
H	-2.92166600	5.79912400	2.23802600
H	-1.52992700	6.89980300	2.47540000
H	-1.89402500	6.25634600	0.85304400
C	-1.78715500	2.39945600	2.23052700
H	-1.67624400	2.40864500	3.31709800
C	-2.31970600	1.24547000	1.61345100
C	-2.90803900	0.15717800	2.50392000
H	-3.27072400	-0.64900000	1.85573900
C	-4.12864500	0.70741300	3.27588000
H	-3.82065800	1.49453500	3.98366600
H	-4.86683200	1.13916700	2.58338400
H	-4.60947900	-0.10218400	3.85039000
C	-1.86575700	-0.43628100	3.46930900
H	-1.02063900	-0.86357200	2.90962600
H	-1.47152400	0.33430600	4.15201100
H	-2.32114500	-1.23045300	4.08427800
C	1.81523100	-0.18695000	0.71082300
C	1.49687900	1.18664700	0.99154100
H	1.48096300	1.56052400	2.01678500
C	1.25237600	2.05580600	-0.07476000

O	3.40176500	2.73743400	-0.61521900
C	3.75566100	1.93260800	-1.52853100
O	3.07111800	1.30715600	-2.37144500
C	5.31801100	1.64043000	-1.52742500
C	5.69175000	0.57942200	-0.44626200
O	6.13718800	0.96436600	0.63014700
F	6.01544700	2.79222800	-1.26440800
F	5.74034500	1.19743600	-2.77194700
C	5.48358200	-0.87723100	-0.74620200
C	6.09549200	-1.81102400	0.12116200
C	4.69973300	-1.34853500	-1.82481200
C	5.95072800	-3.18515600	-0.09442900
H	6.68298700	-1.43689600	0.95994200
C	4.53390100	-2.72831100	-2.01821300
H	4.20501300	-0.63952700	-2.48610900
C	5.16437000	-3.64879500	-1.16435400
H	6.44113700	-3.89527500	0.57457400
H	3.91528500	-3.08386300	-2.84450100
H	5.04316600	-4.72179600	-1.33012900
H	2.24944700	-0.38110000	-0.27337000
C	2.17887000	-1.14583900	1.76063800
C	1.75380000	-0.98940400	3.10231900
C	2.95062300	-2.28037300	1.42536700
C	2.07912800	-1.94557700	4.06984700
H	1.14309300	-0.12803300	3.37411900
C	3.27737300	-3.23585200	2.39456700
H	3.28719300	-2.40617500	0.39685100
C	2.83875500	-3.07726600	3.71975300
H	1.73691500	-1.81324900	5.09876700
H	3.87751500	-4.10356500	2.11339900
H	3.09000800	-3.82427300	4.47583000
H	1.31410000	1.71157700	-1.10381700
H	0.91575500	3.07094900	0.10315500

IM15

Pd	-0.08923200	0.06305500	-0.28259800
P	-2.15089000	0.91661300	0.48559300
C	-3.01083300	2.12645600	-0.73426300
C	-2.26987700	3.47846700	-0.68663700
H	-2.43888500	4.02259200	0.25060000
H	-2.64617800	4.10838700	-1.51127700
H	-1.19318400	3.35440500	-0.82550100
C	-4.51813200	2.36249300	-0.51323300
H	-5.09445400	1.43746300	-0.65450200

H	-4.85682300	3.09070300	-1.27208000
H	-4.73980600	2.77107800	0.47893200
C	-2.83217200	1.52613100	-2.14260300
H	-3.19400200	2.25469600	-2.88926200
H	-3.42619900	0.60762100	-2.25409200
H	-1.77805100	1.30157200	-2.35553100
C	-2.03635000	1.71637000	2.22713300
C	-1.91877700	0.57001400	3.25126900
H	-2.80836100	-0.07792200	3.25237300
H	-1.81053800	1.01126000	4.25702700
H	-1.02224800	-0.03219100	3.05963300
C	-0.71088000	2.51264800	2.24794100
H	-0.69571700	3.31031600	1.49487200
H	0.15362000	1.85651300	2.09625800
H	-0.60791300	2.98207900	3.24183400
C	-3.18004100	2.66277800	2.65137000
H	-3.28105100	3.53245800	1.98874700
H	-2.92823800	3.04695400	3.65547800
H	-4.14338200	2.14884900	2.71302500
C	-3.22380300	-0.60988200	0.49568900
C	-4.57301000	-0.64056800	0.95195100
O	-5.01025200	0.45266100	1.64593900
C	-6.41157200	0.60319000	1.87808700
H	-6.53127100	1.59203200	2.33950000
H	-6.78858900	-0.17150000	2.56813600
H	-6.97780000	0.56060800	0.93168000
C	-5.38339500	-1.76059900	0.71935200
H	-6.42535700	-1.76889400	1.03519200
C	-4.85156000	-2.90019500	0.10398800
H	-5.49421600	-3.76509900	-0.05306100
C	-3.49780000	-2.93358400	-0.25348200
O	-2.87580200	-4.04570000	-0.76493400
C	-3.64981000	-5.23841200	-0.90594200
H	-4.05188500	-5.57084400	0.06732400
H	-2.95633300	-5.99341700	-1.29791700
H	-4.48357500	-5.09510400	-1.61601000
C	-2.67151600	-1.78864100	-0.06407900
C	-1.20168300	-2.02501100	-0.35716100
C	-0.78323200	-2.25929900	-1.72170900
C	-1.56773500	-1.70325000	-2.90047800
H	-2.39789600	-1.11168300	-2.49986600
C	-2.16620900	-2.82733900	-3.77462400
H	-2.82545100	-3.47771900	-3.18331100
H	-1.36832300	-3.45072400	-4.21019300

H	-2.74706100	-2.38901300	-4.60356100
C	-0.68404200	-0.77470700	-3.76057800
H	-1.28241000	-0.30735100	-4.56016800
H	0.13482400	-1.34349700	-4.23189000
H	-0.23654500	0.01724200	-3.14135900
C	0.33046700	-3.07145000	-1.97774000
H	0.62289800	-3.25234500	-3.01478000
C	1.08031500	-3.65662500	-0.94762100
C	2.29720300	-4.51861900	-1.24779600
H	2.33353600	-4.68217000	-2.33884700
C	2.19878000	-5.89854700	-0.56054200
H	1.27077700	-6.42089400	-0.84545100
H	2.21087600	-5.79295400	0.53604100
H	3.05764100	-6.52688300	-0.84834900
C	3.59889300	-3.79751500	-0.82148900
H	4.46811900	-4.45751800	-0.98147000
H	3.56391000	-3.51791900	0.24284300
H	3.75384200	-2.87558600	-1.40320100
C	0.70502700	-3.39434400	0.37939600
H	1.28869300	-3.82931300	1.18943100
C	-0.43463200	-2.64773600	0.70310000
C	-0.92085000	-2.65010200	2.14572900
H	-1.69051500	-1.87847400	2.24826700
C	-1.58338800	-4.01308100	2.46240900
H	-0.84330900	-4.82553500	2.37233600
H	-2.41682200	-4.23094200	1.77940900
H	-1.96691800	-4.00865100	3.49653900
C	0.19746100	-2.35435800	3.16415700
H	-0.24935700	-2.23241500	4.16517700
H	0.75966000	-1.44650100	2.90393200
H	0.91524300	-3.18795300	3.22192500
C	0.71773000	4.84218000	-2.53935200
C	0.92939300	3.51146400	-2.16608700
C	1.24799600	3.17822000	-0.82609600
C	1.36356700	4.22482400	0.11989500
C	1.14801600	5.55666000	-0.25575300
C	0.81929500	5.87109300	-1.58493000
H	0.46529200	5.08008400	-3.57499000
H	0.81831900	2.72360300	-2.91196000
H	1.64175400	3.97918300	1.14459600
H	1.24325900	6.34967600	0.48865200
H	0.64782300	6.90899600	-1.87781500
C	1.49965100	1.80828100	-0.37991900
C	1.79326500	0.74266500	-1.26618800

H	1.79891500	1.68174100	0.66385800
H	1.71491800	0.89334000	-2.34445600
C	1.98519300	-0.55510700	-0.77740200
H	2.08285300	-1.36190800	-1.49700900
H	2.33089100	-0.75355500	0.23840200
O	2.01296200	0.45072900	2.41429100
C	3.15513200	-0.08976100	2.50937800
O	3.51190200	-1.27513500	2.33722100
C	4.28239200	0.96856100	2.86606900
C	4.33451400	2.10438300	1.80914800
O	4.03041000	3.25379200	2.12258300
F	4.01807900	1.51306200	4.10164200
F	5.54603500	0.39214800	2.95223300
C	4.68489000	1.72895800	0.39865000
C	5.06452400	0.42250600	0.01427700
C	4.57512600	2.73219800	-0.59107100
C	5.31156500	0.13247900	-1.33499400
H	5.14257700	-0.36908100	0.75532400
C	4.81766800	2.43718300	-1.93595800
H	4.27408500	3.73384600	-0.28601000
C	5.18591300	1.13279600	-2.31247900
H	5.60152900	-0.88070900	-1.62081600
H	4.71503800	3.21959300	-2.69087900
H	5.37819700	0.90005900	-3.36264700

TS16

Pd	0.17639500	0.65466500	0.91478500
P	1.08553500	2.65377500	0.04657900
C	1.47823800	4.04538800	1.32438300
C	0.17381100	4.79418300	1.67282400
H	0.38699000	5.46969300	2.51859400
H	-0.61968300	4.11058200	1.98508400
H	-0.19582700	5.40771100	0.84226800
C	2.54833600	5.07460000	0.90940600
H	2.26384200	5.64198800	0.01559600
H	3.52298000	4.59776200	0.73285700
H	2.66788600	5.78534500	1.74714000
C	1.97136300	3.34347000	2.60479900
H	2.05091200	4.09253100	3.41210500
H	2.96743300	2.90390700	2.45906200
H	1.27166100	2.56195600	2.92618400
C	-0.01246800	3.35938700	-1.36690300
C	-1.47353800	3.33179600	-0.85435200
H	-2.12126100	3.69513700	-1.67183600

H	-1.63267900	3.98398900	0.01301100
H	-1.79167600	2.31285000	-0.61195600
C	0.31002200	4.78000500	-1.88163000
H	1.24747300	4.80614300	-2.44497100
H	0.36105800	5.52969500	-1.08120300
H	-0.50847900	5.07665000	-2.56091100
C	0.08493100	2.36676800	-2.54321500
H	-0.27554100	1.37411600	-2.24621200
H	1.11158700	2.29037700	-2.93373500
H	-0.56609700	2.72819700	-3.35823500
C	2.72523900	2.05112900	-0.62389400
C	3.64327400	2.86172800	-1.35376400
O	3.20083100	4.09532400	-1.73619500
C	4.14801600	5.04900600	-2.21849000
H	4.96174200	5.20523200	-1.48914200
H	3.58552600	5.98170100	-2.35501900
H	4.57699000	4.73507900	-3.18609400
C	4.92038400	2.38674000	-1.68242400
H	5.62781200	3.01867800	-2.21645300
C	5.29400500	1.07922600	-1.35156500
H	6.28745800	0.72743600	-1.62499600
C	4.37986700	0.23356500	-0.71187900
O	4.64497700	-1.07954900	-0.41105600
C	5.90747700	-1.61643400	-0.80924000
H	6.74275100	-1.09407400	-0.30954000
H	6.04164800	-1.55512800	-1.90365400
H	5.88954200	-2.66835900	-0.49644800
C	3.08642500	0.70839200	-0.34675200
C	2.18631200	-0.36284900	0.24287400
C	2.46165100	-0.84122500	1.57706300
C	3.17750200	0.02808600	2.59676000
H	3.32420800	1.01328000	2.14215100
C	4.57224400	-0.53995300	2.94129100
H	4.48364100	-1.53020400	3.41696000
H	5.09107000	0.13290500	3.64467600
H	5.18598800	-0.64987000	2.03578900
C	2.33241900	0.19797800	3.87562700
H	1.32114300	0.55230600	3.62615300
H	2.80591500	0.92336600	4.55748500
H	2.23651000	-0.76171300	4.41032900
C	2.16525200	-2.16793500	1.91792800
H	2.40653500	-2.52006700	2.92349200
C	1.63696400	-3.07677100	0.99043900
C	1.43913100	-4.53978000	1.35731000

H	1.80265600	-4.67865800	2.38994900
C	2.27308600	-5.45140500	0.42928000
H	2.17238200	-6.50523100	0.73756300
H	3.34054900	-5.17769200	0.45733500
H	1.92507600	-5.36662500	-0.61311300
C	-0.04991200	-4.94431700	1.31209800
H	-0.65167400	-4.33683100	2.00549300
H	-0.16528300	-6.00423200	1.59381300
H	-0.45739700	-4.81381200	0.29882200
C	1.30828800	-2.60154800	-0.29012700
H	0.87111900	-3.28814300	-1.01522200
C	1.58805300	-1.28942600	-0.69517100
C	1.38216800	-0.91471600	-2.15527800
H	1.53816500	0.16572000	-2.25186500
C	2.43740300	-1.61998000	-3.03948900
H	2.29473200	-1.32951800	-4.09382300
H	2.33050600	-2.71492900	-2.96784200
H	3.46142500	-1.35480500	-2.73700200
C	-0.04183100	-1.24005500	-2.64582200
H	-0.22486000	-2.32632500	-2.65592700
H	-0.17058900	-0.87612200	-3.67743200
H	-0.80938900	-0.76828300	-2.01591600
C	-1.58977900	3.63331900	4.74038300
C	-1.36297900	2.48902300	3.96930800
C	-2.08098200	2.27346300	2.76735000
C	-3.03707200	3.23916000	2.37029700
C	-3.26213200	4.38524900	3.14316700
C	-2.53717500	4.58910100	4.32930400
H	-1.02133700	3.78839400	5.66009600
H	-0.60636700	1.76766700	4.28143600
H	-3.59372700	3.07686500	1.44582800
H	-4.00212000	5.12030500	2.81984400
H	-2.70714400	5.48524200	4.92964700
C	-1.87294400	1.10628600	1.91023700
C	-1.30818500	-0.11702900	2.36500800
H	-2.46721200	1.04369500	0.99036100
H	-0.92060300	-0.20997400	3.38294100
C	-1.05093200	-1.12614400	1.42439800
H	-0.49591900	-2.01038900	1.72551200
H	-1.62512200	-1.16258900	0.49577400
O	-3.40092800	-3.40975100	1.50946400
C	-3.06562700	-3.46023500	0.37240900
O	-2.63466800	-3.78021600	-0.68624200
C	-4.32317500	-1.17270300	-0.22767300

C	-3.54179900	-0.59111900	-1.23831500
O	-2.63162600	0.27779400	-0.95183400
F	-5.52567300	-1.79663000	-0.45471100
F	-4.36153800	-0.59561500	1.00900700
C	-3.68337500	-1.05566000	-2.66053700
C	-3.13426900	-0.21895600	-3.66119400
C	-4.31533000	-2.25315800	-3.07115600
C	-3.22256700	-0.55479900	-5.01798800
H	-2.63254800	0.69543500	-3.34453500
C	-4.39587300	-2.59223400	-4.42920300
H	-4.72391600	-2.93437400	-2.32886800
C	-3.85448000	-1.74645000	-5.41191000
H	-2.79453000	0.11309900	-5.77058000
H	-4.87842200	-3.52895900	-4.72012800
H	-3.92016400	-2.01523900	-6.46912700

IM16

C	-3.40222300	2.79542800	3.52715700
C	-2.71918400	1.68330800	3.02640600
C	-3.08592700	1.10932800	1.78280900
C	-4.16522800	1.68327000	1.06640300
C	-4.84464000	2.79904600	1.57007000
C	-4.46533100	3.36311300	2.79988800
H	-3.10003300	3.23086200	4.48232900
H	-1.87610600	1.27283800	3.58383000
H	-4.46193400	1.23718000	0.11614100
H	-5.67407200	3.22739500	1.00298000
H	-4.99172300	4.23654900	3.19052200
C	-2.39249800	-0.03339400	1.19593100
C	-1.59623600	-0.93862800	1.93524400
H	-2.73325600	-0.35125500	0.21186500
H	-1.40426500	-0.73986400	2.99234400
C	-0.87618500	-1.96685500	1.30059000
H	-0.19274100	-2.55849100	1.90260100
H	-1.18159100	-2.38252800	0.34345600
C	-2.46431700	-3.63658400	-1.26196500
C	-2.76076100	-2.30457800	-1.47981400
O	-1.84722300	-1.43464900	-1.79258400
F	-1.21457800	-4.14537800	-1.44136600
F	-3.34769500	-4.64854400	-1.05084400
C	-4.17031000	-1.82251700	-1.27250500
C	-5.06511700	-2.35406900	-0.31581600
C	-4.57879500	-0.68383300	-2.00627400
C	-6.32230300	-1.76860500	-0.10495500

H	-4.76645900	-3.21614800	0.28045900
C	-5.84157800	-0.10972400	-1.80803600
H	-3.87752200	-0.25611000	-2.72217300
C	-6.72025400	-0.64538600	-0.84974600
H	-6.99005500	-2.18529200	0.65338300
H	-6.13838500	0.76314000	-2.39579300
H	-7.69903200	-0.19023500	-0.68101500
Pd	-0.09090900	-0.04381100	0.52882400
P	0.41193700	2.00162200	-0.50876300
C	0.21479200	3.54325300	0.63013200
C	-1.27462600	3.94292700	0.70592000
H	-1.38222700	4.70206000	1.49952300
H	-1.91643900	3.09751900	0.96607700
H	-1.63880400	4.38583700	-0.22982200
C	1.04148200	4.78758700	0.24840400
H	0.77111700	5.18656800	-0.73685800
H	2.11988400	4.57527700	0.26464700
H	0.83933600	5.56776700	1.00453200
C	0.66123000	3.09340700	2.03594600
H	1.74230800	2.89909400	2.06226200
H	0.12756200	2.18795600	2.35344100
H	0.44477000	3.90180400	2.75645700
C	-0.57308300	2.25278200	-2.13411000
C	-2.03648800	1.85327500	-1.82194200
H	-2.61570300	1.95432000	-2.75697800
H	-2.50490100	2.49922400	-1.06847900
H	-2.09080600	0.80435400	-1.50692700
C	-0.55767800	3.65930000	-2.77135400
H	-1.29526600	3.65766500	-3.59327200
H	0.42246100	3.90467500	-3.19173800
H	-0.84785000	4.45367300	-2.07128300
C	-0.02039400	1.23214500	-3.15053700
H	-0.13991000	0.20563300	-2.78090100
H	1.03650400	1.42739600	-3.39065200
H	-0.60520400	1.31925400	-4.08311700
C	2.24708700	1.83802700	-0.82583000
C	3.03690700	2.81694300	-1.49576900
O	2.35807200	3.80902500	-2.14483700
C	3.08072900	4.95233600	-2.60033200
H	3.78601800	4.68530700	-3.40664100
H	3.63263000	5.43041300	-1.77233300
H	2.32418100	5.64459100	-2.99210200
C	4.43598200	2.73246100	-1.50123100
H	5.03875600	3.50173100	-1.98134000

C	5.07764400	1.63674600	-0.91134100
H	6.16492900	1.58365600	-0.93689900
C	4.31837000	0.60774800	-0.34137700
O	4.86644000	-0.54299800	0.17022700
C	6.28000100	-0.71541400	0.06306600
H	6.82535800	0.06208400	0.62727000
H	6.60603100	-0.69672800	-0.99198700
H	6.48909000	-1.70124400	0.49814000
C	2.89657700	0.69615800	-0.29294500
C	2.21462400	-0.55319600	0.23649300
C	2.35260900	-0.88521800	1.63649100
C	2.65152100	0.17858200	2.68318200
H	2.66685300	1.14987000	2.17522700
C	4.03597200	-0.03450700	3.33539600
H	4.06773200	-0.99344400	3.87820900
H	4.23929000	0.77324900	4.05867100
H	4.83185700	-0.04295500	2.57820600
C	1.55770800	0.21847500	3.76969700
H	0.56699700	0.34834800	3.31289500
H	1.74018200	1.05098600	4.46950500
H	1.54806400	-0.72007900	4.34890000
C	2.30574800	-2.22875000	2.03934300
H	2.43061300	-2.46515600	3.09877200
C	2.12343000	-3.27567000	1.12629500
C	2.07562200	-4.72536500	1.58609100
H	2.33847800	-4.74722500	2.65794500
C	3.10185300	-5.59431200	0.82559900
H	2.85471200	-5.64562600	-0.24702100
H	3.09795700	-6.62287600	1.22279800
H	4.12045500	-5.18436000	0.92307700
C	0.65221300	-5.31204800	1.42849400
H	0.30004100	-5.22180700	0.38968000
H	-0.06997200	-4.78549500	2.07197500
H	0.64773100	-6.37930900	1.70743000
C	1.96081900	-2.95331400	-0.23206700
H	1.80564100	-3.75821200	-0.94933600
C	2.05312200	-1.64135300	-0.70773200
C	2.11904400	-1.40617900	-2.21185800
H	1.93610500	-0.34189200	-2.39422400
C	3.53890000	-1.73604800	-2.73549200
H	3.58114500	-1.56305000	-3.82432400
H	3.77635000	-2.79633200	-2.54673500
H	4.31237600	-1.12084600	-2.25600500
C	1.07450300	-2.21471300	-3.00737500

H	1.32327800	-3.28931300	-3.01062600
H	1.08456700	-1.87460300	-4.05694000
H	0.06184100	-2.08788900	-2.59793800

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C	-3.31208500	2.92640300	-7.80679300
C	-2.92584300	2.25956300	-6.64041700
C	-3.23241900	0.88729300	-6.45646000
C	-3.94593400	0.21297900	-7.47741200
C	-4.32791100	0.88344500	-8.64573800
C	-4.01037500	2.24119900	-8.81902000
H	-3.05950600	3.98137200	-7.93596400
H	-2.35090400	2.79063700	-5.87993900
H	-4.20444100	-0.83647400	-7.33193000
H	-4.87877500	0.34599100	-9.42090500
H	-4.30411200	2.76329700	-9.73212700
C	-2.82387100	0.13310500	-5.27446100
C	-2.52468100	0.73506300	-4.02677000
H	-3.05797400	-0.93001500	-5.27273000
H	-2.51712000	1.82509900	-3.94690300
C	-2.03976700	-0.01943800	-2.94818900
H	-1.70757800	0.50617000	-2.05893200
H	-2.17981200	-1.09400500	-2.87768600
C	-3.90542300	-2.62353400	-2.17380600
C	-3.73801300	-2.75546800	-3.54355100
O	-2.57986500	-3.00842900	-4.06796000
F	-2.89727500	-2.87211900	-1.29559100
F	-5.08028000	-2.48860600	-1.50424900
C	-4.90183300	-2.49703700	-4.45799000
C	-5.94214600	-1.57890100	-4.18841100
C	-4.88144300	-3.13061900	-5.72307400
C	-6.92885600	-1.31086200	-5.14872900
H	-5.96472700	-1.05593100	-3.23257300
C	-5.87887300	-2.87837600	-6.67394800
H	-4.06122800	-3.81490800	-5.94158800
C	-6.90632500	-1.95969000	-6.39488800
H	-7.71258600	-0.58216300	-4.92683500
H	-5.85008400	-3.39097300	-7.63926200
H	-7.67552300	-1.74702800	-7.14100800
Pd	-0.56440300	-0.18612400	-4.62310500
P	0.70587800	-0.85920100	-6.46828200
C	0.90696300	0.45307100	-7.85928500
C	-0.44204700	0.57583300	-8.59849800
H	-0.39379000	1.45308500	-9.26646000

H	-1.27048200	0.73012800	-7.90172100
H	-0.66534600	-0.30280800	-9.21696800
C	2.03510600	0.21486900	-8.88397100
H	1.93196000	-0.73486800	-9.42075900
H	3.02369500	0.24940200	-8.40540000
H	1.99077100	1.03543000	-9.62294400
C	1.19726500	1.79389500	-7.15569600
H	2.18775400	1.77897700	-6.67719700
H	0.43559600	2.02864000	-6.40060900
H	1.19916800	2.59861900	-7.91212600
C	0.07184800	-2.50912700	-7.22090400
C	-1.47473900	-2.43280700	-7.20237900
H	-1.86478800	-3.35239000	-7.67426200
H	-1.86466200	-1.57402100	-7.76622400
H	-1.84911700	-2.39917500	-6.17156500
C	0.53294200	-2.85043000	-8.65300500
H	0.05858700	-3.80810500	-8.93101600
H	1.61777100	-2.97217400	-8.72054600
H	0.21028600	-2.10219500	-9.38881000
C	0.49528700	-3.64193200	-6.26376600
H	0.06510700	-3.48904600	-5.26567400
H	1.58967600	-3.73298700	-6.19012400
H	0.09444400	-4.59442700	-6.65249800
C	2.40754000	-1.04075000	-5.72309900
C	3.54826000	-1.50760300	-6.43569100
O	3.31168700	-2.10999300	-7.64036800
C	4.41279200	-2.33098700	-8.52240500
H	4.95787700	-1.39194500	-8.72106900
H	3.97474700	-2.71130200	-9.45438700
H	5.11092900	-3.08166700	-8.11250600
C	4.83453700	-1.37950800	-5.89413400
H	5.71050500	-1.69873600	-6.45660000
C	5.00625300	-0.86288700	-4.60375300
H	6.01301600	-0.78240800	-4.19670800
C	3.88823200	-0.50768000	-3.83804600
O	3.96577200	-0.09297400	-2.53107400
C	5.25371300	-0.06695700	-1.91436400
H	5.71769000	-1.06916200	-1.91596500
H	5.07792500	0.25823100	-0.88077900
H	5.92792300	0.64792900	-2.41901200
C	2.57680100	-0.59435600	-4.38804100
C	1.46098900	-0.33230700	-3.39050500
C	1.25543200	1.00511800	-2.88492500
C	1.67801100	2.23087700	-3.68103700

H	2.07203500	1.88170100	-4.64131800
C	2.79836200	3.01812500	-2.96652100
H	2.44065600	3.42421700	-2.00607400
H	3.12301600	3.86559700	-3.59377300
H	3.66464600	2.37271700	-2.76451200
C	0.47293300	3.15354900	-3.96202700
H	-0.33611400	2.59336800	-4.45610100
H	0.77385700	3.99360100	-4.60999100
H	0.07335700	3.57074500	-3.02250100
C	0.73188200	1.18951600	-1.59522800
H	0.59570100	2.20765500	-1.22302800
C	0.39850500	0.11263900	-0.76424100
C	-0.15645400	0.33437700	0.63528600
H	-0.08083500	1.41246800	0.85960500
C	0.66278200	-0.43225900	1.69722400
H	0.28797400	-0.19849800	2.70744600
H	1.73055100	-0.16300700	1.64808900
H	0.57678900	-1.52086600	1.54950400
C	-1.64860600	-0.06904600	0.71420000
H	-1.79630900	-1.10934100	0.38547600
H	-2.27114300	0.57421300	0.07268200
H	-2.01367900	0.02461900	1.75087200
C	0.56110900	-1.18961900	-1.26838900
H	0.28556300	-2.03548000	-0.63916000
C	1.11357900	-1.44388000	-2.52715600
C	1.44964600	-2.88126900	-2.90273700
H	1.65740000	-2.91348100	-3.97802200
C	2.73724400	-3.33090800	-2.16983300
H	2.58981000	-3.28886700	-1.07773900
H	3.59731300	-2.69529800	-2.42516700
H	2.97841400	-4.37169000	-2.44495600
C	0.30186000	-3.86820500	-2.60487500
H	0.17108100	-4.00889200	-1.51898200
H	0.55568000	-4.85326800	-3.03194700
H	-0.65762200	-3.53434800	-3.02680300

IM17

C	-3.06207600	2.63309700	-6.10607100
C	-2.67607600	1.46163800	-5.44679000
C	-3.02269500	0.18881400	-5.96001300
C	-3.76736700	0.13648600	-7.15849400
C	-4.15616400	1.30996100	-7.81975100
C	-3.80681200	2.56622400	-7.29848500
H	-2.77159500	3.60303400	-5.69467200

H	-2.07325900	1.51856400	-4.53994500
H	-4.05879800	-0.83774400	-7.55720400
H	-4.73977100	1.24195100	-8.74094900
H	-4.10633300	3.48119800	-7.81443500
C	-2.66302900	-1.06197700	-5.26131400
C	-2.40863400	-1.13257500	-3.86486000
H	-3.00884200	-1.97289800	-5.76077200
H	-2.47565900	-0.21844000	-3.26616400
C	-2.74924700	-2.40310800	-3.11050500
H	-2.17816500	-2.48401400	-2.17558700
H	-2.52714000	-3.28872200	-3.72337900
C	-4.23256000	-2.50106500	-2.73647800
C	-5.17768400	-2.49545200	-3.98942400
O	-5.30970900	-3.57988100	-4.55528100
F	-4.44417300	-3.68734800	-2.06060500
F	-4.57120200	-1.49567800	-1.83110200
C	-5.82262500	-1.24901400	-4.50103700
C	-5.53267200	0.05456900	-4.03493200
C	-6.72825800	-1.39806900	-5.58048500
C	-6.13045600	1.16995300	-4.63360000
H	-4.81399300	0.20648800	-3.23697900
C	-7.32889900	-0.28313400	-6.16918800
H	-6.94109900	-2.40258600	-5.94706200
C	-7.02802800	1.00785100	-5.69878600
H	-5.87173800	2.16951400	-4.28212600
H	-8.02412000	-0.41551600	-7.00083600
H	-7.48297200	1.88227800	-6.16840800
Pd	-0.50741400	-1.17857200	-4.86921400
P	0.98110500	-1.46481000	-6.63532900
C	0.67485200	-0.25279600	-8.08471400
C	-0.66821200	-0.65300700	-8.73646700
H	-0.98329500	0.15707900	-9.41738800
H	-1.45170600	-0.77448900	-7.97682600
H	-0.59762200	-1.57709600	-9.32634100
C	1.77207000	-0.11929600	-9.15773700
H	1.99546900	-1.06813600	-9.66017100
H	2.70355700	0.27218300	-8.72499500
H	1.42102700	0.60150500	-9.91914700
C	0.47036800	1.12436900	-7.42362600
H	1.39349600	1.48206300	-6.94661200
H	-0.32916200	1.07696400	-6.67297800
H	0.17792100	1.85805500	-8.19579200
C	0.99534600	-3.27243700	-7.30808500
C	-0.46445900	-3.77659400	-7.18212300

H	-0.50096700	-4.83827100	-7.48677400
H	-1.15254900	-3.21176100	-7.82788400
H	-0.82445900	-3.68988800	-6.14567100
C	1.46009100	-3.50142700	-8.76217600
H	1.37612100	-4.58178500	-8.98072400
H	2.50257300	-3.20191500	-8.90912500
H	0.83420900	-2.97307800	-9.49328600
C	1.87468300	-4.12494000	-6.37099300
H	1.51415300	-4.07196200	-5.33635900
H	2.92893000	-3.81465900	-6.40121500
H	1.81575400	-5.18002900	-6.69266100
C	2.65369200	-1.07372400	-5.89448200
C	3.90051700	-1.26747500	-6.55375800
O	3.84219800	-1.77493500	-7.82483700
C	5.04083200	-1.82730600	-8.59630700
H	5.50191300	-0.82776200	-8.68584000
H	4.73949700	-2.18590900	-9.58928600
H	5.77206000	-2.52950800	-8.15785400
C	5.11131000	-0.97698900	-5.91049300
H	6.06353300	-1.11252500	-6.42122500
C	5.11146400	-0.53427100	-4.58100500
H	6.06353700	-0.33860200	-4.09009800
C	3.90070800	-0.37154500	-3.89683700
O	3.82042300	-0.00206200	-2.57431000
C	5.04269000	0.24319300	-1.87768500
H	5.67697600	-0.66100800	-1.84922100
H	4.74942900	0.52135500	-0.85707600
H	5.61001400	1.07077900	-2.33999700
C	2.65866500	-0.60965000	-4.55260200
C	1.42951800	-0.36071300	-3.69917400
C	1.03944900	0.99807100	-3.41190900
C	1.60862000	2.18632700	-4.18553300
H	2.15178000	1.79780300	-5.05763100
C	2.62111700	2.97340400	-3.31919000
H	2.11927400	3.38573900	-2.42772900
H	3.03959200	3.81563000	-3.89661400
H	3.44433200	2.33212000	-2.97876300
C	0.51683100	3.15620700	-4.68537900
H	-0.24573100	2.64228400	-5.28144800
H	0.97337100	3.94473300	-5.30706800
H	0.01490200	3.65145200	-3.83758500
C	0.18994500	1.24984700	-2.33040800
H	-0.09173900	2.28395500	-2.11603700
C	-0.26792900	0.23847700	-1.46065400

C	-1.06344100	0.63279000	-0.22102300
H	-1.69852500	1.49370000	-0.49719300
C	-0.08793100	1.11059600	0.88160000
H	-0.64167500	1.46204200	1.76922000
H	0.55105700	1.93198200	0.51870100
H	0.56951700	0.27977300	1.18934600
C	-1.98052400	-0.47484500	0.32729300
H	-1.39358000	-1.33672000	0.68622300
H	-2.69040500	-0.83054000	-0.43249300
H	-2.55730300	-0.09160300	1.18503300
C	0.12402600	-1.07254500	-1.72934100
H	-0.18742400	-1.87846700	-1.06492200
C	0.95896300	-1.40334000	-2.82652600
C	1.54354300	-2.81489000	-2.87852000
H	2.14999000	-2.89399600	-3.78953700
C	2.48549900	-3.04981900	-1.67601300
H	1.92143400	-3.01738000	-0.72891300
H	3.26732200	-2.27735800	-1.63499300
H	2.96532200	-4.04025800	-1.75580500
C	0.45409300	-3.90136700	-2.93211300
H	-0.17686000	-3.87929400	-2.02909500
H	0.91435700	-4.90167000	-2.99839400
H	-0.19884600	-3.75058600	-3.80539500

TS18

C	1.49959400	0.66620900	2.11443300
C	1.43189200	2.00471800	1.71866100
H	1.45954900	0.39849100	3.17406700
H	1.69935200	2.26623300	0.69171000
C	0.85354500	2.99480400	2.56471200
H	0.81150800	2.79282800	3.62961000
C	2.70118000	3.19788100	5.17804500
C	2.63428600	1.82160300	4.97783000
O	1.56607900	1.15747900	5.26491000
F	1.70193000	3.86802700	5.81283800
F	3.79983300	3.99349300	5.08805800
C	3.77441100	1.12067500	4.29177700
C	4.69412400	1.73943000	3.41259100
C	3.85145100	-0.28305800	4.45189500
C	5.65940200	0.98191300	2.73288100
H	4.63978400	2.81342300	3.23959800
C	4.82583500	-1.03719200	3.78539800
H	3.11955600	-0.76277400	5.10285700
C	5.73610000	-0.40938300	2.91759600

H	6.34971300	1.48107000	2.04774200
H	4.87309200	-2.11878200	3.93706600
H	6.48937800	-0.99657000	2.38689100
Pd	-0.66093400	1.26287600	1.94294500
P	-2.85187100	1.85941600	2.52747300
C	-3.00610100	2.12715500	4.42879600
C	-1.68964700	2.80997600	4.87673100
H	-1.48344800	3.72994100	4.31175600
H	-1.77901800	3.07739300	5.94431700
H	-0.82919700	2.13461600	4.77724300
C	-4.19478800	2.97807000	4.92502100
H	-4.16777300	4.00762400	4.54494100
H	-5.16002200	2.52917500	4.67050900
H	-4.12074300	3.03551800	6.02527700
C	-3.07407200	0.74216200	5.10085000
H	-3.97408900	0.18300200	4.80647300
H	-2.17972700	0.15300900	4.86710800
H	-3.09548200	0.88580700	6.19521700
C	-3.63773200	3.34828400	1.60153400
C	-3.35195900	3.13989700	0.10109200
H	-3.68007200	4.03936900	-0.44920200
H	-2.28199200	2.99081600	-0.08994000
H	-3.91548300	2.28044500	-0.29222000
C	-2.89089500	4.62233600	2.05259800
H	-3.25298700	5.46940300	1.44479600
H	-3.06199500	4.87132600	3.10751300
H	-1.81319500	4.53057100	1.88949400
C	-5.16033600	3.55353600	1.75002100
H	-5.48135300	3.69154400	2.78793400
H	-5.42627700	4.46538800	1.18505600
H	-5.72160500	2.71523000	1.31524400
C	-3.80701800	0.34730200	1.99237100
C	-5.19332000	0.15251100	2.25156700
O	-5.77884000	1.03617900	3.11593200
C	-7.20007100	1.02229200	3.25151700
H	-7.54773800	0.08297600	3.71609700
H	-7.44360600	1.86705600	3.90878300
H	-7.69569000	1.15385600	2.27402700
C	-5.88893300	-0.91776100	1.67327400
H	-6.95556000	-1.05059200	1.84794600
C	-5.20952100	-1.85020100	0.87881200
H	-5.76706900	-2.67846100	0.44428500
C	-3.82678200	-1.73277000	0.68696600
O	-3.07894000	-2.64592000	-0.01567000

C	-3.75000700	-3.78394800	-0.55852200
H	-4.22795700	-4.38492100	0.23543700
H	-4.51305700	-3.48535600	-1.29936700
H	-2.96893700	-4.37714200	-1.05153100
C	-3.10862100	-0.63497900	1.24536700
C	-1.60072100	-0.72766300	1.06954700
C	-0.91092600	-1.63462600	1.96177300
C	-1.48161900	-2.00300700	3.32256200
H	-2.36277800	-1.37717900	3.50430800
C	-1.95168000	-3.47528900	3.32735100
H	-1.10052400	-4.15587200	3.15954200
H	-2.40630700	-3.72618300	4.30041000
H	-2.69440100	-3.65480400	2.53451200
C	-0.46383800	-1.74422700	4.45358500
H	-0.11686500	-0.70005700	4.46559300
H	-0.92142400	-1.97242400	5.43066200
H	0.42429100	-2.38741200	4.34196100
C	0.27198700	-2.25611900	1.54359500
H	0.76974200	-2.94081300	2.23138200
C	0.81615700	-2.05628900	0.26494300
C	2.07583400	-2.78987200	-0.17084000
H	2.27553800	-2.51945200	-1.22200800
C	3.29647600	-2.36348300	0.67721700
H	4.19303000	-2.92865700	0.37143300
H	3.51247700	-1.29022300	0.56507000
H	3.11483200	-2.55833100	1.74545300
C	1.87992500	-4.32059100	-0.09976400
H	1.71082400	-4.64478700	0.94019700
H	1.01329500	-4.63911700	-0.70188500
H	2.77767200	-4.83945400	-0.47509400
C	0.17511300	-1.14489100	-0.58563300
H	0.59465500	-0.96406200	-1.57787600
C	-1.01889100	-0.50102000	-0.23072200
C	-1.71030500	0.37315800	-1.26271700
H	-2.60624400	0.79243800	-0.79398200
C	-2.15983300	-0.44933500	-2.48963500
H	-2.81519000	-1.27847800	-2.18487000
H	-2.70565400	0.19474600	-3.19975000
H	-1.28912500	-0.87567600	-3.01483100
C	-0.79866800	1.54203300	-1.69159300
H	0.08532500	1.17155800	-2.23631500
H	-1.34415600	2.23486300	-2.35350700
H	-0.44582900	2.09640100	-0.80728400
H	1.87969800	-0.07131200	1.41454900

C	0.61606400	4.37265400	2.13510800
C	0.52215800	4.74078200	0.76838100
C	0.42916100	5.37938100	3.11420600
C	0.23897200	6.05971500	0.39954400
H	0.63433500	3.97965800	-0.00483900
C	0.14517200	6.69842600	2.74144400
H	0.52061800	5.11207600	4.16611900
C	0.04305300	7.04590000	1.38341500
H	0.15883500	6.31923400	-0.65861700
H	0.00488400	7.45866100	3.51297300
H	-0.18586900	8.07354500	1.09355100

IM18

C	1.34470900	0.95386200	1.92365900
C	1.08464700	2.26042900	2.38726400
H	1.74428800	0.19877600	2.60253500
H	1.07678300	3.07863300	1.66232100
C	1.48925700	2.66270600	3.80290600
H	1.30409900	1.81441800	4.47837700
C	3.03066500	2.86274500	3.86257300
C	3.82916700	1.54103900	3.58940400
O	3.77072300	0.69163900	4.47628000
F	3.40351600	3.26639000	5.13235400
F	3.41400400	3.88998400	3.01392500
C	4.63368200	1.33414400	2.34837400
C	4.36715400	1.98009200	1.11943300
C	5.66780400	0.37132900	2.40904100
C	5.11563400	1.65735100	-0.02017100
H	3.55643900	2.69880700	1.04400800
C	6.42822300	0.07028000	1.27499600
H	5.85731600	-0.13348500	3.35650200
C	6.14959500	0.70942300	0.05428100
H	4.89051600	2.14833100	-0.96905000
H	7.23055300	-0.66754200	1.33767200
H	6.73451900	0.46767800	-0.83575100
Pd	-0.76808900	1.09230600	2.14120400
P	-2.95834300	1.87761100	2.18408700
C	-3.66934300	2.43058800	3.89360500
C	-2.44200100	2.95331600	4.67381400
H	-1.99964800	3.84151100	4.20514600
H	-2.75564700	3.22619600	5.69722900
H	-1.65724200	2.18755600	4.73499200
C	-4.74655500	3.53533100	3.91476200
H	-4.39226100	4.47213100	3.46442100

H	-5.66756600	3.22515500	3.41101000
H	-4.98691600	3.75319800	4.97158400
C	-4.21752400	1.19353600	4.63368500
H	-5.08794500	0.75692500	4.12434300
H	-3.44600000	0.42116800	4.75005500
H	-4.53074500	1.50282000	5.64697400
C	-3.12867800	3.32557000	0.93479700
C	-2.44556000	2.84000300	-0.35974700
H	-2.41764400	3.67017300	-1.08864200
H	-1.41560400	2.50929700	-0.16029100
H	-3.00070000	2.00731200	-0.81398000
C	-2.28600300	4.49144300	1.49850800
H	-2.18773100	5.26872600	0.71894000
H	-2.74037600	4.96069700	2.38134400
H	-1.28177300	4.14452800	1.77955100
C	-4.54208800	3.81552900	0.56178500
H	-5.12227900	4.15185300	1.42811200
H	-4.43571200	4.66842300	-0.13409500
H	-5.11304100	3.02934600	0.04769800
C	-3.99020200	0.45114100	1.54258300
C	-5.41308800	0.46345900	1.47184000
O	-6.03126600	1.62008600	1.86987500
C	-7.44065200	1.73936000	1.69136000
H	-7.98971700	1.00930900	2.31284900
H	-7.69499100	2.75818200	2.01181500
H	-7.72272100	1.60142900	0.63232800
C	-6.12771900	-0.66235400	1.04170600
H	-7.21478100	-0.64562500	0.97880500
C	-5.44776700	-1.84224800	0.71271100
H	-6.02372200	-2.71427500	0.40672000
C	-4.05124400	-1.89137200	0.79848500
O	-3.31727500	-3.02746600	0.54540600
C	-4.02727100	-4.20907300	0.17524400
H	-4.72592600	-4.52333300	0.97145200
H	-4.58952400	-4.06472500	-0.76500800
H	-3.25992300	-4.98071300	0.03083300
C	-3.30378000	-0.73843800	1.17999600
C	-1.80075300	-0.93682400	1.17433000
C	-1.15209000	-1.47467300	2.33726300
C	-1.89517900	-1.64220300	3.65951000
H	-2.84834700	-1.10615400	3.57731000
C	-2.22259400	-3.13289200	3.90124100
H	-1.29673500	-3.71867200	4.02835900
H	-2.83035500	-3.24798600	4.81510900

H	-2.77820500	-3.55390300	3.04946400
C	-1.11823500	-1.05030300	4.85058800
H	-0.91212000	0.01807400	4.67887800
H	-1.70181700	-1.15706400	5.78083000
H	-0.15419100	-1.56516100	4.99571300
C	0.13009000	-2.05320200	2.21342800
H	0.59849500	-2.46646800	3.10786300
C	0.78906200	-2.15145300	0.98411600
C	2.15278000	-2.81921400	0.86054600
H	2.36373200	-2.94025900	-0.21663300
C	3.27275500	-1.93993500	1.46096000
H	4.25293000	-2.43088400	1.33969700
H	3.31509200	-0.95686800	0.97158800
H	3.10512300	-1.77614600	2.53743500
C	2.16855100	-4.22176100	1.50567100
H	2.01160000	-4.15502200	2.59477500
H	1.37645800	-4.86304700	1.08562500
H	3.14263000	-4.71108400	1.33693100
C	0.15311100	-1.60621400	-0.14416100
H	0.65639400	-1.67481900	-1.11172500
C	-1.11487700	-1.01263000	-0.08514500
C	-1.75578600	-0.53593000	-1.38486600
H	-2.67441200	0.01032800	-1.13303100
C	-2.15563700	-1.72762700	-2.28487300
H	-2.85215000	-2.40108000	-1.76774800
H	-2.63347800	-1.36290200	-3.21056400
H	-1.26315700	-2.31067700	-2.56755900
C	-0.82728900	0.41400800	-2.17360800
H	0.03370800	-0.13652000	-2.58748100
H	-1.37379300	0.86483100	-3.01886700
H	-0.43920200	1.22051400	-1.53600600
H	1.52565300	0.75758200	0.86203100
C	0.80404500	3.89863100	4.36198000
C	0.55610500	5.03193800	3.56688800
C	0.45844200	3.94089400	5.72516600
C	-0.06676300	6.16530000	4.11152900
H	0.84238600	5.03001300	2.51573300
C	-0.15715300	5.07308100	6.27668100
H	0.66485000	3.07012700	6.35105600
C	-0.42972000	6.18829100	5.46764200
H	-0.26638000	7.03039400	3.47511700
H	-0.42910300	5.08260200	7.33454800
H	-0.91676600	7.06940200	5.89149900

IM19

C	1.70562900	0.12144300	0.29615100
C	1.72793400	-1.28239800	0.07875000
H	2.12752400	-1.65636800	-0.87115100
C	1.86793400	-2.23373700	1.23751600
O	3.30631300	-2.39867600	1.58904300
C	3.81430500	-1.52310100	2.49063300
O	3.16605300	-0.73206500	3.15860400
C	5.33704700	-1.63878300	2.58084900
C	6.00250400	-0.27249600	2.28678900
O	6.57744700	0.33215500	3.18872900
C	5.91904200	0.27042400	0.89398400
C	5.33737800	-0.45394700	-0.17019900
C	6.45065900	1.55653400	0.63957400
C	5.28702800	0.09731200	-1.45767800
H	4.91260900	-1.44096200	0.00171600
C	6.39984400	2.10234200	-0.64547400
H	6.89581500	2.10847600	1.46803000
C	5.81854600	1.37278600	-1.69849900
H	4.82225200	-0.46327800	-2.26947700
H	6.80543400	3.09916100	-0.83059300
H	5.76461900	1.80508500	-2.69848400
H	1.71463600	0.46667300	1.33238000
C	2.10926900	1.12059900	-0.70703300
C	1.96784100	0.89428900	-2.09815400
C	2.65332700	2.35468100	-0.28834400
C	2.34628600	1.86768600	-3.02830700
H	1.51818700	-0.04046100	-2.43550000
C	3.03951300	3.32846900	-1.21902300
H	2.79443000	2.53372300	0.77899800
C	2.88242800	3.09558800	-2.59499900
H	2.21439500	1.67451300	-4.09591300
H	3.46052800	4.27275100	-0.86654400
H	3.17381900	3.85779200	-3.32124400
H	1.33478800	-1.87717300	2.12575300
H	1.54285900	-3.24976200	0.98538800
Pd	-0.31530900	-0.71547900	-0.15265400
P	-1.76659100	-2.39986400	-0.61127200
C	-3.47301900	-1.74391900	-0.39903200
C	-4.61147900	-2.56875500	-0.30767000
C	-5.88675300	-2.00583400	-0.16466300
H	-6.76526200	-2.65040100	-0.09230800
C	-6.02537400	-0.60859300	-0.11490900
H	-7.01475000	-0.15951100	-0.00515600

C	-4.89274100	0.21431800	-0.19367400
C	-3.60107100	-0.33704800	-0.32627300
C	-2.43858500	0.62669600	-0.35896700
C	-2.08223500	1.26883000	-1.58991900
C	-2.47856000	0.66956700	-2.93418800
H	-3.11871900	-0.20510200	-2.75103600
C	-3.28150400	1.66187500	-3.79958500
H	-2.68094100	2.55460800	-4.04014500
H	-3.57866000	1.18680200	-4.74975100
H	-4.19320300	1.99492800	-3.27672300
C	-1.22290800	0.16910900	-3.67886100
H	-0.67801300	-0.55603300	-3.05571300
H	-1.50510100	-0.32015400	-4.62589900
H	-0.54356300	1.00770600	-3.90120900
C	-1.31872200	2.43890000	-1.54870700
H	-1.04404100	2.92118000	-2.48906200
C	-0.89977300	3.02870800	-0.33855500
C	-0.20942000	4.38762300	-0.38683000
H	0.57574800	4.32394800	-1.15793900
C	-1.22130100	5.46997600	-0.83471000
H	-0.72232000	6.44922300	-0.93356000
H	-1.67812000	5.21400500	-1.80409700
H	-2.03173700	5.56870300	-0.09228700
C	0.45443400	4.80730900	0.93425300
H	1.15246900	4.03760000	1.29517900
H	1.01418700	5.74591500	0.79198100
H	-0.30097100	4.98331500	1.71901400
C	-1.17803400	2.34766800	0.85097300
H	-0.83194800	2.75400800	1.80087900
C	-1.93080300	1.15059400	0.87272700
C	-2.32113700	0.53733900	2.21742100
H	-2.80839100	-0.42913600	2.02318100
C	-3.34317000	1.44003500	2.94225800
H	-2.90421900	2.42803200	3.15961900
H	-4.24225400	1.59147000	2.32360700
H	-3.65174700	0.98251500	3.89736300
C	-1.09632400	0.26303500	3.11242700
H	-0.55427800	1.19078600	3.35637900
H	-1.41641100	-0.20104800	4.06073200
H	-0.39189200	-0.41376400	2.60333000
H	-4.99977900	1.29948700	-0.14392800
H	-4.49109300	-3.65341400	-0.34437400
C	-1.73960800	-3.07988600	-2.32367300
C	-0.52988500	-3.65292100	-2.77676100

C	-2.82222300	-2.96831400	-3.21785300
C	-0.41054400	-4.10921400	-4.09572100
H	0.31927300	-3.73534000	-2.09409700
C	-2.69447300	-3.41222400	-4.54458500
H	-3.76201500	-2.52948900	-2.88168500
C	-1.49150000	-3.98295700	-4.98678900
H	0.52816100	-4.55480900	-4.43228200
H	-3.53889500	-3.31270700	-5.23027300
H	-1.39368800	-4.32679500	-6.01860800
C	-1.72392300	-3.89656100	0.46268100
C	-1.31747100	-3.71497800	1.80184900
C	-2.07535800	-5.18599200	0.01437100
C	-1.27840700	-4.80399800	2.68411700
H	-1.01877500	-2.71937000	2.13772700
C	-2.02493100	-6.27667700	0.89746100
H	-2.37649900	-5.33677500	-1.02390100
C	-1.63054200	-6.08739500	2.23220200
H	-0.96139600	-4.65388900	3.71846900
H	-2.29353800	-7.27407000	0.54213800
H	-1.59008400	-6.93797400	2.91595400
H	5.60246600	-1.90496100	3.61286300
H	5.71157400	-2.41015200	1.89298200

TS19

C	1.77001800	0.14783600	0.04667800
C	1.82985800	-1.18631100	-0.41987200
H	2.14980300	-1.39995100	-1.44282900
C	1.48181200	-2.26062900	0.44284700
O	3.47933400	-2.78695000	1.24638800
C	3.69264000	-1.96172700	2.21021700
O	2.85855400	-1.33607300	2.89844400
C	5.21719100	-1.71727300	2.52827000
C	5.57596400	-0.24386800	2.36078400
O	5.77978400	0.47744100	3.33962600
C	5.67142300	0.31188100	0.96267600
C	5.29989100	-0.43418300	-0.17770100
C	6.14780200	1.63144900	0.79245400
C	5.39372700	0.13669900	-1.45561700
H	4.90908900	-1.44443300	-0.06388400
C	6.25819100	2.19030700	-0.48435000
H	6.42661800	2.19921700	1.68116300
C	5.87660700	1.44444600	-1.61376300
H	5.08780200	-0.44131100	-2.33031200
H	6.62931500	3.21070600	-0.60376600

H	5.94360900	1.88661600	-2.60966700
H	1.77867500	0.28643900	1.13049500
C	2.15065800	1.30631700	-0.76202200
C	2.00855100	1.32569500	-2.17022300
C	2.70357800	2.43977500	-0.12650400
C	2.42281800	2.43432000	-2.91491900
H	1.54484200	0.47497200	-2.66976200
C	3.13230100	3.54385500	-0.87330800
H	2.83128400	2.42773700	0.95699000
C	2.99071300	3.54975100	-2.27000200
H	2.29935600	2.43440700	-4.00059200
H	3.57127100	4.40265100	-0.36232100
H	3.31636900	4.41424500	-2.85256100
H	1.25633700	-2.08579700	1.49110800
H	1.37211600	-3.26934400	0.05240100
Pd	-0.30742700	-0.82437400	-0.25883900
P	-1.83582700	-2.49053100	-0.57110900
C	-3.48648800	-1.74188800	-0.30888600
C	-4.67115200	-2.49266400	-0.17680000
C	-5.90013600	-1.84286600	-0.00126900
H	-6.81724400	-2.42579200	0.10342400
C	-5.94369700	-0.43882300	0.04152600
H	-6.89758500	0.07486100	0.17713600
C	-4.76262900	0.30803500	-0.07556700
C	-3.51685700	-0.33155300	-0.24124600
C	-2.29253600	0.55430900	-0.32006800
C	-1.95125300	1.16396100	-1.57761100
C	-2.37701000	0.52657500	-2.89468500
H	-2.95842200	-0.37831300	-2.67036100
C	-3.27791400	1.46632800	-3.72126600
H	-2.73929200	2.38723600	-3.99896700
H	-3.60069200	0.96673800	-4.64995900
H	-4.17562300	1.75406600	-3.15014100
C	-1.14186400	0.08079500	-3.70489900
H	-0.52071000	-0.60458100	-3.10628400
H	-1.45468200	-0.44160300	-4.62381300
H	-0.52470400	0.94882800	-3.98826900
C	-1.21642000	2.35178200	-1.57618100
H	-0.96812600	2.81880200	-2.53108300
C	-0.80843000	2.98833900	-0.38489400
C	-0.18416200	4.37570300	-0.47422900
H	0.62437000	4.32099700	-1.22052800
C	-1.23679100	5.38390800	-0.99764300
H	-0.78325500	6.38166500	-1.12210100

H	-1.64915200	5.06715400	-1.96883900
H	-2.07370100	5.47134400	-0.28393300
C	0.41504700	4.88855000	0.84471900
H	1.14570800	4.17950600	1.26017800
H	0.92533600	5.85006200	0.67436300
H	-0.37328500	5.05531100	1.59844200
C	-1.04246600	2.32594900	0.82654500
H	-0.68582200	2.76166700	1.75926400
C	-1.77326900	1.12087500	0.89160900
C	-2.10159200	0.51055600	2.25247700
H	-2.60507400	-0.45216900	2.08178500
C	-3.07682800	1.41799900	3.03297200
H	-2.62228800	2.40357400	3.22645500
H	-4.00913700	1.57277100	2.46644000
H	-3.33139800	0.96027100	4.00329000
C	-0.82772200	0.22919000	3.07403300
H	-0.26438000	1.15448400	3.27423400
H	-1.09403600	-0.22098900	4.04473400
H	-0.15663300	-0.46188600	2.54089800
H	-4.79521300	1.39798900	-0.03003900
H	-4.62443400	-3.58306600	-0.20507400
C	-1.85502800	-3.16776900	-2.27890300
C	-0.64838700	-3.71144800	-2.77297900
C	-2.97744800	-3.09319700	-3.12640400
C	-0.57171900	-4.18098200	-4.09023000
H	0.23083600	-3.75837100	-2.12653800
C	-2.89208600	-3.55184400	-4.45146200
H	-3.91325900	-2.67287200	-2.75665500
C	-1.69268400	-4.09613800	-4.93528500
H	0.36430200	-4.60379400	-4.46081100
H	-3.76600000	-3.48417900	-5.10282900
H	-1.62849800	-4.45109700	-5.96578200
C	-1.77263500	-3.95781100	0.52767900
C	-1.27639400	-3.77484200	1.83575300
C	-2.20059200	-5.23606900	0.11464500
C	-1.22211300	-4.85685300	2.72526100
H	-0.91783800	-2.79116800	2.14527300
C	-2.13854700	-6.31749300	1.00726800
H	-2.56840800	-5.38528800	-0.90213100
C	-1.65208300	-6.12903300	2.31142600
H	-0.82926000	-4.70947800	3.73303600
H	-2.46596600	-7.30731800	0.68217100
H	-1.59854100	-6.97380600	3.00111700
H	5.39496500	-1.98015000	3.58035100

H	5.83793300	-2.34541000	1.87304500
IM20			
Pd	0.15160000	0.17813300	-1.15481900
P	-0.14102100	-2.05334300	-1.43833700
C	-1.38978600	-2.49365900	-0.17667200
C	-1.66888300	-3.83313300	0.15978000
C	-2.71871400	-4.13896700	1.03542500
H	-2.92437700	-5.17757700	1.30081600
C	-3.50693400	-3.10132300	1.55695400
H	-4.34349100	-3.32775100	2.22094700
C	-3.21531900	-1.76746500	1.23868700
C	-2.13230100	-1.43360600	0.39984500
C	-1.87461300	0.04096000	0.15903800
C	-1.47593900	0.87135000	1.27842100
C	-0.83992100	0.29092600	2.53915400
H	-0.42938000	-0.69918500	2.30141900
C	-1.87168500	0.14589000	3.68323600
H	-2.66973400	-0.56952400	3.44170100
H	-2.33576300	1.12128200	3.91068600
H	-1.36095200	-0.21159800	4.59272800
C	0.32997400	1.15986400	3.05071600
H	0.85884600	0.60548300	3.83950700
H	-0.02665200	2.10903700	3.48523600
H	1.04470900	1.37551700	2.24940800
C	-1.70782800	2.24755900	1.20499100
H	-1.42143000	2.87190300	2.05136000
C	-2.31181600	2.87142200	0.09414800
C	-2.65612500	4.35281600	0.17832300
H	-1.74222400	4.88117300	0.49072900
C	-3.72440500	4.57914300	1.27620600
H	-3.39081200	4.18857200	2.25025900
H	-4.66527800	4.06929600	1.00758600
H	-3.93426500	5.65612800	1.38867700
C	-3.13536900	4.96779500	-1.14608300
H	-3.27154500	6.05447600	-1.02643200
H	-4.10428800	4.53788200	-1.45271600
H	-2.41009500	4.79874500	-1.95585100
C	-2.61958000	2.07695400	-1.01289500
H	-3.07788000	2.52756700	-1.89169200
C	-2.44243000	0.67601300	-1.00171900
C	-3.06836400	-0.12618100	-2.13810100
H	-2.75323600	-1.17056900	-2.05139800
C	-4.60749700	-0.11565000	-2.00287600

H	-5.00048500	0.91115400	-2.08311000
H	-4.91886700	-0.52913400	-1.03009000
H	-5.06212800	-0.72549900	-2.80159600
C	-2.63014700	0.38067900	-3.52467000
H	-2.97600500	-0.31310800	-4.30641200
H	-1.53261700	0.45151200	-3.57669800
H	-3.05302200	1.37605800	-3.73937600
C	0.17165900	5.69639800	-1.28620700
C	0.48776500	4.35736000	-1.53337000
C	1.06888100	3.55486400	-0.52003800
C	1.26941400	4.12411900	0.76270600
C	0.93676800	5.46088700	1.01115100
C	0.39619900	6.25610200	-0.01465900
H	-0.26437600	6.30554100	-2.08011500
H	0.29146000	3.92842800	-2.51725800
H	1.72430000	3.51192700	1.54226500
H	1.10990900	5.88663400	2.00161800
H	0.14407000	7.30148300	0.17488000
C	1.53167100	2.19218700	-0.74331300
C	1.69149000	1.57568700	-1.99331200
H	1.96915100	1.68594400	0.12109900
H	1.38691500	2.09545400	-2.90546600
C	2.08566300	0.20413900	-2.05922600
H	2.18503800	-0.26343100	-3.04115800
H	2.69804100	-0.22325300	-1.26269400
O	1.85986500	-0.63035300	0.98114100
C	2.27601400	-1.04430400	2.10845400
O	1.77803300	-1.91230700	2.85986800
C	3.61328200	-0.35513000	2.63040300
C	4.04762200	0.73660000	1.68290300
O	3.82638700	1.93042100	1.93263600
C	4.68809000	0.34200100	0.37669100
C	4.83872700	-1.00722500	-0.01342400
C	5.09239700	1.35760500	-0.51544000
C	5.36863300	-1.32991900	-1.26963400
H	4.50134300	-1.80825200	0.64139100
C	5.62723200	1.03682500	-1.76908900
H	4.96094900	2.39631600	-0.21030300
C	5.76288100	-0.30932900	-2.15179000
H	5.45420100	-2.37740700	-1.56411400
H	5.93265000	1.83340100	-2.45166700
H	6.17322700	-0.56132400	-3.13266500
H	-1.05469000	-4.63060000	-0.26139300
H	-3.82667700	-0.96378700	1.64955200

C	1.28182100	-3.18322200	-1.19667300
C	2.01540700	-3.67155400	-2.29804600
C	1.69104800	-3.49719000	0.11527900
C	3.15260600	-4.46562700	-2.08664700
H	1.69783800	-3.44507000	-3.31683900
C	2.82738600	-4.29380200	0.31629300
H	1.16223600	-3.09586900	0.97826300
C	3.56190700	-4.77759500	-0.77921900
H	3.71261800	-4.84475400	-2.94439500
H	3.13837000	-4.52166700	1.33752300
H	4.44717600	-5.39668500	-0.61659000
C	-0.83937600	-2.55063300	-3.07194000
C	-1.88489600	-3.48583400	-3.20490700
C	-0.30410100	-1.94727000	-4.22897600
C	-2.38293900	-3.81202000	-4.47544700
H	-2.32289300	-3.94458500	-2.31846800
C	-0.78708200	-2.29286200	-5.49942100
H	0.47808900	-1.19324100	-4.13063700
C	-1.83188700	-3.22259400	-5.62495200
H	-3.20135800	-4.52932000	-4.56561800
H	-0.36095900	-1.82138800	-6.38740100
H	-2.22006600	-3.48049200	-6.61237600
H	4.37712900	-1.14086500	2.74245800
H	3.41757600	0.08399700	3.61851500

IM21

Pd	-0.10260000	0.28558600	1.05619800
P	-0.44446500	-1.96018800	0.73957700
C	0.06822000	-2.67503400	-0.88460600
C	-0.69481600	-3.72460200	-1.44495400
C	-0.29783000	-4.35658600	-2.63006000
H	-0.90582600	-5.16341100	-3.04387100
C	0.88173000	-3.95090300	-3.27014200
H	1.20801100	-4.43819500	-4.19124800
C	1.64243900	-2.90988800	-2.72270100
C	1.25423400	-2.24909200	-1.53753700
C	2.15448100	-1.14280600	-1.06431100
C	1.95941500	0.17665700	-1.55398700
C	0.77617500	0.52619000	-2.45336500
H	-0.04687300	-0.16282600	-2.21242500
C	1.14958200	0.32648600	-3.94089900
H	1.98681200	0.99123700	-4.21518200
H	0.28692300	0.57715300	-4.58118300
H	1.44919600	-0.71058500	-4.15384100

C	0.24563000	1.95541900	-2.24825600
H	-0.66442000	2.08762300	-2.84525000
H	0.97421100	2.71176300	-2.58468300
H	-0.00708000	2.14350800	-1.19789800
C	2.92118700	1.15528900	-1.24614700
C	4.04226100	0.87811500	-0.44892600
C	5.06953400	1.95909200	-0.13458000
H	4.70869100	2.90392300	-0.57745200
C	6.43378300	1.62504600	-0.77728500
H	6.33677100	1.49680900	-1.86756600
H	6.83934600	0.68854400	-0.35941100
H	7.16227500	2.43011900	-0.58239000
C	5.22993800	2.17445900	1.38611600
H	4.27530600	2.45798600	1.85679200
H	5.96516000	2.97187800	1.58568100
H	5.58705200	1.25306700	1.87464700
C	4.19674800	-0.42621000	0.04418200
C	3.27931100	-1.44736800	-0.25677100
C	3.56466000	-2.86634100	0.23166200
H	2.66298400	-3.47335000	0.07644000
C	4.69829600	-3.49541800	-0.60841200
H	5.62954300	-2.91448900	-0.49998800
H	4.43315500	-3.51804800	-1.67762700
H	4.89594700	-4.52932600	-0.27735200
C	3.90422100	-2.92858500	1.73427000
H	4.83328900	-2.38057000	1.96202400
H	4.04995400	-3.97628500	2.04116100
H	-1.60726600	-4.05222500	-0.94733400
H	2.55982900	-2.58654500	-3.21632100
H	2.79263900	2.16883600	-1.62969800
H	5.06559300	-0.66075800	0.66144900
C	0.32322100	-3.08638700	1.98191400
C	0.79157600	-4.37205000	1.64798000
C	0.35883000	-2.66756200	3.32758400
C	1.31942300	-5.21093700	2.64107100
H	0.74716800	-4.71659600	0.61456400
C	0.87583400	-3.51219600	4.32084100
H	-0.03675000	-1.68739800	3.59394200
C	1.36728000	-4.78224200	3.97703700
H	1.69124200	-6.20103100	2.36908400
H	0.89623000	-3.17730400	5.35990700
H	1.78052600	-5.43646600	4.74744100
C	-2.23955800	-2.37376600	0.86351300
C	-2.76586000	-3.11395300	1.94178900

C	-3.11354100	-1.88210900	-0.13013300
C	-4.14696300	-3.35196600	2.02601400
H	-2.10661100	-3.50724100	2.71548000
C	-4.49073800	-2.12366800	-0.04121500
H	-2.72961600	-1.29620200	-0.96176000
C	-5.01161300	-2.85724600	1.03772300
H	-4.54256900	-3.92624300	2.86675600
H	-5.14274200	-1.71074000	-0.81083500
H	-6.08621100	-3.03990400	1.10883000
H	3.09176400	-2.50671400	2.34327700
C	0.30988700	2.36751900	2.02828900
C	1.47235300	1.59394800	1.84611500
H	-0.33890800	2.14102100	2.88007300
H	2.20142400	1.87649200	1.08802100
C	1.54922700	0.28438600	2.41102700
H	1.10730500	0.10480800	3.39727300
O	-2.86798000	1.35312700	1.89602900
C	-2.83996400	1.23597800	0.66081500
O	-1.84148300	0.84695800	-0.07281300
C	-4.13682000	1.56005600	-0.14488900
C	-4.01167800	1.35734100	-1.64919100
O	-4.47045900	0.34398400	-2.18893800
C	-3.32502900	2.41084400	-2.46998000
C	-3.22452400	2.21741500	-3.86617500
C	-2.76698300	3.57480500	-1.89995300
C	-2.58766600	3.16515500	-4.67436900
H	-3.65118500	1.31023200	-4.29528100
C	-2.13566500	4.52761300	-2.71084400
H	-2.79247000	3.73176500	-0.82265200
C	-2.04405500	4.32674700	-4.09704400
H	-2.51250400	3.00154400	-5.75174800
H	-1.69944100	5.41545100	-2.25264200
H	-1.54533900	5.06819800	-4.72556200
H	2.40953800	-0.33682700	2.16177300
C	0.00134500	3.62109700	1.33210600
C	0.88004600	4.22575900	0.40147700
C	-1.22555900	4.26676500	1.61892700
C	0.55467600	5.44812600	-0.19568200
H	1.82269600	3.73955200	0.14947400
C	-1.55050300	5.48931400	1.01819000
H	-1.92570200	3.77923900	2.29834400
C	-0.65651000	6.09157800	0.11614600
H	1.24831500	5.90320600	-0.90600900
H	-2.49983900	5.97446900	1.25539800

H	-0.90272900	7.05079800	-0.34430700
H	-4.92124600	0.88642500	0.22754900
H	-4.42877900	2.59296300	0.10071600

TS20

Pd	-2.02176400	0.31527200	1.04404300
C	-0.99190000	0.58694500	3.27730100
O	-0.88945500	-2.02892200	0.09994500
P	-2.20968000	0.45081600	-1.24232300
C	-1.17754400	1.75496500	2.52310000
C	-0.59321000	1.86987100	1.21867100
H	-0.80236200	2.76979300	0.63549300
H	0.37046400	1.39946000	1.01030200
H	-0.17940100	-0.08322600	2.98618300
H	-1.88877800	2.51334300	2.85570400
C	-3.05379700	-0.98457500	-2.03186600
C	-4.16283000	-1.56995000	-1.36288600
C	2.08985100	0.87162200	-2.96282700
C	1.29361400	2.01211100	-2.76161500
C	-0.02580300	1.88153800	-2.30181300
C	-0.55834100	0.60087900	-2.03457100
C	0.24317900	-0.54283700	-2.24267900
C	1.55860400	-0.40316200	-2.70886000
H	3.11682100	0.97781500	-3.31918100
H	1.69543400	3.00686000	-2.96734300
H	-0.63661400	2.77374500	-2.15607200
H	-0.12926000	-1.54379800	-2.03945900
H	2.14904300	-1.30835800	-2.85674000
C	-4.20434600	4.41037400	-2.63080000
C	-3.98966900	3.37765800	-3.56020400
C	-3.43551500	2.15929700	-3.14271100
C	-3.09873100	1.96542600	-1.78801100
C	-3.34427400	2.99022400	-0.85489200
C	-3.88774700	4.21411600	-1.27696800
H	-4.62878200	5.36064600	-2.96076500
H	-4.24830400	3.52403900	-4.61074700
H	-3.25642900	1.36174000	-3.86634100
H	-3.11251900	2.81481500	0.19665100
H	-4.07217100	5.00683000	-0.54885800
C	-2.60955500	-1.51961600	-3.25585700
H	-1.76086800	-1.07264100	-3.77136300
C	-4.77245200	-2.70261500	-1.92683100
H	-5.62006000	-3.15883700	-1.41580400
C	-3.23520900	-2.64733500	-3.80612400

H	-2.87104100	-3.06046500	-4.74812400
C	-4.30878900	-3.24700000	-3.13432900
H	-4.78981200	-4.13531200	-3.54827700
C	-4.67988500	-0.91000800	-0.12078800
C	-5.58553300	0.17215900	-0.24583700
C	-4.16618700	-1.28685500	1.16316200
C	-5.88787300	0.93153400	0.89880400
C	-4.46396100	-0.45375900	2.26896000
C	-5.30592500	0.66811100	2.14549800
H	-6.57174600	1.77529800	0.81006000
H	-4.07220800	-0.71340800	3.25229500
C	-3.55761400	-2.67297000	1.37408400
C	-4.71553000	-3.68849100	1.53619400
C	-2.61831200	-2.77959100	2.58630500
H	-2.98491100	-2.93652500	0.47690300
H	-5.39398300	-3.67553400	0.67050900
H	-4.30999200	-4.70853000	1.64274000
H	-5.30766100	-3.45479100	2.43759000
H	-1.83249700	-2.01551900	2.55311900
H	-3.16566900	-2.67361700	3.53659300
H	-2.13561100	-3.76932600	2.58502000
C	-6.27473600	0.46545400	-1.57942100
C	-6.76442200	1.91599500	-1.73675300
C	-7.47078000	-0.49904300	-1.76456400
H	-5.55182900	0.26659700	-2.38492100
H	-5.97133500	2.63956100	-1.51103700
H	-7.10125600	2.07964200	-2.77254300
H	-7.62308500	2.11972300	-1.07477900
H	-7.15250800	-1.55087300	-1.74244600
H	-8.20959100	-0.34532300	-0.95974900
H	-7.96866200	-0.30813500	-2.73039600
C	-5.59784300	1.56349200	3.34032300
C	-7.10638500	1.61558400	3.66296600
C	-5.04803900	2.98650500	3.10178100
H	-5.07817600	1.13623100	4.21145600
H	-7.50408800	0.60640500	3.85671200
H	-7.28681600	2.23935300	4.55450100
H	-7.67370800	2.05137700	2.82408900
H	-3.97128700	2.95862600	2.87302500
H	-5.56038600	3.46285200	2.24942700
H	-5.20302000	3.61972900	3.99167000
C	0.00850700	-2.73744700	0.61622100
C	0.97576000	-2.08651700	1.56609400
C	1.55873200	-0.85563000	1.20505000

C	1.27187600	-2.64854100	2.82243100
C	2.42412900	-0.19564400	2.08759800
H	1.33161300	-0.44106200	0.22308500
C	2.10933700	-1.96889900	3.72245500
H	0.83161900	-3.60907800	3.09693800
C	2.68815800	-0.74258200	3.35625200
H	2.89143200	0.74591800	1.79005600
H	2.31730800	-2.40031200	4.70416600
H	3.35003500	-0.22110600	4.05092500
C	-1.65653400	0.26072300	4.53489600
C	-1.33138300	-0.96493600	5.16750700
C	-2.61104800	1.10550500	5.15387400
C	-1.95026100	-1.34204400	6.36498800
H	-0.58972100	-1.61469600	4.70029400
C	-3.22493500	0.72837200	6.35261500
H	-2.87422900	2.05826400	4.69499800
C	-2.90345000	-0.49913200	6.96108400
H	-1.68930600	-2.29294300	6.83380700
H	-3.95847500	1.39216800	6.81497100
H	-3.38866400	-0.79117700	7.89448500
O	0.83690500	-3.67659800	-2.16222600
C	1.39883400	-3.96798500	-1.08922000
O	2.56548800	-4.17415900	-0.73063700
C	0.25776900	-4.11758000	0.21552700
H	-0.63304300	-4.60028600	-0.20405400
H	0.75966400	-4.72053600	0.98018800

IM22

Pd	-0.15285300	0.27353100	1.05213700
P	-0.47300400	-1.95845400	0.61610300
C	0.21128900	-2.82387500	-0.86551600
C	-0.48712500	-3.94633700	-1.36801800
C	0.01742800	-4.69241000	-2.44002500
H	-0.53803900	-5.55698000	-2.80854200
C	1.23636100	-4.32315100	-3.02819700
H	1.64365500	-4.89595200	-3.86382100
C	1.93118700	-3.20968400	-2.53991800
C	1.43789000	-2.44270600	-1.46193800
C	2.27484400	-1.27801800	-1.02295300
C	2.03024800	0.01111600	-1.56634200
C	0.85003100	0.26107500	-2.50504300
H	0.05227700	-0.44753000	-2.23439900
C	1.26266100	-0.03021600	-3.96642000
H	2.07925700	0.64530600	-4.27298300

H	0.40794900	0.13190300	-4.64510200
H	1.60867900	-1.06757300	-4.08815300
C	0.26087700	1.67984700	-2.39761400
H	-0.65468100	1.74051500	-3.00832700
H	0.96223600	2.43875300	-2.78216100
H	-0.00091100	1.93192700	-1.36291000
C	2.94375300	1.04050500	-1.28299700
C	4.06488100	0.83914900	-0.46104600
C	5.04304500	1.97384100	-0.18080100
H	4.64254000	2.88634600	-0.65589100
C	6.42151200	1.67545000	-0.81101700
H	6.33296700	1.50678200	-1.89659800
H	6.86427200	0.77133200	-0.36093400
H	7.11502300	2.51638700	-0.64234000
C	5.19071100	2.24887900	1.33138200
H	4.22434300	2.50887900	1.79092800
H	5.89108800	3.08336300	1.50163600
H	5.58609600	1.36221600	1.85341400
C	4.26238500	-0.43576300	0.09086400
C	3.38817900	-1.50403700	-0.17671100
C	3.68911100	-2.87997200	0.41901200
H	2.83468900	-3.54145800	0.21849000
C	4.92806100	-3.49663800	-0.26675600
H	5.81899300	-2.86956400	-0.09648800
H	4.77563200	-3.58337200	-1.35474500
H	5.13244800	-4.50235400	0.13778200
C	3.87816100	-2.83813800	1.95009100
H	4.71598700	-2.18079900	2.23457400
H	4.10053500	-3.84988100	2.32635200
H	-1.43204200	-4.24212100	-0.91120900
H	2.87802700	-2.91425500	-2.99452800
H	2.78116800	2.03326800	-1.70674200
H	5.12390100	-0.60670500	0.73921900
C	0.03452300	-3.00066800	2.04033600
C	0.65828600	-4.25459900	1.89553400
C	-0.22505400	-2.48729900	3.33040200
C	1.03971400	-4.98280000	3.03372200
H	0.85265100	-4.65846300	0.90180000
C	0.14649200	-3.22780700	4.46182300
H	-0.72222500	-1.51972800	3.43909900
C	0.78753100	-4.47045400	4.31601500
H	1.53499300	-5.94887500	2.91537400
H	-0.05962300	-2.82848600	5.45698300
H	1.08815000	-5.03742700	5.19963100

C	-2.28383500	-2.24707500	0.43303100
C	-3.04312100	-2.96003900	1.37969200
C	-2.93019800	-1.62980400	-0.65963300
C	-4.43851600	-3.04198000	1.24078700
H	-2.55120800	-3.43357700	2.22969400
C	-4.32020400	-1.71944600	-0.79641300
H	-2.34729400	-1.05629100	-1.38106300
C	-5.07873500	-2.42086500	0.15778100
H	-5.02259800	-3.58905500	1.98363800
H	-4.81411100	-1.23140600	-1.63911500
H	-6.16443400	-2.47877400	0.05733000
H	2.96809300	-2.48449900	2.45600700
C	0.37601500	2.33357400	2.09905300
C	1.49516400	1.52874300	1.81984700
H	-0.21736200	2.09624100	2.98689700
H	2.19875700	1.81221800	1.03904800
C	1.54678000	0.19295900	2.32529500
H	1.10964700	-0.03820600	3.30210500
O	-3.26515100	2.33012600	3.73352500
C	-2.74883000	1.29996000	3.25378300
O	-1.78890300	0.58980800	3.65477200
C	-3.43670100	0.75742300	1.86189800
C	-2.94609300	1.51266100	0.68818800
O	-1.88483300	1.18106400	0.07836000
C	-3.65498600	2.72853400	0.20979600
C	-3.32391500	3.28082300	-1.04919100
C	-4.60457900	3.38419500	1.02621900
C	-3.94716600	4.45059100	-1.49331300
H	-2.56594100	2.78863000	-1.65799800
C	-5.20862700	4.56928500	0.58512400
H	-4.80185100	3.00554600	2.02851600
C	-4.89223900	5.09862300	-0.67714600
H	-3.69021200	4.86692700	-2.46972500
H	-5.92583700	5.08178800	1.22977600
H	-5.37422900	6.01643200	-1.02178500
H	2.37721400	-0.43645500	2.01044200
C	0.00751900	3.55832600	1.38860100
C	0.70138400	4.02349400	0.24455000
C	-1.13064700	4.27443400	1.83220300
C	0.27199500	5.17158300	-0.42740400
H	1.56468100	3.47183200	-0.12847000
C	-1.55722900	5.42330500	1.15568600
H	-1.69403700	3.89881900	2.68846200
C	-0.86046100	5.87525200	0.02409200

H	0.81284500	5.51530600	-1.31211100
H	-2.45045900	5.94825200	1.49682700
H	-1.20145400	6.76404000	-0.51104300
H	-3.15407500	-0.29198900	1.75950400
H	-4.52261000	0.85792500	1.97525400
TS21			
Pd	-0.00648100	0.30851400	1.37559700
P	-0.55085500	-1.85430300	0.83963900
C	-0.04382500	-2.46584300	-0.82722900
C	-0.80548700	-3.49466900	-1.42950800
C	-0.41736500	-4.06605700	-2.64697700
H	-1.02130500	-4.85939600	-3.09159100
C	0.75201200	-3.61855200	-3.27922300
H	1.07416500	-4.06028000	-4.22440800
C	1.50932700	-2.59858600	-2.69097100
C	1.12766000	-1.99681700	-1.47124700
C	2.04146700	-0.92929100	-0.94105500
C	1.88299400	0.41837900	-1.36716700
C	0.70693300	0.84768100	-2.24679700
H	-0.14704900	0.19781600	-2.00155800
C	1.05377000	0.65485200	-3.74255700
H	1.92278700	1.27934500	-4.01148600
H	0.20182800	0.96599400	-4.37102900
H	1.29388600	-0.39066500	-3.98320200
C	0.26202200	2.30527700	-2.01725200
H	-0.66228600	2.49712000	-2.58425500
H	1.02150600	3.01682300	-2.37893000
H	0.05676900	2.50436400	-0.96099900
C	2.88067400	1.34752300	-1.02491000
C	4.00635700	0.99273200	-0.26466200
C	5.08550800	2.02200900	0.05115200
H	4.72051300	3.00367800	-0.29708100
C	6.38451400	1.69664100	-0.71983200
H	6.19942600	1.64942500	-1.80518400
H	6.78661300	0.72098100	-0.39965200
H	7.15319300	2.46419100	-0.52798800
C	5.37537700	2.12939000	1.56346800
H	4.47174800	2.39750600	2.13330200
H	6.14206600	2.89909500	1.75184200
H	5.75328900	1.17248800	1.95913200
C	4.11798800	-0.33522100	0.17682300
C	3.16007600	-1.30876000	-0.15553200
C	3.40919700	-2.76427400	0.24402000
H	2.50510900	-3.34731400	0.02247500

C	4.55596100	-3.34808000	-0.61158100
H	5.49637800	-2.80255800	-0.42684400
H	4.32415400	-3.27201800	-1.68613600
H	4.71935800	-4.41091200	-0.36461100
C	3.70392100	-2.94679200	1.74626900
H	4.57215400	-2.34819200	2.06665500
H	3.92997900	-4.00489200	1.95541500
H	-1.70856500	-3.85378300	-0.93633100
H	2.42247000	-2.24985900	-3.17486300
H	2.77717500	2.38317300	-1.34711400
H	4.98668200	-0.63010100	0.76818000
C	0.07134100	-3.13615200	2.00862700
C	0.52425300	-4.40137400	1.58652000
C	0.07755300	-2.82326400	3.38371100
C	0.99437100	-5.33123800	2.52660800
H	0.52056200	-4.65700600	0.52725100
C	0.53232700	-3.76026100	4.32260600
H	-0.27352700	-1.84433700	3.71087200
C	1.00065900	-5.01348900	3.89388200
H	1.35660500	-6.30413100	2.18796800
H	0.52960200	-3.50793600	5.38488400
H	1.36976500	-5.73801200	4.62255600
C	-2.37707500	-2.08796400	0.82279700
C	-3.06105100	-2.70321000	1.88782800
C	-3.11086000	-1.52890500	-0.24468200
C	-4.46413100	-2.74817500	1.88889100
H	-2.50413300	-3.14537200	2.71499900
C	-4.50973000	-1.57644500	-0.23941900
H	-2.58919100	-1.03295200	-1.06194300
C	-5.19050200	-2.18309200	0.82942600
H	-4.98695100	-3.22724600	2.71947100
H	-5.06582700	-1.12123700	-1.06080000
H	-6.28209300	-2.21228800	0.83670500
H	2.83562900	-2.66496900	2.35811200
C	0.64957600	2.32671800	2.31484700
C	1.68532600	1.37016000	2.28562500
H	-0.10207600	2.28099000	3.10894800
H	2.49751700	1.49738800	1.57257600
C	1.51527300	0.08923500	2.88177700
H	0.94410200	-0.00593700	3.81192500
O	-3.57008200	3.54166600	3.30011500
C	-2.87067500	2.64727100	3.67977300
O	-2.13455200	2.09509300	4.44942300
C	-3.14804500	0.93457400	2.07150900

C	-2.78163500	1.33736200	0.78940700
O	-1.60108000	1.15373300	0.25393200
C	-3.76785500	2.01290800	-0.11572300
C	-3.54945900	2.00423900	-1.51195700
C	-4.92533600	2.65148200	0.38141600
C	-4.46926700	2.59902700	-2.38615700
H	-2.65016500	1.52557500	-1.89724300
C	-5.83950500	3.25500900	-0.49324600
H	-5.08977800	2.70093700	1.45654500
C	-5.61967300	3.22768000	-1.88097800
H	-4.28607500	2.57586500	-3.46333200
H	-6.72365900	3.75362800	-0.08894600
H	-6.33476100	3.69688200	-2.56075200
H	2.29146200	-0.65839100	2.72347100
C	0.62427700	3.51407200	1.44930600
C	1.78925200	4.02609500	0.83041900
C	-0.61671800	4.13304800	1.17307000
C	1.70950100	5.11065300	-0.05070800
H	2.75869100	3.57789600	1.04869800
C	-0.69580800	5.20830400	0.28032500
H	-1.52334500	3.74155000	1.63137200
C	0.46568800	5.69937500	-0.33911700
H	2.61960200	5.49792000	-0.51501300
H	-1.66800600	5.65469800	0.06238300
H	0.40444500	6.53791800	-1.03608800
H	-2.47235200	0.26902200	2.60641500
H	-4.20561800	0.86870700	2.32679800

IM23

Pd	0.75496400	-0.55199800	0.44686000
P	0.32113000	1.64006800	0.93913600
C	-1.24684400	2.35893700	0.28066200
C	-1.29218400	3.74224000	-0.00761500
C	-2.48074200	4.35819300	-0.41761000
H	-2.49130100	5.42808600	-0.63468100
C	-3.64993600	3.59306700	-0.53822400
H	-4.58698900	4.05926300	-0.84961500
C	-3.61147700	2.22131600	-0.25897700
C	-2.42061900	1.57685200	0.14172300
C	-2.51623600	0.10312300	0.41645500
C	-2.35775300	-0.82478600	-0.64923200
C	-1.95700100	-0.36815700	-2.05206800
H	-1.34533200	0.54033700	-1.94840200
C	-3.21702800	-0.01862700	-2.87898100

H	-2.92652600	0.31771200	-3.88883400
H	-3.81147400	0.77827100	-2.40870900
H	-3.85821700	-0.91046100	-2.98502000
C	-1.11168300	-1.40032300	-2.82235600
H	-0.77288400	-0.94659800	-3.76679200
H	-1.69992800	-2.29624300	-3.07916600
H	-0.22698800	-1.70054700	-2.25031200
C	-2.65642200	-2.17725700	-0.40780500
C	-3.07743800	-2.63782000	0.84979200
C	-3.42174200	-4.10707200	1.06572300
H	-3.16650800	-4.64832700	0.13811500
C	-4.93691500	-4.27919700	1.31434800
H	-5.52451000	-3.86593600	0.47858200
H	-5.23834200	-3.75294100	2.23544900
H	-5.19315600	-5.34600600	1.42954700
C	-2.61516300	-4.73571100	2.22231500
H	-1.53017800	-4.65820700	2.04924600
H	-2.87240600	-5.80239100	2.33243200
H	-2.84189200	-4.23340900	3.17706200
C	-3.18781600	-1.70683900	1.89469000
C	-2.92403300	-0.33999800	1.70021200
C	-3.17967100	0.63819400	2.84712400
H	-2.77694500	1.62003500	2.56344300
C	-4.70064700	0.80521000	3.06208600
H	-5.15934000	-0.15425200	3.35435300
H	-5.19465800	1.15165600	2.14009400
H	-4.89905800	1.53998600	3.86090000
C	-2.48781500	0.23130200	4.16338800
H	-2.82360200	-0.76000300	4.50966400
H	-2.73053500	0.96105000	4.95250100
H	-0.38761200	4.34161800	0.09463200
H	-4.51782900	1.62144800	-0.35121900
H	-2.54904500	-2.89968900	-1.21745400
H	-3.51541800	-2.04665600	2.87882900
C	0.28652000	2.06403300	2.73392600
C	-0.59882500	3.01492600	3.27742300
C	1.20953400	1.41720700	3.58122900
C	-0.57652300	3.29464100	4.65241900
H	-1.30976700	3.52956200	2.63144200
C	1.24149600	1.71011500	4.95222600
H	1.89988200	0.68729100	3.15772500
C	0.34039600	2.64303100	5.49206000
H	-1.27714100	4.02301100	5.06598700
H	1.96258100	1.20500400	5.59822900

H	0.35381700	2.86079800	6.56194900
C	1.61875500	2.74831100	0.24299000
C	2.59119700	3.36444500	1.05358800
C	1.67078500	2.91818800	-1.15701500
C	3.60941600	4.13436700	0.46905300
H	2.55721300	3.24773100	2.13739700
C	2.68570500	3.69080700	-1.73390900
H	0.94251700	2.41791700	-1.79246300
C	3.65951300	4.29850300	-0.92345400
H	4.35998300	4.60760900	1.10604900
H	2.72564000	3.80025400	-2.81887200
H	4.45425700	4.89529600	-1.37649800
H	-1.39475400	0.21297200	4.04962100
C	1.42920600	-2.76164100	0.39561100
C	0.36389000	-2.53385500	1.29248600
H	2.45576400	-2.52945700	0.69955700
H	-0.62845400	-2.88445400	1.01549600
C	0.45963800	-1.56806700	2.33299400
H	1.40644300	-1.42888100	2.86584800
C	3.73405800	-0.00518900	-0.74086100
C	2.75061500	0.04538300	-1.69250100
O	1.44261700	-0.08401300	-1.49194000
C	3.11148900	0.23676300	-3.13711000
C	2.33092000	-0.37266200	-4.14409500
C	4.21154100	1.03194500	-3.52749000
C	2.65616200	-0.21259200	-5.49895000
H	1.47900300	-0.98084400	-3.84563300
C	4.53392900	1.19627700	-4.88253300
H	4.79688200	1.53633200	-2.75752100
C	3.75873800	0.57275800	-5.87570700
H	2.04611500	-0.70114900	-6.26334100
H	5.38601700	1.82000200	-5.16489400
H	4.00775900	0.70405500	-6.93153200
H	-0.44200000	-1.33740400	2.89952900
C	1.27458200	-3.48868200	-0.87285500
C	0.18696900	-4.35949000	-1.12086400
C	2.21255100	-3.26362200	-1.90717500
C	0.03577500	-4.97273200	-2.37027400
H	-0.53462300	-4.56399800	-0.32859600
C	2.05283900	-3.87134200	-3.15881500
H	3.03874600	-2.57288300	-1.72874500
C	0.96227000	-4.72460200	-3.39838500
H	-0.80680600	-5.64651900	-2.54305000
H	2.77404400	-3.66436700	-3.95187100

H	0.83713400	-5.19675700	-4.37523700
H	3.48144000	-0.09496000	0.31842100
H	4.78569700	0.08921400	-1.01202300

TS22

Pd	-12.28583300	-9.06808200	5.41432300
C	-9.29560200	-7.74463200	5.46480400
C	-9.80096900	-8.91295000	4.94061100
H	-9.78222500	-9.07896100	3.86372100
C	-10.41351800	-9.94653100	5.74454200
H	-10.21158500	-9.90276100	6.82256800
H	-10.39081100	-10.95786800	5.33861900
H	-9.30179800	-7.63071400	6.55276900
P	-13.40327200	-10.72307300	6.37997200
C	-14.16801200	-12.09276100	5.39454400
C	-15.39565000	-12.62868000	5.84730900
C	-15.98342300	-13.73078200	5.21437000
H	-16.93082400	-14.12779100	5.58407700
C	-15.34323700	-14.31859300	4.11360300
H	-15.78519700	-15.18192300	3.61198900
C	-14.13177200	-13.78779700	3.65322500
C	-13.52580400	-12.67138200	4.26966000
C	-12.22926200	-12.19241200	3.68713900
C	-12.21625800	-11.09546900	2.78209600
C	-13.51080700	-10.37809600	2.39761400
H	-14.15533600	-10.35569900	3.29044300
C	-14.24692500	-11.17732900	1.29588300
H	-13.62164700	-11.23159600	0.38851400
H	-15.19370600	-10.67628400	1.03196300
H	-14.47747800	-12.20325300	1.61840200
C	-13.31682100	-8.92324200	1.93303900
H	-14.30445200	-8.45358400	1.79606300
H	-12.79667800	-8.88029400	0.96082400
H	-12.75974300	-8.32546500	2.66731400
C	-10.99680700	-10.73658800	2.18433500
C	-9.80234600	-11.42933700	2.44223800
C	-8.49988900	-11.01399400	1.76902200
H	-8.69175000	-10.07447500	1.22218400
C	-8.05405600	-12.07871400	0.74176400
H	-8.83484800	-12.24951100	-0.01722300
H	-7.85237900	-13.03936200	1.24480600
H	-7.13071400	-11.76020500	0.22903100
C	-7.37397000	-10.74731200	2.79133200
H	-7.66616600	-9.97551300	3.51998500

H	-6.46110000	-10.40984500	2.27274600
H	-7.12570800	-11.66523100	3.34921800
C	-9.84556800	-12.51695000	3.32565700
C	-11.03641800	-12.90442800	3.96722300
C	-10.99495300	-14.06744400	4.95838200
H	-11.96058900	-14.11191600	5.48130500
C	-10.80068000	-15.40858500	4.21890100
H	-9.84988200	-15.40955200	3.66018800
H	-11.61705800	-15.58760400	3.50073600
H	-10.77820800	-16.24651100	4.93637300
C	-9.90183900	-13.87412800	6.03138800
H	-8.89505100	-13.89458800	5.58342500
H	-9.95624100	-14.68622200	6.77463400
H	-15.89181600	-12.18493000	6.71106900
H	-13.63245700	-14.23605100	2.79303300
H	-10.96654300	-9.88880100	1.49800700
H	-8.92724700	-13.06559200	3.54093500
C	-12.57394800	-11.58615600	7.77784400
C	-12.67339800	-12.97320500	7.99906900
C	-11.81582300	-10.79354900	8.66750200
C	-12.00721000	-13.56279800	9.08573500
H	-13.26634100	-13.59250600	7.32614800
C	-11.16355900	-11.38422700	9.75826200
H	-11.74524400	-9.71648500	8.50315100
C	-11.25149800	-12.77200600	9.96478600
H	-12.08171700	-14.64076700	9.24348900
H	-10.58224700	-10.76171200	10.44161400
H	-10.73317800	-13.23362000	10.80776100
C	-14.86593900	-9.90364600	7.15779800
C	-15.14953100	-9.97351700	8.53507500
C	-15.67910600	-9.11027300	6.31852200
C	-16.23013900	-9.24976400	9.06714100
H	-14.52782200	-10.58332900	9.19113000
C	-16.76139600	-8.39958000	6.85197900
H	-15.44521700	-9.02920000	5.25489700
C	-17.03557800	-8.46298500	8.22979900
H	-16.43966200	-9.30279900	10.13771000
H	-17.37975700	-7.78391300	6.19601400
H	-17.87016600	-7.89647300	8.64768200
H	-10.02488200	-12.91663300	6.55859900
C	-12.24505400	-4.81348100	4.68318800
C	-12.39221600	-6.01605000	5.32107000
O	-12.77297500	-7.11926300	4.68879600
C	-12.10883800	-6.10989900	6.79760800

C	-12.91711500	-6.91309600	7.63275700
C	-11.00876700	-5.44069000	7.37555200
C	-12.62943300	-7.05163100	8.99915300
H	-13.78286100	-7.41720600	7.20586600
C	-10.71121900	-5.58611300	8.73947600
H	-10.36864400	-4.83427700	6.73328200
C	-11.51725200	-6.39762400	9.55742600
H	-13.27894000	-7.66866200	9.62449400
H	-9.84478600	-5.07157100	9.16362300
H	-11.28562300	-6.51163400	10.61933600
C	-8.74624600	-6.63255000	4.70810400
C	-8.04860300	-5.60835100	5.39918900
C	-8.88372000	-6.51796000	3.29952100
C	-7.51513400	-4.51062700	4.71465100
H	-7.93788700	-5.68728500	6.48302800
C	-8.35181000	-5.42054600	2.61960100
H	-9.44301900	-7.27570100	2.74945400
C	-7.66661000	-4.40959000	3.32132600
H	-6.98505100	-3.73095800	5.26617000
H	-8.48135700	-5.34045800	1.53803600
H	-7.25906600	-3.54997600	2.78521300
H	-12.41827800	-4.73483400	3.60779600
H	-11.94870500	-3.91677000	5.22853900

IM24

Pd	0.38628500	-0.02298000	-0.22548000
P	0.55486700	0.30471700	1.97054200
C	2.14066100	-0.36689700	2.60106700
C	2.36045800	-0.55909000	3.98156400
C	3.58263900	-1.06242600	4.44431400
H	3.74314000	-1.21034000	5.51396300
C	4.59244900	-1.38222300	3.52181600
H	5.54939500	-1.77566700	3.87059800
C	4.36834400	-1.21450400	2.14883700
C	3.14049300	-0.71595600	1.66228100
C	2.96951100	-0.63851600	0.16970800
C	2.86366800	-1.85255500	-0.57481600
C	2.50100000	-3.17614200	0.09542500
H	2.53336400	-3.03855300	1.18634400
C	3.49412800	-4.30274400	-0.25617800
H	3.48625700	-4.51669600	-1.33727600
H	3.21861200	-5.23090100	0.27192100
H	4.52367000	-4.03186700	0.03076600
C	1.05523300	-3.57906000	-0.27932800

H	0.34062000	-2.78701600	-0.00822200
H	0.77020100	-4.51208500	0.23608100
H	0.96357500	-3.74265600	-1.36423700
C	2.97531000	-1.80242200	-1.97120900
C	3.17130400	-0.59789700	-2.66459000
C	3.27716400	-0.51165100	-4.18360500
H	2.54302000	0.24989600	-4.49806500
C	2.94639300	-1.81840100	-4.92167200
H	2.95727100	-1.64386200	-6.00903800
H	1.95033200	-2.19276500	-4.64841400
H	3.69309500	-2.59944500	-4.69507400
C	4.68302100	-0.01225700	-4.59421800
H	4.92815900	0.94795800	-4.11298300
H	4.73815100	0.12449100	-5.68740700
H	5.45171800	-0.74719500	-4.29954400
C	3.24176500	0.58973200	-1.92046600
C	3.14424600	0.60462400	-0.51975400
C	3.32093000	1.92011400	0.23310900
H	3.01786100	1.77056000	1.27821200
C	4.80936200	2.33203800	0.24154800
H	5.17250200	2.49171800	-0.78733800
H	5.43335300	1.55195700	0.70771800
H	4.94528800	3.26991800	0.80629000
C	2.43659400	3.04433000	-0.33757900
H	2.74724600	3.32698100	-1.35601600
H	2.50531900	3.93835900	0.30300800
H	1.56119500	-0.33133300	4.68879300
H	5.14258900	-1.48804900	1.43000900
H	2.85398700	-2.72795300	-2.53217700
H	3.35558100	1.53571600	-2.45071300
C	0.45939100	2.06638300	2.49695900
C	1.15071600	2.58017800	3.61262900
C	-0.33866300	2.93166700	1.71854800
C	1.03939400	3.93864300	3.94544800
H	1.78972300	1.93030300	4.21046200
C	-0.46128900	4.28517200	2.06488300
H	-0.83750200	2.54597900	0.82844100
C	0.22967000	4.79147000	3.17743900
H	1.58796500	4.33029800	4.80461800
H	-1.08102500	4.94501100	1.45453900
H	0.14592700	5.84818700	3.43941500
C	-0.72257100	-0.57565800	2.95285000
C	-0.60769500	-1.97483400	3.10342200
C	-1.88579000	0.07808600	3.40302900

C	-1.64328400	-2.70647000	3.69987500
H	0.28718500	-2.48791500	2.74802400
C	-2.92524600	-0.66121200	3.99096300
H	-1.97953700	1.15990800	3.29470800
C	-2.80811200	-2.05185700	4.13860400
H	-1.54361800	-3.78763800	3.81660400
H	-3.82552000	-0.14736300	4.33401400
H	-3.61869300	-2.62415800	4.59386600
H	1.38673600	2.71927300	-0.37678900
C	-2.84062000	-5.70908700	0.00196200
C	-2.61202900	-4.33030000	0.04157800
C	-2.65490800	-3.55047200	-1.14461200
C	-2.93302600	-4.21792900	-2.36525300
C	-3.15911100	-5.59985000	-2.40266300
C	-3.11506100	-6.35472900	-1.21883000
H	-2.80062600	-6.28904700	0.92745900
H	-2.38889000	-3.84907400	0.99510200
H	-2.96395100	-3.63225900	-3.28732400
H	-3.36865300	-6.08890700	-3.35700100
H	-3.28868000	-7.43268500	-1.24464600
C	-2.38948800	-2.11602500	-1.17195500
C	-2.13311500	-1.31093500	-0.10071400
H	-2.35098600	-1.66050200	-2.16398900
H	-2.15942300	-1.72197800	0.91101500
C	-1.73130500	0.08810900	-0.22312000
H	-1.94190200	0.55192400	-1.19662000
H	-2.04756900	0.71665300	0.61923200
C	-0.03022300	1.61093800	-3.14287100
C	-0.03106100	0.24264000	-3.22109700
O	0.20071300	-0.57936500	-2.21059000
C	-0.30291100	-0.47332800	-4.51601100
C	-0.14093800	0.15092100	-5.77305500
C	-0.68268700	-1.83509100	-4.49566200
C	-0.37150200	-0.55192100	-6.96352700
H	0.19483900	1.18808600	-5.81668800
C	-0.91928800	-2.53809000	-5.68615400
H	-0.77190100	-2.33698900	-3.53405000
C	-0.76578300	-1.90092900	-6.92774900
H	-0.23181500	-0.04827100	-7.92332700
H	-1.21196500	-3.59037800	-5.64192300
H	-0.93926900	-2.44912800	-7.85670300
H	0.19272900	2.09684000	-2.19183300
H	-0.29132400	2.23877200	-3.99461200

TS23

Pd	0.46642600	-0.60474000	-0.66370700
P	0.65484800	0.22199200	1.40550900
C	2.14650700	-0.28607200	2.37363900
C	2.14189800	-0.24279800	3.78514600
C	3.26810700	-0.63325400	4.52224200
H	3.24552700	-0.59243500	5.61326000
C	4.41658900	-1.07930900	3.85028800
H	5.29863400	-1.39180300	4.41328000
C	4.42855600	-1.12748900	2.44958200
C	3.30587100	-0.73482900	1.69140100
C	3.41256900	-0.82243800	0.19715000
C	3.23387400	-2.07564500	-0.45002700
C	2.80470600	-3.32850900	0.31232200
H	2.57342900	-3.04406900	1.34901000
C	3.95797900	-4.35465700	0.35748200
H	4.23495700	-4.67367900	-0.66100300
H	3.65652200	-5.24995300	0.92744300
H	4.85365500	-3.92427500	0.83458100
C	1.53048700	-3.96423300	-0.28267200
H	0.69475900	-3.24497000	-0.26199100
H	1.24752800	-4.85782400	0.30042300
H	1.68494100	-4.27262200	-1.32908600
C	3.48148000	-2.16216200	-1.83012700
C	3.88563100	-1.05409300	-2.58531100
C	4.17831100	-1.18553300	-4.07375300
H	3.91596000	-2.21408500	-4.37549900
C	5.68389800	-0.97717100	-4.35205800
H	5.90309200	-1.11742000	-5.42426900
H	6.29789100	-1.68741900	-3.77401200
H	5.99184000	0.04444100	-4.07212400
C	3.33043800	-0.21431100	-4.92094000
H	2.25871500	-0.38416200	-4.75174800
H	3.54866000	-0.35460600	-5.99336700
H	3.55695700	0.83370400	-4.66537300
C	4.04813600	0.17611000	-1.92615200
C	3.81443200	0.31911800	-0.54996200
C	4.08029400	1.65841400	0.13400200
H	3.56445400	1.66020500	1.10405200
C	5.59228200	1.81428600	0.41001700
H	6.15981900	1.80123400	-0.53581400
H	5.96429500	0.99345400	1.04429700
H	5.79582900	2.76997500	0.92304800
C	3.53822100	2.86155400	-0.65967300

H	4.06635400	2.98712400	-1.61941200
H	3.67701800	3.78575900	-0.07649100
H	1.24449900	0.09015100	4.30854000
H	5.31653400	-1.47927000	1.92143500
H	3.33425600	-3.11783300	-2.33708100
H	4.37046700	1.04490200	-2.50188500
C	0.72710400	2.06797200	1.36660900
C	1.42955300	2.83639900	2.31615200
C	0.03417100	2.71868600	0.32491300
C	1.44001300	4.23642400	2.22052800
H	1.97812700	2.34154300	3.11909500
C	0.03227400	4.11884200	0.24079200
H	-0.47371200	2.12011400	-0.43313400
C	0.73835700	4.87960700	1.18643200
H	1.99687100	4.82484700	2.95323500
H	-0.49874500	4.60700900	-0.57824600
H	0.75081800	5.96936400	1.11409900
C	-0.71725400	-0.12977600	2.58869700
C	-0.92566300	-1.47350100	2.97296800
C	-1.61192700	0.85965400	3.03927000
C	-1.99884700	-1.81528600	3.80602400
H	-0.24370400	-2.24983300	2.61798000
C	-2.69304000	0.51235100	3.86728500
H	-1.46495800	1.90051300	2.74774000
C	-2.88787100	-0.82190500	4.25431500
H	-2.14586200	-2.85666900	4.10067000
H	-3.38022000	1.28876000	4.21080000
H	-3.72871200	-1.08966700	4.89753400
H	2.46615700	2.73939500	-0.86102500
C	-4.06881700	-4.65527100	-4.36684900
C	-3.27220600	-3.79341800	-3.60312800
C	-3.51071900	-2.39900400	-3.59978200
C	-4.55992000	-1.89994300	-4.40434300
C	-5.35807000	-2.76227700	-5.16928300
C	-5.11801200	-4.14588800	-5.15282800
H	-3.86689000	-5.72893000	-4.35494000
H	-2.44792400	-4.19802100	-3.01273500
H	-4.75113800	-0.82355800	-4.41695900
H	-6.16804100	-2.35341300	-5.77792900
H	-5.73657100	-4.81990900	-5.74922500
C	-2.69251000	-1.45582300	-2.80317600
C	-2.16710400	-1.80759800	-1.54470900
H	-2.96126200	-0.40255100	-2.92611900
H	-2.05858300	-2.86927700	-1.30567600

C	-1.75433800	-0.87220300	-0.56278500
C	-1.04158100	-1.29548800	-4.28049800
C	-0.14838700	-0.48990700	-3.56064900
O	0.67042900	-1.04506300	-2.72231400
C	-0.22842000	1.00366100	-3.61608100
C	-1.35012800	1.68432700	-4.14168000
C	0.84755700	1.77079400	-3.11227200
C	-1.39672600	3.08650700	-4.15953600
H	-2.19723800	1.11591000	-4.52830500
C	0.80904700	3.16938800	-3.14750200
H	1.70804400	1.25046600	-2.69377700
C	-0.31561500	3.83579400	-3.66709700
H	-2.27799900	3.59326600	-4.56002600
H	1.65299400	3.74166500	-2.75811700
H	-0.34831900	4.92763300	-3.68748700
H	-2.09543300	0.16298800	-0.70136900
H	-1.81534500	-1.21952400	0.47288000
H	-1.61591200	-0.89553300	-5.11707500
H	-0.84898900	-2.36758800	-4.29667900

TS24

Pd	-1.08301100	0.00714000	0.32361700
C	-1.32306600	-0.38242900	2.67529900
O	0.95290200	1.06232600	0.97186200
P	-1.15079000	1.10318400	-1.66384900
C	-2.47407000	0.15464400	2.05871900
C	-2.36401300	1.38917800	1.35310000
H	-3.22838900	1.76590500	0.80169000
H	-1.64574600	2.14823400	1.68267000
H	-0.48236600	0.29353200	2.85763500
H	-3.38862800	-0.43512800	1.97614100
C	0.16570300	0.58861300	-2.84877400
C	0.42484900	-0.80119500	-3.01149500
C	-0.58497600	5.66452300	-0.88687900
C	-1.80648600	5.19605600	-1.39454300
C	-1.98097400	3.83005500	-1.66920800
C	-0.93075900	2.91767400	-1.43271800
C	0.29368700	3.39106800	-0.90741000
C	0.46166200	4.75840900	-0.64728800
H	-0.45018300	6.72778400	-0.67609900
H	-2.62747500	5.89150500	-1.58287500
H	-2.93405800	3.48365700	-2.06869500
H	1.09773600	2.69414100	-0.68142400
H	1.41439700	5.11099800	-0.24662700

C	-5.29597600	1.09531700	-3.75294600
C	-4.16810400	1.54460700	-4.46147500
C	-2.89807600	1.48861600	-3.86931300
C	-2.75017200	0.98147900	-2.56254300
C	-3.87660600	0.49914700	-1.86976000
C	-5.14802800	0.56200500	-2.46200900
H	-6.28474700	1.14649800	-4.21330800
H	-4.27899300	1.94294000	-5.47203100
H	-2.02332600	1.85441500	-4.41045500
H	-3.74264900	0.07675500	-0.87212600
H	-6.01933300	0.19044000	-1.91844100
C	0.93526000	1.53643400	-3.55133200
H	0.73981400	2.60019300	-3.41752800
C	1.46548400	-1.19305400	-3.87124900
H	1.67243600	-2.25412400	-4.00527300
C	1.96767200	1.12259700	-4.40533000
H	2.56004600	1.86736600	-4.94037400
C	2.23694800	-0.24425900	-4.55943800
H	3.04526500	-0.57586900	-5.21422900
C	-0.45330500	-1.78587500	-2.29552200
C	-1.67769300	-2.18252000	-2.88860700
C	-0.11123500	-2.21866900	-0.97284800
C	-2.59966100	-2.90703500	-2.11228700
C	-1.09901600	-2.89873000	-0.22249400
C	-2.35287700	-3.22356700	-0.76975000
H	-3.55231600	-3.19988600	-2.55337500
H	-0.87608500	-3.20767100	0.79815500
C	1.34057400	-2.17530200	-0.49872600
C	2.09385000	-3.36579900	-1.14324000
C	1.53157200	-2.24079800	1.02280000
H	1.80288700	-1.24288200	-0.85225400
H	2.00876600	-3.36710100	-2.23919300
H	3.16338900	-3.32021600	-0.87792800
H	1.68398600	-4.32017000	-0.77000900
H	1.01870300	-1.41386400	1.52442500
H	1.16821300	-3.19397900	1.43929800
H	2.60284300	-2.16007900	1.25623700
C	-1.96301100	-1.89153600	-4.36275900
C	-3.45806000	-1.87773400	-4.72800700
C	-1.23668000	-2.93220200	-5.24829200
H	-1.55003400	-0.89837200	-4.59683000
H	-4.03753700	-1.24730600	-4.04302400
H	-3.58451400	-1.49009400	-5.75131300
H	-3.88089300	-2.89658600	-4.70648500

H	-0.15024900	-2.92233100	-5.08344400
H	-1.60930600	-3.94539500	-5.02129400
H	-1.42728200	-2.72573700	-6.31538000
C	-3.41676100	-3.91185100	0.07348500
C	-3.88284400	-5.24372800	-0.55075800
C	-4.61991300	-2.96815000	0.29430500
H	-2.97125300	-4.13264100	1.05590700
H	-3.03332800	-5.92991700	-0.69837900
H	-4.62092200	-5.73772300	0.10346700
H	-4.35940200	-5.07450700	-1.53038500
H	-4.29379600	-2.01423300	0.73810500
H	-5.11360500	-2.74112000	-0.66518600
H	-5.36532900	-3.43157300	0.96293500
C	2.24773900	0.88240000	0.89460500
C	2.99128600	0.92231900	-0.26565700
C	2.94491200	0.63986900	2.21729800
C	2.31727200	1.05113300	3.41426300
C	4.17723100	-0.04437800	2.32310700
C	2.89739700	0.79752200	4.66668200
H	1.36499300	1.57779300	3.34018300
C	4.75776000	-0.30705700	3.57225300
H	4.66628900	-0.40259600	1.41556700
C	4.12021300	0.11135800	4.75343300
H	2.39326300	1.13398800	5.57674900
H	5.70386300	-0.85220400	3.62555500
H	4.56913800	-0.09850800	5.72729700
C	-1.21519500	-1.70178800	3.29006700
C	-0.01630200	-2.03213400	3.97050200
C	-2.24287700	-2.67576000	3.22712700
C	0.15077000	-3.28933200	4.56190200
H	0.78662700	-1.29354000	4.01412600
C	-2.07345100	-3.93153900	3.82035400
H	-3.17267100	-2.45079500	2.70487400
C	-0.87548500	-4.24700800	4.48798200
H	1.08516500	-3.52347000	5.07618000
H	-2.87648600	-4.66967600	3.76009000
H	-0.74534900	-5.22997800	4.94541200
H	2.50283000	1.04010000	-1.23433600
H	4.07906800	0.84142300	-0.25676000

IM25

C	1.54374200	0.00215100	1.56184200
C	2.09759000	0.55093600	0.36894200
H	1.32897300	0.67688600	2.40707900

H	2.62481100	-0.09421600	-0.33953400
C	1.81097400	1.88069800	0.01750900
H	1.45982300	2.55953500	0.79847600
C	1.67909200	4.54957700	2.49005000
C	1.77340400	3.25158000	2.97413500
O	0.77731200	2.47360500	3.26443800
C	3.15808300	2.64397000	3.13715800
C	4.26783900	3.02542000	2.35052800
C	3.33475400	1.58531300	4.05532600
C	5.50657900	2.37945500	2.48058200
H	4.14560400	3.81390700	1.60598300
C	4.57402300	0.94449000	4.19932400
H	2.47065100	1.27440800	4.64505300
C	5.66827100	1.33565800	3.40862200
H	6.34515300	2.68297300	1.84766900
H	4.68703700	0.13463200	4.92582700
H	6.63213500	0.82997000	3.50842600
Pd	-0.12683000	0.43024000	0.27432700
P	-1.43837700	-1.17802500	1.20324700
C	-3.04575200	-1.08745000	0.32871300
C	-4.10978400	-1.97776200	0.57303300
C	-5.30917700	-1.85136300	-0.13838300
H	-6.13250300	-2.54249000	0.05150300
C	-5.44397100	-0.83411100	-1.09911500
H	-6.37490200	-0.73123600	-1.66013100
C	-4.38412800	0.05006400	-1.34295800
C	-3.17193600	-0.06087200	-0.63020500
C	-2.07238900	0.91633100	-0.98137100
C	-1.32663400	0.68832000	-2.19232300
C	-1.23410700	-0.70871200	-2.79689000
H	-1.73915600	-1.40702100	-2.11504200
C	-1.95654700	-0.77311500	-4.15863700
H	-1.49030900	-0.08419700	-4.88196300
H	-1.90395600	-1.79359700	-4.57375400
H	-3.01733100	-0.49401400	-4.05462900
C	0.23045600	-1.17336100	-2.92036200
H	0.72006900	-1.16202200	-1.93265500
H	0.27260800	-2.19918700	-3.32302500
H	0.79791500	-0.51473600	-3.59724100
C	-0.73891700	1.77895200	-2.84522200
H	-0.19364200	1.60571100	-3.77459100
C	-0.84961900	3.09422000	-2.35523200
C	-0.31941000	4.24148600	-3.20549200
H	0.70585100	3.97588700	-3.50612700

C	-1.16547500	4.36323600	-4.49690400
H	-0.75645700	5.15343700	-5.14874200
H	-1.17443900	3.41778400	-5.06252000
H	-2.20880900	4.62396300	-4.25087900
C	-0.27107900	5.59742000	-2.48330500
H	-1.28772300	5.96103100	-2.25621600
H	0.29201000	5.53475300	-1.54079000
H	0.21723400	6.34504400	-3.12850500
C	-1.47924500	3.28959400	-1.11515400
H	-1.52253300	4.28851100	-0.68527500
C	-2.09949500	2.23868300	-0.41590400
C	-2.88972800	2.52156200	0.85774400
H	-3.05483400	1.56291800	1.37288900
C	-4.27377100	3.10901400	0.49456000
H	-4.84999400	2.42457800	-0.14742800
H	-4.85588700	3.29735700	1.41194400
H	-4.15239100	4.06637800	-0.03934800
C	-2.15110900	3.45663600	1.83591900
H	-2.04702400	4.47024300	1.41436800
H	-2.74440500	3.54677600	2.76123300
H	-1.15038100	3.08758300	2.10974700
H	1.72524100	-1.05415800	1.77799300
C	2.27066400	2.51945200	-1.21059900
C	2.55979700	1.80290000	-2.39677000
C	2.49673000	3.91699200	-1.18573200
C	3.08574200	2.46125700	-3.51294200
H	2.35773700	0.73236400	-2.43830200
C	3.03916100	4.57060900	-2.29908300
H	2.26985200	4.46051000	-0.26396900
C	3.33590700	3.84674400	-3.46628700
H	3.30266400	1.89812900	-4.42356900
H	3.22237300	5.64622800	-2.26025600
H	3.75333800	4.35623200	-4.33742900
H	-4.48595500	0.83633800	-2.09251300
H	-3.99258100	-2.77161400	1.31216800
C	-0.85384900	-2.90199900	0.99750100
C	0.04733300	-3.44228900	1.94076800
C	-1.18953100	-3.65057800	-0.14978200
C	0.60150100	-4.71381600	1.73628800
H	0.30453900	-2.87278100	2.83539400
C	-0.63064100	-4.92174000	-0.34920200
H	-1.89143800	-3.24579500	-0.87973000
C	0.26651300	-5.45507900	0.59041200
H	1.29335400	-5.12550500	2.47375000

H	-0.90045400	-5.49626200	-1.23778700
H	0.70021000	-6.44452500	0.43293100
C	-1.76974600	-0.97395100	2.98969400
C	-2.42503000	-1.96859400	3.74849300
C	-1.36753600	0.23087000	3.59842600
C	-2.68732500	-1.74528000	5.10673800
H	-2.71030400	-2.91534700	3.28645400
C	-1.63177200	0.44470100	4.96065400
H	-0.82385900	0.99037800	3.03634100
C	-2.29392200	-0.53736400	5.71254500
H	-3.19178000	-2.51503400	5.69481000
H	-1.29960700	1.37613500	5.42109100
H	-2.49535900	-0.37196800	6.77321600
H	0.69793700	5.02085600	2.38914700
H	2.56201700	5.17898400	2.36187800

TS25

C	3.67234000	-1.50933900	3.02954400
C	2.81718200	-0.66871400	2.30896900
C	3.15949100	-0.23699200	1.00400300
C	4.36861500	-0.69918600	0.43528100
C	5.22954700	-1.52978000	1.16278600
C	4.88761200	-1.93943100	2.46268700
H	3.39088900	-1.83748300	4.03311100
H	1.86511200	-0.35607300	2.73912500
H	4.64866400	-0.35287000	-0.55979600
H	6.16989500	-1.85549900	0.71324600
H	5.55542600	-2.59313800	3.02796100
C	2.33481300	0.70933400	0.25672500
C	1.62223100	1.75046200	0.87908300
H	2.50466600	0.79231500	-0.81947600
H	1.64817500	1.83696300	1.96929200
C	0.78583700	2.62026900	0.13088300
H	0.18916000	3.37116500	0.64782400
H	0.88608600	2.70738100	-0.95093500
C	2.69190200	4.45988000	-0.96382000
C	3.10416400	3.31554600	-1.66398100
O	2.40245400	2.71527900	-2.55230400
C	4.44379100	2.69631100	-1.30597200
C	5.06018300	2.85244600	-0.04484600
C	5.07863700	1.86650500	-2.25705500
C	6.27601900	2.21748000	0.24862400
H	4.56484800	3.45249900	0.72010700
C	6.30583500	1.24911800	-1.97694200

H	4.58152800	1.72256100	-3.21768200
C	6.91068200	1.42054000	-0.71894500
H	6.72416200	2.33463100	1.23848300
H	6.78888200	0.62689700	-2.73533300
H	7.85948300	0.92896000	-0.49046400
Pd	-0.08378200	0.54592400	0.15263300
P	-2.26518600	1.17328100	0.16602200
C	-3.22598300	-0.23811900	-0.49777600
C	-4.58341900	-0.14715700	-0.86314700
C	-5.26298700	-1.27836300	-1.33421700
H	-6.31415500	-1.20533900	-1.61981300
C	-4.58299500	-2.50373800	-1.43881600
H	-5.10566200	-3.39002500	-1.80423000
C	-3.22800600	-2.59094300	-1.08862300
C	-2.52691200	-1.45953500	-0.62286200
C	-1.05628200	-1.63926000	-0.31902800
C	-0.13429600	-1.68943600	-1.41697100
C	-0.49225100	-1.10613900	-2.78065500
H	-1.43988200	-0.55613800	-2.68049100
C	-0.70887200	-2.23299500	-3.81411000
H	0.21296300	-2.82421500	-3.94207800
H	-0.98168800	-1.80561700	-4.79334000
H	-1.51435600	-2.91443400	-3.49573300
C	0.57793700	-0.10769300	-3.26644100
H	0.73227200	0.71006000	-2.54711600
H	0.27366500	0.33180400	-4.23083200
H	1.55106400	-0.60259700	-3.41587700
C	1.09643600	-2.35353900	-1.24740000
H	1.77323300	-2.40027200	-2.09964000
C	1.45184900	-2.96941000	-0.03984600
C	2.71941100	-3.79800600	0.13303900
H	3.25552800	-3.38994600	1.00435300
C	3.67233000	-3.75762100	-1.07186500
H	4.59591100	-4.30908400	-0.83396000
H	3.94851400	-2.72608600	-1.33470400
H	3.21245400	-4.23256500	-1.95563100
C	2.34917900	-5.26604100	0.45658900
H	1.80982100	-5.72256200	-0.39083400
H	1.70445300	-5.33425100	1.34719700
H	3.26091000	-5.85783700	0.64443400
C	0.58061900	-2.81920900	1.05879400
H	0.87734500	-3.23056100	2.02518500
C	-0.65800700	-2.17954000	0.95185700
C	-1.56324300	-2.05045300	2.17114700

H	-2.47865200	-1.52487500	1.86554100
C	-1.97630200	-3.43009200	2.72284900
H	-1.09353700	-4.00107200	3.05425100
H	-2.49774500	-4.02261500	1.95340900
H	-2.65069900	-3.31057700	3.58726500
C	-0.88832000	-1.19234600	3.26143600
H	0.02519200	-1.68260400	3.63631200
H	-1.57544900	-1.03931000	4.10976600
H	-0.61108600	-0.20711500	2.85310100
H	-5.09998400	0.81146300	-0.78392100
H	-2.69601700	-3.53895200	-1.18467400
C	-2.93599300	1.48709000	1.84711900
C	-2.31980100	2.49956000	2.61627400
C	-3.96263600	0.71149700	2.42114800
C	-2.73269200	2.73636000	3.93332700
H	-1.51240100	3.09454900	2.18407500
C	-4.36433700	0.94382500	3.74699400
H	-4.44355100	-0.07432200	1.83809900
C	-3.75283100	1.95449400	4.50432700
H	-2.25294000	3.52427700	4.51754300
H	-5.15775700	0.33419000	4.18451500
H	-4.06586700	2.13237300	5.53507700
C	-2.74199900	2.63506400	-0.83002000
C	-3.84509200	3.44913000	-0.50086700
C	-1.96290700	2.93407500	-1.96757300
C	-4.16878000	4.54829100	-1.31108300
H	-4.43740400	3.22990600	0.38950900
C	-2.29332900	4.03128500	-2.77541200
H	-1.09241200	2.32045100	-2.20541100
C	-3.39553200	4.83881300	-2.44775600
H	-5.02116100	5.17992000	-1.05193800
H	-1.67984400	4.26208700	-3.64823300
H	-3.64576600	5.69940800	-3.07148700
H	1.77541300	4.96749400	-1.27244900
H	3.34277300	4.97544400	-0.25561100

IM26

Pd	0.57741100	-0.80539600	-0.74277700
P	0.65470900	0.11558300	1.26618200
C	2.11836200	-0.26268000	2.34139200
C	2.02697700	-0.18253500	3.74832500
C	3.13003200	-0.46927200	4.56433100
H	3.03668700	-0.39989500	5.65030400
C	4.34791500	-0.84460400	3.97715200

H	5.21442200	-1.07431200	4.60105300
C	4.44933900	-0.92813500	2.58147000
C	3.34956600	-0.64258600	1.74588100
C	3.55051400	-0.76519000	0.26371100
C	3.43457200	-2.03600100	-0.36055300
C	3.03973700	-3.28493200	0.42619200
H	2.67907700	-2.97058600	1.41653600
C	4.27458900	-4.18697000	0.64544700
H	4.68519300	-4.52315400	-0.32145600
H	4.00382100	-5.08013300	1.23407300
H	5.06944700	-3.64496500	1.18316900
C	1.89881800	-4.07597400	-0.24562600
H	1.00878700	-3.43749600	-0.37537700
H	1.62361100	-4.94343800	0.37892000
H	2.19594800	-4.45401600	-1.23713400
C	3.72968500	-2.14344600	-1.73107000
C	4.12146300	-1.03689900	-2.49631200
C	4.45610600	-1.18478400	-3.97467100
H	4.24638400	-2.22963500	-4.26165700
C	5.95576400	-0.91256700	-4.22729100
H	6.20371100	-1.05764300	-5.29272600
H	6.58893600	-1.58588800	-3.62639200
H	6.21077800	0.12565100	-3.95579200
C	3.58311500	-0.26790700	-4.85724500
H	2.51587200	-0.46514100	-4.68474200
H	3.81032300	-0.43346000	-5.92427400
H	3.77631300	0.79395900	-4.63254200
C	4.22102700	0.21088400	-1.85783900
C	3.93682300	0.37198000	-0.49261100
C	4.11031900	1.73839800	0.16656500
H	3.55563900	1.73716200	1.11511600
C	5.59977200	1.97870200	0.49712000
H	6.20513000	1.97518400	-0.42526300
H	5.98694700	1.19137200	1.16385500
H	5.73414900	2.95412100	0.99572100
C	3.53956300	2.89201100	-0.67877800
H	4.10416200	3.02581800	-1.61665100
H	3.60063600	3.83559100	-0.11363800
H	1.07827700	0.10049500	4.20656900
H	5.39282500	-1.22388100	2.11907500
H	3.63676300	-3.11468800	-2.22183700
H	4.53141000	1.07897400	-2.44146500
C	0.62909500	1.96490100	1.18568200
C	1.23786900	2.80048900	2.14344700

C	-0.03977500	2.54795000	0.08925900
C	1.18122500	4.19574600	2.00194400
H	1.76575900	2.36205800	2.99181000
C	-0.11349800	3.94278000	-0.04026500
H	-0.47530800	1.89658600	-0.67245500
C	0.50169800	4.76948000	0.91378400
H	1.66709800	4.83502500	2.74281200
H	-0.62814500	4.37739400	-0.89900800
H	0.46061200	5.85573600	0.80630900
C	-0.76203600	-0.27172800	2.38891900
C	-0.87811700	-1.58909800	2.88812800
C	-1.78969000	0.65288400	2.66208500
C	-1.98846500	-1.96604500	3.65445700
H	-0.09251300	-2.31838300	2.67631800
C	-2.90904200	0.26862800	3.41970500
H	-1.71588700	1.67385100	2.28422000
C	-3.01162800	-1.03818000	3.92017700
H	-2.05957800	-2.98589000	4.03952800
H	-3.69785500	0.99673200	3.62283700
H	-3.88139300	-1.33441900	4.51036300
H	2.48619500	2.70468300	-0.92442100
C	-4.74465100	-4.08330700	-4.69793600
C	-3.61672000	-3.47983500	-4.12388900
C	-3.70005600	-2.19222600	-3.55541200
C	-4.93823700	-1.52318500	-3.57797800
C	-6.06964100	-2.12392900	-4.15308800
C	-5.97653500	-3.40676300	-4.71541600
H	-4.66242800	-5.08206000	-5.13289500
H	-2.66230800	-4.01082800	-4.11499500
H	-5.01298500	-0.52558900	-3.13727400
H	-7.02226300	-1.58911600	-4.16113900
H	-6.85500600	-3.87624500	-5.16337400
C	-2.47663900	-1.52575500	-2.93500100
C	-1.97187800	-2.29232600	-1.74805000
H	-2.75863900	-0.51303300	-2.60376200
H	-1.67604300	-3.33069100	-1.92522000
C	-1.79307800	-1.73338700	-0.52053600
C	-1.36199100	-1.35862200	-4.05834500
C	-0.20195800	-0.56392600	-3.52881900
O	0.71500700	-1.19185700	-2.92594200
C	-0.18112800	0.91695600	-3.63207300
C	-1.27476400	1.65278700	-4.14994100
C	0.97594700	1.62366200	-3.21528200
C	-1.21312700	3.05049700	-4.24695700

H	-2.18141600	1.13717700	-4.46796700
C	1.04138300	3.01286000	-3.33587000
H	1.80595100	1.06088600	-2.78893300
C	-0.05352800	3.73535300	-3.85014100
H	-2.06944600	3.60292400	-4.64002700
H	1.94021800	3.53982000	-3.01270600
H	-0.00174100	4.82297100	-3.93515000
H	-2.18022500	-0.73417200	-0.30446300
H	-1.51221900	-2.33690600	0.34381300
H	-1.83042500	-0.89618600	-4.93840400
H	-1.00554200	-2.35999200	-4.33660900

IM27

C	3.49620000	-0.65114600	2.85321700
C	2.69888300	0.05704300	1.94819300
C	2.97721700	0.03549200	0.55952000
C	4.08125500	-0.72552400	0.11844100
C	4.88485500	-1.43128900	1.02387700
C	4.59744900	-1.40163600	2.39785500
H	3.25562700	-0.62535000	3.91917100
H	1.82732800	0.60911400	2.30217400
H	4.32354900	-0.73128600	-0.94542000
H	5.73688900	-2.00634800	0.65342200
H	5.21858800	-1.95570400	3.10533000
C	2.17885100	0.78965500	-0.42079400
C	1.47325900	1.98736700	-0.13415000
H	2.44615700	0.60756300	-1.46644600
H	1.54334300	2.38463400	0.88655800
C	1.28258600	3.04952600	-1.20180000
H	0.38167500	3.64979900	-0.99766300
H	1.14101100	2.56978400	-2.18272200
C	2.50664600	4.01379800	-1.30221400
C	3.74839600	3.26421700	-1.79153600
O	3.87497200	3.04813100	-3.00129700
C	4.76927000	2.75878600	-0.81173600
C	4.61875800	2.87293500	0.58750600
C	5.90751000	2.08899800	-1.31765000
C	5.57297000	2.32655500	1.45562900
H	3.73785900	3.35407300	1.00844400
C	6.86601100	1.55359400	-0.45209900
H	6.01357500	1.99465900	-2.39891900
C	6.69876300	1.66714900	0.93965300
H	5.42668600	2.39832100	2.53458100
H	7.73847500	1.03662400	-0.85779700

H	7.43651800	1.23384700	1.61797100
Pd	0.00372600	0.43442500	-0.17427700
P	-2.13695100	1.09098400	0.18120800
C	-3.24000600	-0.30215200	-0.30320100
C	-4.62678000	-0.15872600	-0.50665900
C	-5.41197200	-1.26610600	-0.85457700
H	-6.48596800	-1.14817000	-1.01350000
C	-4.80758600	-2.52645100	-0.99717000
H	-5.41082400	-3.39652900	-1.26510600
C	-3.42552000	-2.66952900	-0.80858800
C	-2.61922700	-1.56192600	-0.47178100
C	-1.13471100	-1.80427700	-0.33611900
C	-0.32546800	-1.86562100	-1.51403300
C	-0.84808900	-1.37580300	-2.86450300
H	-1.77629400	-0.81231700	-2.68901400
C	-1.19154600	-2.57432600	-3.77617300
H	-0.29194300	-3.17923300	-3.97849600
H	-1.59481100	-2.22243500	-4.74075100
H	-1.94350300	-3.22581000	-3.30291200
C	0.14436000	-0.42384100	-3.56292400
H	0.36055700	0.44734600	-2.92382900
H	-0.27892200	-0.07034400	-4.51850700
H	1.09959700	-0.92801900	-3.78279100
C	0.92446300	-2.52463100	-1.45534400
H	1.51045200	-2.59508800	-2.37172100
C	1.40585500	-3.10126700	-0.27516300
C	2.68471900	-3.93009700	-0.20347700
H	3.27230500	-3.54786400	0.64765100
C	3.56382300	-3.84685100	-1.46141900
H	4.50292500	-4.40103100	-1.30140100
H	3.81367500	-2.80458400	-1.70868400
H	3.05287600	-4.29548400	-2.33053200
C	2.33273000	-5.40806900	0.09278800
H	1.74693800	-5.83652900	-0.73849500
H	1.73423500	-5.50037900	1.01308800
H	3.25059500	-6.00854700	0.21433300
C	0.64380600	-2.92989700	0.89927600
H	1.04393000	-3.30718500	1.84293800
C	-0.60574000	-2.30293800	0.89958600
C	-1.35685200	-2.10709300	2.21178300
H	-2.31975300	-1.62410900	1.99298600
C	-1.65173200	-3.44567900	2.91771100
H	-0.71633800	-3.96645400	3.18061800
H	-2.24414500	-4.11337600	2.27049500

H	-2.21705300	-3.27143800	3.84881200
C	-0.56861300	-1.15156900	3.13308500
H	0.40982200	-1.58400600	3.39742800
H	-1.13286800	-0.95783200	4.06064100
H	-0.39036200	-0.19410800	2.62008900
H	-5.08503800	0.82585800	-0.39400400
H	-2.95509800	-3.64702500	-0.92968800
C	-2.63198300	1.48864000	1.91167700
C	-1.90787300	2.50470800	2.57480200
C	-3.61878200	0.77725500	2.62231700
C	-2.17299000	2.80733900	3.91649800
H	-1.12979800	3.05159100	2.03704400
C	-3.87172300	1.07176700	3.97258500
H	-4.18617200	-0.01055800	2.12598300
C	-3.15272000	2.08628500	4.62240100
H	-1.60865000	3.59836500	4.41537700
H	-4.63464000	0.50729100	4.51350300
H	-3.35027600	2.31330200	5.67212300
C	-2.76759800	2.51262500	-0.80581600
C	-3.76065200	3.40321500	-0.35143800
C	-2.20494700	2.69435400	-2.08721200
C	-4.18812600	4.45882500	-1.17316000
H	-4.18975100	3.27604100	0.64409500
C	-2.64199500	3.74210900	-2.90989300
H	-1.41500700	2.01674300	-2.42009400
C	-3.63318400	4.62767800	-2.45247100
H	-4.95442200	5.14932600	-0.81358400
H	-2.20037600	3.87603200	-3.89984400
H	-3.96599700	5.45126100	-3.08787900
H	2.28314400	4.78559900	-2.05506300
H	2.66663700	4.51341500	-0.33531100