

Cartesian coordinates of MPWB1K/6-31G(d) optimized geometries  
all-cisoid C2FSO-n, and all-transoid T2FSO-n, n = 1-6.  
Charge and multiplicity are given first.

C2FSO-1

0 1

C	3.41357900	-0.51583100	-0.00024600
C	1.33692300	0.10044800	0.00007200
C	-0.07251200	-0.15358900	0.00006400
C	-2.34051100	-1.15345600	0.00024200
C	2.06953600	1.24222300	0.00040800
C	3.42812600	0.83222100	0.00019000
C	-1.07076200	0.76501200	-0.00008600
C	-2.36005400	0.19565300	-0.00001200
O	2.14994600	-0.97324200	-0.00032200
S	-0.73290700	-1.74216200	0.00006300
F	-3.44686400	0.94516200	-0.00011000
F	-0.87251200	2.07333800	-0.00024700
H	1.67732000	2.24139900	0.00077700
H	4.29806700	1.46194800	0.00033300
H	4.18118200	-1.26450600	-0.00054700
H	-3.18118700	-1.82090300	0.00042400

C2FSO-2

0 1

C	-5.33425000	-2.88310000	0.00034600
C	-4.44814000	-0.90633300	-0.00007800
C	-3.33792200	-0.00579300	0.00004700
C	-1.08863700	1.05373300	0.00031400
C	0.30830900	1.34306000	0.00054900
C	2.40813700	0.77638300	0.00039600
C	-5.79291200	-0.71826700	-0.00075800
C	-6.36664400	-2.01525500	-0.00044300
C	-3.37887400	1.35294400	-0.00047400
C	-2.11132500	1.95028900	-0.00032500
C	2.38033300	2.13503200	0.00111700
C	1.01733300	2.50364200	0.00126500
O	-4.16386500	-2.22286500	0.00068900
O	1.15063700	0.28998900	0.00003700
C	3.47048500	-0.17877300	0.00005000
C	4.86969400	-2.22316300	-0.00050000
C	5.59862200	-1.08734600	-0.00048900
C	4.80455800	0.07613900	-0.00022200
S	-1.70564800	-0.55590800	0.00090600
S	3.19394400	-1.87716900	0.00000000
F	6.91686800	-1.02455700	-0.00081000
F	5.32414200	1.29226400	-0.00025500
F	-1.94387600	3.26198900	-0.00073500
F	-4.49707600	2.05935800	-0.00112200
H	3.23830600	2.78010300	0.00156100
H	0.60155000	3.49301900	0.00181800
H	-6.29473000	0.23043700	-0.00140800
H	-7.41104600	-2.26528400	-0.00079400
H	-5.26661400	-3.95324600	0.00081000
H	5.23250700	-3.23343000	-0.00077100

C2FSO-3

0 1

C	-4.76306000	4.95505300	-0.00052500
C	-5.39875200	2.88420200	-0.00003800
C	-5.15870800	1.47516300	0.00006600
C	-4.17740500	-0.80950800	0.00012500
C	-3.31939600	-1.94887400	0.00012400
C	-1.36769000	-2.91085100	0.00000700
C	-6.53438700	3.62863500	0.00026100
C	-6.11128300	4.98225000	-0.00006900
C	-6.08986500	0.48517300	0.00020700
C	-5.53823200	-0.80262700	0.00025000
C	-2.28814600	-3.91282800	0.00016400
C	-3.55312500	-3.28922500	0.00022300
O	-4.31726200	3.68735500	-0.00051200
O	-1.99129400	-1.71454400	-0.00000900
C	0.05786400	-2.90005300	-0.00007300
C	2.47113400	-2.30279900	-0.00007000
C	2.24392100	-3.64454900	-0.00027800
C	3.73479600	-1.64255800	0.00000200
C	4.99864800	0.12719700	0.00003300
C	5.83896200	-0.94134900	0.00021100
O	3.71794600	-0.29447400	-0.00010400
C	5.01917700	-2.09048500	0.00018400
C	0.88507500	-3.98076700	-0.00028700
C	5.21465200	1.53935500	-0.00004000
C	5.00394900	4.00768200	-0.00035900
C	6.28722600	3.58998500	0.00016000
C	6.40881500	2.18643700	0.00035300
S	-3.57225300	0.80500200	-0.00007400
S	0.97739400	-1.44273700	0.00016500
S	3.92539200	2.67934200	-0.00066800
F	7.34729800	4.37590900	0.00049300
F	7.58114900	1.57446400	0.00085600
F	3.20245300	-4.55471800	-0.00048200
F	0.46372100	-5.23392800	-0.00049400
F	-6.28467800	-1.89401800	0.00041600
F	-7.39491000	0.69863400	0.00032700
H	6.91129700	-0.89520500	0.00033200
H	5.32557800	-3.11910400	0.00028200
H	-2.07087000	-4.96381800	0.00022700
H	-4.51748500	-3.75941800	0.00033400
H	-7.53759300	3.24673800	0.00065300
H	-6.73253900	5.85823800	0.00004200
H	-4.00740200	5.71575700	-0.00087000
H	4.64507200	5.01938400	-0.00057300

C2FSO-4

0 1

C	-0.44376100	5.33554200	1.20276900
C	-2.44984000	4.72070300	0.65661800
C	-3.44226600	3.73284000	0.36841000
C	-4.69780600	1.62716600	-0.03307300
C	-5.09258700	0.26585600	-0.19471300
C	-4.66073600	-1.86811500	-0.26500500
C	-2.47281300	6.07685200	0.71621900
C	-1.15811000	6.47267100	1.07246900
C	-4.75954800	3.93139200	0.09594300

C	-5.46929900	2.74295900	-0.12905000
C	-5.99923600	-1.74140200	-0.47033500
C	-6.27912300	-0.35801800	-0.42521100
O	-1.21621600	4.26454800	0.94975600
O	-4.10760600	-0.64904500	-0.09727400
C	-3.75750300	-2.96932300	-0.20025000
C	-1.73697800	-4.40630200	-0.04197900
C	-2.89436900	-5.11159400	-0.16523400
C	-0.40118700	-4.89359300	0.06496800
C	1.75070400	-4.57706600	0.18631900
C	1.55834400	-5.92261200	0.23543800
O	0.56220700	-3.94958300	0.08327100
C	0.16339200	-6.12790500	0.15707700
C	-4.03457100	-4.30033700	-0.25500200
C	2.90079200	-3.73452000	0.20615900
C	4.46856100	-1.80929400	0.15155900
C	5.09056000	-3.00976400	0.30697700
C	4.20561400	-4.09643600	0.33897800
C	5.06662300	-0.51707600	0.07095600
C	4.97172500	1.64121500	-0.18552100
C	6.28496100	1.33430500	-0.01377000
C	4.27413600	2.86848400	-0.40858400
C	2.59587300	4.64234000	-0.82675000
C	3.85282800	5.12282500	-0.71486000
O	4.22736200	0.51889200	-0.13405500
C	6.34690500	-0.06626000	0.15396300
C	4.80821000	4.11557100	-0.47629700
S	-3.07127100	2.05229700	0.34547000
S	-2.06272800	-2.71470500	-0.03522800
S	2.76411300	-2.02543500	0.04099500
S	2.57018700	2.94115100	-0.64079200
F	4.19654500	6.39339800	-0.80977000
F	6.09712500	4.37608900	-0.33495400
F	6.39995000	-3.15186700	0.41772000
F	4.61266400	-5.34578300	0.48091800
F	-2.95725500	-6.43108700	-0.20028600
F	-5.25317700	-4.79603800	-0.38108900
F	-6.76162300	2.72553100	-0.40586900
F	-5.33162800	5.12239300	0.04778500
H	7.09692400	2.03631300	-0.01062400
H	7.21750000	-0.67323100	0.31417700
H	2.32955900	-6.66476200	0.31625300
H	-0.36006200	-7.06463100	0.16913000
H	-6.69040300	-2.54574000	-0.63602800
H	-7.23088300	0.12313300	-0.54479800
H	-3.32523000	6.70152700	0.52925400
H	-0.79717400	7.47361600	1.21845800
H	0.57469000	5.12518800	1.46555100
H	1.69390900	5.19682500	-1.00727700

C2FSO-5

0 1

C	-4.54410200	-2.30712100	-1.97125000
C	-5.20388400	-0.30249700	-1.47991700
C	-4.97967800	1.06387300	-1.12647600
C	-4.02669300	3.28275700	-0.52679900
C	-3.19382700	4.40015900	-0.22149300

C	-1.27634800	5.37489400	0.10781600
C	-6.32979600	-1.02368200	-1.71844400
C	-5.89101500	-2.33334900	-2.03965600
C	-5.92161500	2.02511700	-0.93708500
C	-5.38600000	3.27468400	-0.59988100
C	-2.22694200	6.33700200	0.25888700
C	-3.46810600	5.70593600	0.04596700
O	-4.11435600	-1.08083300	-1.62627500
O	-1.86051100	4.19333300	-0.18291200
C	0.14696000	5.41302100	0.19181400
C	2.59086400	4.94297600	0.24047200
C	2.28397500	6.25581800	0.43121600
C	3.90087800	4.38042200	0.20279400
C	5.32616100	2.74295100	0.05890900
C	6.06130200	3.88266400	0.16848400
O	4.00963200	3.04088500	0.07973800
C	5.13910300	4.94257900	0.26174800
C	0.91120500	6.51972800	0.40408400
C	5.68969700	1.36943800	-0.06203200
C	5.75821200	-1.11147900	-0.22567200
C	6.98747900	-0.52978400	-0.27113500
C	6.94972200	0.86565700	-0.17862700
C	5.47032300	-2.50575800	-0.29964100
C	4.13106000	-4.21991500	-0.26615900
C	5.38140200	-4.71562100	-0.46882700
C	2.84581800	-4.82545200	-0.14992500
C	0.42984900	-5.30959600	0.16209300
C	1.16984000	-6.41393800	-0.12867900
O	4.18069000	-2.87578000	-0.16248400
C	6.24969300	-3.60510200	-0.49081800
C	2.53272300	-6.14120100	-0.30370700
S	-3.40258200	1.71384500	-0.88174600
S	1.14980900	4.02018800	0.02401800
S	4.53330600	0.09082000	-0.06742800
S	1.43365300	-3.91146600	0.22011200
C	-0.97744900	-5.23758000	0.38125900
C	-1.99076000	-6.13652800	0.26545000
O	-1.46711300	-4.04140600	0.76766400
C	-3.17485500	-5.44447600	0.60140800
C	-2.80271200	-4.17134400	0.90037800
C	-3.52509600	-3.00544700	1.30066900
C	-4.87409300	-2.84903000	1.33045000
S	-2.74853800	-1.54093300	1.75941000
C	-5.28033900	-1.55754600	1.71707400
C	-4.24099600	-0.73912800	1.98861800
H	-4.28046200	0.28786200	2.29892800
F	-6.55497100	-1.22548300	1.79078600
F	-5.73495500	-3.79781000	1.00398100
F	0.66691900	-7.63127800	-0.24215900
F	3.41589100	-7.08183700	-0.59098400
F	8.11919600	-1.20159800	-0.39169900
F	8.04498000	1.60509100	-0.20342600
F	3.18254000	7.20647700	0.62180100
F	0.42284200	7.73703600	0.56975000
F	-6.14798600	4.33269900	-0.38054900
F	-7.22196500	1.82109500	-1.05765000
H	-4.17614000	-5.82950400	0.62879300

H	-1.88913200	-7.16345800	-0.02883900
H	5.63613500	-5.75132800	-0.58508300
H	7.31362300	-3.60524800	-0.63124200
H	7.13213700	3.94385200	0.18245700
H	5.35183000	5.98962200	0.35742200
H	-2.04672100	7.36857200	0.49236000
H	-4.44349400	6.15091000	0.08025200
H	-7.33675800	-0.65587300	-1.66897600
H	-6.50159600	-3.18181900	-2.28507500
H	-3.78071700	-3.04660000	-2.11555200

# 2FSO-6

0 1

C	3.56327700	-1.72656100	2.01216000
C	3.84846000	0.70672800	1.58844600
C	3.67969000	2.10872600	1.39036600
C	2.47253600	3.89848300	1.12895000
C	1.22831800	4.57568200	0.97933300
C	-1.16016400	5.18234100	0.66895200
C	-2.57808400	5.18994200	0.52599000
C	-4.51041900	4.21062500	0.31897600
C	1.47586800	-4.48774000	2.54759600
C	2.62650300	-5.19115500	2.59419100
C	3.67168600	-4.25157500	2.40744500
C	3.06588200	-3.04482100	2.25590200
C	3.77112000	4.30670100	1.10058400
C	4.55403800	3.14432400	1.26431300
C	5.01346100	0.00764100	1.54358600
C	4.85246500	-1.36340700	1.78074200
C	1.03045700	5.90759500	0.77835800
C	-0.31716100	6.24960400	0.60631300
C	-4.75450300	5.54927800	0.29395100
C	-3.50195600	6.18402400	0.42796800
O	2.41392900	2.56337300	1.30937400
O	-3.18777400	3.98839600	0.46031400
O	1.72863800	-3.18430800	2.34543600
C	-5.34550000	3.05969100	0.21462000
C	-6.27441000	0.76071500	0.03370600
C	-7.22649300	1.73389300	0.02872100
C	-6.48691700	-0.64649400	-0.05166900
C	-5.81585800	-2.71312200	-0.17194100
C	-7.17618400	-2.75136000	-0.16648900
O	-5.39237400	-1.43374200	-0.10250700
C	-7.61096900	-1.41285700	-0.08947800
C	-6.70397400	3.02857600	0.12996500
H	0.44047200	-4.75673800	2.62597000
C	-4.81446300	-3.72642300	-0.23834800
C	-2.70402900	-5.03418700	-0.39431100
C	-3.81885400	-5.81049000	-0.30218700
C	-5.00645700	-5.07433300	-0.21465500
C	-1.35093400	-5.47335600	-0.49803000
C	0.78224400	-5.14022400	-0.78412600
C	0.62291200	-6.48102700	-0.61724000
C	1.91847700	-4.30707700	-1.00078600
C	3.47797200	-2.41310600	-1.38370000
C	4.10964600	-3.60055200	-1.18021900
O	-0.41574800	-4.52409400	-0.71164800

C	-0.75789800	-6.69664800	-0.42945400
C	3.22983500	-4.66857800	-0.96269100
S	2.53052600	-0.35013500	1.93332100
S	-0.27394700	3.73366100	0.95729800
S	-4.70551000	1.45962100	0.16626400
S	-3.13413600	-3.36535300	-0.37049700
S	1.76953000	-2.62027700	-1.31416100
C	4.06887600	-1.12881500	-1.56756300
C	5.34978500	-0.66951800	-1.57737100
O	3.21186500	-0.10170400	-1.73463900
C	5.26611800	0.73063300	-1.74907700
C	3.94235000	1.02454600	-1.84390500
C	3.21364000	2.23938500	-2.02408500
C	3.70493800	3.50405500	-2.01012200
S	1.51232400	2.26803400	-2.28333300
C	2.71796400	4.49073100	-2.20182300
C	1.48229000	3.97597000	-2.37030400
H	0.56225100	4.51189700	-2.51055500
F	3.01312300	5.77759500	-2.17793000
F	4.97664900	3.79937700	-1.80157900
F	5.42331500	-3.74322300	-1.16262100
F	3.65092500	-5.89578800	-0.71159000
F	-3.80167200	-7.13246600	-0.29455300
F	-6.19231300	-5.65057800	-0.12122200
F	-8.52345400	1.49567400	-0.06147400
F	-7.46962300	4.10589800	0.13950200
F	-0.71787400	7.49184000	0.39753100
F	2.00435700	6.79881400	0.73638600
F	6.18701900	0.54559600	1.25922600
F	5.86878900	-2.21008700	1.75323700
H	6.07076500	1.43984900	-1.79456000
H	6.23331400	-1.26704400	-1.45338600
H	1.40537800	-7.21477300	-0.63086200
H	-1.26004400	-7.63065100	-0.26696700
H	-7.78169400	-3.63551900	-0.21603100
H	-8.62015600	-1.04847400	-0.06256400
H	-5.71779100	6.01019600	0.18933300
H	-3.29273400	7.23660800	0.45227500
H	4.10927300	5.31584600	0.95964100
H	5.62411100	3.06870500	1.29087200
H	4.72894800	-4.43413200	2.37964600
H	2.72236900	-6.25058700	2.74071200

T2SO-1

0 1

C	3.22400500	-0.94251300	-0.01791200
C	3.56642000	0.36126400	0.01496700
O	1.88856000	-1.08135300	-0.02606400
C	2.34710800	1.08414100	0.02804600
C	1.35836400	0.15546600	0.00197200
H	2.22136800	2.15117200	0.05523900
C	-0.07336300	0.25411600	-0.00105700
C	-0.99331700	-0.74471600	0.00484700
S	-0.86874000	1.78300600	-0.01185600
C	-2.32700500	-0.27765900	0.00203100
C	-2.42294400	1.06598900	-0.00565000
H	-3.31554800	1.66207600	-0.00897100

F	-0.71357900	-2.03248800	0.01425600
H	4.56230100	0.76264000	0.02867100
F	-3.34639000	-1.11583400	0.00766700
H	3.78736700	-1.85479200	-0.03748900

# T2SO-2

0 1

C	-4.87523900	-0.08538600	0.00014600
C	-5.73866800	-1.13350700	-0.00064700
C	-7.03953400	-0.57036400	0.00022500
C	-6.86461700	0.76724300	0.00126800
O	-5.55889600	1.07428900	0.00127300
H	-5.47962000	-2.17652000	-0.00172100
C	-3.44607800	0.00654800	-0.00007500
C	-2.66942300	1.12119700	-0.00052000
C	-1.28792300	0.84962200	-0.00061400
C	-0.99320000	-0.47751300	-0.00023900
F	-3.12447500	2.35699000	-0.00087000
C	0.28824100	-1.11117900	-0.00022300
C	0.67601200	-2.41479300	-0.00032900
O	1.37023500	-0.31007200	-0.00009400
C	2.08580800	-2.40711200	-0.00020300
C	2.45989100	-1.10024200	-0.00007100
H	2.74061000	-3.25912500	-0.00024600
C	3.73725200	-0.45279500	0.00007900
C	4.01489500	0.87796300	0.00011300
C	5.39892600	1.15932300	0.00030600
C	6.16986500	0.05410900	0.00042800
F	3.11701300	1.83999500	-0.00001300
S	-2.45117800	-1.40217100	0.00014400
S	5.20463100	-1.35841900	0.00025900
H	0.03037500	-3.27378400	-0.00050800
H	-7.97679200	-1.09435600	-0.00000300
F	5.84539100	2.40051100	0.00037100
F	-0.40016400	1.82031200	-0.00103800
H	-7.53950900	1.60062100	0.00210300
H	7.24187300	-0.00007700	0.00058100

# T2SO-3

0 1

C	-8.29462200	0.56362200	0.00528100
C	-9.31840300	-0.32841300	0.02427800
C	-10.50919100	0.43997700	0.01874200
C	-10.11732200	1.73061600	-0.00287700
O	-8.77862300	1.81945400	-0.01131500
H	-9.23356900	-1.39967100	0.04087400
C	-6.87032300	0.41359900	0.00054100
C	-5.91248200	1.37713100	-0.00751100
C	-4.59905000	0.87036100	-0.00865000
C	-4.53866200	-0.48787800	-0.00135100
F	-6.14506900	2.67297600	-0.01326500
C	-3.37888100	-1.32249000	-0.00005300
C	-3.19913000	-2.67102100	0.00322100
O	-2.18513200	-0.70052200	-0.00223300
C	-1.80561700	-2.88367300	0.00309000
C	-1.23142800	-1.65030400	-0.00032300
H	-1.29242200	-3.82779600	0.00527500

C	0.12633200	-1.20578400	-0.00184500
C	0.60100400	0.06863400	-0.00335400
C	2.00607500	0.14791300	-0.00414800
C	2.62183100	-1.06440400	-0.00320900
C	4.02049500	-1.35629700	-0.00376500
C	4.72431800	-2.52014800	-0.00661200
O	4.86560000	-0.30850000	-0.00086800
C	6.08710400	-2.15682600	-0.00524400
C	6.11867400	-0.79785100	-0.00179800
H	6.93551800	-2.81625400	-0.00657100
C	7.19017800	0.15159500	0.00089800
C	7.11948100	1.50882000	0.00750400
C	8.38624000	2.13344400	0.00874400
C	9.41305200	1.26045900	0.00316800
F	-0.14843100	1.14938000	-0.00403700
F	6.00452800	2.20803400	0.01260900
S	-6.13375800	-1.14694600	0.00630800
S	1.44113800	-2.32392800	-0.00126300
S	8.83895900	-0.35157100	-0.00398700
H	4.31700100	-3.51450400	-0.00945900
H	-3.97055900	-3.41897100	0.00531200
H	-11.51962200	0.07673900	0.02962700
F	8.50245300	3.44717900	0.01493100
F	2.62500700	1.30826400	-0.00579000
F	-3.55492400	1.67031300	-0.01596400
H	-10.64619600	2.66342800	-0.01412000
H	10.46355600	1.48089000	0.00275900

T2SO-4

0 1

C	-11.37133400	1.70903100	0.07119100
C	-12.53803500	1.05221800	0.29817700
C	-13.56030100	2.03139000	0.22544800
C	-12.93759700	3.19864800	-0.03819600
O	-11.61192900	3.01729100	-0.13447000
H	-12.65359300	0.00192100	0.49451900
C	-10.00471800	1.28506200	0.01625100
C	-8.89230800	2.03542800	-0.19610900
C	-7.69654400	1.29267800	-0.18297600
C	-7.88199100	-0.03547800	0.04029600
F	-8.88774100	3.33632800	-0.39941000
C	-6.90141000	-1.07202900	0.11797700
C	-6.98572600	-2.41964100	0.28569900
O	-5.61137200	-0.70243200	0.01252800
C	-5.66132900	-2.90150600	0.28331700
C	-4.86035500	-1.81507800	0.11334000
H	-5.34029300	-3.92095200	0.39482600
C	-3.44328000	-1.65226600	0.03245600
C	-2.72681700	-0.50348300	-0.09877900
C	-1.33523100	-0.70756700	-0.13806800
C	-0.97166800	-2.01413700	-0.03695900
C	0.34359400	-2.57151700	-0.04183200
C	0.81494800	-3.84777400	-0.03118300
O	1.37146300	-1.70284900	-0.05668900
C	2.22142000	-3.74907900	-0.03844200
C	2.51029600	-2.41947800	-0.05463500
H	2.92905900	-4.55769600	-0.03232900



C	3.73778400	-1.68853400	-0.06387200
C	3.92375700	-0.34154300	-0.04582000
C	5.27746100	0.04203300	-0.05294100
C	6.14205000	-1.00718800	-0.07584600
F	-3.24582500	0.70166300	-0.18382600
F	2.95902900	0.55152200	-0.02241500
S	-9.56465000	-0.36834600	0.23754000
S	-2.37578600	-3.00655200	0.11148600
S	5.26526300	-2.49350600	-0.08850800
C	7.57077400	-0.97695600	-0.08882800
C	8.52457500	-1.94371800	-0.16282000
O	8.15165600	0.23474900	-0.01230000
C	9.76690100	-1.27613500	-0.12745200
C	9.48405400	0.05027800	-0.03589800
H	10.74443600	-1.72065900	-0.16434400
C	10.29630600	1.22730600	0.03758200
C	9.88989900	2.51848300	0.16513900
S	12.01721900	1.15546000	-0.02769000
C	10.96070600	3.43805100	0.21074700
C	12.17148600	2.85327400	0.11925900
H	13.13364400	3.32894100	0.12940800
F	8.63678600	2.91232900	0.24417400
H	8.35755700	-3.00273300	-0.23571100
H	0.22675700	-4.74702600	-0.02312200
H	-7.88676200	-2.99469000	0.39552900
H	-14.61598200	1.88252200	0.35344100
F	10.74759800	4.73379900	0.33308900
F	5.63176000	1.30836500	-0.03953800
F	-0.49890100	0.29934300	-0.26433900
F	-6.53030100	1.86937700	-0.37517800
H	-13.28195300	4.20422700	-0.18038200

T2SO-5

0 1

C	-13.95294900	3.30462100	-0.05233300
C	-15.24205500	2.89375000	0.06531400
C	-16.03653700	4.06435700	-0.02099900
C	-15.17251600	5.08762000	-0.18236500
O	-13.90770500	4.64136800	-0.20350600
H	-15.58142900	1.88291000	0.19987200
C	-12.70198700	2.60775000	-0.04519500
C	-11.44446500	3.11685800	-0.11799200
C	-10.43369300	2.13790400	-0.07963000
C	-10.90806400	0.86798200	0.02339700
F	-11.15193400	4.39708700	-0.21268900
C	-10.16869300	-0.35304000	0.08852400
C	-10.53362200	-1.65958500	0.19458900
O	-8.82724900	-0.25416100	0.03930700
C	-9.33643800	-2.40373600	0.21131300
C	-8.32406600	-1.50010300	0.11412300
H	-9.23576000	-3.47086500	0.28769500
C	-6.90138400	-1.62610300	0.08070100
C	-5.96553400	-0.64121600	0.01315700
C	-4.64251800	-1.11966500	0.00163400
C	-4.55157500	-2.47561000	0.06037800
C	-3.37312800	-3.28297000	0.06515000
C	-3.16097100	-4.62660400	0.09518700

O	-2.19479900	-2.63347900	0.03388900
C	-1.76263200	-4.80606200	0.08182500
C	-1.21852700	-3.55943700	0.04391000
H	-1.22715200	-5.73756000	0.09911000
C	0.12693700	-3.08022600	0.01488200
C	0.56588100	-1.79300100	0.00847600
C	1.96774200	-1.67471700	-0.02073200
C	2.61638600	-2.86994500	-0.03659200
F	-6.22979500	0.64577600	-0.03697500
F	-0.21305600	-0.73372200	0.02743500
S	-12.63351000	0.88760500	0.06923800
S	-6.13026600	-3.16973300	0.12996000
S	1.47124000	-4.16186200	-0.01449000
C	4.02174900	-3.12377000	-0.07066000
C	4.75467200	-4.26876100	-0.12870000
O	4.84037400	-2.05552900	-0.04223400
C	6.10709400	-3.87189300	-0.13497100
C	6.10550000	-2.51247300	-0.08155900
H	6.97134800	-4.50935700	-0.17289000
C	7.15179000	-1.54016700	-0.06143100
C	7.05534900	-0.18697700	0.03331800
S	8.81080600	-2.00684600	-0.16079800
C	8.29997900	0.46986900	0.02822600
C	9.36183900	-0.37406800	-0.07001600
F	5.92768900	0.48303800	0.12551700
H	4.37192100	-5.27222400	-0.16407400
H	-3.91378400	-5.39282700	0.12251300
H	-11.53669000	-2.04026800	0.25429100
H	-17.10692900	4.13138300	0.03176600
F	8.38560600	1.77930000	0.11396400
F	2.55539100	-0.49868700	-0.03251900
F	-3.61747300	-0.29865800	-0.06156800
F	-9.16094500	2.46450700	-0.13819800
H	-15.29464000	6.14730300	-0.29252700
C	10.75394000	-0.05298800	-0.10228700
C	11.87975400	-0.80994900	-0.19719700
O	11.08209200	1.25036400	-0.02570400
C	12.96416500	0.09118600	-0.17584900
H	11.92570500	-1.88095400	-0.27203200
C	12.42442900	1.33438700	-0.07033800
H	14.01007800	-0.14920400	-0.22938300
C	12.99578500	2.64565900	-0.00265200
C	12.35926600	3.83669600	0.15348600
S	14.69721300	2.89924100	-0.11830700
C	13.23989600	4.94057900	0.18092400
C	14.53532000	4.59448400	0.04725700
H	15.39119000	5.24223100	0.03669000
F	11.05802200	3.98959000	0.27377600
F	12.79093900	6.17206200	0.32677700

T2SO-6

0 1

C	-11.33734500	-0.62713700	0.28521100
C	-12.50276700	-1.28337600	0.53425600
C	-13.52090500	-0.30905200	0.49435400
C	-12.90565200	0.87418300	0.22412000
O	-11.57980100	0.68316000	0.09609000

H	-12.61669200	-2.33493300	0.72394200
C	-9.97640500	-1.05164500	0.19652700
C	-8.86923000	-0.29855700	-0.04197000
C	-7.67400800	-1.04068400	-0.05765000
C	-7.85342600	-2.36980300	0.16894000
F	-8.87232300	1.00089800	-0.24367000
C	-6.86968100	-3.40422900	0.22372900
C	-6.94734000	-4.75274300	0.38876300
O	-5.58275100	-3.03100100	0.09583600
C	-5.62208900	-5.23098300	0.36078600
C	-4.82711000	-4.14165800	0.17965400
H	-5.29634900	-6.24987700	0.46315500
C	-3.41221200	-3.97383500	0.07477300
C	-2.70299000	-2.82186000	-0.06805900
C	-1.31146100	-3.01972500	-0.12974200
C	-0.94045100	-4.32475300	-0.03451000
C	0.37799300	-4.87406300	-0.05932800
C	0.85967200	-6.14656500	-0.05563000
O	1.39863500	-3.99756900	-0.08911600
C	2.26525300	-6.03665600	-0.08349600
C	2.54311700	-4.70475700	-0.10371300
H	2.97938700	-6.83954200	-0.08817500
C	3.76198100	-3.96023100	-0.12995500
C	3.92825800	-2.61035800	-0.12128900
C	5.27564100	-2.20694900	-0.14450000
C	6.15553600	-3.24385700	-0.17059900
F	-3.22794700	-1.61899600	-0.14462200
F	2.95120800	-1.73116600	-0.09296700
S	-9.53010300	-2.70567200	0.40644800
S	-2.33752500	-5.32353000	0.13631000
S	5.30050900	-4.74318900	-0.16584900
C	7.58301400	-3.19025200	-0.19739200
C	8.55361500	-4.14088000	-0.27217900
O	8.14291800	-1.96810200	-0.13648000
C	9.78374600	-3.45216100	-0.25464000
C	9.47870100	-2.12882900	-0.17122800
H	10.76843600	-3.87998200	-0.29850500
C	10.26712100	-0.93869100	-0.11449200
C	9.83778300	0.34877200	-0.02098900
S	11.99184000	-0.98266000	-0.15715100
C	10.88191200	1.29105700	0.01711300
C	12.12132600	0.73519600	-0.04687100
F	8.57735100	0.71947000	0.03287200
H	8.40428800	-5.20318700	-0.33456800
H	0.27896100	-7.05054200	-0.03903500
H	-7.84469900	-5.33063800	0.51298100
H	-14.57366600	-0.46236600	0.64544300
F	10.63683900	2.57970000	0.10791900
F	5.61118200	-0.93579200	-0.14159100
F	-0.48235700	-2.00878000	-0.26921000
F	-6.51290200	-0.46434600	-0.27706100
C	13.39460100	1.38398100	-0.03104600
C	14.67197500	0.91962400	-0.08267000
O	13.39765800	2.72691500	0.05236700
C	15.50711600	2.05478200	-0.02692400
H	14.97666600	-0.10856800	-0.15167500
C	14.68092900	3.13151700	0.05485800

H	16.58132100	2.07251400	-0.04498600
C	14.91767100	4.54123100	0.13838600
C	14.00793800	5.54829900	0.21389600
S	16.51494100	5.19093900	0.15311200
C	14.59743200	6.82971600	0.28262000
C	15.94459500	6.80083600	0.25951500
H	16.62142000	7.63296600	0.29977200
F	12.70161400	5.39162700	0.22422600
F	13.85918700	7.91973700	0.36072900
C	-13.38708000	2.20956700	0.06186800
C	-12.68281200	3.33505400	-0.22965200
S	-15.06191200	2.59234500	0.23160100
C	-13.47891200	4.49279900	-0.31703600
C	-14.79965400	4.26653000	-0.09299500
C	-15.88319300	5.20303100	-0.09952900
C	-17.21898600	5.07546700	0.11083500
O	-15.57936300	6.48858700	-0.35993900
C	-17.76506400	6.37528000	-0.03214900
H	-17.74709500	4.16771900	0.33918700
C	-16.72470300	7.18537900	-0.31615000
H	-18.79475000	6.66407300	0.06447700
H	-16.63773800	8.23716300	-0.50637500
F	-11.38223500	3.38195300	-0.41998100
F	-12.95101200	5.66674700	-0.59332900