

Cartesian coordinates of B3LYP/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	0.06727900	-0.14603500	0.00008900
C	2.36995100	-1.16880400	0.00046100
C	-3.45765800	-0.51822700	-0.00117600
C	-3.46744300	0.84354700	0.00112500
C	-2.09930600	1.25707100	0.00176700
C	-1.34911900	0.10777200	0.00010300
C	2.38554300	0.19286000	-0.00009700
C	1.08688100	0.77203800	-0.00035000
O	-2.17566900	-0.98508600	-0.00205400
H	-4.22826100	-1.27339100	-0.00245600
S	0.73583400	-1.76695100	0.00088500
F	3.48830000	0.95206900	-0.00052600
F	0.89879600	2.10143000	-0.00092000
H	-1.71278600	2.26511700	0.00344100
H	-4.34111300	1.48016300	0.00217900
H	3.21353900	-1.84280200	0.00059400

C2FSO-2

0 1			
C	-3.38843400	-0.00804500	-0.00000600
C	-1.09657700	1.06813000	-0.00000500
C	0.30627400	1.35455000	0.00006000
C	2.44188800	0.77939500	0.00006200
C	3.51294300	-0.17506200	-0.00001300
C	4.94620200	-2.24652400	-0.00019200
C	-5.41543900	-2.91218600	0.00029000
C	-6.45045800	-2.02625000	-0.00005100
C	-5.86659200	-0.72282300	-0.00017400
C	-4.50527400	-0.90962700	0.00003200
C	2.40267000	2.15468400	0.00020000
C	1.03220900	2.52467900	0.00025400
C	-2.13822700	1.96739200	-0.00010700
C	-3.41614100	1.36673400	-0.00010000
C	4.86336100	0.07814100	0.00005800
C	5.66926400	-1.09181200	-0.00003700
O	1.16324100	0.28374200	-0.00005200
O	-4.22236200	-2.25076500	0.00033700
H	-5.35096900	-3.98918000	0.00050500
S	-1.72634800	-0.57135600	0.00003300
S	3.23971200	-1.90767300	-0.00023600
F	7.00566300	-1.01879800	0.00002800
F	5.39349400	1.31101400	0.00021700
F	-1.97517300	3.29928300	-0.00017300
F	-4.54559400	2.09181100	-0.00017900
H	3.26119400	2.80941200	0.00028800
H	0.61927200	3.52217500	0.00038300
H	-6.37364800	0.23022700	-0.00042100
H	-7.50387100	-2.26885800	-0.00017400
H	5.31565200	-3.26116400	-0.00028400

## C2FSO-3

0 1

C	5.26529200	1.49146900	-0.00000800
C	4.23395800	-0.82097500	0.00002000
C	3.36348100	-1.95644200	-0.00004400
C	1.37739400	-2.93048100	-0.00009400
C	-0.05256000	-2.92225600	-0.00008200
C	-2.51147500	-2.31700900	-0.00001700
C	-3.78171400	-1.65858800	0.00005300
C	-5.08125200	0.13094400	0.00009900
C	4.89719700	5.01332500	-0.00059200
C	6.25956000	5.02146800	0.00011300
C	6.67188500	3.65415900	0.00044700
C	5.52056800	2.90370000	-0.00004900
C	2.31513400	-3.94035700	-0.00015900
C	3.58782900	-3.31614400	-0.00011800
C	5.61064100	-0.82058400	0.00021100
C	6.18492100	0.46877100	0.00019300
C	-0.89833500	-4.00971000	-0.00010400
C	-2.26734000	-3.67246600	-0.00008300
C	-5.91537400	-0.96369600	0.00021100
C	-5.08237800	-2.11248400	0.00018800
O	2.01337000	-1.71471500	-0.00004000
O	-3.77543400	-0.28690800	0.00000200
O	4.42860400	3.73231000	-0.00068300
C	-5.31548900	1.54609700	0.00008200
C	-5.13154700	4.05787300	0.00014800
C	-6.41934000	3.61287000	0.00004200
C	-6.52603400	2.19638200	-0.00000100
H	4.14328000	5.78513100	-0.00106500
S	3.63881600	0.83135900	-0.00017600
S	-0.99096200	-1.43791800	-0.00001800
S	-4.01540100	2.72360700	0.00013700
F	-7.50530400	4.39496000	-0.00002100
F	-7.71224500	1.56907700	-0.00008300
F	-3.23239700	-4.60418800	-0.00010800
F	-0.47570300	-5.28315700	-0.00016000
F	6.35757800	-1.93538800	0.00037700
F	7.51344300	0.65785100	0.00035900
H	-6.99461100	-0.93333500	0.00031200
H	-5.38896100	-3.14768900	0.00027200
H	2.09999900	-4.99828300	-0.00023200
H	4.55623400	-3.79316000	-0.00015600
H	7.67972100	3.26715400	0.00099000
H	6.89687200	5.89460500	0.00035400
H	-4.78257200	5.07974100	0.00020300

## C2FSO-4

0 1

C	-4.65046500	3.36300800	0.36775100
C	-5.33523800	0.96262700	-0.05697600
C	-5.39711400	-0.45641900	-0.22912700
C	-4.50715000	-2.47995100	-0.31564700
C	-3.41394100	-3.39959000	-0.25505000

C	-1.15251700	-4.52586100	-0.09075000
C	0.23610000	-4.84223200	0.03540000
C	2.37734300	-4.31289700	0.20715600
C	-2.15653600	5.74349600	1.17642000
C	-3.17253600	6.64512100	1.07148100
C	-4.34218000	5.89852000	0.73350300
C	-3.95176000	4.58306200	0.65625600
C	-5.86077500	-2.63200600	-0.52506600
C	-6.43103900	-1.33521200	-0.47056900
C	-6.37171600	1.86479200	-0.13988500
C	-5.98919200	3.20269900	0.09642800
C	-3.46535600	-4.77457100	-0.32853200
C	-2.20618500	-5.40176300	-0.23533300
C	2.30395700	-5.68890400	0.24355600
C	0.93215300	-6.02813400	0.13219600
O	-4.21833100	-1.15093600	-0.13500000
O	1.11527300	-3.79056500	0.08085100
O	-2.61154400	4.48206000	0.92626900
C	3.46304900	-3.38398100	0.26165200
C	4.95023400	-1.33513600	0.24297800
C	5.62764100	-2.51799600	0.44055400
C	5.49716300	-0.01489400	0.17393700
C	5.34980400	2.17126400	-0.12542300
C	6.67417500	1.89492300	0.12694600
O	4.62462300	1.00832700	-0.09687700
C	6.76975700	0.49216500	0.31898300
C	4.79962500	-3.65928600	0.44991600
H	-1.10669300	5.82160600	1.41296500
C	4.63395700	3.38208300	-0.40656200
C	2.91397700	5.13630600	-0.95859500
C	4.16638600	5.64570600	-0.78908400
C	5.13895200	4.65817900	-0.47757100
S	-3.84258000	1.80537300	0.32635900
S	-1.74892000	-2.87419500	-0.06779300
S	3.23249600	-1.65395900	0.06689500
S	2.91125600	3.41126000	-0.73469500
F	4.49308100	6.93915900	-0.89610800
F	6.43012500	4.96391500	-0.27676000
F	6.95608300	-2.59740600	0.60858400
F	5.28857300	-4.89587300	0.62614400
F	-2.06550600	-6.73496200	-0.28447900
F	-4.60254300	-5.47121500	-0.47458300
F	-7.63909300	1.52265300	-0.41668600
F	-6.87042600	4.21371200	0.05698100
H	7.47231200	2.62097200	0.16470800
H	7.65667000	-0.08367600	0.53686300
H	3.14313900	-6.36199800	0.33564800
H	0.49605100	-7.01576200	0.12505500
H	-6.36929200	-3.56877500	-0.69693700
H	-7.47009100	-1.06716400	-0.58950400
H	-5.34120200	6.27347000	0.56916700
H	-3.10114200	7.71375000	1.21814800
H	2.00797600	5.67028300	-1.20380400

C2FSO-5

0 1

C	-4.65249100	1.68814500	-1.30034800
C	-3.42525300	3.81535500	-0.68147000
C	-2.46392200	4.82418500	-0.35702400
C	-0.41420300	5.55996900	0.03308900
C	1.00139300	5.40506500	0.16229500
C	3.39073000	4.57163000	0.28401700
C	4.60166000	3.81148200	0.27916500
C	5.76628500	1.93553000	0.14676000
C	-4.61437100	-1.75666100	-2.12265700
C	-5.96751600	-1.61450300	-2.19980900
C	-6.24845100	-0.24819300	-1.89439000
C	-5.03515600	0.35005500	-1.65007900
C	-1.25560500	6.64562000	0.14995900
C	-2.56839700	6.17431200	-0.09965000
C	-4.78929800	3.96622800	-0.79455600
C	-5.47263500	2.78076800	-1.13948000
C	1.92995700	6.39345700	0.40724300
C	3.25870400	5.93017400	0.47369700
C	6.67752400	2.95952700	0.29363600
C	5.93184800	4.16089200	0.37964800
O	-1.14873800	4.44250000	-0.27559100
O	4.49478900	2.45128700	0.13778100
O	-4.02940200	-0.57057500	-1.78845700
C	5.90245500	0.51889200	0.01181200
C	5.55251100	-1.97953100	-0.20181300
C	6.87583500	-1.59573900	-0.21105700
C	5.02703100	-3.30443100	-0.31316200
C	3.38331100	-4.78495500	-0.32851800
C	4.54943600	-5.48385300	-0.55568600
O	3.67015400	-3.45188900	-0.17988800
C	5.60292000	-4.53546000	-0.54451400
C	7.07076100	-0.20515400	-0.09014700
H	-3.93951400	-2.58657600	-2.26196900
C	2.01038900	-5.16911000	-0.21997100
C	-0.49510200	-5.26539200	0.12626900
C	0.06756400	-6.46995900	-0.23324900
C	1.46388500	-6.41701500	-0.42402900
C	-1.87437100	-4.98217300	0.38006200
C	-3.53627900	-3.65796900	0.99660800
C	-4.09891200	-4.86629800	0.65286000
C	-4.07913100	-2.41810300	1.47233000
C	-4.45997800	-0.09656000	2.36344900
C	-5.61654300	-0.75993900	2.08114500
O	-2.17703000	-3.72230600	0.83141000
C	-3.03290500	-5.71700300	0.25811000
C	-5.40430400	-2.07106600	1.57803700
S	-2.98274500	2.14805200	-1.01364300
S	1.81031200	3.85263200	0.01416900
S	4.52257100	-0.56577800	-0.04108500
S	0.74971300	-4.03118100	0.22625800
S	-3.07524100	-1.08600500	2.01034800
F	-6.84898300	-0.26453400	2.24329500
F	-6.41834200	-2.87867100	1.23237400
F	-0.63418400	-7.60186200	-0.39442800
F	2.17947800	-7.49625100	-0.77395300
F	7.89995100	-2.45464600	-0.32455700
F	8.29336600	0.34684400	-0.07811000

F	4.29174800	6.75539300	0.70020000
F	1.61662800	7.68791200	0.56840900
F	-5.43070800	5.12868500	-0.59996500
F	-6.80509900	2.74461500	-1.29275200
H	-5.15176800	-5.10258300	0.69025700
H	-3.09665700	-6.74143300	-0.07717300
H	4.62460200	-6.55017000	-0.70780900
H	6.65677000	-4.71958700	-0.68995300
H	7.75033400	2.84561300	0.33426300
H	6.31178300	5.16458000	0.49664200
H	-0.95255800	7.65441900	0.38663300
H	-3.48464600	6.74521300	-0.09676000
H	-7.21209300	0.23696300	-1.85585600
H	-6.68201100	-2.38823200	-2.44289400
H	-4.34712300	0.90544200	2.74971900

C2FSO-6

0 1

C	-3.78346800	-1.81320000	-2.30143200
C	-4.09287600	0.66255000	-1.87152300
C	-3.93798700	2.06407300	-1.62804600
C	-2.75353600	3.89340400	-1.24885300
C	-1.53421900	4.61200500	-1.04573500
C	0.86490100	5.35153500	-0.70578600
C	2.28213400	5.44433700	-0.54169500
C	4.31242500	4.59231100	-0.32543600
C	-1.66883500	-4.62076100	-2.74404200
C	-2.83713500	-5.30918800	-2.87852200
C	-3.88833200	-4.35331000	-2.73438700
C	-3.27983200	-3.13946700	-2.51964400
C	-4.07707700	4.27741900	-1.28667700
C	-4.83575400	3.10554600	-1.52928600
C	-5.27193500	-0.03445500	-2.01208700
C	-5.09886800	-1.41370000	-2.25222000
C	-1.38042000	5.97444900	-0.90502900
C	-0.04583300	6.38569100	-0.71710600
C	4.45131000	5.96357300	-0.29468900
C	3.15111700	6.50942700	-0.43192500
O	-2.66336100	2.53992300	-1.45667000
O	2.98740800	4.26946000	-0.47634800
O	-1.91852600	-3.29771900	-2.52489400
C	5.24416200	3.51255800	-0.22944400
C	6.40220200	1.26739900	-0.06244700
C	7.26259100	2.34391400	-0.06139800
C	6.74146900	-0.11935500	0.00873700
C	6.25187500	-2.27326800	0.13010400
C	7.62682200	-2.17973500	0.09053000
O	5.70594600	-1.01572000	0.08055100
C	7.94051500	-0.79998100	0.01382600
C	6.61793300	3.59377800	-0.15226400
H	-0.62724600	-4.90011300	-2.77174800
C	5.34428300	-3.37466900	0.21123200
C	3.32494000	-4.88958200	0.40384700
C	4.52122500	-5.56209600	0.27976000
C	5.64570300	-4.71879300	0.17477800
C	2.01452100	-5.45015600	0.51520500

C	-0.17712500	-5.31514700	0.79269400
C	0.11991400	-6.64943200	0.61238500
C	-1.39661800	-4.60428500	1.02140400
C	-3.19012200	-2.88252600	1.48802800
C	-3.67755800	-4.14936100	1.25240900
O	0.97793800	-4.57791300	0.73361900
C	1.52385400	-6.73603400	0.43603200
C	-2.67822700	-5.10850400	0.99177900
S	-2.73094600	-0.43260600	-2.04398700
S	0.03109400	3.82228500	-0.93805900
S	4.74285100	1.83012000	-0.18391400
S	3.61051000	-3.15669300	0.38659800
S	-1.43826900	-2.88763200	1.38416500
C	-3.94108900	-1.69707000	1.76653100
C	-5.28945500	-1.43450400	1.87162900
O	-3.23210700	-0.54176400	1.97485400
C	-5.41429200	-0.05006100	2.15754200
C	-4.13708000	0.45999900	2.21185800
C	-3.61005700	1.77155100	2.45556900
C	-4.31358700	2.93178900	2.67301000
S	-1.89007700	2.10679900	2.50868200
C	-3.49260400	4.07198000	2.88022100
C	-2.15938000	3.79552700	2.82321000
H	-1.33345400	4.48046300	2.94408000
F	-4.02073500	5.28134900	3.10438700
F	-5.65356800	3.00256500	2.68980200
F	-4.98268200	-4.45946400	1.25803700
F	-2.96827300	-6.39182700	0.73137300
F	4.62532700	-6.89936200	0.25640300
F	6.89145500	-5.20004700	0.04946800
F	8.59694600	2.23094500	0.01758600
F	7.29765300	4.75034100	-0.16158300
F	0.28936800	7.67572500	-0.56441700
F	-2.39744500	6.84805000	-0.94215500
F	-6.48704900	0.52852200	-1.93028000
F	-6.13979600	-2.24638900	-2.40910400
H	-6.32392200	0.51227200	2.30579500
H	-6.08260200	-2.15739900	1.75385300
H	-0.59538200	-7.45807400	0.61523400
H	2.11284600	-7.62546000	0.26898000
H	8.31524000	-3.01109300	0.11672100
H	8.91993000	-0.34835600	-0.03516800
H	5.38233200	6.49881200	-0.18383500
H	2.87384400	7.55265600	-0.45254600
H	-4.44552200	5.28356600	-1.15402000
H	-5.90792600	3.02338500	-1.62433300
H	-4.95265500	-4.52791400	-2.78079500
H	-2.94084100	-6.36997400	-3.05839000

T2FSO-1

0 1

C	-2.45640200	1.07711900	-0.00073100
C	-2.35121000	-0.27876400	0.00035700
S	-0.87799000	1.81038300	-0.00209000
C	-1.00653000	-0.75035300	0.00076600
C	-0.06793300	0.25180300	-0.00011000

C	1.37066000	0.15671800	0.00039500
C	2.37471400	1.09299000	0.00466900
O	1.91441100	-1.10068600	-0.00432100
C	3.60546500	0.36778100	0.00249100
H	2.25109900	2.16720800	0.00914700
C	3.26848700	-0.95187300	-0.00291100
H	4.60545000	0.77809700	0.00474700
H	3.83675700	-1.86917300	-0.00610800
F	-3.38313600	-1.13098500	0.00127500
F	-0.73138500	-2.05868800	0.00225600
H	-3.35357300	1.67777200	-0.00111000

#### T2FSO-2

0 1

C	-2.49240300	-1.10292600	-0.00044000
C	-2.10001200	-2.42172400	-0.00159500
C	-0.68115700	-2.42462300	-0.00165000
C	-0.28385500	-1.10625100	-0.00058100
O	-1.38717900	-0.29523200	0.00019600
H	-2.75172400	-3.28441700	-0.00246000
C	-3.77790200	-0.45889000	0.00017200
C	-4.07951600	0.88240700	-0.00110000
C	-5.47762500	1.15499400	-0.00014200
C	-6.25415600	0.03790400	0.00184000
F	-3.17993100	1.86889400	-0.00319900
S	-5.26597600	-1.39397200	0.00273900
H	-0.03281900	-3.28982900	-0.00251300
F	-5.93847500	2.41080000	-0.00123500
C	1.00122900	-0.46832700	-0.00018900
C	1.31297700	0.87086200	0.00006900
S	2.48510000	-1.41362900	0.00006400
C	2.70510400	1.14327600	0.00024100
C	3.49981400	0.02227400	0.00014200
C	4.93399800	-0.08452600	0.00003400
C	5.79671200	-1.15434700	-0.00227900
O	5.65071100	1.08350200	0.00272700
C	7.11667000	-0.61033700	-0.00092300
H	5.52236100	-2.20026700	-0.00480800
C	6.96960600	0.74422100	0.00207600
H	8.04875600	-1.15760700	-0.00209200
H	7.66227900	1.57161500	0.00394400
F	0.41765500	1.86063100	-0.00000300
F	3.15986900	2.39937000	0.00029900
H	-7.33204500	-0.02522500	0.00287400

#### T2FSO-3

0 1

C	-1.24018100	-1.58033200	-0.00036600
C	-1.82370100	-2.82854600	-0.00067700
C	-3.22586500	-2.62265900	-0.00065600
C	-3.42567800	-1.25937800	-0.00035100
O	-2.21555900	-0.61865100	-0.00016400
H	-1.30661200	-3.77809300	-0.00091100
C	0.12313400	-1.13786500	-0.00022600
C	0.62935200	0.14186900	-0.00021200

C	2.04515100	0.20663300	-0.00007300
C	2.66618000	-1.02128200	0.00001900
F	-0.11167300	1.25141200	-0.00033500
C	4.06475200	-1.33757500	0.00017500
C	4.75998800	-2.52650700	0.00044700
O	4.94757900	-0.29064500	0.00005400
C	6.13813700	-2.19163700	0.00048600
C	6.21101700	-0.81728700	0.00024300
H	6.97343100	-2.87812200	0.00067500
C	7.31119900	0.10814600	0.00016800
C	7.29319200	1.48293200	-0.00007100
C	8.58985400	2.07240900	-0.00006600
C	9.60430000	1.16577100	0.00017500
F	6.18923700	2.23340600	-0.00029100
S	1.45032200	-2.29291000	-0.00004000
S	8.97553300	-0.45630500	0.00039600
H	4.33231300	-3.51949800	0.00060600
H	-3.99450000	-3.38300400	-0.00087200
F	8.74707500	3.40064700	-0.00028100
F	2.68157400	1.37932100	-0.00004600
C	-4.60486900	-0.44365700	-0.00019200
C	-4.72286100	0.92671700	-0.00013500
S	-6.20851800	-1.16826200	-0.00006500
C	-6.06178100	1.39425300	0.00002300
C	-7.00800300	0.39752200	0.00008400
C	-8.44242100	0.49679400	0.00026600
C	-9.44960700	-0.43842800	0.00061700
O	-8.98443000	1.75546700	0.00006800
C	-10.67790300	0.28899300	0.00063000
H	-9.32822000	-1.51291000	0.00085400
C	-10.33831700	1.60855800	0.00028900
H	-11.67878500	-0.11906600	0.00086600
H	-10.90535900	2.52662600	0.00017300
F	-3.69556700	1.77840800	-0.00021500
F	-6.33378000	2.70204500	0.00011200
H	10.66740800	1.35453800	0.00022800

T2FSO-4

0 1

C	-4.93527400	-1.76171700	0.01047100
C	-5.73480800	-2.88396900	0.01993900
C	-7.07679500	-2.42809300	0.01898700
C	-7.02691300	-1.05108100	0.00903300
O	-5.72105200	-0.63987200	0.00374800
H	-5.39749700	-3.91119600	0.02710300
C	-3.51491600	-1.57067400	0.00660100
C	-2.78931500	-0.40089300	0.00164800
C	-1.38502300	-0.58840900	-0.00072800
C	-0.99159400	-1.90750700	0.00234300
F	-3.32124300	0.82253700	-0.00063600
C	0.32912500	-2.46379100	0.00091200
C	0.80668300	-3.75671800	0.00012100
O	1.38117500	-1.58709700	0.00004400
C	2.22089800	-3.66834600	-0.00124300
C	2.53388800	-2.32623000	-0.00130300
H	2.92337300	-4.49023500	-0.00199900



C	3.77525800	-1.61009000	-0.00240900
C	4.00203000	-0.25251000	0.00073700
C	5.37261000	0.10740500	-0.00133400
C	6.23710100	-0.96330600	-0.00610100
C	7.67087000	-0.97747800	-0.00976100
C	8.60221800	-1.99216400	-0.01900200
O	8.31207700	0.23272500	-0.00310900
C	9.87819600	-1.37298100	-0.01784100
C	9.65826200	-0.01442100	-0.00809300
H	10.84005100	-1.86669000	-0.02345700
C	10.53694500	1.12339300	-0.00246100
C	10.22661600	2.46276300	0.01101200
C	11.36787500	3.31483700	0.01335100
C	12.55213600	2.64508300	0.00183800
F	3.04520200	0.67697900	0.00538000
F	8.98830500	2.96085700	0.02149200
S	-2.41399000	-2.94324800	0.00826800
S	5.31507500	-2.46152100	-0.00795400
S	12.28329100	0.92637600	-0.01267900
H	8.39503000	-3.05330100	-0.02599000
H	0.21207900	-4.65974000	0.00033300
H	-7.97010900	-3.03708000	0.02514500
F	11.23808700	4.64590400	0.02602500
F	5.74946700	1.38719300	0.00103600
F	-0.55038300	0.45221900	-0.00563300
C	-8.03765600	-0.03410100	0.00353100
C	-7.90162300	1.33460900	-0.00474700
S	-9.74694400	-0.45158700	0.00721400
C	-9.13166500	2.04037600	-0.00819000
C	-10.24505800	1.23454200	-0.00266900
C	-11.63692600	1.59549700	-0.00418500
C	-12.79856700	0.86089600	-0.00182700
O	-11.93897000	2.93218400	-0.00886300
C	-13.87264400	1.80122700	-0.00523400
H	-12.87611900	-0.21762300	0.00171300
C	-13.29677600	3.03614500	-0.00945600
H	-14.93139200	1.58369000	-0.00467400
H	-13.68574000	4.04266100	-0.01306800
F	-6.73514100	1.98252700	-0.00935100
F	-9.15829500	3.37578100	-0.01628500
H	13.55064300	3.05594600	0.00086200

T2FSO-5

0 1

C	-8.45891600	-1.44763100	0.00513000
C	-9.44708900	-2.40800400	0.00819300
C	-10.68519200	-1.71852400	0.00709100
C	-10.38880300	-0.37282700	0.00341800
O	-9.03021500	-0.20267200	0.00221700
H	-9.30015400	-3.47919400	0.01097700
C	-7.02750400	-1.51622100	0.00440500
C	-6.10196900	-0.49729900	0.00247800
C	-4.75482300	-0.93622200	0.00229600
C	-4.60712600	-2.30480800	0.00408600
F	-6.40397600	0.80214800	0.00091300
C	-3.41095700	-3.09377500	0.00422800

C	-3.18172400	-4.45289100	0.00521000
O	-2.21470700	-2.42729600	0.00305700
C	-1.77603700	-4.62863000	0.00464000
C	-1.21913300	-3.36781100	0.00330100
H	-1.23876300	-5.56690000	0.00527100
C	0.13425100	-2.89710600	0.00207200
C	0.61319000	-1.60649100	0.00329900
C	2.02681700	-1.51159800	0.00150300
C	2.67398700	-2.72658300	-0.00113700
C	4.07818000	-3.01228100	-0.00373400
C	4.79868800	-4.18718600	-0.00821500
O	4.93881900	-1.94713100	-0.00162100
C	6.16832500	-3.82481200	-0.00885400
C	6.21363000	-2.44732500	-0.00477800
H	7.01742800	-4.49412800	-0.01190900
C	7.29263000	-1.50405000	-0.00344900
C	7.25322000	-0.12825900	0.00203700
C	8.52872500	0.48937700	0.00168300
C	9.58351900	-0.39450700	-0.00404900
F	-0.15165300	-0.51360600	0.00603800
F	6.13490100	0.59893700	0.00742200
S	-6.19388800	-3.06552000	0.00602700
S	1.48542500	-4.02400000	-0.00142600
S	8.96763400	-2.04244000	-0.00926200
C	10.99330900	-0.13294500	-0.00610800
C	12.10192900	-0.95025400	-0.01186500
O	11.39057400	1.17765500	-0.00173000
C	13.23549600	-0.09796600	-0.01095100
C	12.75910400	1.19328700	-0.00470600
H	14.27413300	-0.39821400	-0.01443000
C	13.40361900	2.47830200	-0.00097700
C	12.84300800	3.73369200	0.00612600
S	15.15541000	2.61845600	-0.00537000
C	13.80050100	4.78820500	0.00806800
C	15.09090900	4.35692200	0.00253400
F	11.53221600	3.98557100	0.01100000
H	12.10177000	-2.03142100	-0.01620700
H	4.39130500	-5.18868400	-0.01082400
H	-3.93385100	-5.22958600	0.00623000
H	-11.67342600	-2.15702200	0.00882600
F	13.41906800	6.07006700	0.01483900
F	8.65146100	1.81778600	0.00663500
F	2.63851300	-0.32619800	0.00232500
F	-3.74529100	-0.06427500	0.00047700
C	-11.20165900	0.80828300	0.00069900
C	-10.82461100	2.13112200	-0.00272800
S	-12.95808100	0.70120300	0.00136500
C	-11.90980500	3.04416300	-0.00487100
C	-13.14855200	2.44880800	-0.00314200
C	-14.45417300	3.05110900	-0.00453900
C	-15.72777900	2.53432100	-0.00399300
O	-14.51411600	4.42019400	-0.00694300
C	-16.61781100	3.65039500	-0.00617600
H	-15.99565800	1.48671100	-0.00230800
C	-15.83189800	4.76348000	-0.00791500
H	-17.69835800	3.62424100	-0.00643900
H	-16.03608400	5.82305100	-0.00984500

F	-9.56169100	2.56174700	-0.00408100
F	-11.69939700	4.36318400	-0.00834600
H	15.99256500	4.95095600	0.00261600

T2FSO-6

0 1

C	-11.66189200	-0.67268000	0.16100700
C	-12.81494600	-1.41588500	0.29098600
C	-13.89567400	-0.49941000	0.26309800
C	-13.34628500	0.75596500	0.11803700
O	-11.98238300	0.65479800	0.05520600
H	-12.87676400	-2.49030700	0.39502400
C	-10.27198000	-1.01972300	0.12041000
C	-9.16921000	-0.20361000	0.00717300
C	-7.93272300	-0.89524700	0.00297900
C	-8.05026500	-2.26234200	0.11303100
F	-9.21568200	1.12596300	-0.09110800
C	-7.02685000	-3.26499100	0.14274700
C	-7.05788200	-4.64002900	0.23301000
O	-5.72713600	-2.83996300	0.07193800
C	-5.71096600	-5.07947100	0.21775100
C	-4.92692900	-3.95028100	0.11828300
H	-5.35984300	-6.10043900	0.27540300
C	-3.51009500	-3.74382400	0.06030800
C	-2.79932800	-2.56630000	0.00087600
C	-1.39367000	-2.73786800	-0.03920000
C	-0.98445400	-4.05200000	-0.01176300
C	0.34204800	-4.59341400	-0.03858000
C	0.83313800	-5.88124800	-0.05497200
O	1.38463900	-3.70555600	-0.04953800
C	2.24596000	-5.77793200	-0.07649000
C	2.54486200	-4.43246000	-0.07268500
H	2.95692700	-6.59232000	-0.09291300
C	3.77888500	-3.70427300	-0.08514600
C	3.99310100	-2.34449900	-0.06701600
C	5.35981800	-1.97169500	-0.08302100
C	6.23427600	-3.03441400	-0.11384700
F	-3.34617900	-1.34984100	-0.01716100
F	3.02762900	-1.42469600	-0.03670700
S	-9.75159400	-2.69727200	0.22428500
S	-2.39315000	-5.10332600	0.06603700
S	5.32611500	-4.54127100	-0.12218900
C	7.66704900	-3.03521100	-0.13772000
C	8.60630900	-4.04209600	-0.19733800
O	8.29914600	-1.82108100	-0.09328600
C	9.87665500	-3.41485600	-0.18863100
C	9.64764000	-2.05732200	-0.12446500
H	10.84170900	-3.90089900	-0.22583400
C	10.51797300	-0.91939600	-0.08514400
C	10.20623800	0.41959400	-0.01910300
S	12.26644600	-1.11334700	-0.11656000
C	11.33362700	1.27777600	0.00698600
C	12.54275500	0.62216600	-0.03821900
F	8.96597100	0.90906300	0.01947100
H	8.40616300	-5.10360200	-0.24368600
H	0.24809700	-6.79049500	-0.05394600

H	-7.94235100	-5.25799300	0.30209100
H	-14.94842900	-0.73335500	0.33986900
F	11.19055700	2.60259600	0.07104800
F	5.72529800	-0.68892600	-0.06986700
F	-0.57214100	-1.68876700	-0.09938000
F	-6.77592400	-0.23920300	-0.10080600
C	13.87217000	1.15919200	-0.02849300
C	15.12134100	0.58012600	-0.06526700
O	14.00031400	2.52156100	0.02849500
C	16.06232300	1.64061800	-0.02927100
H	15.33666700	-0.47835500	-0.11250900
C	15.33827800	2.80971700	0.02790200
H	17.13992100	1.55391200	-0.04418300
C	15.71424300	4.19616700	0.08414500
C	14.91528400	5.31427900	0.12807700
S	17.40324400	4.68142700	0.10495200
C	15.64408100	6.53705700	0.17676900
C	16.99444100	6.37097800	0.17069200
H	17.75996300	7.13182800	0.20106400
F	13.58060000	5.30108000	0.12609200
F	15.01565900	7.71674200	0.22271100
C	-13.91399400	2.06944000	0.02683700
C	-13.28847400	3.28312800	-0.13951700
S	-15.65337900	2.31673400	0.12410500
C	-14.17323200	4.39020000	-0.19007800
C	-15.50095100	4.05813500	-0.06392500
C	-16.66128500	4.90732800	-0.06786100
C	-18.00734700	4.66062000	0.05995700
O	-16.45405700	6.25256700	-0.22717800
C	-18.66120900	5.92668200	-0.02600500
H	-18.47268800	3.69451700	0.19912400
C	-17.67633400	6.85226700	-0.19908600
H	-19.72317500	6.11886500	0.03368400
H	-17.67027100	7.92518400	-0.31397800
F	-11.96918100	3.44970700	-0.24950100
F	-13.71128800	5.63338900	-0.34853700