

Cartesian coordinates of MPWB1K/6-31G(d) optimized geometries
all-cisoid CFSFO-n, and all-transoid TFSFO-n, n = 1-6.
Charge and multiplicity are given first.

CFSFO-1

0 1			
C	-2.53888900	-1.19792200	0.00007600
C	-0.65312800	-0.10561900	0.00004500
C	-1.62295000	0.84427000	0.00013700
C	-2.83229700	0.11662100	0.00012800
O	-1.19671800	-1.33539000	0.00001500
C	0.77760600	-0.03270000	-0.00002800
C	3.20000800	-0.48095400	0.00035900
C	2.93873200	0.84888300	-0.00001200
C	1.55227700	1.08552800	-0.00015300
S	1.77919200	-1.42841800	-0.00022300
H	-3.12737400	-2.09220800	0.00005700
H	4.16157600	-0.96100900	0.00066700
F	1.03620200	2.30801200	-0.00026600
F	-4.04102600	0.64584500	0.00017900
H	3.67945900	1.62942600	0.00001000
H	-1.49173800	1.90823300	0.00018200

CFSFO-2

0 1			
C	-2.79893400	0.34400200	0.00002400
C	-0.46682000	1.15858400	0.00002700
C	0.95376400	1.25973800	0.00001100
C	2.99740300	0.47972700	-0.00001100
C	3.95264800	-0.58217900	-0.00002700
C	5.14398700	-2.73626800	0.00003400
C	-5.08324700	-2.32275000	-0.00006400
C	-5.99703100	-1.33295300	0.00001400
C	-5.31772400	-0.09632800	0.00006200
C	-4.00063200	-0.43040600	0.00000900
C	3.12596200	1.83493400	-0.00001300
C	1.80766900	2.31601900	0.00000000
C	-1.36682500	2.18725100	0.00004900
C	-2.67896100	1.70072500	0.00004400
C	5.30986300	-0.47031000	-0.00001500
C	6.00673700	-1.69048200	0.00000600
O	1.69676100	0.13042300	0.00000600
O	-3.85387800	-1.76807600	-0.00006700
H	-5.14348500	-3.39156000	-0.00012100
S	-1.23804400	-0.38042800	0.00002900
S	3.50949500	-2.24255300	-0.00012400
F	5.92335000	0.70566900	0.00000700
F	-3.73460400	2.50294600	0.00005300
H	7.07994900	-1.76797400	0.00004200
H	-1.10096700	3.22973100	0.00005800
F	1.43830900	3.58299800	0.00000000
F	-7.30805300	-1.48283500	0.00004200
H	4.03759300	2.39935000	-0.00002600
H	-5.74091300	0.88862900	0.00012900
H	5.38336000	-3.78407500	0.00008200

CFSFO-3

0 1

C	-5.06594000	0.68042300	-0.00009900
C	-3.73706800	-1.40367200	-0.00042400
C	-2.68876700	-2.36717600	-0.00038000
C	-0.60470600	-3.03591000	-0.00005800
C	0.80180900	-2.80918800	0.00022600
C	3.09126900	-1.88205500	0.00041700
C	4.22744600	-1.02491900	0.00040200
C	5.25933800	0.90348400	0.00001700
C	-5.25058600	4.18873100	0.00151800
C	-6.57792500	3.95856500	0.00078200
C	-6.78999700	2.56354300	-0.00001700
C	-5.54061900	2.02864300	0.00031200
C	-1.35291900	-4.17500900	-0.00041500
C	-2.68138200	-3.72622400	-0.00059800
C	-5.08155500	-1.65352500	-0.00097800
C	-5.81050600	-0.46032000	-0.00078200
C	1.78971300	-3.74998100	0.00052600
C	3.09415200	-3.25023900	0.00065000
C	6.24502800	-0.03578300	0.00054900
C	5.56509000	-1.26269000	0.00079200
O	-1.40226300	-1.94999700	-0.00004300
O	4.04816600	0.31534100	-0.00006700
O	-4.61114000	3.00085600	0.00123600
C	5.28916600	2.33124800	-0.00042700
C	4.79074300	4.74125100	-0.00114300
C	6.12692500	4.50956200	-0.00100700
C	6.39239100	3.13017800	-0.00056300
H	-4.64857700	5.07395400	0.00223400
S	-3.39169300	0.28371500	0.00029700
S	1.49609600	-1.23411500	0.00009000
S	3.87194100	3.30244000	-0.00075500
F	7.62369000	2.63781600	-0.00031700
F	1.52428400	-5.04859600	0.00065400
F	-7.13643200	-0.43711900	-0.00120400
H	6.89095700	5.26716100	-0.00120800
H	3.97979700	-3.86071700	0.00087100
H	-5.52260100	-2.63432300	-0.00147200
F	6.11777800	-2.46033900	0.00129400
F	-3.75994700	-4.48685600	-0.00092700
F	-7.52717000	4.87523600	0.00079000
H	7.30342200	0.13556300	0.00073400
H	-0.99617000	-5.18622700	-0.00051000
H	-7.72302100	2.03511200	-0.00071900
H	4.29014200	5.69231000	-0.00147800

CFSFO-4

0 1

C	-4.42176600	2.64667200	0.21671300
C	-4.98823600	0.26274700	-0.09807000
C	-4.93300000	-1.15624100	-0.19803900
C	-3.91254200	-3.09376200	-0.20888900
C	-2.73561800	-3.89347500	-0.14289500
C	-0.41837800	-4.73621300	-0.00837300
C	1.00021200	-4.80548600	0.08255000
C	2.99610800	-3.90787400	0.18229900
C	-2.06416700	5.13273900	0.98836600

C	-3.10379400	5.96241400	0.76941700
C	-4.23098600	5.18719200	0.42304000
C	-3.78537800	3.90352000	0.45711400
C	-5.23541100	-3.37806800	-0.36776400
C	-5.87113900	-2.12640400	-0.35852000
C	-6.08208000	1.06993100	-0.23988300
C	-5.73587200	2.41351500	-0.05768700
C	-2.63166400	-5.25295500	-0.16181600
C	-1.32796300	-5.75532400	-0.08543700
C	3.19791400	-5.25417600	0.24960900
C	1.91035900	-5.81085000	0.18389000
O	-3.72888200	-1.76359000	-0.10671700
O	1.68265600	-3.63744100	0.08317300
O	-2.48385000	3.86518800	0.79486900
C	3.87170600	-2.78497900	0.18688600
C	4.89088600	-0.53757000	0.11480000
C	5.83050200	-1.52010500	0.27031100
C	5.11051900	0.86614900	0.02829200
C	4.49878400	2.95179900	-0.22872600
C	5.84932800	2.98671800	-0.05733700
O	4.05239500	1.68293700	-0.17660300
C	6.22228100	1.64356200	0.10510800
C	5.23028500	-2.78153200	0.30747000
H	-1.04585900	5.27532200	1.28778800
C	3.52062200	3.96841300	-0.45377100
C	1.48059800	5.27993600	-0.87721200
C	2.57472100	6.07609400	-0.78765900
C	3.72871600	5.31194000	-0.54686000
S	-3.56054400	1.15802000	0.25592900
S	-1.17157200	-3.18807000	-0.02770300
S	3.29419600	-1.17210100	0.02005100
S	1.84942300	3.62609900	-0.66867000
F	4.93218400	5.85353400	-0.42165900
F	5.92428900	-3.90187200	0.44652400
F	-3.69593600	-6.03768800	-0.24952000
F	-6.62249000	3.39548000	-0.14587200
H	2.57540700	7.14735800	-0.88869100
H	6.88909600	-1.35038900	0.35004900
H	-1.08300600	-6.80255200	-0.08995500
H	-7.07576400	0.72301200	-0.46154400
F	7.44631600	1.19271200	0.30005100
F	1.61680500	-7.09581000	0.21490400
F	-7.16632100	-1.90816200	-0.48166700
F	-3.08134900	7.27853100	0.86172100
H	6.48339500	3.85096000	-0.05145700
H	4.13840500	-5.76283900	0.33258200
H	-5.68316700	-4.34619500	-0.47663500
H	-5.22006700	5.52672800	0.18638600
H	0.46421700	5.57817300	-1.06191400

CFSFO-5

0 1

C	3.58581800	-2.68255600	-1.21714600
C	1.90829400	-4.40474200	-0.64950100
C	0.69837100	-5.10042600	-0.37026400
C	-1.45915300	-5.25743700	-0.03267800
C	-2.76203000	-4.69439300	0.08239400

C	-4.73637300	-3.21637000	0.21365600
C	-5.60239200	-2.08808000	0.22015100
C	-6.05742300	0.05199300	0.11640400
C	4.40444500	0.66897200	-1.86999100
C	5.66384700	0.18941400	-1.90291400
C	5.61780800	-1.20224600	-1.67469200
C	4.29632600	-1.47704400	-1.50653900
C	-0.97776600	-6.52684600	0.08912600
C	0.40308000	-6.40487900	-0.12954000
C	3.17773000	-4.91366600	-0.66303200
C	4.10836900	-3.91854000	-0.98190800
C	-3.94049100	-5.34831600	0.29378300
C	-5.07300400	-4.53329600	0.37080100
C	-7.26288900	-0.57290900	0.23941700
C	-6.95111200	-1.93852600	0.30445600
O	-0.45702700	-4.40104300	-0.30851800
O	-5.06101400	-0.85396200	0.10485500
O	3.56328000	-0.35475800	-1.62393000
C	-5.67065200	1.41879200	0.00593800
C	-4.45156700	3.55991400	-0.16315600
C	-5.80763300	3.73946000	-0.20150600
C	-3.44693600	4.56335400	-0.24591900
C	-1.39226100	5.31647300	-0.22178300
C	-2.17661400	6.40423700	-0.46862500
O	-2.15013400	4.21153400	-0.08874700
C	-3.48542300	5.90212500	-0.47990600
C	-6.47521600	2.51574800	-0.10275900
H	3.97721900	1.64601400	-1.97529100
C	0.01558200	5.15397000	-0.07767300
C	2.31652300	4.34970400	0.32135500
C	2.29197400	5.66954100	-0.03949000
C	0.98132700	6.10075500	-0.25765700
C	3.46429700	3.56254800	0.61857500
C	4.51746700	1.75644700	1.26253600
C	5.49275600	2.66695100	0.98874800
C	4.56044000	0.39224300	1.68137000
C	4.07915000	-1.92171100	2.36108400
C	5.40332600	-1.73606600	2.13319300
O	3.30069600	2.28864100	1.04342900
C	4.79967900	3.81458100	0.57710400
C	5.65868000	-0.41025900	1.74497400
S	1.87651400	-2.72720200	-1.03623800
S	-3.04585600	-2.99991300	-0.02763700
S	-4.01779300	1.90150500	-0.01133500
S	0.73975900	3.66054500	0.38177100
S	3.15899900	-0.50907300	2.09874800
F	6.86885400	0.02310000	1.42277900
F	0.68838900	7.34327300	-0.61307000
F	-7.79697600	2.42170500	-0.11209400
F	-3.99923400	-6.66649400	0.41852100
F	5.41340600	-4.15360600	-1.03601800
H	6.16307500	-2.49264300	2.22319200
H	3.16402300	6.29132300	-0.13878100
H	-6.29407800	4.69418700	-0.29390700
H	-6.07245300	-4.89596500	0.53211700
H	3.42780200	-5.93878000	-0.45339900
F	5.33659800	4.96136500	0.20828100

F	-4.58727600	6.59808700	-0.68325300
F	-7.81259600	-2.92968500	0.42635000
F	1.28826300	-7.38349400	-0.10780500
F	6.75985900	0.89499900	-2.10834800
H	6.55265800	2.52221500	1.05937500
H	-1.85350400	7.41612000	-0.61541700
H	-8.23208200	-0.11743600	0.28033200
H	-1.53824700	-7.41488600	0.30589100
H	6.43531000	-1.89503500	-1.63457200
H	3.58618100	-2.82896000	2.66038900

CFSFO-6

0 1

C	-3.32918300	1.32504000	1.96920900
C	-3.60084500	-1.10692900	1.62175600
C	-3.34500200	-2.49179400	1.40944900
C	-2.02658800	-4.21104900	1.08557300
C	-0.73329800	-4.78711300	0.93024300
C	1.68203600	-5.19419300	0.60934200
C	3.08655000	-5.02511400	0.45936000
C	4.91481400	-3.83870200	0.24973000
C	-1.22896100	4.11288100	2.33599800
C	-2.39462200	4.78598700	2.40740000
C	-3.45337100	3.86088500	2.29381500
C	-2.83895100	2.65624800	2.14364100
C	-3.29348300	-4.71365500	1.06237900
C	-4.12342700	-3.59753800	1.25809500
C	-4.80594400	-0.46473900	1.69401300
C	-4.62536200	0.91129900	1.87940200
C	-0.40436100	-6.09876400	0.75266000
C	0.95938600	-6.35616500	0.57378700
C	5.31895000	-5.14076100	0.22197000
C	4.13676400	-5.88280000	0.35637900
O	-2.05680900	-2.88390700	1.30441900
O	3.57820300	-3.76658400	0.39474200
O	-1.50255400	2.80406100	2.17148900
C	5.61167700	-2.60178200	0.14050900
C	6.28981900	-0.23515600	-0.06338500
C	7.36845700	-1.07898900	-0.06577800
C	6.30774400	1.18329800	-0.16005200
C	5.40850000	3.17343500	-0.29459000
C	6.75692600	3.38265700	-0.27320900
O	5.13729900	1.85686800	-0.22667700
C	7.31296000	2.09897300	-0.18509200
C	6.95948200	-2.40976800	0.04954100
H	-0.19836600	4.40415000	2.36381200
C	4.29555200	4.05790000	-0.37837700
C	2.06953000	5.11524900	-0.56281000
C	3.06896700	6.04376700	-0.45343200
C	4.31597500	5.42255000	-0.35173400
C	0.67402400	5.36157500	-0.67088600
C	-1.42112000	4.79154800	-0.93827500
C	-1.43039200	6.14651700	-0.77726400
C	-2.45544200	3.82910100	-1.10724600
C	-3.81185500	1.78770500	-1.38282000
C	-4.59184000	2.89503800	-1.18784500
O	-0.16264700	4.31960600	-0.87914900

C	-0.08210500	6.48973800	-0.60424200
C	-3.80138600	4.03584500	-1.03663000
S	-2.27565500	-0.02232800	1.80735100
S	0.68528400	-3.81610000	0.87382400
S	4.79947400	-1.08402000	0.08413100
S	2.67298700	3.50245700	-0.53457600
S	-2.13281500	2.16048700	-1.37541200
F	-4.31524100	5.23413500	-0.80158700
F	5.44578600	6.10632100	-0.23985200
F	7.81529200	-3.42171400	0.06361500
F	-1.32149700	-7.05601200	0.73189000
F	-5.64381000	1.76053900	1.94229700
H	-5.66614800	2.88694500	-1.13866400
H	2.91689000	7.10893500	-0.44892600
H	8.39311700	-0.76217700	-0.14869000
H	1.37905100	-7.33483200	0.42210400
H	-5.76464900	-0.94115700	1.59765500
F	0.39786100	7.70234500	-0.41031800
F	8.59803700	1.80507900	-0.13449800
F	4.03948700	-7.19787100	0.37820100
F	-5.44262200	-3.60313900	1.28415900
F	-2.52980200	6.09210100	2.54214800
H	-2.28616400	6.79263400	-0.76139500
H	7.26910200	4.32373200	-0.31730800
H	6.32099700	-5.50629100	0.11456700
H	-3.58549500	-5.73358000	0.90609000
H	-4.50693500	4.05665800	2.30660500
C	-4.25089700	0.44256000	-1.55567400
C	-5.47670600	-0.14427300	-1.56950800
O	-3.32723000	-0.53283900	-1.71547200
C	-5.31693300	-1.52864700	-1.73505300
C	-3.97077700	-1.71063100	-1.82583400
H	-6.07990900	-2.28138700	-1.78862500
C	-3.15760000	-2.87052700	-2.01625300
C	-3.57093900	-4.16854600	-2.08104000
S	-1.45399400	-2.79439000	-2.22442800
C	-2.54763100	-5.10632200	-2.29340300
C	-1.34364900	-4.48790700	-2.39433200
H	-2.70942700	-6.16852100	-2.35617500
H	-0.38151100	-4.94553700	-2.54170200
F	-4.84266200	-4.51387500	-1.92162500
F	-6.62169700	0.49625900	-1.42724300

TFSFO-1

0 1

C	3.12889600	-0.80449100	-0.00002200
C	3.02109600	0.54395500	-0.00002900
C	1.67065500	0.94757400	-0.00002000
H	3.84679600	1.23410500	-0.00002200
C	0.76889900	-0.07274300	-0.00002000
C	-0.66453700	-0.00393200	0.00000800
C	-1.62712800	-0.96211800	0.00018100
O	-1.22035300	1.21892300	-0.00017200
C	-2.84380100	-0.24811800	0.00009700
H	-1.49672100	-2.02785600	0.00035600
C	-2.55915300	1.06823500	-0.00011500
H	-3.15492700	1.95782600	-0.00023700

F	1.32410800	2.22238100	0.00000100
F	-4.04735200	-0.78949600	0.00021100
S	1.60503900	-1.57665100	-0.00006900
H	4.02669400	-1.39517500	-0.00001600

TFSFO-2

0 1

C	-6.72831000	-0.60596700	0.00046000
C	-5.94631700	-1.71046900	0.00010500
C	-4.58042400	-1.36750700	-0.00006300
H	-6.30352800	-2.72552800	0.00012300
C	-4.32728000	-0.02787900	0.00002300
C	-3.06523900	0.64704200	-0.00001500
C	-2.73335400	1.96725000	-0.00008900
O	-1.95755300	-0.11520300	0.00001200
C	-1.33049300	1.98168100	-0.00008300
H	-3.39463900	2.81293600	-0.00013900
C	-0.88068900	0.70054300	-0.00003700
C	0.41444900	0.10664500	-0.00003200
C	0.70320100	-1.22551200	-0.00000800
C	2.08789700	-1.44823400	0.00000200
H	-0.03689200	-2.00647800	0.00001000
C	2.85525900	-0.32122300	-0.00001700
C	4.28319700	-0.20808700	0.00000900
C	5.11911600	0.86399600	0.00020100
O	4.98871700	-1.35166700	-0.00018500
C	6.41511000	0.30764400	0.00011100
H	4.85684300	1.90515400	0.00039400
C	6.29745400	-1.03461600	-0.00011900
H	7.00018300	-1.84236500	-0.00024900
F	-3.63059400	-2.28519300	-0.00022000
F	-0.55930900	3.05252800	-0.00013700
F	2.59447200	-2.66768500	0.00004000
F	7.54194700	0.99464200	0.00024000
S	1.84138400	1.07224500	-0.00006000
S	-5.81572600	0.83704000	-0.00003400
H	-7.80191500	-0.55779200	0.00076400

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C	6.68572800	0.22360300	-0.00004300
C	6.69022700	1.58521800	-0.00008900
C	5.33398400	1.94518700	-0.00002500
C	4.58291600	0.81415400	0.00002200
O	5.42462200	-0.24188600	0.00001600
H	7.53992500	2.24132800	-0.00014800
C	3.18091000	0.56232800	0.00007100
C	2.56554300	-0.65513200	0.00013000
C	1.17062600	-0.52206500	0.00015100
H	3.08667300	-1.59657600	0.00014900
C	0.71168400	0.76349800	0.00011200
C	-0.63665300	1.23287300	0.00011300
C	-1.17180700	2.48638200	0.00013700
O	-1.61204900	0.30640300	0.00008200
C	-2.55912600	2.28001700	0.00011200
H	-0.65077100	3.42503300	0.00016800
C	-2.80235500	0.94438000	0.00008500

C	7.74031800	-0.74354700	-0.00007000
C	7.65090700	-2.10413000	-0.00004500
C	8.88742700	-2.77767300	0.00004200
C	9.92053000	-1.90317400	0.00025800
H	8.97952100	-3.84979500	0.00014300
C	-3.99179000	0.16116800	0.00006100
C	-4.08015600	-1.19909000	0.00005900
C	-5.41681600	-1.62433600	0.00002200
H	-3.23224600	-1.86157900	0.00007600
C	-6.34259100	-0.62373400	-0.00000200
C	-7.77156300	-0.71942000	-0.00006100
C	-8.75082000	0.22335200	-0.00028800
O	-8.30744300	-1.95158000	0.00013900
C	-9.95482300	-0.51065600	-0.00021500
H	-8.63777300	1.29111200	-0.00049200
C	-9.64865500	-1.82253700	0.00004100
H	-10.22998900	-2.72161100	0.00017200
F	6.50296100	-2.75702200	-0.00001600
F	4.84719100	3.17146700	-0.00003200
F	0.36851600	-1.57115400	0.00019700
F	-3.49370600	3.21211000	0.00011900
F	-5.73916700	-2.90490200	0.00000100
F	-11.16752400	0.01023200	-0.00037600
S	-5.54693300	0.90481600	0.00003400
S	2.04357700	1.85721800	0.00007100
S	9.39742800	-0.27786100	-0.00041500
H	10.97217000	-2.12475400	0.00049800

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C	-3.09164500	-1.93353700	-0.00043900
C	-2.84151400	-3.27358600	-0.00068400
C	-1.44232300	-3.37351200	-0.00061300
C	-0.91471200	-2.12227900	-0.00030800
O	-1.93855200	-1.24174100	-0.00021100
H	-3.55339100	-4.07710900	-0.00089000
C	0.41360400	-1.61007100	-0.00009300
C	0.78419700	-0.29710200	0.00028200
C	2.17843400	-0.16006300	0.00032200
H	0.09227300	0.52695200	0.00046000
C	2.87630900	-1.33319700	0.00000500
C	4.28911400	-1.53842900	-0.00009300
C	5.04855200	-2.67001800	-0.00033600
O	5.07517600	-0.44663400	0.00008500
C	6.37295300	-2.20955600	-0.00030900
H	4.71169300	-3.68937300	-0.00050400
C	6.36440500	-0.85154600	-0.00004300
C	-4.30186200	-1.17692600	-0.00037800
C	-4.45665200	0.17958300	-0.00016800
C	-5.78375000	0.62708400	-0.00010700
C	-6.65987400	-0.41873000	-0.00026200
H	-6.07707900	1.66234300	0.00009000
C	7.38419400	0.14312800	0.00013200
C	7.20969500	1.49533700	0.00044600
C	8.43963000	2.16934600	0.00052500
H	6.25037000	1.98257600	0.00060000
C	9.54035700	1.36498000	0.00028900

C	10.92320000	1.73747600	0.00028600
C	12.06986600	1.00735800	-0.00012500
O	11.20466500	3.05122700	0.00076900
C	13.10472500	1.96568200	0.00015200
H	12.17070000	-0.06160000	-0.00057200
C	12.54460100	3.19089100	0.00068200
H	12.93610300	4.18736900	0.00102300
F	-3.43940800	1.02109900	0.00002000
F	-0.73454300	-4.48665700	-0.00079100
F	2.76183800	1.02430400	0.00059500
F	7.46103300	-2.95671200	-0.00049300
F	8.51022600	3.48822500	0.00080100
F	14.39671700	1.69565900	-0.00009000
C	-8.08141700	-0.33933200	-0.00018900
C	-9.07657700	-1.26273000	-0.00030200
O	-8.65193200	0.88396700	0.00003900
C	-10.31086500	-0.59525500	-0.00016200
C	-9.98753300	0.72774000	0.00004400
H	-11.29052200	-1.03408100	-0.00020400
C	-10.77427400	1.92324500	0.00026100
C	-10.34148000	3.21685500	0.00048600
C	-11.36625600	4.18223900	0.00052000
C	-12.58723300	3.59836600	0.00035400
H	-11.18378600	5.24270900	0.00058100
F	-8.88800800	-2.56858300	-0.00050600
F	-9.06495100	3.55571200	0.00051100
S	9.05317200	-0.28760600	-0.00003800
S	1.77796000	-2.66265800	-0.00018800
S	-5.84894600	-1.93892800	-0.00062500
S	-12.49496100	1.89344100	0.00036500
H	-13.54818600	4.07960000	0.00026200

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0 1

C	0.61018400	-3.27581600	-0.00034600
C	1.12824500	-4.53735000	-0.00063500
C	2.51858600	-4.34964600	-0.00061900
C	2.77967700	-3.01740900	-0.00033300
O	1.59857900	-2.36371100	-0.00016200
H	0.59393200	-5.46845600	-0.00083400
C	3.97615800	-2.24686500	-0.00021100
C	4.07274700	-0.88606700	0.00009100
C	5.41020200	-0.46976100	0.00010300
H	3.22833900	-0.21919800	0.00029000
C	6.33115900	-1.47759000	-0.00018100
C	7.75550200	-1.38224900	-0.00027100
C	8.74175900	-2.32285500	-0.00059600
O	8.28698000	-0.14656700	-0.00001800
C	9.93540400	-1.58658100	-0.00052800
H	8.63271900	-3.39084900	-0.00085400
C	9.63293700	-0.26295000	-0.00017800
C	-0.72722600	-2.77715000	-0.00022700
C	-1.14740200	-1.47761700	0.00003800
C	-2.53614600	-1.30132000	0.00006800
C	-3.18866300	-2.49975600	-0.00018500
H	-3.02892300	-0.34479900	0.00025800
C	10.41071500	0.92961600	0.00003100

C	9.94147800	2.20972300	0.00043900
C	10.99155900	3.13896200	0.00052300
H	8.89781100	2.47169900	0.00066500
C	12.24327900	2.59906500	0.00018900
C	13.51257900	3.26261300	0.00016700
C	14.78876600	2.79379000	-0.00023800
O	13.50760000	4.60590300	0.00062400
C	15.59555600	3.95090200	0.00000200
H	15.11552900	1.77097800	-0.00065400
C	14.78655600	5.02827800	0.00052100
H	14.95614900	6.08540500	0.00084600
F	-0.31709800	-0.45092100	0.00025100
F	3.44340600	-5.29099800	-0.00084800
F	5.74227300	0.80819600	0.00037000
F	11.16018500	-2.07792800	-0.00076600
F	10.76484900	4.43993400	0.00090000
F	16.91539400	3.96285800	-0.00024700
C	-4.59801200	-2.69696500	-0.00025200
C	-5.39945400	-3.79340600	-0.00051000
O	-5.39197200	-1.60462300	-0.00004400
C	-6.73781900	-3.37445700	-0.00046700
C	-6.67347500	-2.01265600	-0.00017600
H	-7.61602600	-3.99190000	-0.00063300
C	-7.67484200	-0.99529400	-0.00000500
C	-7.50670100	0.35987000	0.00026400
C	-8.69171800	1.10632900	0.00035600
C	-9.78893200	0.29559300	0.00015100
H	-8.73209000	2.18147000	0.00056100
C	-11.15258200	0.70524600	0.00016400
C	-12.33580900	0.03969200	-0.00002200
O	-11.42173500	2.02797100	0.00039500
C	-13.38027100	0.97670600	0.00009500
C	-12.75659800	2.18771200	0.00035200
H	-14.43529300	0.77850500	-0.00000100
C	-13.24716800	3.53187100	0.00057100
C	-12.53212600	4.69309500	0.00079700
C	-13.31078200	5.86593700	0.00097200
C	-14.63285300	5.57436400	0.00087600
H	-12.89231200	6.85727000	0.00115600
F	-4.96639700	-5.03936000	-0.00076400
F	-6.32124900	0.94037300	0.00042700
F	-12.45668400	-1.27371600	-0.00027100
F	-11.21205200	4.73189900	0.00084800
S	12.13339000	0.87845900	-0.00024500
S	5.52547500	-3.00217300	-0.00047600
S	-2.09328100	-3.83009600	-0.00045100
S	-9.35713000	-1.37243000	-0.00015100
S	-14.92949000	3.89312100	0.00057500
H	-15.45933600	6.26134600	0.00096500

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C	4.28939600	-3.94361000	-0.00044100
C	5.04143300	-5.08094300	-0.00098200
C	6.36878200	-4.62922300	-0.00102700
C	6.36913200	-3.27109100	-0.00053500
O	5.08281200	-2.85765300	-0.00017300

H	4.69742600	-6.09787000	-0.00131800
C	7.39232200	-2.28154700	-0.00036000
C	7.21800600	-0.92835900	0.00028500
C	8.44652100	-0.25588200	0.00023800
H	6.25864800	-0.44131900	0.00075800
C	9.54882900	-1.06178100	-0.00042100
C	10.92513000	-0.68244300	-0.00067400
C	12.08336600	-1.40129500	-0.00147500
O	11.19272500	0.63567600	-0.00006300
C	13.10112500	-0.43565900	-0.00131400
H	12.19553400	-2.46894600	-0.00210200
C	12.53326100	0.79773800	-0.00045800
C	2.87915700	-3.72357300	-0.00017000
C	2.19815900	-2.54017800	0.00009800
C	0.80263300	-2.65637600	0.00025300
C	0.41311100	-3.96416100	0.00009800
H	0.12239600	-1.82266300	0.00045800
C	13.05005600	2.12458000	0.00006600
C	12.32872800	3.28155300	0.00115900
C	13.16669600	4.40577600	0.00137700
H	11.25348400	3.32365300	0.00178100
C	14.50243700	4.13287200	0.00047300
C	15.60819500	5.04294400	0.00041900
C	16.95369100	4.84701300	-0.00055100
O	15.32660800	6.35655300	0.00152000
C	17.50472000	6.14549000	0.00003000
H	17.48486400	3.91395300	-0.00155000
C	16.49131000	7.03302800	0.00127800
H	16.43979500	8.10242600	0.00206500
F	2.79827500	-1.36434800	0.00020000
F	7.45327300	-5.38080100	-0.00148500
F	8.51792300	1.06276600	0.00079800
F	14.40145700	-0.66312600	-0.00189200
F	12.68101200	5.63387700	0.00240300
F	18.79387200	6.42893100	-0.00056500
C	-0.92282400	-4.45470900	0.00016800
C	-1.47186800	-5.69684900	0.00013200
O	-1.93153100	-3.55690000	0.00028000
C	-2.86895600	-5.57312700	0.00022100
C	-3.09634400	-4.22870400	0.00031100
H	-3.59448600	-6.36429900	0.00021000
C	-4.29199600	-3.44970600	0.00038900
C	-4.41907300	-2.09016300	0.00031500
C	-5.73653900	-1.61526000	0.00036800
C	-6.63442400	-2.64316400	0.00048500
H	-6.00765700	-0.57404400	0.00031700
C	-8.05372300	-2.53843800	0.00055200
C	-9.06375800	-3.44689200	0.00070800
O	-8.60579400	-1.30594600	0.00043500
C	-10.28697700	-2.76250900	0.00068400
C	-9.94407500	-1.44280100	0.00051100
H	-11.27313900	-3.18660200	0.00077500
C	-10.71884800	-0.24406500	0.00038400
C	-10.28325000	1.05009400	0.00014700
C	-11.29570200	2.01823300	0.00004000
C	-12.53290400	1.44286600	0.00020100
H	-11.12104600	3.07991400	-0.00015000

F	-0.78279500	-6.82157200	0.00002400
F	-3.38446800	-1.26999500	0.00019600
F	-8.89527600	-4.75556800	0.00085100
F	-9.00470500	1.37924800	0.00001700
S	14.74651800	2.42619300	-0.00070300
S	9.06027400	-2.71536100	-0.00102100
S	1.76140200	-5.03722100	-0.00023700
S	-5.85401300	-4.17989500	0.00053400
S	-12.44210500	-0.27802400	0.00049200
C	-13.78955100	2.11311400	0.00014600
C	-15.08024500	1.69103700	0.00029300
O	-13.79590000	3.46312900	-0.00011300
C	-15.92170800	2.81346500	0.00011800
C	-15.07397200	3.87964300	-0.00013300
H	-16.99512700	2.82451200	0.00016800
C	-15.29878900	5.29262400	-0.00040100
C	-14.38006900	6.30032300	-0.00067000
S	-16.88448700	5.96244100	-0.00042200
C	-14.92610600	7.59796500	-0.00089800
C	-16.27925700	7.55878600	-0.00079700
H	-14.32945600	8.49346500	-0.00112400
H	-16.96305600	8.38791500	-0.00091900
F	-13.07568200	6.09466000	-0.00072200
F	-15.45759700	0.42716100	0.00055500