

Electronic Supporting Information For

Theoretical Investigation on A Chiral Brønsted acid (CBA)-Catalyzed Isomerization Reaction of BCB: Mechanism and Origin of Stereoselectivity

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Part 1: Structures and energies for intermediates involved in Pathway A

Pathway A

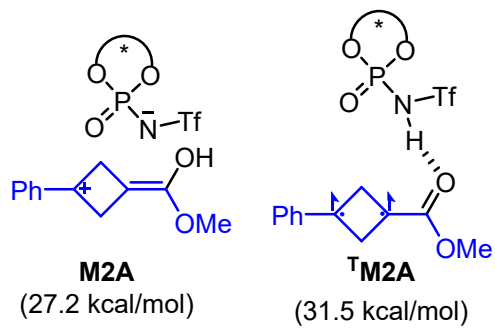


Fig. S1 Structures and energies for intermediates involved in Pathway A

Part 2: Derivations for the computed ee values

In the equations, the ΔG^\ddagger is the energy difference of the two enantioselective transition states, R and T represent the gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) and temperature of the reaction. In this reaction, the energy difference between TS2R and TS2S is 2.0 kcal/mol, the value of $[R]/[S]$ is 29.68. Then, we can obtain the predicted ee value of 93.4%, which aligns with the experimental observations.

Moreover, we have provided the detailed derivations in ESI and added the sentence “The detailed derivations for the computed ee value is provided in Part X of ESI.” in Page 3 Line 39 of the revised manuscript. In addition, the following sentences is provided in Part X of ESI:

The predicted ee value can be calculated using Boltzmann distribution with the equations:

$$\frac{[R]}{[S]} = \frac{e^{\frac{-G_R^\ddagger}{RT}}}{e^{\frac{-G_S^\ddagger}{RT}}} = e^{\Delta G^\ddagger / RT} \quad (1)$$

$$ee\% = \frac{[S] - [R]}{[S] + [R]} \times 100\% = \frac{\frac{[S]}{[R]} - 1}{\frac{[S]}{[R]} + 1} \times 100\% \quad (2)$$

In the equations, the ΔG^\ddagger is the energy difference of the two enantioselective transition states, R and T represent the gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) and temperature of the reaction. As depicted in Fig. 1 of the main text, the energy barriers of R- and S-configured pathways are 12.5 and 10.5 kcal/mol, respectively. Based on the equation (1), the energy difference (ΔG^\ddagger) between TS2R and TS2S is 2.0 kcal/mol, the value of $[R]/[S]$ is 29.68. Then, we can obtain the predicted ee value by equation (2), which is calculated to be 93.4%.

Part 3: Test of different methods and solvation model

Table S1. Text of different methods and solvation models involved in rate-determining step

	M06-2X/6-31G(d, p)		B3LYP/6-31G(d, p)		ω B97X-D/6-31G(d, p)	
	IEF-PCM	SMD	IEF-PCM	SMD	IEF-PCM	SMD
CBA+React	0.0	0.0	0.0	0.0	0.0	0.0
M1	-7.5	1.0	4.0	5.1	-7.0	-4.7
TS1	5.2	13.6	18.4	18.7	5.6	8.2

Part 4: Energies and Cartesian coordinates of all the stationary points

1. Energies of all the stationary points

	G (a.u.)	G-correct (a.u.)	Imaginary frequency (cm ⁻¹)
M06-2X/IEF-PCM			
React	-614.483551	0.17387	–
CBA	-8534.802728	0.594153	–
M1	-9149.292179	0.796498	–
TS1	-9149.269168	0.794448	-540.37
M2	-9149.281698	0.79447	–
M2A	-9149.238396	0.793563	–
[‡]M2A	-9149.231452	0.788005	–
TS2R	-9149.272255	0.791362	-764.92
TS2S	-9149.275412	0.791753	-1072.96
PR	-614.495606	0.172963	–
PS	-614.496156	0.172246	–
M06-2X/SMD			
React	-614.494796	0.174449	–
CBA	-8534.846677	0.594199	–
M1	-9149.339893	0.797996	–
TS1	-9149.319849	0.793057	-765.11
B3LYP/IEF-PCM			
React	-614.74174	0.170719	–
CBA	-8535.713393	0.584238	–
M1	-9150.448754	0.776059	–
TS1	-9150.425771	0.772089	-922.48
B3LYP/SMD			
React	-614.753221	0.170519	–
CBA	-8535.757251	0.583698	–
M1	-9150.502321	0.775004	–
TS1	-9150.480639	0.776572	-945.95
ω B97X-D/IEF-PCM			
React	-614.542954	0.173076	–
CBA	-8534.920894	0.596835	–
M1	-9149.475032	0.798957	–
TS1	-9149.459857	0.792482	-985.37
ω B97X-D/SMD			
React	-614.554004	0.173807	–
CBA	-8534.964805	0.596816	–
M1	-9149.526292	0.797025	–

TS1	-9149.505806	0.79095	-1059.80
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2. Cartesian coordinates of all the stationary points

M06-2X/IEF-PCM

React

C	-2.94975100	-0.26932800	-1.08036600
C	-1.82650300	0.55244900	-1.11981600
C	-1.01776300	0.70372700	0.01065700
C	-1.35636500	0.02072400	1.18624200
C	-2.47826900	-0.79964600	1.22165700
C	-3.27930600	-0.94755900	0.08992600
H	-3.56949600	-0.37541900	-1.96489900
H	-1.57562200	1.09072700	-2.02878000
H	-0.73284400	0.11942500	2.06931000
H	-2.72756300	-1.32706800	2.13675200
H	-4.15604900	-1.58592000	0.12251400
C	0.18406000	1.55404700	-0.06184000
C	1.09822400	1.72761100	-1.22579800
C	1.08580800	2.03294700	1.02545200
C	1.62505600	1.07706400	0.01497500
H	1.47151200	2.72219500	-1.46575700
H	0.92606700	1.07627600	-2.07866300
H	1.44369800	3.06093600	0.98764700
H	0.91849500	1.63744300	2.02325200
C	1.87294100	-0.34225600	0.27453500
O	1.92129800	-0.83467400	1.38206600
O	1.97813000	-1.04956700	-0.86002700
C	2.10694600	-2.46199100	-0.67706700
H	2.17886100	-2.88565400	-1.67647700
H	3.00363200	-2.68955200	-0.09804400
H	1.23340500	-2.85620200	-0.15452000

2a

C	3.75743700	1.38788400	-0.25655600
C	2.40364300	1.29249500	0.03694700
C	1.78792800	0.03824100	0.14557000
C	2.55531400	-1.11515100	-0.04675900
C	3.91265300	-1.01865000	-0.34054900
C	4.51614100	0.23175700	-0.44563700
H	4.22506700	2.36376700	-0.33984000
H	1.81285600	2.19226000	0.18514400
H	2.08240800	-2.09007100	0.03590800
H	4.49858600	-1.92028400	-0.48789300
H	5.57422300	0.30758000	-0.67462600

C	0.36471400	-0.07723400	0.45729200
C	-0.63157500	0.78929300	0.70092700
C	-0.51089100	-1.30352300	0.64192300
C	-1.66475000	-0.30278500	0.93075100
H	-0.71601600	1.87012100	0.73516900
H	-0.67139600	-1.91167300	-0.25143200
H	-0.25195600	-1.94456400	1.48938300
H	-2.08355700	-0.33976300	1.94113100
C	-2.78434800	-0.29219500	-0.08058800
O	-2.82217700	-0.93193600	-1.10545500
O	-3.74025100	0.57719600	0.27969500
C	-4.82174200	0.71212800	-0.64671100
H	-5.31913100	-0.24862300	-0.79165000
H	-5.50549000	1.43428000	-0.20545500
H	-4.45330800	1.07133800	-1.60941900

CBA

C	-2.12222500	2.00616500	-0.56894100
C	-3.22001500	2.74615300	-0.11297300
C	-4.36280100	2.08879700	0.30790200
C	-4.42788400	0.69968000	0.30499200
C	-3.31971100	-0.05743900	-0.08167600
C	-2.16337800	0.62260300	-0.49786900
C	-1.38775600	4.23848400	-0.29151200
C	-2.91735700	4.22120400	-0.12052400
H	-5.33001100	0.19479200	0.63289900
H	-0.90745300	4.15349200	0.68846800
H	-1.01325200	5.14167300	-0.77940400
H	-3.43238000	4.71856400	-0.95096400
C	-1.07160300	2.95831200	-1.11547800
C	0.41154700	2.64252200	-1.10425800
C	-1.29188600	3.23658300	-2.63097400
C	1.03468200	3.27230700	-2.18468700
C	1.17506700	1.91185700	-0.21036100
C	0.01698600	3.89955100	-3.10017100
H	-1.42384700	2.28053700	-3.14806200
H	-2.17922600	3.84849400	-2.81090400
C	2.41437500	3.21866800	-2.29601200
C	2.56878700	1.82403000	-0.31949800
H	-0.00236700	4.98811300	-2.96934500
C	3.17984300	2.51912500	-1.36954100
H	4.25961100	2.49060400	-1.46800700
H	-3.25100400	4.70564300	0.80072700
H	0.24209400	3.70579800	-4.15187100

Br	-5.84150700	3.09716100	0.91828000
C	-3.35600100	-1.53977500	0.04074000
C	-3.66354400	-2.09064900	1.29252500
C	-3.08646700	-2.39430300	-1.04903100
C	-3.67131600	-3.46357300	1.49787600
H	-3.87265700	-1.42181800	2.12288300
C	-3.10041300	-3.80354900	-0.84040900
C	-2.82505600	-1.90149600	-2.37908100
C	-3.38567600	-4.33987100	0.44503700
H	-3.89382700	-3.86418800	2.48213300
C	-2.82534500	-4.69141900	-1.92666400
C	-2.57244700	-2.74607300	-3.40675700
H	-2.84551000	-0.83095900	-2.55221600
C	-3.37696000	-5.76783200	0.62996600
C	-2.82499300	-6.09731300	-1.71713400
C	-2.55329900	-4.17258100	-3.21996700
H	-2.38149300	-2.35564000	-4.40217700
C	-3.10836100	-6.60512100	-0.39977400
H	-3.59224300	-6.15723000	1.62057900
C	-2.55055900	-6.94811600	-2.79419900
C	-2.28565800	-5.05649600	-4.27129900
H	-3.10318700	-7.68104700	-0.25127300
C	-2.28349600	-6.43107700	-4.05775300
H	-2.54850000	-8.02195000	-2.63127800
H	-2.07848200	-4.65552300	-5.25919100
H	-2.07266400	-7.10435300	-4.88195800
C	3.37552500	1.05374900	0.66230700
C	3.22266100	1.34004200	2.02168700
C	4.30078500	0.06975600	0.25314400
C	3.99713100	0.70942100	2.98304100
H	2.48331700	2.07400700	2.32568100
C	5.11129900	-0.56281900	1.23848600
C	4.43846200	-0.35771500	-1.11807200
C	4.96253100	-0.23161100	2.61285100
H	3.86066800	0.95037700	4.03300200
C	6.08050700	-1.54088600	0.85242700
C	5.35263000	-1.28963900	-1.47978900
H	3.77424200	0.06264200	-1.86445000
C	5.80412100	-0.87801200	3.58655400
C	6.90424700	-2.15773300	1.83378000
C	6.22253800	-1.90424100	-0.51304300
H	5.43334500	-1.60360600	-2.51656900
C	6.73271100	-1.79110900	3.21604800
H	5.67483900	-0.61107100	4.63145500

C	7.85338700	-3.10476800	1.43206700
C	7.18147100	-2.85823500	-0.87370200
H	7.36519300	-2.27081400	3.95756000
C	7.99050200	-3.44913300	0.09098800
H	8.48308900	-3.57202200	2.18382300
H	7.28418600	-3.13451300	-1.91919700
H	8.73019300	-4.18647500	-0.20325600
O	-1.02295600	-0.12437000	-0.79495200
O	0.50894100	1.17983500	0.78224200
P	0.11485600	-0.30656500	0.33208000
O	1.17365000	-1.20251800	-0.13527200
Br	3.26007700	4.09880300	-3.74156700
N	-0.75524100	-0.76253700	1.71571400
H	-1.30901200	-1.61967400	1.64661200
S	-0.63730800	-0.22641100	3.27599800
O	-1.22798800	-1.25765200	4.10068500
O	0.66133600	0.34465700	3.53627000
C	-1.83900900	1.17674400	3.30684600
F	-3.04346800	0.72737800	2.98508000
F	-1.47657000	2.12058400	2.45519600
F	-1.85975700	1.66510200	4.53547200

M1

C	2.62164900	2.57791800	0.02408100
C	3.69800700	3.08941000	-0.70536300
C	4.69341100	2.23309500	-1.14202400
C	4.63387900	0.87345700	-0.86345300
C	3.53866700	0.33341600	-0.17980700
C	2.51622500	1.20928300	0.22000100
C	2.07471000	4.80697600	-0.54926600
C	3.54831600	4.57151300	-0.92526900
H	5.43776500	0.21762000	-1.17969100
H	1.44155400	4.61582700	-1.42191200
H	1.87017400	5.81847800	-0.18843100
H	4.23473600	5.13110700	-0.27822300
C	1.76938000	3.72872600	0.52739000
C	0.28159600	3.59418000	0.77379000
C	2.24974800	4.21217900	1.92704900
C	-0.10638100	4.43528500	1.81950500
C	-0.67131100	2.83709900	0.11456000
C	1.09384000	5.07591300	2.46478200
H	2.38111100	3.33711700	2.57253400
H	3.20343000	4.74339400	1.87338600
C	-1.44953700	4.54376100	2.13985400

C	-2.03284800	2.93445100	0.42597700
H	1.18314500	6.12385500	2.15388600
C	-2.40928300	3.81665800	1.44420900
H	-3.45917000	3.91658400	1.69863400
H	3.77651600	4.85236400	-1.95660500
H	1.02438700	5.06833400	3.55558900
Br	6.15775500	2.93473800	-2.11340000
C	3.49781200	-1.13221200	0.07476300
C	3.70277100	-1.99597400	-1.00644600
C	3.32746700	-1.66647700	1.37057400
C	3.70751700	-3.37305400	-0.84220600
H	3.83216200	-1.57203200	-1.99743300
C	3.31421500	-3.08071300	1.53703500
C	3.19652200	-0.84367100	2.54856000
C	3.50284400	-3.93858800	0.41948100
H	3.85103700	-4.02378200	-1.70052900
C	3.09159100	-3.65115400	2.82976400
C	3.00718900	-1.38673600	3.77564900
H	3.26413600	0.23381000	2.44490500
C	3.44077500	-5.36504100	0.60945600
C	3.01550800	-5.06223600	2.98522600
C	2.92315700	-2.81040100	3.96150300
H	2.91329100	-0.74715300	4.64882500
C	3.19795300	-5.90095500	1.82896100
H	3.57339800	-6.00197600	-0.26109500
C	2.76416300	-5.59693000	4.25350100
C	2.67903100	-3.38421400	5.21490400
H	3.13716900	-6.97768300	1.95988400
C	2.59677000	-4.76515900	5.35643200
H	2.70157600	-6.67537000	4.36832600
H	2.55192500	-2.73557800	6.07710000
H	2.40409500	-5.19735500	6.33301900
C	-3.06695700	2.17895400	-0.33051300
C	-3.17344400	2.39829300	-1.70596600
C	-3.97064400	1.30998200	0.31230800
C	-4.18550700	1.81462500	-2.45369200
H	-2.45424100	3.05345400	-2.18852500
C	-5.02770200	0.73364200	-0.44635100
C	-3.85708900	0.95907500	1.70664600
C	-5.14030800	0.99758100	-1.83883300
H	-4.25550400	2.00767700	-3.52041200
C	-5.98639200	-0.11595500	0.18949200
C	-4.75535900	0.13828600	2.30155700
H	-3.01382000	1.34410900	2.26909500

C	-6.23439100	0.41885000	-2.57631200
C	-7.05948900	-0.67028200	-0.56110100
C	-5.86279400	-0.41983600	1.57106100
H	-4.64688700	-0.12572600	3.34970500
C	-7.15443000	-0.36746900	-1.96660200
H	-6.30603100	0.63357300	-3.63878600
C	-7.98212200	-1.50557500	0.07950500
C	-6.80530200	-1.26080600	2.17384400
H	-7.97762900	-0.79690900	-2.53076200
C	-7.85441700	-1.79632400	1.43391400
H	-8.80122800	-1.92749900	-0.49611000
H	-6.70577200	-1.49345600	3.23029300
H	-8.57716500	-2.44708700	1.91534400
O	1.35182300	0.68458000	0.78172100
O	-0.24077800	1.89180000	-0.82359400
P	0.06135100	0.45293400	-0.16560700
O	-1.02261200	-0.18523400	0.58404100
Br	-1.97489900	5.67830300	3.55908300
N	0.58112100	-0.37101700	-1.54458900
H	0.70168100	-1.38724300	-1.37625900
S	1.21882100	0.16928800	-2.95950000
O	1.77296700	1.49701000	-2.83460700
O	1.96503500	-0.93402100	-3.53230700
C	-0.28363100	0.35642800	-4.01462300
F	-1.20672100	1.05399100	-3.37211900
F	-0.76818900	-0.84092100	-4.31495900
F	0.06281900	0.98412700	-5.12592700
C	-4.14813900	-3.75377700	-1.04219200
C	-3.06045600	-4.62221900	-1.05870200
C	-1.86124700	-4.24089700	-1.66956400
C	-1.77860200	-2.98025000	-2.27419600
C	-2.86291000	-2.11118600	-2.24739800
C	-4.05215300	-2.49690900	-1.63309600
H	-5.07542200	-4.05796100	-0.56603200
H	-3.14292000	-5.60527500	-0.60513500
H	-0.86367000	-2.68119000	-2.77458800
H	-2.77999700	-1.12820400	-2.70307400
H	-4.90207400	-1.82493200	-1.62687400
C	-0.68704600	-5.13037000	-1.62507500
C	-0.36476100	-6.17163500	-0.60129500
C	0.68556000	-4.88936100	-2.15367700
C	0.49474800	-4.95422800	-0.67500700
H	0.06814600	-7.11590000	-0.92913800
H	-1.03058700	-6.24047400	0.25498100

H	1.21684900	-5.71897700	-2.61908600
H	0.90367800	-3.91110100	-2.57459500
C	0.46626900	-3.78498800	0.19699500
O	0.68028500	-2.64929500	-0.19567500
O	0.12523500	-4.06531300	1.44800400
C	-0.10350400	-2.92088600	2.28956400
H	-0.19104000	-3.31786100	3.29963900
H	0.73266300	-2.22305100	2.21633700
H	-1.01630300	-2.41186500	1.97430800

TS1

C	4.06354200	-0.46442900	-0.02919400
C	5.07123500	-1.03566100	-0.80833500
C	4.99462800	-2.38098200	-1.13059100
C	3.91425900	-3.15607300	-0.72373700
C	2.86822900	-2.58766900	0.00966700
C	2.96917200	-1.22704100	0.34193600
C	5.35820400	1.31482700	-0.89008800
C	6.09482400	-0.00271900	-1.20015000
H	3.86722600	-4.20532000	-0.99499400
H	4.74185000	1.59774500	-1.74929300
H	6.02953600	2.14644200	-0.65999600
H	7.00671000	-0.11421800	-0.60066700
C	4.42014100	0.97352600	0.30470800
C	3.36816200	2.05266900	0.51328100
C	5.20429900	1.08217500	1.64322300
C	3.85495000	3.01764900	1.40083700
C	2.10836200	2.22240800	-0.03955900
C	5.16637500	2.58051900	1.99960800
H	4.67062200	0.51022800	2.40953000
H	6.21737300	0.68022000	1.55904000
C	3.11032000	4.15946600	1.64679600
C	1.35373900	3.38255700	0.18259600
H	5.99981200	3.13240800	1.54837300
C	1.87804800	4.36095700	1.02919700
H	1.31501900	5.26946700	1.21552200
H	6.38584200	-0.09323100	-2.24988600
H	5.20330300	2.76553400	3.07616000
Br	6.38159700	-3.17208600	-2.14896600
C	1.62780300	-3.35926800	0.29253700
C	0.98710600	-3.97655800	-0.78605800
C	1.02485900	-3.39175300	1.56707500
C	-0.26927200	-4.54869900	-0.65291300
H	1.45077800	-3.92963900	-1.76730000

C	-0.26391000	-3.98088700	1.70800700
C	1.66772400	-2.86790100	2.74696300
C	-0.92291300	-4.54677800	0.58233600
H	-0.77041700	-4.96468700	-1.52154700
C	-0.91168300	-3.99554800	2.98375100
C	1.05963200	-2.89485200	3.95635000
H	2.66520700	-2.45196300	2.65086600
C	-2.24048200	-5.10782700	0.74666200
C	-2.21062700	-4.56003600	3.12086500
C	-0.26021000	-3.44556800	4.11974800
H	1.56305400	-2.49866600	4.83361800
C	-2.85332500	-5.11730200	1.95626700
H	-2.73241000	-5.51486000	-0.13128200
C	-2.82851800	-4.55430200	4.37656600
C	-0.91048200	-3.46438500	5.35872500
H	-3.84430700	-5.54818300	2.07223300
C	-2.18324400	-4.01161900	5.48319600
H	-3.82135300	-4.98340900	4.47853100
H	-0.40810300	-3.04377700	6.22519300
H	-2.67573800	-4.01732800	6.45020000
C	0.07027800	3.57975100	-0.55459500
C	0.15242400	3.78352300	-1.93500300
C	-1.18983200	3.56128100	0.07350200
C	-0.98212300	3.97786400	-2.70775400
H	1.13108600	3.78207300	-2.40539400
C	-2.35901000	3.73911400	-0.72167600
C	-1.35126900	3.33780400	1.48972800
C	-2.25111400	3.95340400	-2.12189300
H	-0.89125500	4.13512200	-3.77876300
C	-3.65444800	3.69143900	-0.11502900
C	-2.57900200	3.28711200	2.06018200
H	-0.46208800	3.17401300	2.08793500
C	-3.45086300	4.12526300	-2.90064400
C	-4.82290600	3.86797200	-0.90733500
C	-3.77895900	3.46043400	1.28169900
H	-2.68122600	3.10557400	3.12623700
C	-4.67573000	4.08509000	-2.32386200
H	-3.34743800	4.28801100	-3.96972000
C	-6.08056600	3.82603800	-0.29155100
C	-5.05514500	3.41272000	1.85655500
H	-5.57438400	4.21613400	-2.91998600
C	-6.19290500	3.60052000	1.07733300
H	-6.97077300	3.96926200	-0.89802500
H	-5.14701200	3.23315000	2.92387300

H	-7.17444800	3.56413900	1.53913300
O	1.93695700	-0.60493200	1.02592000
O	1.53118700	1.17722900	-0.75624900
P	0.75074200	0.10658400	0.18857600
O	-0.21169300	0.66012200	1.16357800
Br	3.78568100	5.45774400	2.84780100
N	0.08324000	-0.92725500	-0.87650300
H	-1.35088300	-1.05243600	-0.61011300
S	0.41473600	-1.14940100	-2.42407700
O	1.83432700	-1.15082400	-2.73878800
O	-0.43471900	-2.22826100	-2.91262800
C	-0.29356800	0.37643000	-3.23516500
F	0.66898600	1.23291400	-3.54102000
F	-1.15977700	0.96446800	-2.41252900
F	-0.92966200	0.02504700	-4.34691800
C	-7.35291600	0.01576100	-0.20278800
C	-5.98898100	0.20072400	-0.01008900
C	-5.17082900	-0.88950300	0.30312700
C	-5.72432900	-2.17047800	0.42346300
C	-7.08562500	-2.35039100	0.21281100
C	-7.90044800	-1.26037400	-0.09631000
H	-7.98256300	0.86864200	-0.43457100
H	-5.55928700	1.19583200	-0.07794200
H	-5.09418900	-3.02365600	0.65509700
H	-7.51468400	-3.34322700	0.29349400
H	-8.96425700	-1.40918200	-0.25034900
C	-3.74349900	-0.61560800	0.54748300
C	-2.99639300	0.37144700	-0.20899900
C	-2.75456000	-1.56682400	1.01446500
C	-2.56769200	-1.13031100	-0.48416600
H	-2.17525200	0.90424500	0.26800600
H	-3.51633600	0.88934000	-1.01034000
H	-1.91320400	-1.19458600	1.59690900
H	-3.06646400	-2.58738000	1.21782200
C	-3.10389700	-1.93751100	-1.62089100
O	-3.37687300	-3.11135500	-1.55522600
O	-3.18291200	-1.18167900	-2.71480100
C	-3.47741600	-1.88756900	-3.92700600
H	-3.52017200	-1.12819700	-4.70443500
H	-2.67524800	-2.59961100	-4.12738300
H	-4.43209100	-2.40796300	-3.83833600
M2			
C	3.83278200	0.11177200	0.06833000

C	4.99292200	-0.35980500	-0.55399600
C	5.13189800	-1.71378900	-0.80615100
C	4.12239800	-2.60815300	-0.47452900
C	2.92951900	-2.14614100	0.08614900
C	2.79291300	-0.77083400	0.33070200
C	5.01036700	2.00162900	-0.73157300
C	5.92431600	0.77371500	-0.89450200
H	4.24372900	-3.66676700	-0.67690000
H	4.45685300	2.17117400	-1.66065500
H	5.55042700	2.91805200	-0.47950600
H	6.77672300	0.79894800	-0.20474000
C	4.00210200	1.59229800	0.37863400
C	2.83179800	2.55348200	0.45814800
C	4.64400700	1.81826300	1.77876100
C	3.12123500	3.58349300	1.35717800
C	1.62086300	2.54601000	-0.21212300
C	4.41655300	3.31329300	2.07730300
H	4.10420100	1.21268500	2.51425100
H	5.69688700	1.52564100	1.80104500
C	2.22445600	4.62917100	1.49985000
C	0.68238100	3.57716200	-0.03998600
H	5.22221300	3.93943900	1.67532900
C	1.01943000	4.63963400	0.80320700
H	0.32370900	5.46142700	0.93539900
H	6.33052100	0.67284100	-1.90416100
H	4.34215400	3.53179800	3.14570000
Br	6.71915500	-2.34621400	-1.62510100
C	1.80603600	-3.09631500	0.30934000
C	1.36402300	-3.84697300	-0.78458900
C	1.18513500	-3.26395500	1.56444900
C	0.28906400	-4.71691900	-0.68035600
H	1.84847100	-3.70438600	-1.74529200
C	0.10224400	-4.18168700	1.68298400
C	1.62695400	-2.57407000	2.75153400
C	-0.36178300	-4.89681900	0.54484500
H	-0.05630900	-5.25942200	-1.55582200
C	-0.51682900	-4.40431900	2.95352400
C	1.03831400	-2.78393800	3.95292600
H	2.45911100	-1.88340300	2.66968000
C	-1.47930600	-5.79497900	0.68755100
C	-1.59571400	-5.32462000	3.07343800
C	-0.05473400	-3.70867400	4.10266500
H	1.39131800	-2.25945500	4.83605500
C	-2.06728900	-6.00122700	1.89194500

H	-1.83126900	-6.31846700	-0.19715900
C	-2.17377100	-5.54276100	4.33102600
C	-0.66339000	-3.94977000	5.34031300
H	-2.90174900	-6.68948100	1.99095200
C	-1.70780300	-4.86329500	5.45301400
H	-2.99272400	-6.25077900	4.42001700
H	-0.30526800	-3.41792500	6.21706100
H	-2.16364700	-5.04466100	6.42084100
C	-0.63342200	3.49294300	-0.72890600
C	-0.64786500	3.33073800	-2.11640100
C	-1.84918100	3.48097000	-0.01316700
C	-1.83294700	3.15160000	-2.81447000
H	0.29590100	3.32437200	-2.65017600
C	-3.06825600	3.29950100	-0.72731600
C	-1.91385500	3.58456400	1.42399500
C	-3.05702400	3.12887500	-2.13928200
H	-1.81433600	3.01340900	-3.89139500
C	-4.31545800	3.25577400	-0.02567900
C	-3.09727500	3.57455400	2.08395200
H	-0.98886200	3.65787900	1.98321000
C	-4.30110000	2.91233100	-2.83171300
C	-5.52955200	3.03491500	-0.73378100
C	-4.34567400	3.41153600	1.38715500
H	-3.12027400	3.66511000	3.16685800
C	-5.47905000	2.86398100	-2.16351500
H	-4.27008000	2.78333900	-3.90989200
C	-6.73573900	2.98377500	-0.02479600
C	-5.57299800	3.35392300	2.05849400
H	-6.41154100	2.69685500	-2.69489400
C	-6.75568700	3.14380300	1.35682900
H	-7.66041600	2.81472000	-0.56892600
H	-5.59040400	3.47418500	3.13832500
H	-7.69923000	3.10055500	1.89066300
O	1.58276100	-0.29304800	0.80255000
O	1.31391300	1.45947800	-1.01271500
P	0.48413500	0.26258800	-0.27272300
O	-0.69819700	0.70125700	0.49735200
Br	2.63385000	6.04723000	2.68822000
N	0.17239600	-0.79799700	-1.43625200
H	-2.50507100	-1.59193100	-3.28492100
S	0.84256900	-1.18771400	-2.79589100
O	2.30135900	-1.13433200	-2.84515700
O	0.17633600	-2.38034100	-3.32390700
C	0.30263600	0.11919900	-3.98150500

F	0.94303900	1.26374600	-3.77600200
F	-1.01068000	0.33982900	-3.85972700
F	0.54641700	-0.28688300	-5.22356200
C	-3.56223500	0.19821000	2.97976500
C	-3.36712600	0.07688800	1.61894500
C	-3.06389000	-1.19295100	1.07134000
C	-2.94233300	-2.32914000	1.90648600
C	-3.13129500	-2.19301100	3.26797900
C	-3.44498400	-0.93392800	3.79418200
H	-3.79393500	1.16430900	3.41343800
H	-3.40733100	0.94295500	0.96554000
H	-2.70333900	-3.29591700	1.47027300
H	-3.03532400	-3.05102500	3.92419300
H	-3.59469900	-0.83353100	4.86486600
C	-2.82690800	-1.30391800	-0.30163700
C	-3.00239900	-0.36327200	-1.43410500
C	-2.47965100	-2.44085500	-1.18328000
C	-3.08173800	-1.61696200	-2.36357900
H	-2.06570600	0.18097400	-1.60324100
H	-3.84094000	0.33773400	-1.38927700
H	-1.38484000	-2.47640000	-1.29949300
H	-2.87180500	-3.43075400	-0.93873000
C	-4.52481700	-1.99660200	-2.56596700
O	-5.30598000	-2.10727100	-1.64584300
O	-4.84124400	-2.18618800	-3.84369100
C	-6.20836400	-2.54169600	-4.08942900
H	-6.29356000	-2.66070700	-5.16683200
H	-6.45171200	-3.47360700	-3.57695800
H	-6.87096000	-1.75118200	-3.73374900

M2A

C	0.28575900	3.48104700	0.39000900
C	0.88294500	4.62561100	-0.14287900
C	2.20889200	4.58225900	-0.53592100
C	2.95194900	3.41531400	-0.40290300
C	2.34952500	2.24734400	0.07417300
C	0.99100500	2.28782000	0.42298200
C	-1.44960200	5.03513000	-0.00242300
C	-0.10721400	5.75707200	-0.23288600
H	3.99908100	3.39877900	-0.68576600
H	-1.82381600	4.64853200	-0.95567900
H	-2.21853000	5.67532200	0.43842900
H	0.09196500	6.51354100	0.53608400
C	-1.09276700	3.83301700	0.91413700

C	-2.21574700	2.81934900	0.98998800
C	-1.02041800	4.29344900	2.40002600
C	-3.04341200	3.10563400	2.07781800
C	-2.52123200	1.75887100	0.15257200
C	-2.47203500	4.22451600	2.90799000
H	-0.40627300	3.57688900	2.95657100
H	-0.56684700	5.28265600	2.50270300
C	-4.19783600	2.36431700	2.26679300
C	-3.68537600	0.99829300	0.33527500
H	-3.01812100	5.15745800	2.72191400
C	-4.53020700	1.32869100	1.40072800
H	-5.44353300	0.76288500	1.55258900
H	-0.05520300	6.26056300	-1.20177700
H	-2.54295900	4.01923600	3.97938300
Br	3.00675300	6.13515100	-1.26434900
C	3.15328500	0.99896700	0.16998600
C	3.81149400	0.54361000	-0.97928000
C	3.32072900	0.30880900	1.38983200
C	4.58802900	-0.60468900	-0.95792400
H	3.66671500	1.08038500	-1.91192300
C	4.13376900	-0.86217900	1.41611000
C	2.74921100	0.76480900	2.63388900
C	4.74449800	-1.33555300	0.22426900
H	5.05684700	-0.95687100	-1.87252900
C	4.37204400	-1.54933300	2.64785900
C	3.00239300	0.13003000	3.80434700
H	2.12835100	1.65411200	2.62646300
C	5.50516300	-2.55675800	0.26291800
C	5.17280900	-2.72499000	2.66876600
C	3.83154700	-1.04469600	3.86013100
H	2.58274900	0.50676300	4.73307700
C	5.70334900	-3.22581700	1.42612500
H	5.90558800	-2.93407000	-0.67495900
C	5.42523600	-3.35983400	3.89203400
C	4.11339900	-1.70273700	5.06223300
H	6.28412400	-4.14387600	1.44520800
C	4.90580000	-2.84821300	5.07577200
H	6.03952300	-4.25589200	3.90392300
H	3.70972300	-1.30634900	5.98965700
H	5.11758300	-3.34486600	6.01720900
C	-4.03646700	-0.09011800	-0.61501400
C	-4.15375300	0.23225200	-1.97024000
C	-4.26442100	-1.41332900	-0.19012100
C	-4.52222900	-0.71762500	-2.90969500

H	-3.95049100	1.25127900	-2.28471400
C	-4.66025100	-2.38703800	-1.15053500
C	-4.07906200	-1.83790500	1.17570200
C	-4.79604000	-2.03240900	-2.51968600
H	-4.60540700	-0.44255400	-3.95714300
C	-4.91788900	-3.73376000	-0.74454800
C	-4.32056700	-3.11504400	1.55742400
H	-3.71550800	-1.11508100	1.89775500
C	-5.20348700	-3.03597000	-3.46862700
C	-5.32546500	-4.70305100	-1.70125800
C	-4.76331200	-4.11006200	0.61619200
H	-4.16824200	-3.41741200	2.58981200
C	-5.45987400	-4.30736600	-3.07930400
H	-5.29930200	-2.74475300	-4.51075500
C	-5.57914800	-6.01365200	-1.28064800
C	-5.02445400	-5.43170700	0.99595300
H	-5.76794300	-5.05745600	-3.80233000
C	-5.43062600	-6.37238300	0.05512100
H	-5.89332400	-6.75124400	-2.01390600
H	-4.90572700	-5.71580900	2.03780200
H	-5.63199700	-7.39305400	0.36414800
O	0.34071900	1.10820600	0.74448500
O	-1.62709900	1.43332000	-0.85609500
P	-0.47171200	0.35195200	-0.47026200
O	-0.96471900	-0.92548800	0.09111900
Br	-5.32357800	2.77306400	3.73410700
N	0.47057700	0.24005300	-1.76774800
H	2.64370500	-0.96867300	-3.31595600
S	0.74737000	1.21285300	-2.95755600
O	0.50955800	2.63538500	-2.73680300
O	2.01883700	0.82923500	-3.59553600
C	-0.50166400	0.71889400	-4.21325000
F	-1.73018800	0.84795500	-3.71926800
F	-0.31565200	-0.54722700	-4.57093000
F	-0.38523800	1.49194300	-5.28880100
C	2.27164700	-4.55393100	3.61411600
C	2.46931200	-4.52298800	2.24936000
C	1.87918200	-3.48637200	1.48208300
C	1.08761100	-2.48470000	2.10709500
C	0.88400500	-2.54220400	3.47080700
C	1.48345800	-3.56439800	4.21667600
H	2.72977700	-5.32615800	4.22074900
H	3.07875300	-5.27307400	1.75378800
H	0.62668600	-1.70524800	1.50237400

H	0.28119800	-1.78906200	3.96459800
H	1.33589900	-3.59222900	5.29213300
C	2.10134900	-3.40911200	0.10932700
C	2.83162600	-4.25879100	-0.88789300
C	1.74820900	-2.36172800	-0.88662100
C	2.64829000	-3.10362000	-1.85137100
H	2.24609900	-5.16360200	-1.11697500
H	3.84157300	-4.57262100	-0.60030300
H	0.66837400	-2.33975900	-1.10356600
H	2.01333600	-1.34075800	-0.57930300
C	3.25685100	-2.81227300	-3.00332300
O	3.15983400	-1.69116000	-3.72616700
O	4.06886000	-3.74049900	-3.55510800
C	5.00342900	-3.30249000	-4.53830700
H	5.57863000	-4.18781300	-4.80561900
H	4.49560200	-2.90734500	-5.41906700
H	5.67621700	-2.53930800	-4.13450700

^TM2A

C	-2.62173800	-2.57747200	0.02384400
C	-3.69798800	-3.08910600	-0.70565800
C	-4.69326600	-2.23287100	-1.14275800
C	-4.63375600	-0.87315700	-0.86451800
C	-3.53867200	-0.33301000	-0.18076200
C	-2.51632000	-1.20879800	0.21944500
C	-2.07479800	-4.80669200	-0.54880400
C	-3.54833800	-4.57128300	-0.92508400
H	-5.43757800	-0.21736700	-1.18101700
H	-1.44150800	-4.61576100	-1.42140000
H	-1.87033100	-5.81810800	-0.18768300
H	-4.23485900	-5.13062400	-0.27792400
C	-1.76963700	-3.72818200	0.52764300
C	-0.28189500	-3.59365500	0.77431700
C	-2.25029700	-4.21125700	1.92732900
C	0.10583200	-4.43458800	1.82027000
C	0.67116800	-2.83676200	0.11511400
C	-1.09456600	-5.07497000	2.46547000
H	-2.38169400	-3.33602600	2.57257700
H	-3.20401600	-4.74240300	1.87362900
C	1.44892500	-4.54311100	2.14085100
C	2.03265800	-2.93418700	0.42675200
H	-1.18390400	-6.12297000	2.15478200
C	2.40884700	-3.81623800	1.44520300
H	3.45868400	-3.91622700	1.69980700

H	-3.77642600	-4.85246900	-1.95635100
H	-1.02532400	-5.06716200	3.55628800
Br	-6.15751500	-2.93481300	-2.11406400
C	-3.49781000	1.13260900	0.07377900
C	-3.70216700	1.99641700	-1.00749100
C	-3.32796500	1.66678900	1.36968300
C	-3.70671600	3.37349700	-0.84320000
H	-3.83120600	1.57251800	-1.99854700
C	-3.31449800	3.08100500	1.53620400
C	-3.19769900	0.84390000	2.54768300
C	-3.50247400	3.93895500	0.41859700
H	-3.84973100	4.02428900	-1.70156000
C	-3.09227700	3.65134800	2.82904600
C	-3.00881600	1.38687500	3.77488400
H	-3.26549600	-0.23356100	2.44393900
C	-3.44009700	5.36538500	0.60864700
C	-3.01589200	5.06240200	2.98458500
C	-2.92454500	2.81051200	3.96083100
H	-2.91545000	0.74723500	4.64807500
C	-3.19760700	5.90120100	1.82826200
H	-3.57215000	6.00238100	-0.26194800
C	-2.76495400	5.59699300	4.25298500
C	-2.68081000	3.38422600	5.21435900
H	-3.13655900	6.97790800	1.95923500
C	-2.59825500	4.76514500	5.35596300
H	-2.70213600	6.67541300	4.36787000
H	-2.55424000	2.73552800	6.07658600
H	-2.40588400	5.19726700	6.33264200
C	3.06691000	-2.17897300	-0.32981600
C	3.17342600	-2.39861800	-1.70522400
C	3.97071200	-1.31001300	0.31285700
C	4.18556400	-1.81521300	-2.45304400
H	2.45419200	-3.05382300	-2.18767700
C	5.02783400	-0.73392900	-0.44590300
C	3.85717600	-0.95885900	1.70713900
C	5.14043200	-0.99813700	-1.83833000
H	4.25553200	-2.00845300	-3.51973200
C	5.98656300	0.11573800	0.18978200
C	4.75552100	-0.13805200	2.30190900
H	3.01382500	-1.34366200	2.26962300
C	6.23454600	-0.41961300	-2.57591900
C	7.05967600	0.66989000	-0.56091900
C	5.86299500	0.41985800	1.57130500
H	4.64707100	0.12617500	3.35000600

C	7.15461100	0.36679800	-1.96636200
H	6.30614800	-0.63451100	-3.63836000
C	7.98236300	1.50523900	0.07953800
C	6.80556000	1.26086900	2.17393700
H	7.97782100	0.79610000	-2.53060900
C	7.85469500	1.79621100	1.43390400
H	8.80148900	1.92701600	-0.49615400
H	6.70605000	1.49370800	3.23034600
H	8.57748100	2.44701900	1.91521500
O	-1.35206100	-0.68393100	0.78134600
O	0.24081200	-1.89166100	-0.82333600
P	-0.06136100	-0.45258900	-0.16575000
O	1.02256500	0.18559700	0.58393100
Br	1.97391900	-5.67743600	3.56039100
N	-0.58091300	0.37083800	-1.54516200
H	-0.70061900	1.38725900	-1.37801500
S	-1.21807200	-0.17020400	-2.96008700
O	-1.77183800	-1.49802400	-2.83467900
O	-1.96449600	0.93262500	-3.53352000
C	0.28474000	-0.35726400	-4.01477600
F	1.20800500	-1.05408000	-3.37170500
F	0.76880800	0.84019100	-4.31557100
F	-0.06115300	-0.98566400	-5.12584300
C	-1.04719549	8.72601022	-5.89690574
C	-1.11583565	7.78441026	-4.86124170
C	-0.58721631	8.09032272	-3.59993242
C	0.01003917	9.33783685	-3.37428589
C	0.07867950	10.27943675	-4.40994997
C	-0.44993624	9.97352276	-5.67126040
H	-1.45080625	8.49243849	-6.85994395
H	-1.57185432	6.83190590	-5.03352756
H	0.41365018	9.57140847	-2.41124775
H	0.53469789	11.23194122	-4.23766403
H	-0.39752638	10.69245457	-6.46201338
C	-0.65585244	7.14872106	-2.56426966
C	-0.17710661	7.09490664	-1.10156448
C	-1.18240415	5.70784665	-2.42927249
C	-0.32469684	5.56305143	-1.15845680
H	-0.84868378	7.56458072	-0.41360346
H	0.79484712	7.48776632	-0.88739818
H	-2.23481425	5.65206621	-2.24428190
H	-0.98362492	5.03391823	-3.23624666
C	0.14908706	4.52281100	-0.43044876
O	-0.17537172	3.18141826	-0.80500453

O	0.89928476	4.74461116	0.60945017
C	1.39922291	3.64695470	1.37763774
H	1.51855409	3.94995681	2.39687755
H	0.70808948	2.83171382	1.32648211
H	2.34510474	3.33787009	0.98435125

TS2R

C	-3.94182900	0.07959100	-0.07806800
C	-5.06217200	-0.29933600	0.66374400
C	-5.20167200	-1.62187400	1.05061700
C	-4.22654000	-2.56179000	0.74490400
C	-3.06330500	-2.18772700	0.06190900
C	-2.94300800	-0.84706800	-0.33686600
C	-5.02333200	2.06897300	0.60625000
C	-5.94748700	0.88492500	0.94788600
H	-4.34988100	-3.59128800	1.06298300
H	-4.41624200	2.32206400	1.48122900
H	-5.56270400	2.96647500	0.29197400
H	-6.84194900	0.86303600	0.31342600
C	-4.08618700	1.52900000	-0.51160100
C	-2.89138600	2.44041100	-0.72852200
C	-4.78820700	1.64738900	-1.89427700
C	-3.19360500	3.39136600	-1.70900600
C	-1.65054600	2.46957600	-0.11323900
C	-4.52739000	3.09703800	-2.34549600
H	-4.30635600	0.95521900	-2.59274100
H	-5.84986200	1.39290900	-1.83810600
C	-2.27609300	4.38813600	-1.99652000
C	-0.71393400	3.47315900	-0.39551800
H	-5.29350600	3.78803700	-1.97329500
C	-1.05100300	4.44655300	-1.33790800
H	-0.34301700	5.23561700	-1.56928200
H	-6.28987800	0.89570100	1.98596400
H	-4.49358300	3.20882600	-3.43226100
Br	-6.73633200	-2.13933500	2.03220800
C	-1.95046800	-3.16572200	-0.08112300
C	-1.56131400	-3.86225900	1.06844500
C	-1.25138600	-3.38149700	-1.28889700
C	-0.48229800	-4.73292500	1.06307300
H	-2.08710600	-3.66924100	1.99881100
C	-0.12868900	-4.25952000	-1.29194800
C	-1.64172800	-2.77605200	-2.53845800
C	0.25660500	-4.94073100	-0.10453100
H	-0.18832000	-5.23669200	1.97937400

C	0.61757800	-4.47137500	-2.49440500
C	-0.93523500	-2.97948700	-3.67599000
H	-2.52876000	-2.15314300	-2.55838600
C	1.41188700	-5.80187700	-0.12999300
C	1.74069900	-5.34496000	-2.49808400
C	0.22885200	-3.82442900	-3.69685900
H	-1.24875900	-2.51391000	-4.60601400
C	2.12316300	-5.98941900	-1.26784000
H	1.69947400	-6.29920000	0.79228400
C	2.43428800	-5.56096900	-3.69411500
C	0.96114300	-4.05324900	-4.86703600
H	2.99270100	-6.64153600	-1.27645800
C	2.04994300	-4.91712300	-4.86524600
H	3.27907700	-6.24502000	-3.69857500
H	0.66005100	-3.55318400	-5.78318800
H	2.60167600	-5.09195000	-5.78302300
C	0.58415500	3.51926700	0.33489800
C	0.54854600	3.74848400	1.71295900
C	1.82298800	3.35215100	-0.31526300
C	1.71278300	3.85659700	2.45839700
H	-0.41626100	3.85095200	2.19995800
C	3.01973000	3.44533300	0.45144000
C	1.93205300	3.05512700	-1.72306100
C	2.96147200	3.71808000	1.84535900
H	1.66083600	4.04944900	3.52609800
C	4.29158600	3.26404600	-0.17877900
C	3.13680900	2.87155700	-2.31413800
H	1.01900800	2.94314400	-2.29613900
C	4.19032400	3.84675100	2.58547100
C	5.48957400	3.37691200	0.58089700
C	4.36383600	2.96999900	-1.56701600
H	3.19741400	2.63207800	-3.37190900
C	5.39461600	3.68837300	1.98460700
H	4.12691200	4.07475100	3.64620500
C	6.72249300	3.18094500	-0.05253300
C	5.61666200	2.77882600	-2.16182400
H	6.31591700	3.78911800	2.55229900
C	6.78284500	2.88267400	-1.40986500
H	7.63534000	3.26611800	0.53019800
H	5.66717800	2.54954700	-3.22241000
H	7.74635000	2.73299700	-1.88611600
O	-1.78852000	-0.41678300	-0.96970100
O	-1.27763300	1.41670400	0.72004300
P	-0.56960100	0.20068100	-0.09655000

O	0.49952300	0.58681200	-1.03602400
Br	-2.68555300	5.67745800	-3.32235400
N	-0.08820000	-0.83378800	1.06364700
H	1.68805700	-1.42097200	-1.75965800
S	-0.59230100	-1.00851000	2.56550300
O	-2.03373000	-0.90432800	2.74138800
O	0.12311600	-2.14083200	3.14374300
C	0.10634000	0.46593800	3.45998700
F	-0.75277100	1.47463200	3.46007200
F	1.23922600	0.85782700	2.88525800
F	0.35889000	0.11794700	4.71768500
C	3.49894400	-1.35781500	4.52622000
C	3.15171500	-1.70173700	3.23058300
C	3.52911900	-0.86546000	2.16211200
C	4.26393900	0.30992300	2.40333100
C	4.62443500	0.63416300	3.70184900
C	4.23842000	-0.19572300	4.75674900
H	3.19832100	-1.98639000	5.35666900
H	2.56352300	-2.59174800	3.03440900
H	4.53709800	0.95980500	1.57444100
H	5.19176900	1.53682400	3.89623500
H	4.51423800	0.06915800	5.77272100
C	3.09451700	-1.17712400	0.84019500
C	2.23148500	-2.15309900	0.30201800
C	3.29393800	-0.49141300	-0.47822300
C	2.53576300	-1.70025100	-1.13454500
H	1.19309500	-1.54077400	0.65366700
H	2.04702500	-3.16284400	0.66661500
H	2.74388600	0.45231400	-0.57409700
H	4.34143200	-0.34537800	-0.76287500
C	3.47804000	-2.57209000	-1.92342100
O	3.56174600	-2.57250000	-3.12727800
O	4.27613400	-3.29681600	-1.12249100
C	5.26205800	-4.08112000	-1.79714300
H	5.80076300	-4.61813400	-1.01902600
H	4.77905200	-4.77664400	-2.48598100
H	5.93982800	-3.43590600	-2.36008100

TS2S

C	3.75603600	0.60986000	0.20013900
C	4.98991600	0.30845700	-0.38422500
C	5.34924900	-1.01435200	-0.57663500
C	4.48265000	-2.04562300	-0.23756100
C	3.21344600	-1.76066100	0.27195400

C	2.86483700	-0.41712700	0.47361700
C	4.62667500	2.63279900	-0.65796800
C	5.73126900	1.56461100	-0.76006900
H	4.77253000	-3.07750300	-0.40303200
H	4.06763200	2.67167000	-1.59856800
H	5.00579900	3.63439300	-0.43890800
H	6.55640400	1.75579600	-0.06342400
C	3.68222200	2.10688200	0.45839200
C	2.37235700	2.87157000	0.50226700
C	4.26616800	2.46864900	1.85569500
C	2.48301700	3.95132000	1.38306400
C	1.18401800	2.66576200	-0.17824900
C	3.79829500	3.91265900	2.11523200
H	3.82468400	1.80191600	2.60359500
H	5.35193300	2.34963900	1.89028800
C	1.42783500	4.84017800	1.50481700
C	0.08996400	3.53112000	-0.02978500
H	4.49411000	4.65179500	1.70025100
C	0.24337800	4.64434900	0.80239700
H	-0.57945700	5.34163400	0.91894000
H	6.16532300	1.49177000	-1.76050100
H	3.68019700	4.14213000	3.17720100
Br	7.03947500	-1.41461300	-1.33089300
C	2.22983500	-2.86213300	0.45342900
C	1.95905900	-3.67109800	-0.65577300
C	1.56614800	-3.10725800	1.67280500
C	1.01754400	-4.68701300	-0.59949000
H	2.47421900	-3.46552100	-1.58945800
C	0.61707100	-4.16746100	1.74127600
C	1.83433600	-2.35283800	2.87261500
C	0.32923300	-4.95084100	0.59007300
H	0.80609800	-5.28133000	-1.48380400
C	-0.04400400	-4.46211900	2.97521400
C	1.20581200	-2.63193900	4.03900300
H	2.56747500	-1.55461500	2.82967400
C	-0.65561600	-5.99847900	0.68145100
C	-0.98707800	-5.52499400	3.04601800
C	0.24309000	-3.69762400	4.13738900
H	1.42655200	-2.05559200	4.93272300
C	-1.28234800	-6.27373300	1.85130300
H	-0.87562500	-6.57378900	-0.21344300
C	-1.60506400	-5.81175200	4.27017700
C	-0.40184900	-4.01052200	5.33983600
H	-2.01652800	-7.07186300	1.91204000

C	-1.31178700	-5.06187600	5.40544200
H	-2.32034600	-6.62756500	4.32212400
H	-0.17826900	-3.42461500	6.22662900
H	-1.79789200	-5.29646200	6.34672700
C	-1.19523600	3.26540100	-0.73106200
C	-1.19261800	3.14184300	-2.12236200
C	-2.40572500	3.11787900	-0.01952400
C	-2.36381800	2.90963200	-2.83046600
H	-0.24965300	3.22237000	-2.65411600
C	-3.60847100	2.88266800	-0.74472900
C	-2.47473400	3.14453800	1.42109900
C	-3.58561800	2.78389900	-2.16333000
H	-2.33483200	2.81542600	-3.91197800
C	-4.84999300	2.72680000	-0.05005000
C	-3.65270500	3.01071400	2.07671500
H	-1.55488500	3.25070400	1.98386400
C	-4.81414400	2.52724300	-2.87028300
C	-6.04801600	2.47060200	-0.77271300
C	-4.88845700	2.80748700	1.36842500
H	-3.67939500	3.03007400	3.16283900
C	-5.98682700	2.37648800	-2.20915900
H	-4.77532100	2.45449300	-3.95340600
C	-7.24919200	2.31258700	-0.07140400
C	-6.11091500	2.64452600	2.03192500
H	-6.90741400	2.18095700	-2.75142400
C	-7.27882800	2.40075300	1.31666400
H	-8.16220200	2.11706900	-0.62625500
H	-6.13582300	2.71030200	3.11637700
H	-8.21833500	2.27548100	1.84463400
O	1.57787000	-0.11721600	0.90215600
O	1.05442900	1.52609300	-0.96543900
P	0.44053700	0.23556000	-0.19857000
O	-0.84498800	0.42305900	0.49617800
Br	1.59388300	6.32268600	2.67101800
N	0.37106100	-0.88194900	-1.39127600
H	-1.84099600	-1.50798300	-3.37576700
S	1.22176200	-1.04841500	-2.73538900
O	2.64831600	-0.80701300	-2.59081500
O	0.75210400	-2.26250700	-3.39069200
C	0.63922500	0.31410400	-3.85677700
F	1.34019500	1.42338300	-3.67811200
F	-0.64935100	0.57491500	-3.63635400
F	0.78590900	-0.08807900	-5.11270700
C	-4.04861800	-0.46374700	2.77437300

C	-3.69928000	-0.48206800	1.43401000
C	-3.03114900	-1.59815200	0.90425100
C	-2.70793200	-2.69176900	1.72523100
C	-3.05049200	-2.66198900	3.06841700
C	-3.72243100	-1.55189500	3.58644500
H	-4.56751800	0.39521400	3.18688100
H	-3.91523800	0.36652700	0.79088900
H	-2.19598700	-3.55329900	1.30282200
H	-2.79899900	-3.49757500	3.71292200
H	-3.99192100	-1.53542300	4.63789600
C	-2.65262100	-1.58731900	-0.47282600
C	-3.00273300	-0.65373700	-1.59408700
C	-1.87600100	-2.41620200	-1.30004500
C	-2.50597700	-1.77921700	-2.55817600
H	-2.34375300	0.22277600	-1.60213000
H	-4.04720400	-0.33988500	-1.66730600
H	-0.78801500	-1.73023000	-1.25950300
H	-1.58564500	-3.45271300	-1.13445000
C	-3.67900900	-2.60011600	-3.03937300
O	-4.57949900	-2.96958500	-2.32025400
O	-3.60710300	-2.87043600	-4.34283900
C	-4.68621900	-3.65546800	-4.86394900
H	-4.47293100	-3.78686300	-5.92217000
H	-4.72888000	-4.62027600	-4.35602900
H	-5.63394900	-3.13338000	-4.72266100

PR

H	-2.08349200	0.34069300	1.94121200
C	3.75725600	-1.38805400	-0.25637300
C	2.40349400	-1.29254200	0.03718300
C	1.78780200	-0.03826000	0.14544200
C	2.55525400	1.11508600	-0.04696300
C	3.91256600	1.01846600	-0.34080000
C	4.51600000	-0.23199000	-0.44572200
H	4.22484900	-2.36397200	-0.33938200
H	1.81272300	-2.19225400	0.18575100
H	2.08242300	2.09004200	0.03561000
H	4.49852800	1.92006500	-0.48824000
H	5.57407400	-0.30788400	-0.67470900
C	0.36459700	0.07733700	0.45714800
C	-0.63179400	-0.78897100	0.70112900
C	-0.51075600	1.30381100	0.64171100
C	-1.66472300	0.30340500	0.93083300
H	-0.71638400	-1.86978300	0.73573800

H	-0.25148000	1.94470300	1.48918400
H	-0.67128800	1.91204000	-0.25156700
C	-2.78444400	0.29254400	-0.08041800
O	-2.82290100	0.93287400	-1.10491000
O	-3.73961700	-0.57778400	0.27946500
C	-4.82095900	-0.71314900	-0.64696300
H	-5.50404400	-1.43611000	-0.20599100
H	-5.31920100	0.24723100	-0.79135400
H	-4.45232200	-1.07160000	-1.60992500

PS

H	2.07848500	-1.88478500	-1.19078900
C	-3.68168100	-0.32919000	1.22060300
C	-2.33934200	-0.62510500	1.00112900
C	-1.68534900	-0.14903300	-0.13992700
C	-2.39952000	0.63095000	-1.05944100
C	-3.73868700	0.92580900	-0.83971900
C	-4.38364900	0.44582400	0.30124000
H	-4.17942300	-0.70422300	2.10913100
H	-1.78974800	-1.23008500	1.71727600
H	-1.89729100	1.00269800	-1.94830100
H	-4.28399500	1.52988800	-1.55779300
H	-5.43038600	0.67633600	0.47126200
C	-0.27739000	-0.47472600	-0.35825700
C	0.67822900	-1.30500300	0.47395600
C	0.63476200	-0.19919200	-1.30355500
C	1.73687300	-1.00259700	-0.64460700
H	0.43167300	-2.36550000	0.57616600
H	0.92940700	-0.88887600	1.45373800
H	0.62620900	0.37795800	-2.22191700
C	2.96052000	-0.25101800	-0.18141600
O	4.10083700	-0.62294100	-0.33688500
O	2.64133800	0.89011400	0.44630400
C	3.74983400	1.64111200	0.94608000
H	3.32271100	2.51915300	1.42615800
H	4.31790300	1.04831100	1.66586200
H	4.40945600	1.93475400	0.12733600

M06-2X/SMD

React

C	2.82088900	0.43033200	-1.11709800
C	1.68768200	-0.37231900	-1.21346800
C	0.97917400	-0.74323000	-0.06474800
C	1.43719300	-0.30419800	1.18483100

C	2.56901200	0.49863600	1.27659900
C	3.26471200	0.87064400	0.12722900
H	3.36022200	0.70740600	-2.01764100
H	1.35357800	-0.72406600	-2.18480700
H	0.90728000	-0.58935400	2.08802200
H	2.90968300	0.83395100	2.25127300
H	4.15002200	1.49393100	0.20247000
C	-0.24421000	-1.55741200	-0.18695600
C	-1.18494400	-1.60210400	-1.34217400
C	-1.14629600	-2.08314000	0.87859300
C	-1.66938500	-1.03517200	-0.04532200
H	-1.59699900	-2.56209000	-1.65068600
H	-1.00608900	-0.89272600	-2.14588400
H	-1.54220500	-3.09201000	0.76931200
H	-0.95140100	-1.76996900	1.90062400
C	-1.83687100	0.37155500	0.32653600
O	-1.85852500	0.77692900	1.46950900
O	-1.90400400	1.17032400	-0.74817100
C	-1.94604200	2.57001000	-0.45599100
H	-1.99718900	3.07324500	-1.42024800
H	-2.82607800	2.80941500	0.14463000
H	-1.04607500	2.87261900	0.08404500

CBA

C	-2.09387800	-2.03131000	0.55410100
C	-3.16743900	-2.80005500	0.08704100
C	-4.31616100	-2.16878600	-0.35743000
C	-4.41329900	-0.78137300	-0.36617900
C	-3.32975500	0.00323000	0.03620900
C	-2.16522800	-0.64985900	0.47242100
C	-1.30416100	-4.24812000	0.30680600
C	-2.83068200	-4.26746700	0.11293800
H	-5.32179000	-0.29813800	-0.70972600
H	-0.81101200	-4.16048900	-0.66682000
H	-0.91714900	-5.13817200	0.80927600
H	-3.34530500	-4.76805900	0.94187800
C	-1.02977700	-2.95419300	1.12430700
C	0.44695000	-2.60643800	1.13152500
C	-1.26591000	-3.22573500	2.63790800
C	1.06726700	-3.22009400	2.22388500
C	1.20966400	-1.86800000	0.24284500
C	0.04845300	-3.85953500	3.12959300
H	-1.42359300	-2.26881300	3.14657600
H	-2.14303800	-3.85509100	2.80825200

C	2.44498500	-3.14581000	2.34750600
C	2.60215400	-1.76602000	0.36202300
H	0.05146900	-4.94898600	3.00437100
C	3.21188800	-2.44529100	1.42309800
H	4.29080200	-2.40528600	1.52894000
H	-3.13682600	-4.76934800	-0.80888000
H	0.25291800	-3.65336600	4.18338300
Br	-5.76920900	-3.21351900	-0.97721300
C	-3.40250700	1.48531600	-0.07982300
C	-3.71225500	2.03610700	-1.33054900
C	-3.16762000	2.34033700	1.01857600
C	-3.75551200	3.40937700	-1.52778900
H	-3.89421600	1.36804800	-2.16765200
C	-3.21712000	3.75030100	0.81803400
C	-2.90757900	1.84806600	2.34948600
C	-3.50374600	4.28679100	-0.46726000
H	-3.97984800	3.81076400	-2.51169500
C	-2.97823400	4.63939800	1.91237300
C	-2.68972200	2.69329800	3.38493900
H	-2.90248700	0.77666600	2.51954500
C	-3.53130900	5.71575700	-0.64415700
C	-3.01370300	6.04633500	1.71056800
C	-2.70669500	4.12089100	3.20617200
H	-2.50036900	2.30288000	4.38094000
C	-3.29620400	6.55432300	0.39292200
H	-3.74638000	6.10409300	-1.63558200
C	-2.77443900	6.89824100	2.79539000
C	-2.47519500	5.00586700	4.26561400
H	-3.31782100	7.63119600	0.25096100
C	-2.50786200	6.38124200	4.05922200
H	-2.79972000	7.97271100	2.63697100
H	-2.26849400	4.60425900	5.25360900
H	-2.32448400	7.05563100	4.88956200
C	3.41202200	-1.00547700	-0.62594600
C	3.27028300	-1.31641500	-1.98168500
C	4.33177700	-0.01082900	-0.22821700
C	4.04772100	-0.69893700	-2.94937000
H	2.53846700	-2.06139900	-2.27782800
C	5.14428600	0.60977100	-1.22022200
C	4.46125300	0.43956000	1.13676300
C	5.00538800	0.25438200	-2.58979800
H	3.92038400	-0.95940100	-3.99608700
C	6.10528000	1.60079400	-0.84579800
C	5.36733300	1.38400700	1.48718000

H	3.79822000	0.02661200	1.88873300
C	5.84859600	0.88897700	-3.57005200
C	6.93028000	2.20639300	-1.83358400
C	6.23744800	1.98871700	0.51420900
H	5.44157100	1.71568400	2.51916000
C	6.76924700	1.81465200	-3.21041400
H	5.72608700	0.60264500	-4.61092200
C	7.87050500	3.16736700	-1.44318800
C	7.18767100	2.95591800	0.86347800
H	7.40325800	2.28605100	-3.95630800
C	7.99749800	3.53586600	-0.10738500
H	8.50077400	3.62600500	-2.20009000
H	7.28253200	3.25084500	1.90485000
H	8.73027800	4.28397000	0.17805900
O	-1.04639800	0.12194100	0.78645700
O	0.54479400	-1.14752100	-0.75974600
P	0.10695500	0.32911400	-0.31917400
O	1.13116300	1.25391200	0.16988400
Br	3.29213900	-4.00677600	3.80728500
N	-0.73896500	0.77084000	-1.72219500
H	-1.25721600	1.65276600	-1.67159200
S	-0.58895700	0.22614600	-3.27576500
O	-1.16526000	1.24935000	-4.12105000
O	0.71526200	-0.34351600	-3.51219400
C	-1.77965800	-1.18438300	-3.32254300
F	-2.99929600	-0.74397900	-3.05452500
F	-1.43784900	-2.11024900	-2.44333400
F	-1.75042100	-1.69478900	-4.54329800

M1

C	-2.51835100	-2.64755400	0.04133000
C	-3.58367500	-3.19126400	-0.68345000
C	-4.60538900	-2.36302800	-1.11244200
C	-4.59078100	-1.00390700	-0.82477700
C	-3.51030900	-0.43260000	-0.14288100
C	-2.45397400	-1.27698500	0.23888900
C	-1.90183600	-4.85475300	-0.54830100
C	-3.38480900	-4.66569600	-0.91377100
H	-5.41803200	-0.37248800	-1.13066700
H	-1.28051100	-4.64021600	-1.42407300
H	-1.66399900	-5.86038000	-0.19160400
H	-4.04750700	-5.25184400	-0.26556900
C	-1.62630500	-3.77327000	0.53308500
C	-0.14259600	-3.59002000	0.77643100

C	-2.08645900	-4.28319000	1.92997500
C	0.27500800	-4.42748600	1.81472100
C	0.78474800	-2.79961900	0.11883200
C	-0.90184700	-5.11337100	2.45595400
H	-2.24472100	-3.41947200	2.58448900
H	-3.02147300	-4.84622600	1.87213300
C	1.62277700	-4.49898700	2.12599800
C	2.15068000	-2.86048400	0.42317900
H	-0.95782600	-6.16001200	2.13290200
C	2.55836500	-3.73923200	1.43299700
H	3.61266700	-3.81203900	1.67908200
H	-3.60805700	-4.94693800	-1.94612600
H	-0.83133200	-5.11397600	3.54669700
Br	-6.04862100	-3.10051200	-2.09399800
C	-3.52479400	1.02982700	0.13322600
C	-3.79934900	1.90192100	-0.92663200
C	-3.34364100	1.55057300	1.43400600
C	-3.87378800	3.27355400	-0.73585800
H	-3.93486200	1.49006900	-1.92230700
C	-3.39417800	2.96176400	1.62548000
C	-3.13717900	0.71712000	2.59391700
C	-3.66248600	3.82775300	0.53044600
H	-4.07851400	3.93050300	-1.57699400
C	-3.16153300	3.52171900	2.92148300
C	-2.93286600	1.24892500	3.82356000
H	-3.15881100	-0.36063700	2.47631500
C	-3.67619400	5.25205300	0.74654600
C	-3.16061700	4.93250900	3.10226500
C	-2.91436800	2.67181100	4.03243300
H	-2.77919400	0.60091400	4.68203400
C	-3.42749900	5.77971300	1.96884100
H	-3.87858400	5.89527400	-0.10583900
C	-2.90158100	5.45852200	4.37330200
C	-2.66392000	3.23664300	5.28900600
H	-3.42700100	6.85559900	2.12003400
C	-2.65418500	4.61770100	5.45437900
H	-2.89714400	6.53674600	4.50656000
H	-2.47512600	2.58092600	6.13449200
H	-2.45551300	5.04262100	6.43320200
C	3.15984700	-2.07343300	-0.33488800
C	3.26427200	-2.28101400	-1.71309900
C	4.04553300	-1.18594500	0.30946200
C	4.25551200	-1.66435800	-2.46279900
H	2.56370700	-2.95554500	-2.19646800

C	5.07800100	-0.57042200	-0.45340100
C	3.93415800	-0.85058300	1.70820800
C	5.18853700	-0.82120700	-1.84880300
H	4.32567000	-1.84913700	-3.53112600
C	6.00808800	0.31282300	0.17953600
C	4.80871300	-0.00343100	2.30182900
H	3.11435300	-1.27141200	2.27975700
C	6.25245200	-0.19557500	-2.59217900
C	7.04957800	0.91680400	-0.57819000
C	5.88649600	0.60217100	1.56492500
H	4.70220700	0.24691000	3.35364400
C	7.14312100	0.62686800	-1.98658800
H	6.32289700	-0.40223800	-3.65645100
C	7.94444600	1.78460000	0.05989500
C	6.80100400	1.47576100	2.16511400
H	7.94284900	1.09340100	-2.55512000
C	7.81989200	2.05882100	1.41824600
H	8.73918100	2.24387400	-0.52129000
H	6.70285900	1.69628000	3.22442600
H	8.52094500	2.73454400	1.89788400
O	-1.29968800	-0.71418700	0.78599900
O	0.32456800	-1.86891500	-0.82018800
P	-0.03607100	-0.43547000	-0.18267000
O	1.02636300	0.27278400	0.53432700
Br	2.19234400	-5.64559100	3.52306000
N	-0.61517500	0.34320300	-1.56417100
H	-0.74446100	1.36257500	-1.42410500
S	-1.26855300	-0.24249600	-2.95193200
O	-1.76735700	-1.58838100	-2.79324200
O	-2.07054200	0.82069900	-3.52478900
C	0.21331600	-0.38721500	-4.04091800
F	1.17849500	-1.03922900	-3.41260900
F	0.64254900	0.82218300	-4.37383900
F	-0.13571600	-1.04738700	-5.13369600
C	3.92163300	3.86670000	-1.06557300
C	2.82076800	4.71767900	-1.11177700
C	1.64426100	4.31654500	-1.75478600
C	1.59931200	3.05596000	-2.36482500
C	2.69501800	2.20266700	-2.30372600
C	3.86037300	2.60739700	-1.65615200
H	4.83085900	4.18536000	-0.56442600
H	2.87414300	5.70052100	-0.65345900
H	0.70386900	2.74561100	-2.89339300
H	2.64192600	1.21942000	-2.76222800

H	4.71969900	1.94720600	-1.62197400
C	0.44696100	5.17665400	-1.72624200
C	0.09640700	6.21576400	-0.71030800
C	-0.91987100	4.87361900	-2.23674200
C	-0.72035800	4.96663500	-0.75993500
H	-0.37598700	7.13801400	-1.04585700
H	0.76904500	6.32115800	0.13682000
H	-1.48683100	5.67580500	-2.70767100
H	-1.10118500	3.88163200	-2.64257500
C	-0.61439500	3.80421300	0.11718600
O	-0.77656900	2.65615500	-0.26434300
O	-0.25137700	4.10978300	1.35646400
C	0.08349300	2.98641500	2.19025600
H	0.21513500	3.39655000	3.19080700
H	-0.71737400	2.24480900	2.17601500
H	1.00288800	2.52232500	1.82712500

TS1

C	4.04162600	-0.52701700	-0.02956800
C	5.04078800	-1.11566300	-0.80885900
C	4.93965800	-2.45862800	-1.13430000
C	3.84460700	-3.21533500	-0.73242400
C	2.80685100	-2.62800700	-0.00142600
C	2.92959700	-1.26935200	0.33222700
C	5.36950200	1.22892600	-0.88765700
C	6.08198900	-0.10045200	-1.19962300
H	3.77679300	-4.26315700	-1.00528000
H	4.75529300	1.52113300	-1.74560200
H	6.05630100	2.04803700	-0.65849100
H	6.99226100	-0.22974500	-0.60142600
C	4.43027900	0.90239900	0.30951600
C	3.40469600	2.00383000	0.52844200
C	5.22575700	0.98631000	1.64306400
C	3.91831800	2.95337000	1.41891300
C	2.15060500	2.20733500	-0.02554800
C	5.22242900	2.48262900	2.00817800
H	4.68684000	0.42118200	2.41089700
H	6.22998000	0.56539000	1.54619600
C	3.20185900	4.11293600	1.66599100
C	1.42559900	3.38626900	0.20004500
H	6.06500900	3.01787500	1.55392300
C	1.97527600	4.34808900	1.04974000
H	1.43452900	5.26986000	1.23727200
H	6.36779000	-0.19340100	-2.25060100

H	5.26963000	2.65897500	3.08589300
Br	6.31429300	-3.26852600	-2.15985300
C	1.55462200	-3.38381500	0.27443100
C	0.91023600	-3.98124300	-0.81377300
C	0.95415800	-3.43672200	1.55062200
C	-0.34250500	-4.56249700	-0.68730700
H	1.37508200	-3.92290900	-1.79379500
C	-0.33126700	-4.03629200	1.68440600
C	1.59397700	-2.92459500	2.73779300
C	-0.99043400	-4.58742200	0.55125500
H	-0.84263200	-4.97179400	-1.55986500
C	-0.97638400	-4.07661400	2.96158500
C	0.98782500	-2.97531200	3.94782800
H	2.58959400	-2.50226600	2.64962300
C	-2.30506500	-5.15637100	0.70850400
C	-2.27126700	-4.65189700	3.09166800
C	-0.32653900	-3.54042500	4.10559300
H	1.48953200	-2.58834900	4.83034400
C	-2.91521300	-5.18948000	1.91874300
H	-2.79576700	-5.55528600	-0.17414500
C	-2.88513600	-4.67518000	4.34992000
C	-0.97339500	-3.58607700	5.34643200
H	-3.90422000	-5.62625900	2.03016300
C	-2.24067600	-4.14742800	5.46453400
H	-3.87481600	-5.11318300	4.44602300
H	-0.47166300	-3.17572000	6.21834400
H	-2.73010800	-4.17478100	6.43294700
C	0.14240700	3.62055200	-0.52628000
C	0.21533900	3.83615800	-1.90586400
C	-1.11179800	3.62343900	0.11575200
C	-0.92297600	4.06166100	-2.66539500
H	1.18935600	3.82266700	-2.38569700
C	-2.28487700	3.83440100	-0.66614000
C	-1.26418500	3.39008400	1.53163500
C	-2.18649300	4.05955100	-2.06614800
H	-0.84054500	4.22806300	-3.73589100
C	-3.57509700	3.80559000	-0.04720500
C	-2.48674400	3.36266500	2.11425400
H	-0.37407900	3.20281000	2.12146100
C	-3.39020600	4.26202400	-2.83131700
C	-4.74797700	4.00798300	-0.82741000
C	-3.69027400	3.56561400	1.34911800
H	-2.58241600	3.17426500	3.17991000
C	-4.61009000	4.23813400	-2.24316200

H	-3.29326100	4.43400900	-3.89972100
C	-6.00083100	3.97496800	-0.20070700
C	-4.96177600	3.53114200	1.93554200
H	-5.51215500	4.39181400	-2.82900100
C	-6.10376500	3.73843200	1.16720300
H	-6.89417700	4.13595800	-0.79814400
H	-5.04545100	3.34438400	3.00249400
H	-7.08167500	3.71226900	1.63777900
O	1.90163700	-0.63295200	1.00995100
O	1.55111100	1.18055400	-0.75272300
P	0.73951100	0.12105000	0.17577400
O	-0.21401800	0.68897500	1.14945500
Br	3.90778400	5.39976000	2.86707900
N	0.04748700	-0.88347700	-0.90693500
H	-1.36440400	-1.00194900	-0.64165000
S	0.38490900	-1.09531000	-2.45631600
O	1.80624300	-1.11362200	-2.76209000
O	-0.47946500	-2.15431600	-2.95956200
C	-0.29333600	0.44839800	-3.25571300
F	0.68282600	1.30074100	-3.52880500
F	-1.17198200	1.03190500	-2.44480900
F	-0.90698600	0.11886900	-4.38680200
C	-7.39701500	0.03431700	-0.19927000
C	-6.03399100	0.23182600	-0.00784100
C	-5.20134200	-0.85496000	0.28160700
C	-5.74271400	-2.14325800	0.38069200
C	-7.10291200	-2.33495200	0.17203700
C	-7.93091300	-1.24918100	-0.11466100
H	-8.03834100	0.88365800	-0.41215000
H	-5.61652400	1.23368800	-0.05712300
H	-5.10478500	-2.99448400	0.59673100
H	-7.51977400	-3.33449200	0.23638700
H	-8.99396700	-1.40612800	-0.26775200
C	-3.77235200	-0.57847800	0.52449800
C	-3.02484700	0.41728700	-0.22322400
C	-2.77955100	-1.53187600	0.98159900
C	-2.59837800	-1.07944800	-0.51063900
H	-2.20572500	0.94729400	0.26044100
H	-3.54748400	0.94379200	-1.01726600
H	-1.94111100	-1.16351200	1.57018900
H	-3.09157100	-2.55410800	1.17626500
C	-3.12973500	-1.88084500	-1.65246300
O	-3.40127000	-3.05601400	-1.59317000
O	-3.20972600	-1.12367500	-2.74505500

C	-3.51376600	-1.82783100	-3.95536500
H	-3.54502200	-1.07132600	-4.73717100
H	-2.72723700	-2.55711700	-4.15768400
H	-4.47926000	-2.33003600	-3.86990700

B3LYP/IEF-PCM

React

C	2.82038500	1.05052800	-1.02215500
C	1.71008200	0.23476500	-1.23459000
C	1.18811200	-0.55276300	-0.19368600
C	1.82993900	-0.52077600	1.05676600
C	2.93931500	0.29645200	1.26594000
C	3.43823600	1.08868500	0.22948700
H	3.20732300	1.65203900	-1.83950700
H	1.25065000	0.20054300	-2.21714400
H	1.46336900	-1.14227400	1.86710500
H	3.41856900	0.30915100	2.24043800
H	4.30585600	1.72072700	0.39273000
C	0.01007100	-1.40581700	-0.41813500
C	-0.96706200	-1.40068300	-1.55528200
C	-0.78602300	-2.22077700	0.55595700
C	-1.49102300	-1.11966200	-0.17693400
H	-1.24124400	-2.35054200	-2.01863900
H	-0.92821300	-0.56168700	-2.24510700
H	-1.04033200	-3.25009000	0.29599100
H	-0.60470900	-2.05662700	1.61515600
C	-2.02207300	0.11235400	0.40899800
O	-2.15044800	0.30983900	1.60574600
O	-2.34554300	1.01984500	-0.54065300
C	-2.83513200	2.28036900	-0.04824000
H	-3.05397600	2.87595400	-0.93367700
H	-3.73943900	2.13489000	0.54700700
H	-2.07888100	2.77438300	0.56614000

CBA

C	-1.92107500	-2.15695200	0.51629400
C	-2.90375500	-3.04578900	0.04588600
C	-4.10731800	-2.54603700	-0.43107500
C	-4.34900700	-1.17495100	-0.46666100
C	-3.35840900	-0.26622500	-0.06750100
C	-2.13268700	-0.78725700	0.39284900
C	-0.91300400	-4.30354900	0.37623000
C	-2.42584900	-4.47378100	0.12580100
H	-5.30036700	-0.79907100	-0.82404000

H	-0.39120400	-4.20205600	-0.58081300
H	-0.46574700	-5.14135000	0.91638500
H	-2.92126000	-5.00740300	0.94675300
C	-0.79223700	-2.95668300	1.16421800
C	0.65624700	-2.48160600	1.23279800
C	-1.08107700	-3.20494900	2.68376700
C	1.26902700	-3.01491800	2.37792700
C	1.40998700	-1.71113500	0.35370300
C	0.26018500	-3.70049000	3.26368500
H	-1.35612200	-2.25469600	3.15285600
H	-1.90455600	-3.90595200	2.83927600
C	2.63392800	-2.84056400	2.56094600
C	2.79514100	-1.52747500	0.52009700
H	0.35804400	-4.79153700	3.19671300
C	3.39559600	-2.12953700	1.63797800
H	4.46359700	-2.02323200	1.78487800
H	-2.64802400	-5.03056000	-0.78906200
H	0.39332000	-3.43759900	4.31698500
Br	-5.45504500	-3.75310800	-1.05270700
C	-3.60879600	1.19839500	-0.20820700
C	-3.90483600	1.70057800	-1.48677600
C	-3.58943500	2.08595800	0.89838900
C	-4.14276000	3.05398800	-1.70448100
H	-3.93599100	1.01200100	-2.32564700
C	-3.83595300	3.47910500	0.67655700
C	-3.36237900	1.64519100	2.24890200
C	-4.10620700	3.96618100	-0.63973600
H	-4.35495900	3.41116700	-2.70784500
C	-3.81694300	4.39501000	1.77331200
C	-3.35102200	2.51924900	3.29258000
H	-3.20775600	0.58855300	2.43364100
C	-4.33734700	5.37128700	-0.83334400
C	-4.05049400	5.78746800	1.55139100
C	-3.56717400	3.92451500	3.09739800
H	-3.17925000	2.15863600	4.30299600
C	-4.30873300	6.24159300	0.21256400
H	-4.53633500	5.72552600	-1.84081100
C	-4.02219100	6.66816000	2.64494100
C	-3.55058100	4.84178600	4.16108000
H	-4.48425800	7.30163700	0.05152000
C	-3.77421200	6.19835300	3.93390700
H	-4.19695300	7.72683400	2.47482100
H	-3.36005500	4.48062900	5.16781500
H	-3.75618100	6.89463100	4.76683600

C	3.63417500	-0.78499500	-0.46327000
C	3.66537100	-1.23576900	-1.79037500
C	4.44679100	0.31305800	-0.08068500
C	4.49934100	-0.65554400	-2.73710800
H	3.03109800	-2.06723200	-2.07839900
C	5.31640800	0.90499000	-1.05247300
C	4.42206500	0.88654100	1.23962000
C	5.34512200	0.40867200	-2.39163500
H	4.50594200	-1.03256600	-3.75565000
C	6.16302800	1.99813600	-0.69015900
C	5.22581400	1.93130000	1.58087700
H	3.73083000	0.48352000	1.96992900
C	6.23528000	1.01467000	-3.34318300
C	7.04221300	2.57865500	-1.65656000
C	6.13464300	2.51921000	0.63859100
H	5.18036300	2.34755900	2.58356200
C	7.04803900	2.04865300	-2.99243200
H	6.24483300	0.62576700	-4.35767100
C	7.86976800	3.64718900	-1.27386700
C	6.97850100	3.59063800	0.97531900
H	7.71673800	2.49599200	-3.72286300
C	7.83710100	4.14506900	0.02790700
H	8.53922500	4.08580600	-2.00874600
H	6.95273700	3.98590000	1.98709900
H	8.48339800	4.97269400	0.30466900
O	-1.09881800	0.11148900	0.69623900
O	0.73919900	-1.06365300	-0.70557700
P	0.10926700	0.38065200	-0.35421800
O	1.00264600	1.43358400	0.15807500
Br	3.48528000	-3.58867300	4.10292800
N	-0.70240100	0.67996300	-1.82822500
H	-1.41769800	1.40803700	-1.79806600
S	-0.34199100	0.23937800	-3.40322400
O	-0.99552900	1.22165600	-4.26068300
O	1.06105400	-0.11772000	-3.53593400
C	-1.32431300	-1.34751400	-3.61179500
F	-2.61337400	-1.10655400	-3.36536900
F	-0.87867900	-2.28473700	-2.77876800
F	-1.17864100	-1.75748800	-4.86970200
M1			
C	-3.35180700	-1.76769900	-0.53565100
C	-4.43128800	-1.84971900	-1.42992000
C	-5.13073700	-0.69794400	-1.76002600

C	-4.77708700	0.53435800	-1.21698400
C	-3.66207800	0.65059200	-0.37294900
C	-2.93061000	-0.51971100	-0.08882100
C	-3.32510100	-3.95725300	-1.45533800
C	-4.62482600	-3.26376200	-1.91744500
H	-5.35637000	1.41917800	-1.45271300
H	-2.54989400	-3.83195400	-2.21788800
H	-3.44744200	-5.02745200	-1.27088600
H	-5.51606700	-3.71743100	-1.46540600
C	-2.89925100	-3.17749100	-0.16743700
C	-1.47755300	-3.52844100	0.26026900
C	-3.70562200	-3.71186800	1.06536200
C	-1.51075800	-4.61836400	1.14608900
C	-0.24896000	-3.00015200	-0.12247200
C	-2.92652800	-4.95612500	1.53808300
H	-3.69522900	-2.95096800	1.85273500
H	-4.74859300	-3.92266000	0.81741400
C	-0.31970900	-5.20402200	1.55139000
C	0.96769000	-3.59193100	0.26852000
H	-3.26499500	-5.86910000	1.03155400
C	0.90549500	-4.71777900	1.10421200
H	1.82548000	-5.20217900	1.40873100
H	-4.76743900	-3.30462100	-3.00114900
H	-3.02257500	-5.13898100	2.61217600
Br	-6.61448200	-0.80266500	-2.96499100
C	-3.30030700	1.99352400	0.16855700
C	-3.03417900	3.03154100	-0.73580200
C	-3.28773200	2.26442400	1.56149800
C	-2.72762700	4.31616100	-0.30272700
H	-3.04121400	2.81657800	-1.79904200
C	-2.97064800	3.58693900	2.01020900
C	-3.61441500	1.27638400	2.55531700
C	-2.68217700	4.61995400	1.06543300
H	-2.51195300	5.09430600	-1.02928100
C	-2.94856400	3.88749400	3.40797700
C	-3.59713800	1.56535600	3.88569200
H	-3.89086700	0.28053300	2.22952300
C	-2.35754700	5.93572000	1.54498700
C	-2.62308400	5.20579000	3.85598200
C	-3.25583800	2.87416300	4.36541700
H	-3.84996100	0.79858300	4.61290900
C	-2.32649800	6.21551600	2.87678600
H	-2.13569500	6.70850700	0.81421000
C	-2.60467700	5.47462000	5.23445100

C	-3.22671500	3.18978200	5.73403400
H	-2.07875600	7.21490100	3.22399000
C	-2.90273200	4.47619900	6.16080700
H	-2.35572700	6.47637600	5.57369600
H	-3.46133500	2.41623700	6.46000500
H	-2.88396200	4.70334400	7.22250300
C	2.28977700	-3.11444900	-0.23092600
C	2.53046500	-3.15433900	-1.61122300
C	3.32286000	-2.69442800	0.64442500
C	3.76500900	-2.81044200	-2.14691800
H	1.73302800	-3.47636200	-2.27250600
C	4.60089600	-2.35129900	0.09640500
C	3.14280100	-2.57184400	2.06724700
C	4.82165300	-2.41479600	-1.31355000
H	3.92174900	-2.85857200	-3.22077000
C	5.66640200	-1.94312800	0.95705900
C	4.15884000	-2.18033300	2.88458500
H	2.16669600	-2.78181500	2.48789400
C	6.11689400	-2.07266100	-1.83465800
C	6.94596500	-1.61229700	0.41192200
C	5.45933500	-1.86206500	2.36721000
H	3.99276800	-2.09130900	3.95467500
C	7.13252500	-1.69159400	-1.01115800
H	6.27104700	-2.13070500	-2.90872500
C	7.97948900	-1.22156800	1.27934500
C	6.52172800	-1.46443800	3.19582700
H	8.10810000	-1.44183200	-1.41949500
C	7.76725500	-1.15009400	2.65537800
H	8.95278400	-0.97477000	0.86395800
H	6.36064900	-1.40256600	4.26854300
H	8.57795900	-0.84560400	3.31054300
O	-1.74414500	-0.41043000	0.64802500
O	-0.22530700	-1.82163000	-0.89262400
P	-0.28772800	-0.42608900	-0.07407900
O	0.76043100	-0.13867400	0.92090400
Br	-0.35703500	-6.70534100	2.73850300
N	-0.29001900	0.67530700	-1.36537300
H	0.08644900	1.61221700	-1.11541700
S	-0.77071500	0.56900500	-2.95230700
O	-1.69214100	-0.54074400	-3.14935000
O	-1.07100900	1.92443600	-3.40620500
C	0.80813500	0.10420200	-3.84964600
F	1.23159100	-1.09369300	-3.46007700
F	1.75482200	1.01544700	-3.59539400

F	0.55269700	0.08811000	-5.15676800
C	6.39832900	4.17263500	-0.49543300
C	5.26387400	4.86646400	-0.91539200
C	4.23799900	4.20822300	-1.61434200
C	4.39164600	2.84082700	-1.90382300
C	5.52466900	2.14988700	-1.47960700
C	6.53141600	2.81109400	-0.77144600
H	7.17930400	4.69915900	0.04530600
H	5.17529400	5.92816100	-0.70844500
H	3.62138200	2.31039100	-2.45254700
H	5.62185300	1.09096700	-1.69939500
H	7.41137600	2.26807100	-0.44054100
C	3.03987400	4.95671600	-2.03136200
C	2.47705600	6.21176000	-1.44158400
C	1.84119000	4.52267600	-2.82062900
C	1.61920300	4.97639000	-1.40827900
H	2.16537900	7.01753600	-2.10847000
H	2.89447500	6.54628900	-0.49552400
H	1.48155300	5.17432200	-3.61891300
H	1.72327600	3.46330900	-3.02620700
C	1.22444600	4.14581600	-0.27801300
O	0.74596800	3.01966100	-0.37426900
O	1.46213300	4.73174600	0.90388900
C	1.15901700	3.93869300	2.07344000
H	1.50023700	4.53278700	2.91963000
H	0.08454100	3.76010400	2.13882800
H	1.68298900	2.98247100	2.03235500

TS1

C	3.71481500	0.67903700	-0.30384900
C	4.83393000	0.39181300	-1.10185600
C	5.15064100	-0.92990700	-1.38007100
C	4.37215600	-1.97290000	-0.88458800
C	3.21087100	-1.70520500	-0.14546100
C	2.87446800	-0.35743600	0.08959100
C	4.46958600	2.74277500	-1.20282000
C	5.51008300	1.65935700	-1.56216600
H	4.65011800	-3.00157800	-1.08164000
H	3.75832000	2.85771700	-2.02684800
H	4.91513800	3.72040100	-1.00185100
H	6.46158300	1.81276300	-1.03713400
C	3.71560000	2.16618700	0.04055500
C	2.45617000	2.96503900	0.36574300
C	4.55791400	2.42995600	1.33584800

C	2.77423600	3.99622900	1.26565500
C	1.15273000	2.85222600	-0.10834600
C	4.19194900	3.86637600	1.76078800
H	4.24239400	1.72608100	2.11305000
H	5.62834500	2.28720600	1.16983400
C	1.80797400	4.93591900	1.59565200
C	0.16281100	3.80114100	0.21640900
H	4.84191800	4.61266300	1.28606200
C	0.52314000	4.85842900	1.06584700
H	-0.21341100	5.61227400	1.31688700
H	5.74279200	1.63054100	-2.63061600
H	4.26660900	4.02623300	2.84029700
Br	6.68782100	-1.33103100	-2.45028000
C	2.37260800	-2.84082500	0.34025700
C	1.80796900	-3.71135500	-0.60210600
C	2.16905200	-3.08492300	1.72289400
C	1.02452100	-4.79369900	-0.21812000
H	1.95646900	-3.51214600	-1.65793700
C	1.36129900	-4.19765800	2.12199800
C	2.76089400	-2.27688000	2.75619200
C	0.77949800	-5.05471800	1.13777300
H	0.57121700	-5.42654600	-0.97385100
C	1.13071600	-4.46028800	3.50815500
C	2.54673700	-2.53254100	4.07628400
H	3.40022100	-1.45041500	2.46805500
C	-0.04266800	-6.15403400	1.56629100
C	0.31008600	-5.56180000	3.90552900
C	1.71892600	-3.62424300	4.50482100
H	3.00876800	-1.90634500	4.83472300
C	-0.26962400	-6.39486400	2.88720800
H	-0.47999900	-6.79434300	0.80519700
C	0.09577500	-5.79645300	5.27368000
C	1.47808700	-3.89868000	5.86144900
H	-0.89172500	-7.23067900	3.19600600
C	0.67427100	-4.97283400	6.23853100
H	-0.52874200	-6.63322100	5.57455900
H	1.92763900	-3.26100900	6.61762600
H	0.49778700	-5.17055700	7.29163300
C	-1.21183300	3.74536200	-0.35941800
C	-1.35320000	3.80227900	-1.75307300
C	-2.37129700	3.69395900	0.45547800
C	-2.60226000	3.83086500	-2.35994600
H	-0.46112100	3.83591100	-2.36820400
C	-3.66107000	3.73883400	-0.16649500

C	-2.31794900	3.57106000	1.88910100
C	-3.77408500	3.81311000	-1.58876400
H	-2.67679200	3.88158400	-3.44253900
C	-4.84681100	3.70871200	0.63159600
C	-3.44877800	3.53889800	2.64669800
H	-1.34995500	3.48515800	2.36775000
C	-5.08071400	3.86636100	-2.18473800
C	-6.13389900	3.76712800	0.01155900
C	-4.75348000	3.61786000	2.05341600
H	-3.37758700	3.44034500	3.72647500
C	-6.20784200	3.84764900	-1.42156500
H	-5.14946300	3.92551800	-3.26757600
C	-7.28377900	3.74252400	0.81816900
C	-5.93084900	3.59422200	2.81938300
H	-7.18895900	3.89250200	-1.88666800
C	-7.18067600	3.65798900	2.20586300
H	-8.26113900	3.79025900	0.34579700
H	-5.85621400	3.52419500	3.90108200
H	-8.08086300	3.64003400	2.81299500
O	1.65954400	-0.06710800	0.71558300
O	0.81217000	1.75178200	-0.90680000
P	0.34694900	0.38855400	-0.14576300
O	-0.79702000	0.49272000	0.79284000
Br	2.24241700	6.36194200	2.79835400
N	0.03929800	-0.66116600	-1.39155400
H	-1.05265700	-1.45904900	-1.18893000
S	0.63906000	-0.74704300	-2.90220300
O	1.96248600	-0.14254800	-3.05924200
O	0.38354200	-2.10394500	-3.39930800
C	-0.52636100	0.33053300	-3.90544200
F	-1.79348800	0.10484500	-3.54135700
F	-0.38260700	0.02720600	-5.19860900
F	-0.24397100	1.62273000	-3.72818500
C	-6.88310200	-3.67174200	-0.69644500
C	-5.79922000	-2.80179900	-0.63590800
C	-4.60534000	-3.19286800	0.00214900
C	-4.53547300	-4.46825400	0.59693600
C	-5.62153300	-5.33489900	0.53008300
C	-6.79487400	-4.94104300	-0.11880100
H	-7.79822500	-3.35853200	-1.18835000
H	-5.88460400	-1.81150700	-1.06888300
H	-3.63663800	-4.77999500	1.11603400
H	-5.55562600	-6.31611600	0.98868100
H	-7.64236300	-5.61791900	-0.16495300

C	-3.48635300	-2.25570600	0.10360200
C	-3.26379600	-1.08907500	-0.75581400
C	-2.12128900	-2.57737800	0.52854100
C	-2.13824700	-2.16987800	-0.98659300
H	-2.83137000	-0.19923600	-0.30213400
H	-3.96537900	-0.89674300	-1.56104100
H	-1.58773800	-1.82914400	1.11088100
H	-1.87885400	-3.60574400	0.77511500
C	-2.26708400	-3.24127200	-2.02142400
O	-1.91117400	-4.39258700	-1.86268100
O	-2.79502700	-2.75403900	-3.15603500
C	-2.84932200	-3.67582500	-4.26416600
H	-3.32179300	-3.12643500	-5.07687200
H	-1.83858800	-3.97897900	-4.54343200
H	-3.43794200	-4.55682500	-4.00130100

B3LYP/SMD

React

C	2.78640000	1.06947500	-1.01579000
C	1.67740300	0.25294100	-1.23247900
C	1.17282000	-0.56139300	-0.20293600
C	1.83155700	-0.55395600	1.03957100
C	2.93983600	0.26416700	1.25243500
C	3.42114000	1.08251500	0.22807200
H	3.15906300	1.69200100	-1.82442600
H	1.20492700	0.24045200	-2.20951100
H	1.47908500	-1.19550400	1.84065700
H	3.43197700	0.25697500	2.22088700
H	4.28791500	1.71545100	0.39433200
C	-0.00383900	-1.41741100	-0.43037800
C	-0.98765800	-1.39801500	-1.56102000
C	-0.79899700	-2.22929900	0.54647800
C	-1.50431100	-1.12262000	-0.17849700
H	-1.27042100	-2.34413000	-2.02723400
H	-0.94445600	-0.55618400	-2.24728100
H	-1.06173100	-3.25596300	0.28381500
H	-0.60767600	-2.07027500	1.60488500
C	-2.00337500	0.11868500	0.41635600
O	-2.11509800	0.31525000	1.61528100
O	-2.32124700	1.03419300	-0.52643600
C	-2.78068400	2.30369300	-0.02686100
H	-2.99732700	2.90510500	-0.91014700
H	-3.68404300	2.17820000	0.57548100
H	-2.00829800	2.78564000	0.57808300

CBA

C	-1.89609500	-2.17741200	0.49007500
C	-2.86146300	-3.08041500	0.00895900
C	-4.06540300	-2.59436500	-0.48119000
C	-4.32664700	-1.22698000	-0.51802100
C	-3.35383700	-0.30499800	-0.10496000
C	-2.12473000	-0.81055000	0.36389900
C	-0.85835300	-4.31103600	0.36613300
C	-2.36498600	-4.50141200	0.09688500
H	-5.27959000	-0.86257300	-0.88353000
H	-0.32566300	-4.20402800	-0.58455000
H	-0.40833200	-5.14206700	0.91450000
H	-2.86293400	-5.03973400	0.91333400
C	-0.76509000	-2.96198500	1.15393400
C	0.67718900	-2.46970600	1.24104700
C	-1.07073600	-3.21254700	2.66940400
C	1.28116000	-2.99753900	2.39430300
C	1.43508500	-1.69273100	0.37099500
C	0.26769000	-3.69267900	3.26697400
H	-1.36196300	-2.26519800	3.13498800
H	-1.88729900	-3.92419300	2.81287100
C	2.64272500	-2.81216400	2.59080200
C	2.81801300	-1.50317400	0.55021700
H	0.37852900	-4.78251700	3.20044800
C	3.41093400	-2.09868300	1.67540700
H	4.47701400	-1.98507900	1.83178300
H	-2.56576900	-5.06285900	-0.82034400
H	0.38169200	-3.42684300	4.32196100
Br	-5.39499900	-3.81893700	-1.11766900
C	-3.63213200	1.15597200	-0.23597200
C	-3.92580100	1.66214700	-1.51319800
C	-3.64592400	2.03358800	0.87906600
C	-4.19541900	3.01088000	-1.72141300
H	-3.92427700	0.98168900	-2.35923400
C	-3.92430600	3.42260000	0.66665300
C	-3.42110000	1.58737300	2.22855900
C	-4.19367700	3.91436000	-0.64826800
H	-4.40482100	3.37258700	-2.72408700
C	-3.93899300	4.32936000	1.77151000
C	-3.44126400	2.45248400	3.27977000
H	-3.24380900	0.53312500	2.40803400
C	-4.45810000	5.31510100	-0.83210400
C	-4.20538400	5.71776100	1.55898700

C	-3.69034000	3.85376000	3.09432400
H	-3.27060300	2.08772100	4.28908600
C	-4.46174000	6.17696400	0.22135000
H	-4.65585000	5.67252100	-1.83895900
C	-4.21037100	6.58936800	2.66051000
C	-3.70765900	4.76198500	4.16604100
H	-4.66198900	7.23391500	0.06772300
C	-3.96337600	6.11440800	3.94782000
H	-4.41058800	7.64484100	2.49735400
H	-3.51848600	4.39653700	5.17170500
H	-3.97145200	6.80378200	4.78707400
C	3.66513300	-0.76319600	-0.42940600
C	3.72688700	-1.23549300	-1.74826600
C	4.45530800	0.35267100	-0.05065400
C	4.56710800	-0.65711200	-2.69093200
H	3.11396500	-2.08489700	-2.03180100
C	5.32955100	0.94459300	-1.01885200
C	4.40423800	0.94289500	1.26172400
C	5.38782500	0.42808900	-2.34966300
H	4.59793200	-1.05072100	-3.70292600
C	6.15160900	2.05804000	-0.66103400
C	5.18481300	2.00676700	1.59850100
H	3.71272700	0.53714100	1.99057900
C	6.28155100	1.03513500	-3.29739400
C	7.03435700	2.63983100	-1.62382200
C	6.09476600	2.59835200	0.65939300
H	5.11968000	2.43546900	2.59501500
C	7.07008600	2.08931200	-2.95104000
H	6.31303400	0.63048200	-4.30545800
C	7.83637200	3.72965700	-1.24606000
C	6.91389500	3.69051400	0.99140800
H	7.74201800	2.53783900	-3.67801800
C	7.77530500	4.24653300	0.04736000
H	8.50805500	4.16937300	-1.97850700
H	6.86610800	4.10005100	1.99683600
H	8.40198900	5.09071900	0.32035700
O	-1.10617700	0.10026100	0.68327800
O	0.77128000	-1.04457500	-0.69346000
P	0.11763800	0.38918000	-0.34223800
O	0.98883100	1.44919000	0.19433500
Br	3.48627800	-3.55316100	4.14449100
N	-0.66740600	0.69719300	-1.82833500
H	-1.36082100	1.44760400	-1.80303600
S	-0.27152500	0.28238500	-3.39895600

O	-0.91850200	1.26841400	-4.25784500
O	1.13699600	-0.06010400	-3.51423800
C	-1.22947800	-1.31116100	-3.64951000
F	-2.52532600	-1.09422700	-3.42067800
F	-0.78275300	-2.25848700	-2.82868600
F	-1.05816300	-1.69550000	-4.91339500

M1

C	-3.56533800	-1.27062200	-0.64885200
C	-4.62124200	-1.14663200	-1.56750000
C	-5.12767900	0.11295900	-1.85417900
C	-4.60470800	1.25259000	-1.24879700
C	-3.50779200	1.15841900	-0.37877600
C	-2.97154400	-0.12190200	-0.13563600
C	-3.84717300	-3.39495500	-1.67387400
C	-5.01417600	-2.49164200	-2.12526200
H	-5.03474800	2.22596300	-1.45416800
H	-3.04242700	-3.35416800	-2.41504000
H	-4.13593500	-4.44100000	-1.54360500
H	-5.97427600	-2.82380000	-1.71003900
C	-3.34351700	-2.74946700	-0.34080200
C	-2.00505300	-3.33599100	0.09960600
C	-4.25781800	-3.21082900	0.84477100
C	-2.23271500	-4.45102100	0.92467300
C	-0.69824600	-2.98603600	-0.22445700
C	-3.69470600	-4.58264800	1.26640300
H	-4.15253600	-2.50125300	1.67222300
H	-5.31264800	-3.24442100	0.56195300
C	-1.15781100	-5.23395800	1.32150600
C	0.40106800	-3.77723700	0.16248300
H	-4.15433800	-5.40485900	0.70312200
C	0.14140100	-4.92206300	0.93143500
H	0.96718800	-5.55702600	1.22979200
H	-5.13262300	-2.46320700	-3.21244600
H	-3.85142300	-4.79950500	2.32713200
Br	-6.58331500	0.29193500	-3.08910400
C	-2.95643400	2.40499500	0.23154800
C	-2.48678500	3.41674000	-0.61831700
C	-2.95620500	2.61974100	1.63453400
C	-1.99155900	4.61685400	-0.12138900
H	-2.48933500	3.24656700	-1.68972000
C	-2.44747200	3.85585700	2.14895900
C	-3.47660800	1.66218500	2.57454900
C	-1.95563700	4.86062600	1.25927600

H	-1.62151600	5.37422400	-0.80671700
C	-2.43206400	4.09763700	3.55816500
C	-3.46491900	1.89568700	3.91600700
H	-3.89826700	0.73715200	2.19854600
C	-1.44069200	6.08714500	1.80434200
C	-1.91484600	5.32788700	4.07199400
C	-2.93606100	3.11343300	4.46143600
H	-3.86599400	1.15444300	4.60217300
C	-1.41914500	6.31032600	3.14695000
H	-1.06542000	6.83762300	1.11379900
C	-1.90737400	5.53970100	5.46066100
C	-2.90969100	3.36984000	5.84264800
H	-1.02641700	7.24223100	3.54493400
C	-2.39892700	4.56993000	6.33359400
H	-1.51254500	6.47445600	5.84967200
H	-3.29432600	2.61852700	6.52707700
H	-2.38507900	4.75222100	7.40430300
C	1.79748400	-3.47514900	-0.26901800
C	2.08385800	-3.47889200	-1.64132300
C	2.84428300	-3.24760000	0.66041000
C	3.37280500	-3.27744200	-2.11886300
H	1.27680000	-3.65703100	-2.34428600
C	4.17651500	-3.05104400	0.17136600
C	2.62985200	-3.18014800	2.08255700
C	4.43999400	-3.06827400	-1.23275100
H	3.56308200	-3.29145500	-3.18845500
C	5.25410900	-2.83563900	1.08562000
C	3.65824900	-2.97423600	2.95103400
H	1.62066000	-3.28238900	2.46352100
C	5.78690200	-2.87137000	-1.69460100
C	6.58539400	-2.64850300	0.59840100
C	5.00756900	-2.80450300	2.49164100
H	3.46641000	-2.92368800	4.01951900
C	6.81232400	-2.67279000	-0.82086700
H	5.97057900	-2.88947300	-2.76564700
C	7.62850200	-2.44680900	1.51752300
C	6.08185900	-2.59813900	3.37327700
H	7.82666100	-2.53072100	-1.18442400
C	7.37688300	-2.42354000	2.88857900
H	8.64008900	-2.30764900	1.14558900
H	5.89027600	-2.57407100	4.44265900
H	8.19607100	-2.26587100	3.58422600
O	-1.80627300	-0.22721400	0.63477800
O	-0.46903300	-1.78789700	-0.92903300

P	-0.34369200	-0.44068600	-0.04044500
O	0.69514900	-0.37060200	1.00194500
Br	-1.46002600	-6.77410200	2.42296700
N	-0.11752000	0.70863500	-1.26943700
H	0.43273400	1.54134100	-0.97025100
S	-0.53575500	0.74886500	-2.87579400
O	-1.62427400	-0.17525000	-3.15945300
O	-0.57894300	2.15239500	-3.27873100
C	0.97825900	0.05652000	-3.73661600
F	1.11771700	-1.23746800	-3.46658400
F	2.06748900	0.71678800	-3.33135200
F	0.82157600	0.22507700	-5.04959900
C	7.00579500	3.97549600	-0.82461500
C	5.83452100	4.67058400	-1.12545800
C	4.73916200	4.01222100	-1.70996500
C	4.85694200	2.64150100	-2.00279300
C	6.02649400	1.94939900	-1.69539400
C	7.10573500	2.61187300	-1.10451200
H	7.84139400	4.50284900	-0.37314100
H	5.77006900	5.73355100	-0.91478800
H	4.03091700	2.10972900	-2.46204500
H	6.09278600	0.88728200	-1.91325000
H	8.01680100	2.06981000	-0.86860800
C	3.50718300	4.76589500	-2.00629300
C	2.99322800	5.99503400	-1.32813800
C	2.24583500	4.34029000	-2.69548400
C	2.14662700	4.75150600	-1.25614400
H	2.61443700	6.81723300	-1.93794400
H	3.49646700	6.30410700	-0.41552900
H	1.81017300	5.01025600	-3.43890800
H	2.12434700	3.28571200	-2.92164300
C	1.88993900	3.87329000	-0.12153800
O	1.40334700	2.74833000	-0.20511100
O	2.27267600	4.40930600	1.04502700
C	2.13936400	3.56195500	2.20830600
H	2.49797200	4.16300500	3.04356800
H	1.09663200	3.27944600	2.36163500
H	2.74694600	2.66139800	2.09561600
TS1			
C	3.59394500	1.23315700	-0.34356800
C	4.72284200	1.15544000	-1.17674700
C	5.24601700	-0.08888600	-1.49701100
C	4.66780200	-1.25858400	-1.01094700

C	3.50186900	-1.20596900	-0.23353200
C	2.95219100	0.06109100	0.04555100
C	3.96501900	3.41106100	-1.21550000
C	5.16445200	2.52789000	-1.61967200
H	5.10681400	-2.22199900	-1.24269700
H	3.22476600	3.41631000	-2.02207200
H	4.24277200	4.44651000	-1.00236100
H	6.08706200	2.82906700	-1.10706200
C	3.35063300	2.69381300	0.03175400
C	1.98173700	3.26613200	0.39301900
C	4.16419500	3.08052100	1.31361400
C	2.14460400	4.33190400	1.29526100
C	0.70511500	2.94423800	-0.05750100
C	3.57407700	4.43231900	1.76263400
H	3.98645700	2.32714200	2.08825300
H	5.23956600	3.12052400	1.12357000
C	1.04364200	5.10113900	1.64444200
C	-0.41977700	3.72125900	0.28565500
H	4.08201400	5.27961500	1.28415100
C	-0.22088600	4.82096700	1.13438000
H	-1.06515800	5.44627900	1.39965700
H	5.37298600	2.56200800	-2.69311100
H	3.64410500	4.59039600	2.84290500
Br	6.79984900	-0.20678700	-2.61614300
C	2.88630100	-2.48215400	0.24045400
C	2.45832800	-3.41550400	-0.71413900
C	2.77627600	-2.79786500	1.61970100
C	1.90439400	-4.63631200	-0.34551500
H	2.53771700	-3.16582200	-1.76687400
C	2.20953700	-4.05628100	2.00283800
C	3.23699500	-1.92083000	2.66383800
C	1.76702300	-4.98108300	1.00709900
H	1.55996700	-5.32608900	-1.11032200
C	2.08712700	-4.40042200	3.38518100
C	3.12211300	-2.25104000	3.97988300
H	3.69590300	-0.97812500	2.38896100
C	1.19434000	-6.23354500	1.42059400
C	1.51467900	-5.65409200	3.76727100
C	2.53828400	-3.49551900	4.39344900
H	3.48009700	-1.56894600	4.74652800
C	1.07201500	-6.55486500	2.73787900
H	0.86043100	-6.92343300	0.65017400
C	1.40350600	-5.96769700	5.13215200
C	2.40745500	-3.85240500	5.74619200

H	0.63855000	-7.50599600	3.03583700
C	1.84505800	-5.07511900	6.10812400
H	0.96794000	-6.92059300	5.42089200
H	2.75248000	-3.16134400	6.51059600
H	1.75127400	-5.33556200	7.15850900
C	-1.77513600	3.44369900	-0.27261300
C	-1.93760500	3.46411200	-1.66564500
C	-2.90363100	3.21035900	0.55489100
C	-3.18045100	3.28552500	-2.25962800
H	-1.06895800	3.63534500	-2.29163900
C	-4.18949300	3.03945900	-0.05445300
C	-2.81790100	3.10573200	1.98859100
C	-4.32669500	3.08365000	-1.47607100
H	-3.27245600	3.31392300	-3.34179100
C	-5.34710200	2.82063700	0.75588700
C	-3.92142400	2.89334700	2.75776000
H	-1.84523200	3.18179500	2.45974500
C	-5.62995100	2.91879200	-2.05915200
C	-6.63225400	2.66328600	0.14841100
C	-5.22699000	2.75447100	2.17733200
H	-3.82494700	2.81316400	3.83726300
C	-6.73195900	2.72153000	-1.28439900
H	-5.71669200	2.95871700	-3.14176500
C	-7.75507000	2.45473700	0.96683800
C	-6.37753200	2.54204600	2.95528200
H	-7.71199400	2.60274000	-1.73900500
C	-7.62641600	2.39625600	2.35383500
H	-8.73129600	2.33845900	0.50363800
H	-6.28189300	2.49113100	4.03652400
H	-8.50597900	2.23365200	2.97012500
O	1.73020200	0.13031800	0.71965800
O	0.52967800	1.79855800	-0.84699500
P	0.32220400	0.37934200	-0.07031200
O	-0.77505900	0.30626000	0.92321400
Br	1.26034900	6.57882200	2.84847300
N	0.12130400	-0.69920100	-1.31796700
H	-0.82926600	-1.54207700	-1.14506500
S	0.66117500	-0.63825700	-2.85660600
O	1.89201700	0.13246700	-3.03259700
O	0.55576000	-1.99320100	-3.40635300
C	-0.67463600	0.34039400	-3.76674400
F	-0.33689500	1.63034700	-3.83154200
F	-1.85371000	0.22874400	-3.14750400
F	-0.78683700	-0.14153400	-5.00770100

C	-6.59686900	-4.24332700	-0.69808700
C	-5.56701900	-3.31413500	-0.62113000
C	-4.35557300	-3.64450900	0.02674200
C	-4.21641800	-4.92360400	0.61014400
C	-5.25106200	-5.84755400	0.52808100
C	-6.43929200	-5.51102100	-0.12803500
H	-7.52432500	-3.98248600	-1.19796600
H	-5.69718000	-2.32770500	-1.05226900
H	-3.30171300	-5.18352500	1.13119300
H	-5.13592700	-6.82909600	0.97670400
H	-7.24693500	-6.23462200	-0.18839300
C	-3.30236600	-2.66131400	0.15475200
C	-3.11379700	-1.44498900	-0.67143400
C	-1.87866200	-2.91846100	0.47911500
C	-1.84671900	-2.34765700	-0.99158900
H	-2.79069200	-0.54819300	-0.14260200
H	-3.83240100	-1.23972700	-1.46117300
H	-1.40427700	-2.20899500	1.15673600
H	-1.56526200	-3.94615900	0.64456400
C	-1.91933900	-3.33921300	-2.10309500
O	-1.51082500	-4.48482900	-2.04652900
O	-2.43688300	-2.77628500	-3.21408200
C	-2.38521900	-3.58042000	-4.40717800
H	-2.81194700	-2.96081200	-5.19615600
H	-1.35103200	-3.83741300	-4.64610300
H	-2.97134900	-4.49475300	-4.28477000

ωB97X-D/IEF-PCM

React

C	2.88435000	0.58542600	-1.12083700
C	1.77703500	-0.25113500	-1.22026600
C	1.09045200	-0.66302000	-0.07342800
C	1.54796900	-0.23261200	1.17800400
C	2.65387700	0.60365200	1.27444800
C	3.32556200	1.01798300	0.12623700
H	3.40552100	0.89503000	-2.02110900
H	1.44671400	-0.59592600	-2.19493600
H	1.03587600	-0.54717000	2.08120100
H	2.99282900	0.93250900	2.25160600
H	4.19063600	1.66837000	0.20461100
C	-0.10200600	-1.51858400	-0.19947500
C	-1.04437600	-1.61936700	-1.35463800
C	-0.96457500	-2.12999700	0.85711300
C	-1.56631000	-1.10172700	-0.04759900

H	-1.38336200	-2.60245600	-1.68140800
H	-0.92325900	-0.89088400	-2.15210500
H	-1.28632100	-3.16439600	0.73628000
H	-0.79064700	-1.82674600	1.88581300
C	-1.92953700	0.26148500	0.34011900
O	-2.01508700	0.64691800	1.48901300
O	-2.11773700	1.05005700	-0.72824000
C	-2.38443300	2.42378300	-0.43665800
H	-2.51355500	2.91021700	-1.40184200
H	-3.29202900	2.52037900	0.16251400
H	-1.54784200	2.86994200	0.10506800

CBA

C	-2.11301300	-2.00284800	0.54824000
C	-3.20203500	-2.75239700	0.09211400
C	-4.34854300	-2.10605200	-0.33431200
C	-4.42192100	-0.71830100	-0.33676600
C	-3.31971900	0.04722300	0.04379500
C	-2.16036800	-0.62172800	0.46344200
C	-1.36647900	-4.23546600	0.31987400
C	-2.89122600	-4.22438900	0.11923000
H	-5.32592200	-0.21952500	-0.66670500
H	-0.86524000	-4.17179200	-0.65052400
H	-1.00379600	-5.13110300	0.82918300
H	-3.41882800	-4.71717400	0.94422200
C	-1.06737000	-2.94010100	1.12733800
C	0.41716800	-2.62681000	1.13883400
C	-1.31634700	-3.18649000	2.64414300
C	1.01710400	-3.24417900	2.23861900
C	1.20219300	-1.91355000	0.24928000
C	-0.02004700	-3.84199800	3.15044700
H	-1.45927500	-2.22110600	3.14010500
H	-2.20690500	-3.79336700	2.82305500
C	2.39508200	-3.21027800	2.36929600
C	2.59485300	-1.85985900	0.36956400
H	-0.04429800	-4.93327700	3.04764600
C	3.18155900	-2.54523000	1.43662000
H	4.26000000	-2.53052500	1.54501400
H	-3.20299600	-4.72235200	-0.80235600
H	0.18480600	-3.62412700	4.20157300
Br	-5.82561900	-3.12221900	-0.94195000
C	-3.36136700	1.52903700	-0.08561700
C	-3.61049100	2.07604800	-1.34971600
C	-3.13887200	2.38596500	1.01069200

C	-3.60120300	3.44741700	-1.56024500
H	-3.79174500	1.40777100	-2.18592800
C	-3.12852700	3.79245500	0.79644500
C	-2.94095200	1.89654800	2.35194000
C	-3.35194800	4.32503100	-0.50162000
H	-3.77937100	3.84280700	-2.55528700
C	-2.88730800	4.68165500	1.88989600
C	-2.72023200	2.74057800	3.38525400
H	-2.98286800	0.82794900	2.52971800
C	-3.31850300	5.75194700	-0.69092500
C	-2.85971100	6.08546900	1.67479600
C	-2.67440200	4.16547200	3.19437000
H	-2.57610000	2.34957100	4.38810500
C	-3.08258700	6.58960400	0.34460300
H	-3.48692900	6.14181900	-1.69021800
C	-2.61739000	6.93692400	2.75774200
C	-2.43725800	5.05036300	4.25118700
H	-3.05801000	7.66416600	0.18947100
C	-2.40807600	6.42261500	4.03220700
H	-2.59372100	8.01007200	2.59255900
H	-2.27483000	4.65338000	5.24890600
H	-2.22103400	7.09700400	4.86136000
C	3.43493900	-1.12287200	-0.61152300
C	3.39121800	-1.50769100	-1.95214100
C	4.28310300	-0.07122400	-0.21194300
C	4.19148500	-0.89627000	-2.90332000
H	2.71771700	-2.30400600	-2.25046300
C	5.11504500	0.54871600	-1.18503700
C	4.32655700	0.42849400	1.14004300
C	5.07063200	0.12685200	-2.54034100
H	4.13974700	-1.21462400	-3.93991700
C	6.00144100	1.60455700	-0.80444600
C	5.16313000	1.42976600	1.49683000
H	3.65553000	0.00034600	1.87524100
C	5.92965600	0.76756500	-3.50224900
C	6.84246500	2.21508700	-1.77351100
C	6.04342800	2.04926900	0.54272800
H	5.17251900	1.79462400	2.51977300
C	6.77522700	1.75847300	-3.13765600
H	5.88255700	0.43375400	-4.53466600
C	7.70709400	3.24113400	-1.37784200
C	6.92072000	3.07956500	0.89748700
H	7.41940100	2.23254900	-3.87256500
C	7.74530900	3.66689500	-0.05489500

H	8.35077600	3.70617000	-2.11899700
H	6.94933900	3.41943000	1.92875700
H	8.42090800	4.46510600	0.23516400
O	-1.02842000	0.13280700	0.75982200
O	0.56743700	-1.18077400	-0.75876200
P	0.13389600	0.30566600	-0.34394800
O	1.16075600	1.23538400	0.13485800
Br	3.21667500	-4.07024900	3.84314400
N	-0.71003800	0.72645400	-1.75236500
H	-1.32390300	1.53867500	-1.67815200
S	-0.54056200	0.21867600	-3.31789300
O	-1.14251500	1.24774000	-4.13845300
O	0.78449500	-0.30007800	-3.55442600
C	-1.70192900	-1.23205500	-3.41082100
F	-2.92794900	-0.83639300	-3.09388900
F	-1.32063200	-2.19439800	-2.58710800
F	-1.68888400	-1.68043500	-4.65688300

M1

C	-2.58149900	-2.62055100	0.00047300
C	-3.65432900	-3.15431600	-0.71676600
C	-4.67939700	-2.32252900	-1.12828500
C	-4.64797200	-0.96599900	-0.83786100
C	-3.55369600	-0.40019600	-0.17734500
C	-2.50235100	-1.25095200	0.19812900
C	-1.99315900	-4.83733600	-0.57891800
C	-3.47045800	-4.62904000	-0.95054800
H	-5.47141500	-0.32720200	-1.13556300
H	-1.36330100	-4.63918300	-1.45170700
H	-1.77261200	-5.84603300	-0.22144400
H	-4.14295900	-5.21133200	-0.30953500
C	-1.70559800	-3.75550100	0.49979700
C	-0.21849300	-3.60839500	0.75023700
C	-2.18360400	-4.24632500	1.89795500
C	0.17200100	-4.46025500	1.78562900
C	0.73237000	-2.84017800	0.10051700
C	-1.02455000	-5.10511600	2.43072500
H	-2.32531700	-3.37626900	2.54730700
H	-3.13257200	-4.78479700	1.84398100
C	1.51555800	-4.58154000	2.09575400
C	2.09405400	-2.94946600	0.40321300
H	-1.11292000	-6.15264400	2.11916400
C	2.47171300	-3.85044400	1.40242400
H	3.52235400	-3.95572000	1.64782000

H	-3.69247700	-4.90712000	-1.98386500
H	-0.95553600	-5.09999700	3.52140400
Br	-6.14505300	-3.04271000	-2.08790700
C	-3.55490800	1.06866800	0.06396000
C	-3.76652600	1.91495300	-1.02719900
C	-3.42069900	1.62085800	1.35392900
C	-3.81418300	3.29120800	-0.87848800
H	-3.86512200	1.48193400	-2.01678200
C	-3.45175800	3.03517600	1.50620900
C	-3.27572200	0.81396600	2.53958800
C	-3.64531800	3.87543600	0.37781600
H	-3.96009300	3.92533500	-1.74781000
C	-3.26709200	3.62387800	2.79630600
C	-3.11778100	1.37215800	3.76228900
H	-3.30366400	-0.26535300	2.44464700
C	-3.63321700	5.30406200	0.55522400
C	-3.24391400	5.03740500	2.94015700
C	-3.08674600	2.79916500	3.93720000
H	-3.00924800	0.74201000	4.64018500
C	-3.43455400	5.85822900	1.77285200
H	-3.77271200	5.92995000	-0.32123200
C	-3.03387900	5.59092800	4.20708200
C	-2.88253200	3.39188800	5.18780200
H	-3.41449200	6.93752800	1.89204000
C	-2.85393100	4.77509300	5.31857600
H	-3.01187600	6.67143400	4.31521500
H	-2.74409900	2.75768900	6.05864500
H	-2.69153400	5.22149600	6.29423900
C	3.14018600	-2.17784900	-0.32160800
C	3.32846300	-2.41976300	-1.68268400
C	3.98466300	-1.27416100	0.35129400
C	4.35882600	-1.81568900	-2.38627600
H	2.66108300	-3.10756100	-2.19144800
C	5.05867900	-0.67373700	-0.36119700
C	3.79653300	-0.91520500	1.73475600
C	5.25116100	-0.95594300	-1.73970200
H	4.49103400	-2.02734900	-3.44306400
C	5.95411900	0.21780100	0.30838400
C	4.63130000	-0.05423300	2.35976000
H	2.94712200	-1.32792600	2.26563000
C	6.36345900	-0.35388400	-2.42879300
C	7.04446900	0.79683500	-0.39546500
C	5.74909400	0.53892400	1.67522700
H	4.46195200	0.21397600	3.39846700

C	7.22301100	0.47186500	-1.78744400
H	6.50046400	-0.58268200	-3.48157100
C	7.89866300	1.67961200	0.27401000
C	6.62498500	1.42693900	2.30798300
H	8.05945500	0.91716800	-2.31803600
C	7.68830100	1.99099300	1.61244800
H	8.73033700	2.12342200	-0.26556500
H	6.46383200	1.67527700	3.35299500
H	8.35821700	2.67942700	2.11728000
O	-1.34584900	-0.70565400	0.75057100
O	0.30265400	-1.88825200	-0.82754600
P	-0.04669700	-0.45719700	-0.17915600
O	1.01054400	0.20995100	0.58661600
Br	2.05541000	-5.74884500	3.48663200
N	-0.55461500	0.36988200	-1.55929100
H	-0.68934000	1.37979600	-1.36643000
S	-1.16422800	-0.14619100	-2.99741800
O	-1.72033300	-1.47594700	-2.90051700
O	-1.90606500	0.96469500	-3.56084100
C	0.35689300	-0.31626100	-4.05247000
F	1.29753900	-0.98601800	-3.40477000
F	0.81627400	0.88675000	-4.37468400
F	0.02165300	-0.96843500	-5.15554300
C	4.20230700	3.88064500	-1.03463500
C	3.09236600	4.71905800	-1.06292600
C	1.90419500	4.29961700	-1.66967200
C	1.85715300	3.03019500	-2.25746400
C	2.96269500	2.19055700	-2.21852200
C	4.13978500	2.61538400	-1.60952800
H	5.11979100	4.21436700	-0.56011500
H	3.14854400	5.70719600	-0.61719600
H	0.95102000	2.69715500	-2.74829300
H	2.90772200	1.20117600	-2.66047700
H	5.00641000	1.96718900	-1.59434400
C	0.70692500	5.15817000	-1.63184800
C	0.35185900	6.18745800	-0.60399400
C	-0.65903000	4.89431800	-2.17436800
C	-0.49182400	4.95374000	-0.68827900
H	-0.09349100	7.12772300	-0.92776600
H	1.00874600	6.26869100	0.25798600
H	-1.20035500	5.71423800	-2.64560300
H	-0.85694200	3.91730300	-2.60638700
C	-0.46668200	3.78561500	0.17950900
O	-0.70685700	2.65309400	-0.21179600

O	-0.09926200	4.05945800	1.42336600
C	0.10128200	2.91920100	2.27631000
H	0.34012500	3.33198000	3.25448300
H	-0.80801500	2.31977000	2.32638800
H	0.91195700	2.29997500	1.89075400

TS1

C	3.98940600	-0.66050600	0.02317400
C	4.98935800	-1.30591000	-0.70577700
C	4.85768300	-2.65436100	-0.99161000
C	3.73005400	-3.36257700	-0.59370200
C	2.68679300	-2.71709100	0.07295900
C	2.83811600	-1.35186400	0.35589600
C	5.41394900	1.02313700	-0.82085500
C	6.07525300	-0.33945600	-1.09570800
H	3.64012400	-4.41734100	-0.82755300
H	4.83718600	1.33459500	-1.69736200
H	6.13192700	1.81343300	-0.58836000
H	6.97143700	-0.49187100	-0.48245700
C	4.43099400	0.75522000	0.35590400
C	3.46141600	1.91198700	0.54357700
C	5.19333600	0.80753000	1.71169900
C	4.00370900	2.83984400	1.43758400
C	2.23262500	2.17664700	-0.03722400
C	5.26182600	2.30317800	2.06641500
H	4.60576900	0.27630100	2.46737600
H	6.17528300	0.33218600	1.65153900
C	3.35109900	4.04147000	1.65578000
C	1.56834500	3.39450100	0.16123300
H	6.14648100	2.78648400	1.63504000
C	2.15428500	4.33404700	1.00840800
H	1.65941800	5.28403200	1.17570400
H	6.37622900	-0.46304500	-2.13904900
H	5.29097300	2.48516200	3.14367300
Br	6.22933000	-3.54286300	-1.95313800
C	1.40464500	-3.42261300	0.34416900
C	0.75842700	-4.03262000	-0.73317800
C	0.78566800	-3.42086300	1.61082900
C	-0.50848500	-4.57791000	-0.60560300
H	1.23700300	-4.02010900	-1.70661100
C	-0.52258900	-3.96361700	1.74120000
C	1.42473400	-2.89622100	2.79162400
C	-1.17794400	-4.53551900	0.61862900
H	-1.00488400	-5.00270200	-1.47152900

C	-1.19931300	-3.91261100	3.00120500
C	0.79041000	-2.86210000	3.98535400
H	2.44172100	-2.52885300	2.71200900
C	-2.51782700	-5.04125300	0.76953000
C	-2.52363300	-4.41443300	3.12191000
C	-0.55514100	-3.34950000	4.13363800
H	1.29324500	-2.46173200	4.86073400
C	-3.15976800	-4.98248900	1.95996700
H	-3.00906600	-5.45383600	-0.10503100
C	-3.17410600	-4.33475100	4.35779700
C	-1.23824500	-3.29350200	5.35308200
H	-4.17180800	-5.36462400	2.06043900
C	-2.53597500	-3.77954900	5.46105000
H	-4.18801800	-4.71396000	4.44778800
H	-0.74293900	-2.86267500	6.21838400
H	-3.05428000	-3.72618800	6.41297300
C	0.29613900	3.67413300	-0.56694200
C	0.36954900	3.87675600	-1.94576700
C	-0.95613600	3.70103900	0.07524900
C	-0.76749400	4.09008500	-2.70751400
H	1.34123800	3.84993100	-2.42739800
C	-2.12815700	3.89795600	-0.70797200
C	-1.10897500	3.49766200	1.49407600
C	-2.03009400	4.09011200	-2.11098100
H	-0.68241100	4.23542400	-3.78009100
C	-3.41805300	3.87489700	-0.08901600
C	-2.32843600	3.48292500	2.07808700
H	-0.22040100	3.32443700	2.08872800
C	-3.23462300	4.25976000	-2.88149300
C	-4.59101100	4.04489300	-0.87403500
C	-3.53230500	3.66404000	1.31027200
H	-2.41991800	3.31615600	3.14721100
C	-4.45342600	4.23717700	-2.29483500
H	-3.14155100	4.40298100	-3.95404700
C	-5.84293500	4.01516700	-0.24820500
C	-4.80274300	3.63131600	1.89576200
H	-5.35426900	4.36352500	-2.88817000
C	-5.94484000	3.81030000	1.12358900
H	-6.73841100	4.14982900	-0.84817100
H	-4.88841100	3.46563900	2.96559400
H	-6.92265400	3.78310100	1.59329300
O	1.80047200	-0.66875800	0.96169300
O	1.60274300	1.18590400	-0.78088800
P	0.71281900	0.14786700	0.09059800

O	-0.25549200	0.72101700	1.04664000
Br	4.09482600	5.30475700	2.85795800
N	-0.00033300	-0.78175600	-1.05116700
H	-1.34745500	-0.93462300	-0.82060100
S	0.42212400	-1.10837400	-2.56774600
O	1.85619100	-1.22717300	-2.76947000
O	-0.47215800	-2.14851700	-3.05386200
C	-0.10639800	0.41233200	-3.51453400
F	0.88136900	1.29352000	-3.57939100
F	-1.16017200	0.97123000	-2.92585300
F	-0.44352500	0.05146800	-4.74899400
C	-7.40945900	0.16599700	-0.09793400
C	-6.03660100	0.35685700	-0.00675700
C	-5.19948000	-0.71019400	0.33703100
C	-5.75138400	-1.97240800	0.59211200
C	-7.12250200	-2.16022600	0.48345700
C	-7.95262900	-1.09323700	0.14172700
H	-8.05197700	1.00182300	-0.35356700
H	-5.61736200	1.34299000	-0.17622500
H	-5.11347400	-2.81083000	0.85020500
H	-7.54648900	-3.14114600	0.66864100
H	-9.02447400	-1.24485200	0.06718800
C	-3.75962100	-0.44683400	0.46675300
C	-3.02900200	0.49092100	-0.37177100
C	-2.74548700	-1.39572600	0.89394300
C	-2.61173000	-1.01548800	-0.62323400
H	-2.19376000	1.03781000	0.05957900
H	-3.57594600	1.00257700	-1.15759600
H	-1.88714000	-1.01659800	1.44380900
H	-3.05515700	-2.40377500	1.14744600
C	-3.22966100	-1.85713300	-1.68494500
O	-3.50299900	-3.02955200	-1.56010200
O	-3.39815700	-1.14803000	-2.80060700
C	-3.82227500	-1.89129400	-3.94735500
H	-3.90479900	-1.16444600	-4.75284700
H	-3.07450000	-2.64769600	-4.19123900
H	-4.78576200	-2.36877400	-3.76049300

ωB97X-D/SMD

React

C	-2.08879900	-2.02970400	0.53208800
C	-3.15843300	-2.80218400	0.06744700
C	-4.31200900	-2.17618200	-0.37074900
C	-4.41292900	-0.79008600	-0.37654500

C	-3.33024200	-0.00231300	0.01578900
C	-2.16222600	-0.65004500	0.44470500
C	-1.29642800	-4.24814200	0.32101600
C	-2.81843500	-4.26758000	0.10363200
H	-5.32358600	-0.30837400	-0.71436300
H	-0.78550500	-4.17907700	-0.64416100
H	-0.92315900	-5.13407600	0.83993400
H	-3.34437200	-4.76660100	0.92609800
C	-1.03127200	-2.94409700	1.12613900
C	0.44775700	-2.60392500	1.15296100
C	-1.29244600	-3.18934500	2.64030700
C	1.04593300	-3.21048000	2.26065300
C	1.23136300	-1.88030500	0.27022400
C	0.00813300	-3.82241600	3.16221100
H	-1.45544500	-2.22460900	3.13180400
H	-2.17482100	-3.81076400	2.81010100
C	2.42233700	-3.15711500	2.40183300
C	2.62295900	-1.81248900	0.39947900
H	0.00237000	-4.91400600	3.05973400
C	3.20953300	-2.48661000	1.47373100
H	4.28726600	-2.45987100	1.58868600
H	-3.10799700	-4.77616200	-0.81972100
H	0.19569200	-3.59811800	4.21544400
Br	-5.77004000	-3.22081800	-0.98534500
C	-3.40451700	1.47931500	-0.10825100
C	-3.66298700	2.02417200	-1.37097800
C	-3.20598900	2.33850800	0.99174400
C	-3.68850700	3.39562100	-1.57754600
H	-3.82144100	1.35440200	-2.21032100
C	-3.23012500	3.74588600	0.78125900
C	-2.99798400	1.85188700	2.33285400
C	-3.46444900	4.27648600	-0.51589300
H	-3.87366100	3.78999300	-2.57209900
C	-3.01330600	4.63865500	1.87744400
C	-2.80012300	2.69890400	3.36874700
H	-3.01505600	0.78253000	2.51125800
C	-3.46672900	5.70447400	-0.70155200
C	-3.02082200	6.04362900	1.66575900
C	-2.78941900	4.12502400	3.18135600
H	-2.64863300	2.30971100	4.37146800
C	-3.25404500	6.54565000	0.33636700
H	-3.64255500	6.09158600	-1.70096800
C	-2.80156300	6.89845000	2.75125500
C	-2.57644800	5.01326200	4.24094100

H	-3.25600700	7.62118700	0.18430200
C	-2.58148600	6.38638300	4.02494000
H	-2.80453700	7.97231800	2.58752200
H	-2.40594600	4.61741800	5.23801300
H	-2.41275000	7.06373400	4.85609100
C	3.46485600	-1.07906800	-0.58394900
C	3.43603500	-1.48369500	-1.91958700
C	4.30456900	-0.01710600	-0.19246100
C	4.24211400	-0.88237000	-2.87260600
H	2.77285100	-2.29114900	-2.21198300
C	5.14120400	0.59386200	-1.16776700
C	4.33430900	0.50197500	1.15289400
C	5.11167000	0.15179800	-2.51723800
H	4.20291600	-1.21721200	-3.90479500
C	6.01811200	1.66070500	-0.79509200
C	5.16155900	1.51401700	1.50197200
H	3.66169600	0.07950600	1.89034100
C	5.97550600	0.78320900	-3.48117700
C	6.86421300	2.26188800	-1.76604200
C	6.04548800	2.12565300	0.54592100
H	5.16067400	1.89361000	2.51980100
C	6.81212600	1.78456800	-3.12394700
H	5.93895700	0.43333400	-4.50894800
C	7.71928000	3.29916200	-1.37810400
C	6.91332000	3.16687600	0.89288100
H	7.46059700	2.25189400	-3.85973600
C	7.74270500	3.74485200	-0.06124900
H	8.36678800	3.75678100	-2.12084700
H	6.93030700	3.52224100	1.91935000
H	8.41076800	4.55198600	0.22273700
O	-1.04767800	0.12383800	0.75611500
O	0.59671800	-1.15333500	-0.74270900
P	0.12724500	0.32207800	-0.32857900
O	1.12603000	1.27098300	0.17295000
Br	3.24613500	-4.00403800	3.88549200
N	-0.69577200	0.73822700	-1.75055100
H	-1.28638600	1.56930000	-1.68677100
S	-0.50156500	0.23257400	-3.31261600
O	-1.10256900	1.25547500	-4.14217200
O	0.83069300	-0.27363400	-3.53803900
C	-1.64191900	-1.23212400	-3.42353200
F	-2.87971200	-0.85684400	-3.13354800
F	-1.26132700	-2.18888100	-2.59347200
F	-1.59671400	-1.68127700	-4.67004800

CBA

C	-2.60755400	-2.61395400	-0.03023900
C	-3.67749800	-3.13694100	-0.76049200
C	-4.69584700	-2.29486500	-1.16876300
C	-4.66349200	-0.94155700	-0.86249200
C	-3.57168400	-0.38738400	-0.18768800
C	-2.52516900	-1.24684200	0.18138800
C	-2.02233200	-4.82687900	-0.62641600
C	-3.49599100	-4.61009300	-1.00636600
H	-5.48355300	-0.29640700	-1.15674000
H	-1.38567700	-4.62301100	-1.49319800
H	-1.80919700	-5.83970600	-0.27585200
H	-4.17378400	-5.19546600	-0.37358900
C	-1.73893500	-3.75657700	0.46486600
C	-0.25234300	-3.61851300	0.72860800
C	-2.23009100	-4.25926500	1.85384100
C	0.12481100	-4.48700700	1.75624800
C	0.70954100	-2.84990900	0.09478400
C	-1.08072800	-5.13072400	2.38507700
H	-2.37034100	-3.39563000	2.51223200
H	-3.18157200	-4.79197000	1.78598600
C	1.46597600	-4.62507800	2.06948000
C	2.06978600	-2.98208800	0.39773400
H	-1.17317900	-6.17382500	2.05963800
C	2.43381200	-3.89894800	1.38756900
H	3.48290800	-4.02085800	1.63274800
H	-3.70948900	-4.87911800	-2.04404600
H	-1.02158800	-5.13721200	3.47650400
Br	-6.16145300	-2.99794100	-2.14635500
C	-3.56746500	1.07834700	0.07553600
C	-3.78229600	1.94099300	-1.00258200
C	-3.42367000	1.61273000	1.37277300
C	-3.82895900	3.31507200	-0.83444900
H	-3.88936000	1.52198600	-1.99751800
C	-3.44917700	3.02546500	1.54417200
C	-3.27246800	0.79044400	2.54755900
C	-3.65179100	3.88149700	0.42924600
H	-3.98192000	3.96153200	-1.69364200
C	-3.25215700	3.59668900	2.84074200
C	-3.09983100	1.33203100	3.77569400
H	-3.30990100	-0.28764500	2.44178200
C	-3.63905900	5.30774700	0.62646900
C	-3.22626400	5.00838700	3.00364500

C	-3.06204000	2.75646100	3.96891000
H	-2.98689500	0.69012700	4.64479300
C	-3.42857700	5.84541400	1.84983100
H	-3.78950300	5.94555500	-0.23986600
C	-3.00190300	5.54472200	4.27593700
C	-2.84401500	3.33194900	5.22541200
H	-3.40814400	6.92303200	1.98466000
C	-2.81145200	4.71347800	5.37423900
H	-2.97736400	6.62388200	4.39817200
H	-2.69788500	2.68528000	6.08605200
H	-2.63829900	5.14664200	6.35440700
C	3.12921800	-2.22135600	-0.32086100
C	3.31441400	-2.45779100	-1.68385400
C	3.98820600	-1.33495800	0.35779400
C	4.35154200	-1.86177400	-2.38480700
H	2.63892700	-3.13486000	-2.19693000
C	5.06609900	-0.73914400	-0.35375200
C	3.81047400	-0.98713800	1.74579900
C	5.25182700	-1.01246200	-1.73512100
H	4.48016600	-2.06752900	-3.44348300
C	5.96958600	0.14247500	0.31854500
C	4.65540900	-0.13836500	2.37451200
H	2.96326400	-1.39980700	2.28067900
C	6.36187900	-0.40794700	-2.42581000
C	7.05845400	0.72318100	-0.38679700
C	5.77278100	0.45429500	1.68903200
H	4.49434300	0.12059100	3.41707300
C	7.22691200	0.41108800	-1.78312900
H	6.49105800	-0.62857400	-3.48158800
C	7.91987300	1.59707400	0.28560300
C	6.65601100	1.33322600	2.32485700
H	8.06113500	0.86009600	-2.31464600
C	7.71807000	1.89805500	1.62791200
H	8.75014400	2.04254300	-0.25516700
H	6.50040900	1.57361900	3.37281400
H	8.39387300	2.57988000	2.13465100
O	-1.37149200	-0.71209800	0.74758200
O	0.29524700	-1.87974300	-0.82208200
P	-0.06131200	-0.45569200	-0.16258500
O	0.98095200	0.20499100	0.62869400
Br	1.99040600	-5.81553600	3.45012500
N	-0.54590500	0.39095800	-1.53839900
H	-0.64008400	1.40788400	-1.35355000
S	-1.14158400	-0.10241500	-2.98822900

O	-1.69914400	-1.43311900	-2.91333200
O	-1.87676300	1.01484600	-3.54746200
C	0.38592300	-0.26168000	-4.03428300
F	1.32290400	-0.93717700	-3.38815900
F	0.84543100	0.94294700	-4.34775700
F	0.05675800	-0.90672300	-5.14506900
C	4.24217900	3.93797400	-0.98828500
C	3.13811600	4.78436600	-1.02600700
C	1.95333100	4.37486000	-1.64670200
C	1.90298100	3.10654900	-2.23750000
C	3.00327200	2.26052100	-2.19095700
C	4.17730700	2.67512000	-1.56881800
H	5.15642500	4.26367500	-0.50144200
H	3.19577200	5.77038300	-0.57518600
H	0.99636000	2.77587200	-2.72965200
H	2.94369400	1.27302100	-2.63611200
H	5.03827000	2.01819300	-1.54299500
C	0.76245000	5.24425700	-1.62360200
C	0.39558700	6.26058400	-0.58819800
C	-0.59265600	4.99748000	-2.19900900
C	-0.45822100	5.03501400	-0.70770400
H	-0.03630400	7.20874200	-0.90773300
H	1.03811100	6.32392900	0.28629700
H	-1.11714200	5.82932400	-2.66877800
H	-0.78467300	4.02856300	-2.65181000
C	-0.45346100	3.85311800	0.14345300
O	-0.68770900	2.72651700	-0.26781600
O	-0.11253900	4.11120800	1.39840900
C	0.09637800	2.96421100	2.23940300
H	0.23003500	3.36392600	3.24361800
H	-0.76419900	2.29601000	2.20316700
H	0.98339500	2.42027700	1.91052500

M1

C	-2.60755400	-2.61395400	-0.03023900
C	-3.67749800	-3.13694100	-0.76049200
C	-4.69584700	-2.29486500	-1.16876300
C	-4.66349200	-0.94155700	-0.86249200
C	-3.57168400	-0.38738400	-0.18768800
C	-2.52516900	-1.24684200	0.18138800
C	-2.02233200	-4.82687900	-0.62641600
C	-3.49599100	-4.61009300	-1.00636600
H	-5.48355300	-0.29640700	-1.15674000
H	-1.38567700	-4.62301100	-1.49319800

H	-1.80919700	-5.83970600	-0.27585200
H	-4.17378400	-5.19546600	-0.37358900
C	-1.73893500	-3.75657700	0.46486600
C	-0.25234300	-3.61851300	0.72860800
C	-2.23009100	-4.25926500	1.85384100
C	0.12481100	-4.48700700	1.75624800
C	0.70954100	-2.84990900	0.09478400
C	-1.08072800	-5.13072400	2.38507700
H	-2.37034100	-3.39563000	2.51223200
H	-3.18157200	-4.79197000	1.78598600
C	1.46597600	-4.62507800	2.06948000
C	2.06978600	-2.98208800	0.39773400
H	-1.17317900	-6.17382500	2.05963800
C	2.43381200	-3.89894800	1.38756900
H	3.48290800	-4.02085800	1.63274800
H	-3.70948900	-4.87911800	-2.04404600
H	-1.02158800	-5.13721200	3.47650400
Br	-6.16145300	-2.99794100	-2.14635500
C	-3.56746500	1.07834700	0.07553600
C	-3.78229600	1.94099300	-1.00258200
C	-3.42367000	1.61273000	1.37277300
C	-3.82895900	3.31507200	-0.83444900
H	-3.88936000	1.52198600	-1.99751800
C	-3.44917700	3.02546500	1.54417200
C	-3.27246800	0.79044400	2.54755900
C	-3.65179100	3.88149700	0.42924600
H	-3.98192000	3.96153200	-1.69364200
C	-3.25215700	3.59668900	2.84074200
C	-3.09983100	1.33203100	3.77569400
H	-3.30990100	-0.28764500	2.44178200
C	-3.63905900	5.30774700	0.62646900
C	-3.22626400	5.00838700	3.00364500
C	-3.06204000	2.75646100	3.96891000
H	-2.98689500	0.69012700	4.64479300
C	-3.42857700	5.84541400	1.84983100
H	-3.78950300	5.94555500	-0.23986600
C	-3.00190300	5.54472200	4.27593700
C	-2.84401500	3.33194900	5.22541200
H	-3.40814400	6.92303200	1.98466000
C	-2.81145200	4.71347800	5.37423900
H	-2.97736400	6.62388200	4.39817200
H	-2.69788500	2.68528000	6.08605200
H	-2.63829900	5.14664200	6.35440700
C	3.12921800	-2.22135600	-0.32086100

C	3.31441400	-2.45779100	-1.68385400
C	3.98820600	-1.33495800	0.35779400
C	4.35154200	-1.86177400	-2.38480700
H	2.63892700	-3.13486000	-2.19693000
C	5.06609900	-0.73914400	-0.35375200
C	3.81047400	-0.98713800	1.74579900
C	5.25182700	-1.01246200	-1.73512100
H	4.48016600	-2.06752900	-3.44348300
C	5.96958600	0.14247500	0.31854500
C	4.65540900	-0.13836500	2.37451200
H	2.96326400	-1.39980700	2.28067900
C	6.36187900	-0.40794700	-2.42581000
C	7.05845400	0.72318100	-0.38679700
C	5.77278100	0.45429500	1.68903200
H	4.49434300	0.12059100	3.41707300
C	7.22691200	0.41108800	-1.78312900
H	6.49105800	-0.62857400	-3.48158800
C	7.91987300	1.59707400	0.28560300
C	6.65601100	1.33322600	2.32485700
H	8.06113500	0.86009600	-2.31464600
C	7.71807000	1.89805500	1.62791200
H	8.75014400	2.04254300	-0.25516700
H	6.50040900	1.57361900	3.37281400
H	8.39387300	2.57988000	2.13465100
O	-1.37149200	-0.71209800	0.74758200
O	0.29524700	-1.87974300	-0.82208200
P	-0.06131200	-0.45569200	-0.16258500
O	0.98095200	0.20499100	0.62869400
Br	1.99040600	-5.81553600	3.45012500
N	-0.54590500	0.39095800	-1.53839900
H	-0.64008400	1.40788400	-1.35355000
S	-1.14158400	-0.10241500	-2.98822900
O	-1.69914400	-1.43311900	-2.91333200
O	-1.87676300	1.01484600	-3.54746200
C	0.38592300	-0.26168000	-4.03428300
F	1.32290400	-0.93717700	-3.38815900
F	0.84543100	0.94294700	-4.34775700
F	0.05675800	-0.90672300	-5.14506900
C	4.24217900	3.93797400	-0.98828500
C	3.13811600	4.78436600	-1.02600700
C	1.95333100	4.37486000	-1.64670200
C	1.90298100	3.10654900	-2.23750000
C	3.00327200	2.26052100	-2.19095700
C	4.17730700	2.67512000	-1.56881800

H	5.15642500	4.26367500	-0.50144200
H	3.19577200	5.77038300	-0.57518600
H	0.99636000	2.77587200	-2.72965200
H	2.94369400	1.27302100	-2.63611200
H	5.03827000	2.01819300	-1.54299500
C	0.76245000	5.24425700	-1.62360200
C	0.39558700	6.26058400	-0.58819800
C	-0.59265600	4.99748000	-2.19900900
C	-0.45822100	5.03501400	-0.70770400
H	-0.03630400	7.20874200	-0.90773300
H	1.03811100	6.32392900	0.28629700
H	-1.11714200	5.82932400	-2.66877800
H	-0.78467300	4.02856300	-2.65181000
C	-0.45346100	3.85311800	0.14345300
O	-0.68770900	2.72651700	-0.26781600
O	-0.11253900	4.11120800	1.39840900
C	0.09637800	2.96421100	2.23940300
H	0.23003500	3.36392600	3.24361800
H	-0.76419900	2.29601000	2.20316700
H	0.98339500	2.42027700	1.91052500

TS1

C	3.99529300	-0.63044800	-0.00999500
C	4.99960500	-1.25566600	-0.75234400
C	4.87922700	-2.60154100	-1.05515300
C	3.76094900	-3.32707600	-0.66186200
C	2.71542900	-2.70159800	0.02042900
C	2.85272700	-1.33817100	0.31984300
C	5.39852800	1.07844500	-0.83875600
C	6.07375200	-0.27250400	-1.13210400
H	3.67938600	-4.37995100	-0.90803700
H	4.81385700	1.39200400	-1.70949700
H	6.10863000	1.87396000	-0.59956400
H	6.97206600	-0.42317600	-0.52133300
C	4.42480500	0.78513700	0.33937200
C	3.44599900	1.93112000	0.54585200
C	5.19481000	0.82767200	1.69067800
C	3.98980700	2.85472400	1.44432400
C	2.21149100	2.19339000	-0.02490000
C	5.25436400	2.31942900	2.06087900
H	4.61624300	0.28401000	2.44474800
H	6.18035700	0.36145800	1.61698500
C	3.33319700	4.05225200	1.67250100
C	1.54551400	3.40895200	0.18320100

H	6.13320700	2.81324000	1.62940000
C	2.13290400	4.34580100	1.03274400
H	1.63466700	5.29307700	1.20687700
H	6.37309900	-0.37723000	-2.17816000
H	5.28734700	2.48807800	3.14041200
Br	6.25701800	-3.46689800	-2.03350600
C	1.44585700	-3.42931000	0.29396900
C	0.79695800	-4.03033700	-0.78714100
C	0.84307700	-3.46226100	1.56840100
C	-0.45710000	-4.60358100	-0.65412300
H	1.26375500	-3.99368800	-1.76581700
C	-0.45161700	-4.03612700	1.70518100
C	1.48470600	-2.94261300	2.75034800
C	-1.10950500	-4.60128800	0.58038000
H	-0.95556900	-5.02291800	-1.52197500
C	-1.11188200	-4.02556500	2.97505700
C	0.86547700	-2.94535600	3.95286900
H	2.49244400	-2.55093700	2.66687300
C	-2.43527500	-5.14091200	0.73946700
C	-2.42211400	-4.56181800	3.10390000
C	-0.46570800	-3.46844500	4.10969100
H	1.36982300	-2.54840600	4.82924800
C	-3.06131100	-5.12159500	1.93961800
H	-2.92683200	-5.55409200	-0.13524900
C	-3.05643400	-4.52305300	4.35041500
C	-1.13283100	-3.45252400	5.33954500
H	-4.06202300	-5.53115500	2.04732900
C	-2.41647900	-3.97311000	5.45552700
H	-4.05952000	-4.92930900	4.44666600
H	-0.63574600	-3.02549600	6.20597500
H	-2.92273200	-3.95097700	6.41553400
C	0.26920500	3.69588500	-0.53559400
C	0.33461400	3.91470500	-1.91287000
C	-0.97880200	3.72164800	0.11586300
C	-0.80621200	4.14889200	-2.66346300
H	1.30278600	3.88835700	-2.40223400
C	-2.15489000	3.93722300	-0.65684900
C	-1.12379200	3.50019300	1.53317600
C	-2.06475300	4.15251500	-2.05747400
H	-0.72793100	4.31022300	-3.73458400
C	-3.44116800	3.90909500	-0.03043500
C	-2.34003400	3.48192500	2.12444800
H	-0.23304800	3.31773900	2.12211900
C	-3.27308100	4.34439500	-2.81713900

C	-4.61831000	4.09530300	-0.80584100
C	-3.54785000	3.67653300	1.36622200
H	-2.42592500	3.30103900	3.19200400
C	-4.48852900	4.31619400	-2.22339100
H	-3.18493000	4.50829000	-3.88742200
C	-5.86703100	4.05075500	-0.17434600
C	-4.81521400	3.63244500	1.95800200
H	-5.39314100	4.45835700	-2.80798300
C	-5.96151100	3.82053400	1.19403000
H	-6.76587700	4.19578700	-0.76723100
H	-4.89439100	3.44890600	3.02571600
H	-6.93721500	3.78297300	1.66818700
O	1.81335300	-0.67630000	0.94653600
O	1.57877800	1.20241800	-0.76820800
P	0.70810900	0.15202600	0.10890000
O	-0.24321200	0.71377800	1.08737200
Br	4.07898700	5.31407500	2.87865000
N	-0.02370900	-0.77036200	-1.02952600
H	-1.35509200	-0.93452500	-0.77912700
S	0.37624200	-1.07752000	-2.55587000
O	1.80822400	-1.16573800	-2.78451500
O	-0.50683000	-2.12928100	-3.03568000
C	-0.19509500	0.44272500	-3.47991600
F	0.79224100	1.32027600	-3.59434600
F	-1.21675000	1.00944400	-2.84614100
F	-0.59153800	0.08001700	-4.69695900
C	-7.43812200	0.10741200	-0.14520500
C	-6.06926300	0.30623500	-0.01634400
C	-5.23231700	-0.75866600	0.33690700
C	-5.78412900	-2.02592500	0.56622200
C	-7.15114200	-2.22153000	0.42103100
C	-7.97953600	-1.15748200	0.06733700
H	-8.07934000	0.94206000	-0.40938400
H	-5.65299200	1.29695600	-0.16619900
H	-5.15073600	-2.86330100	0.83777700
H	-7.57272200	-3.20739700	0.58673000
H	-9.04832100	-1.31552600	-0.03724500
C	-3.79438800	-0.49210600	0.49839100
C	-3.05429200	0.46870600	-0.30620000
C	-2.77965200	-1.44647400	0.91676100
C	-2.62953800	-1.02881300	-0.58557800
H	-2.22853300	1.01019100	0.14995300
H	-3.59125700	0.99686000	-1.08783400
H	-1.93308600	-1.07641200	1.49073100

H	-3.08452000	-2.46279900	1.14288000
C	-3.22331900	-1.84621000	-1.67898800
O	-3.49881100	-3.02159000	-1.58881300
O	-3.36464800	-1.11120900	-2.78150300
C	-3.75665100	-1.82294300	-3.95891000
H	-3.78137600	-1.08034400	-4.75514500
H	-3.02353900	-2.59861700	-4.18806100
H	-4.74390700	-2.27147800	-3.82749300