

Cartesian coordinates of B3LYP/6-31G(d) optimized geometries
all-cisoid C2FOS-n, and all-transoid T2FOS-n, n = 1-6.
Charge and multiplicity are given first.

C2FOS-1

0 1

C	2.21078400	-1.46558200	0.00010900
C	0.40964800	-0.15789900	0.00004400
C	1.51157500	0.65844800	-0.00001300
C	2.66056700	-0.18095100	-0.00003400
O	0.84329300	-1.45827700	0.00004500
C	-1.00331000	0.11018900	0.00006500
C	-3.49076200	-0.04948000	-0.00027900
C	-3.04478300	1.24429500	0.00006300
C	-1.62520200	1.34109100	0.00022300
H	-1.07503300	2.27451100	0.00038600
F	1.51249500	1.99589100	-0.00007200
S	-2.17973900	-1.18650800	0.00000900
F	3.92661100	0.23811300	-0.00011700
H	-3.70561900	2.10417100	0.00009200
H	2.69803400	-2.42629100	0.00017700
H	-4.51096300	-0.40874400	-0.00052600

C2FOS-2

0 1

C	5.11285900	-2.20746800	0.00010100
C	3.88757500	-0.34951500	-0.00007200
C	5.20814000	0.02665500	-0.00020800
C	5.98678300	-1.16325800	-0.00007700
O	3.83552900	-1.71972700	0.00013900
C	2.66324000	0.39771400	-0.00010700
C	0.27264100	1.13188300	-0.00010600
C	1.16672500	2.18780900	-0.00024500
C	-1.15609100	1.20195800	-0.00004800
C	-3.22669700	0.34632900	0.00008000
C	-3.34556200	1.71637100	0.00003300
O	-1.88806400	0.03945100	0.00003300
C	-2.03961200	2.25676300	-0.00004500
C	2.51672000	1.77218300	-0.00024400
H	3.36155700	2.45037400	-0.00033800
F	5.67880500	1.27796100	-0.00041500
F	-4.48572100	2.41253300	0.00005800
C	-4.19006400	-0.71525800	0.00016100
C	-5.35260000	-2.92016900	0.00031400
C	-6.22376500	-1.86400800	0.00029300
C	-5.56690700	-0.60332500	0.00021200
H	-6.07810400	0.35196500	0.00019300
S	1.10814500	-0.40837400	0.00001000
S	-3.69848000	-2.39662400	0.00019900
F	7.31880500	-1.21797800	-0.00014000
F	-1.72268800	3.55454300	-0.00010600
H	0.84934700	3.22355600	-0.00033700
H	-7.30210100	-1.97926700	0.00034300
H	5.23097000	-3.27818800	0.00023700
H	-5.57914400	-3.97778300	0.00037700

C2FOS-3

0 1

C	5.48460100	3.99191300	-0.00055500
C	5.61778000	1.77048300	-0.00005300
C	6.90039900	2.26110500	0.00041200
C	6.81016500	3.68021100	0.00013300
O	4.75467500	2.83598600	-0.00059800
C	5.08585500	0.43862000	-0.00001900
C	3.61344100	-1.58223400	0.00003400
C	4.96272400	-1.89119000	0.00024800
C	2.51327100	-2.49468300	-0.00003000
C	0.34343500	-3.05417400	-0.00014100
C	1.07315000	-4.22247600	-0.00023400
O	1.22996100	-2.00442300	0.00000700
C	2.43993600	-3.86990500	-0.00014500
C	5.79331600	-0.74928000	0.00023300
H	6.87607300	-0.78496200	0.00038700
F	8.02709700	1.54171500	0.00105300
F	0.57859100	-5.46300100	-0.00037500
C	-1.05989800	-2.78606700	-0.00018400
C	-3.32478500	-1.72338400	-0.00010200
C	-3.37167300	-3.10751200	-0.00030700
C	-2.09462600	-3.70679000	-0.00032100
H	-1.92660200	-4.77703800	-0.00043600
C	-4.42814800	-0.81468700	0.00005100
C	-5.38248800	1.21264000	0.00015800
C	-6.39340200	0.27990000	0.00047300
C	-5.38068200	2.64587700	0.00000900
C	-4.75877300	5.05928500	-0.00052500
C	-6.11390500	4.86342400	0.00003500
O	-4.18640800	0.53805000	-0.00011200
C	-5.79228800	-0.99866900	0.00047300
C	-6.47525100	3.48875100	0.00038700
H	-7.49557200	3.12439000	0.00087600
F	-7.70505600	0.53335700	0.00077600
S	3.35821000	0.15151800	-0.00022600
S	-1.67118100	-1.14335400	-0.00005300
S	-3.88626500	3.55969200	-0.00074300
F	7.84315900	4.52280700	0.00045700
F	3.47335100	-4.71613200	-0.00018800
F	-6.43269700	-2.17066600	0.00078800
H	5.32984300	-2.91035500	0.00041400
H	-4.30212800	-3.66241500	-0.00041600
H	-6.83448200	5.67387300	0.00024700
H	4.93732600	4.91975100	-0.00101600
H	-4.21541100	5.99447800	-0.00084500

C2FOS-4

0 1

C	3.43205200	5.25894000	-0.82675300
C	4.89978300	3.63990800	-0.40518900
C	5.58967400	4.82701500	-0.42871700
C	4.64817700	5.85798800	-0.69848300
O	3.57800000	3.91137300	-0.64949400

C	5.30537800	2.28110400	-0.19051500
C	5.39968100	-0.19945500	0.10679700
C	6.63906400	0.40874500	0.20763800
C	5.10366900	-1.59374400	0.21314000
C	3.75514900	-3.38277300	0.23609100
C	5.04582400	-3.83413000	0.40441900
O	3.79936600	-2.01446000	0.12088800
C	5.89524800	-2.70689600	0.39014500
C	6.58462900	1.80983900	0.04009400
H	7.44938600	2.46095800	0.08447800
F	6.90219000	4.98858800	-0.23499600
F	5.42428100	-5.10597400	0.55470200
C	2.49446600	-4.05104800	0.16934600
C	0.06802700	-4.64064600	0.02237000
C	0.89377600	-5.74867500	0.12280800
C	2.26151300	-5.41617500	0.20655800
H	3.05946100	-6.14394200	0.29126100
C	-1.35582000	-4.62504100	-0.08906300
C	-3.36782900	-3.64768800	-0.22663200
C	-3.56321700	-5.01018400	-0.28719300
C	-4.26552500	-2.53680900	-0.25330900
C	-5.31791100	-0.26853200	-0.18308000
C	-6.23291600	-1.28823300	-0.38632200
O	-2.01802100	-3.42119700	-0.10618400
C	-2.29637400	-5.62555100	-0.20056500
C	-5.63968300	-2.56729500	-0.42531700
H	-6.19143500	-3.48785400	-0.57292000
F	-4.73725500	-5.63575700	-0.40352200
S	4.13742300	0.97630000	-0.20108300
S	0.99556000	-3.15362300	0.02996200
S	-3.68820700	-0.89586700	-0.03828300
C	-5.58340800	1.13289900	-0.09103800
C	-6.73512800	1.87690800	-0.21360400
O	-4.54982200	1.99821500	0.17527000
C	-6.38835300	3.23198200	-0.01455700
C	-5.03462700	3.28188100	0.22443000
C	-4.13541700	4.36259700	0.50294400
C	-4.43745200	5.70830400	0.58255200
S	-2.43334400	4.08300700	0.80830300
C	-3.30519400	6.51148800	0.88762800
H	-5.43782000	6.09426300	0.42763900
C	-2.15712500	5.78058300	1.03751100
H	-1.16240400	6.13403000	1.27304100
F	-7.22470000	4.27313300	-0.05031900
F	4.92914700	7.15708400	-0.80107200
F	7.22429000	-2.71791800	0.52126700
F	-2.05398500	-6.93852800	-0.22435800
F	-7.95739600	1.40533400	-0.47311600
H	7.55017100	-0.14649100	0.39496000
H	0.51348100	-6.76299100	0.13514400
H	-7.29499300	-1.10764400	-0.50029300
H	-3.34461400	7.59019200	0.99222000
H	2.43974400	5.62344300	-1.03380400

C2FOS-5

0 1

C	5.18097800	-0.19558400	2.14919700
C	5.06887000	1.92818800	1.49730100
C	4.39599600	3.11617600	1.05863500
C	2.71553600	4.82278400	0.33608600
C	1.52802600	5.53665700	-0.01496000
C	-0.67444300	5.77320300	-0.35234500
C	6.38938100	1.63979300	1.73900000
C	6.45621500	0.28197400	2.15447800
C	4.95766000	4.34849300	0.77949600
C	4.00994900	5.31259600	0.37153400
C	-0.08413400	6.99524300	-0.59007800
C	1.30245300	6.84600400	-0.37774500
O	4.33378500	0.80007900	1.75235500
O	0.31667700	4.88755000	-0.00355400
H	6.01950900	4.54242600	0.87267100
C	-2.03380500	5.33658100	-0.39934700
C	-4.17434900	4.04135200	-0.35279500
C	-4.35552500	5.38738700	-0.62803500
C	-5.19219700	3.04619900	-0.23403900
C	-5.98981500	0.97237500	0.05149600
C	-7.06995500	1.81982900	-0.06765900
O	-4.84674800	1.72852400	-0.05104800
C	-6.56796300	3.12490500	-0.24747400
C	-3.15010800	6.11638500	-0.65555300
H	-3.08831600	7.17948600	-0.85374800
F	7.42379200	2.47616100	1.60517100
F	-0.70892900	8.11793600	-0.95437200
F	-8.35789600	1.46932800	-0.02482500
C	-5.89717100	-0.44155800	0.23135900
C	-5.15854000	-2.82350700	0.43332500
C	-6.52923800	-2.66396900	0.55967400
C	-6.94522700	-1.32280600	0.44464900
H	-7.97665100	-0.99916400	0.51264900
C	-4.42610100	-4.04777500	0.49919700
C	-2.59245200	-5.32884900	0.37444100
C	-3.65412500	-6.15296000	0.67803700
C	-1.20372900	-5.58219600	0.15736800
C	1.24010200	-5.42137200	-0.35056500
C	0.82899500	-6.70987300	-0.05248200
O	-3.07167900	-4.04538100	0.26855000
C	-4.80860500	-5.34644800	0.75660100
C	-0.54902200	-6.80074200	0.23362000
H	-1.05700900	-7.72342600	0.48681700
F	-3.60055000	-7.47468200	0.86156600
S	2.66115900	3.13681300	0.81282300
S	-2.47803200	3.66347100	-0.12153000
S	-4.36123000	-1.28433000	0.17035100
S	-0.09871300	-4.29290700	-0.27644400
C	2.55872600	-4.98291800	-0.68419700
C	3.76288500	-5.63891800	-0.80433800
O	2.77523400	-3.65373200	-0.95686600
C	4.73625400	-4.67831300	-1.16031400
C	4.10321000	-3.46019600	-1.24856900
C	4.56466900	-2.13983700	-1.56147600
C	5.85866700	-1.74300600	-1.83976300
S	3.46361900	-0.77963700	-1.62524300
C	5.96366300	-0.34991300	-2.10110400

H	6.69468900	-2.43212700	-1.85151900
C	4.76067800	0.30051000	-2.02242200
H	4.55382000	1.35195100	-2.16887000
F	6.03426700	-4.91341700	-1.37094300
F	7.56984100	-0.37461000	2.48040700
F	2.22615500	7.80234000	-0.50247900
F	-7.29474300	4.23486100	-0.39892100
F	-6.04673200	-5.76561900	1.03036600
F	3.97446400	-6.94447900	-0.61843300
H	4.25729800	6.33533000	0.11390800
H	-5.33192000	5.82311900	-0.80133200
H	-7.20157500	-3.49642000	0.72786200
H	1.50793600	-7.55403000	-0.04415300
H	6.89750600	0.14821800	-2.33735100
H	4.74225000	-1.15199300	2.37905800

C2FOS-6

0 1

C	4.44300900	0.09853200	-2.10305800
C	4.03164900	-2.31660400	-1.60623400
C	3.46201300	-3.59409400	-1.31237900
C	1.79177800	-5.01884400	-0.87023100
C	0.43194300	-5.39438200	-0.64662800
C	-2.04824300	-5.46754300	-0.31646300
C	-3.44144300	-5.17839600	-0.19064300
C	-5.24996100	-3.85893000	-0.10517700
C	3.20770900	3.41757000	-2.58589100
C	4.52308000	3.70466500	-2.78925800
C	5.23892400	2.48512300	-2.64302100
C	4.32139800	1.50525200	-2.35379900
C	2.96273100	-5.74440600	-0.88687300
C	4.01452600	-4.84717400	-1.16530000
C	5.36917300	-2.02242300	-1.81108400
C	5.60057100	-0.65824000	-2.09146600
C	-0.05387500	-6.67450300	-0.43269800
C	-1.45013000	-6.71578500	-0.24723400
C	-5.68112400	-5.16266200	0.01184100
C	-4.54321200	-5.99287000	-0.04160600
O	2.10526800	-3.70741500	-1.13115000
O	-3.88087300	-3.87661400	-0.22737500
O	3.07878700	2.08339100	-2.32106000
H	6.57980000	-0.23504100	-2.28079800
H	0.58687700	-7.54767200	-0.41665300
C	-5.95386200	-2.61620000	-0.11489300
C	-6.64445800	-0.21123400	-0.12509300
C	-7.71732300	-1.08775700	-0.09827400
C	-6.70456400	1.21547000	-0.15134900
C	-5.85731200	3.28911200	-0.12633600
C	-7.22640900	3.40176800	-0.23387400
O	-5.54669300	1.95118700	-0.07708800
C	-7.75991800	2.09646800	-0.24939900
C	-7.32865600	-2.44170200	-0.09119000
H	-8.02324800	-3.27247100	-0.06987100
H	2.30711500	4.00811800	-2.58545500
F	6.56066500	2.32756200	-2.76455500
F	3.08196100	-7.05809700	-0.67449300

F	-6.94616000	-5.56709200	0.15211800
F	-7.92204700	4.53913600	-0.30664600
C	-4.81241900	4.25959000	-0.05061000
C	-2.63372800	5.46439000	0.19067000
C	-3.70724000	6.31505500	-0.01810500
C	-4.93528800	5.63614300	-0.15313700
H	-5.88556700	6.12884300	-0.31974800
C	-1.26147000	5.82206000	0.35898600
C	0.90851800	5.40750900	0.73888400
C	0.77322900	6.76474400	0.54323400
C	2.03291800	4.57243900	1.02050900
C	3.56139200	2.66689200	1.55501500
C	4.22696500	3.87146100	1.39563100
O	-0.33761400	4.83990600	0.62423700
C	-0.59315300	7.02560500	0.30431600
C	3.36480100	4.94647600	1.09493500
H	3.69768000	5.96516000	0.93572100
F	1.75529100	7.66923400	0.57553500
S	3.03490300	-0.88431800	-1.76084900
S	-0.86195300	-4.21109300	-0.61539600
S	-5.11868200	-1.07499800	-0.14420100
S	-3.14623100	3.78843900	0.21994600
S	1.83525700	2.85873200	1.32995100
C	4.13202900	1.39196400	1.85782400
C	5.43009800	0.96307900	2.01815900
O	3.30533500	0.31080800	2.04336000
C	5.38736400	-0.41858400	2.30874900
C	4.06518100	-0.79841900	2.31913600
C	3.41483200	-2.05346700	2.55594200
C	4.01010000	-3.26965000	2.83216200
S	1.67043500	-2.20203100	2.52329900
C	3.06640800	-4.31620400	3.01696100
H	5.08420700	-3.39581700	2.89694200
C	1.76964300	-3.89562600	2.88246600
H	0.86240000	-4.47808200	2.96790800
F	6.44044700	-1.20955100	2.53268600
F	5.06264900	4.89106900	-3.07126400
F	5.30968800	-5.15773500	-1.26726100
F	-4.53566900	-7.32635000	0.03459500
F	-9.05234600	1.77363200	-0.34444300
F	-1.13768400	8.22120800	0.06540900
F	6.52932900	1.71479500	1.91532600
H	6.14927900	-2.77222800	-1.75916000
H	-2.01259500	-7.62461700	-0.07157800
H	-8.74668700	-0.75099600	-0.08419700
H	-3.60017600	7.39188300	-0.06945800
H	5.30169600	3.96362200	1.49527300
H	3.34158200	-5.34080700	3.24192200

T2FOS-1

0 1			
C	-3.41336200	-0.37104700	-0.00001300
C	-3.26509200	0.98896100	0.00000700
C	-1.90177600	1.39839100	0.00001800
C	-1.02187000	0.33784200	-0.00000200
C	0.41634200	0.38493400	0.00001800

C	1.39505700	-0.57463300	-0.00000600
O	1.02609700	1.61431700	0.00007500
C	2.65004600	0.09671800	0.00003600
C	2.38113300	1.43044300	0.00008100
H	2.99752900	2.31404100	0.00012100
S	-1.88327800	-1.18839900	-0.00008500
F	1.20782000	-1.89859700	-0.00005800
H	-1.57182500	2.43054100	0.00005100
F	3.84599100	-0.49326800	0.00002900
H	-4.10073000	1.68022800	0.00003100
H	-4.32848300	-0.94783900	-0.00001400

T2FOS-2

0 1

C	6.90727700	-1.10413500	-0.00011000
C	6.09218900	-2.20350900	-0.00004100
C	4.70986500	-1.86916700	-0.00001200
C	4.48486400	-0.50785700	-0.00005700
C	3.22244000	0.17331400	-0.00005100
C	2.85923700	1.49823000	-0.00008900
O	2.07436500	-0.58213200	0.00000200
C	1.44613500	1.55138800	-0.00005700
C	0.98474400	0.25668000	0.00000000
C	-0.32208500	-0.32790900	0.00005300
C	-0.64713400	-1.67067700	0.00011400
C	-2.04096400	-1.90778400	0.00013500
C	-2.79144400	-0.74927800	0.00009100
C	-4.22193400	-0.62999400	0.00008000
C	-5.08399600	0.43735300	0.00004300
O	-4.96968700	-1.78117700	0.00010900
C	-6.40727500	-0.08467100	0.00005300
C	-6.29381100	-1.44107000	0.00009700
H	-7.00858300	-2.24719500	0.00011900
S	-1.76411200	0.67180600	0.00006200
S	6.00032900	0.37503500	-0.00012000
F	-4.74361800	1.72950100	0.00000400
F	3.68975500	2.54404900	-0.00014600
H	-2.49019500	-2.89381800	0.00017000
H	3.90468800	-2.59424800	0.00003600
F	-7.52702100	0.63842100	0.00002600
F	0.69571800	2.65578700	-0.00007800
H	0.10279600	-2.45260600	0.00013100
H	6.46395600	-3.22224700	-0.00001600
H	7.98828100	-1.06818400	-0.00014800

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0 1

C	6.85777700	-0.26351400	-0.00007300
C	6.83074300	1.11041000	-0.00013300
C	5.47446200	1.50850400	-0.00012900
C	4.70897200	0.36639500	-0.00006800
O	5.55948000	-0.71433300	-0.00003400
C	3.29911800	0.12372100	-0.00003600
C	2.64972400	-1.09686900	0.00002200
C	1.24229000	-0.98104600	0.00003700

C	0.80122800	0.32934900	-0.00000900
C	-0.54920100	0.79977800	-0.00001000
C	-1.11616700	2.05337300	-0.00004800
O	-1.56569700	-0.12630000	0.00003400
C	-2.51844800	1.88482200	-0.00002600
C	-2.77227500	0.53286800	0.00002500
C	7.91536100	-1.23227400	-0.00004800
C	7.80233000	-2.60757800	0.00001400
C	9.06176800	-3.26799000	0.00001800
C	10.11973600	-2.39973900	-0.00004500
C	-3.97390700	-0.24353200	0.00006500
C	-4.09390400	-1.62033800	0.00011400
C	-5.43610900	-2.06370000	0.00014000
C	-6.35203700	-1.03064000	0.00011100
C	-7.78412400	-1.12535800	0.00012300
C	-8.79373900	-0.19615700	0.00010000
O	-8.35444800	-2.37395400	0.00016400
C	-10.02586800	-0.90675900	0.00013000
C	-9.71417500	-2.23183300	0.00017000
H	-10.30288200	-3.13415500	0.00020200
S	-5.55004400	0.52855600	0.00005700
S	2.15123200	1.45121700	-0.00007200
S	9.60008800	-0.74453400	-0.00009100
F	-8.64611800	1.13182800	0.00005800
F	-0.45782100	3.21468400	-0.00009600
F	7.89201800	1.92081900	-0.00018400
H	-5.73242300	-3.10592700	0.00017700
H	0.56310700	-1.82521700	0.00007900
H	6.84511600	-3.11535500	0.00005300
F	-11.23957500	-0.35612900	0.00012100
F	-3.43346500	2.85682900	-0.00004900
F	5.01742300	2.76288000	-0.00017700
H	-3.23530000	-2.28113900	0.00012800
H	3.18206200	-2.04049300	0.00005200
H	9.17470100	-4.34653200	0.00006000
H	11.17703700	-2.62784400	-0.00006000

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0 1

C	-3.20562600	-1.46342400	-0.00005500
C	-2.92617400	-2.81081800	-0.00010300
C	-1.52131800	-2.95283800	-0.00009900
C	-0.97777200	-1.68859100	-0.00004900
O	-2.01158900	-0.78171700	-0.00002200
C	0.36289700	-1.19223200	-0.00002200
C	0.77703600	0.12737700	0.00003300
C	2.18122900	0.27204400	0.00004400
C	2.85589600	-0.93523600	-0.00000100
C	4.26997900	-1.14679500	-0.00000500
C	5.06095100	-2.27254800	-0.00004700
O	5.09604200	-0.04740000	0.00004100
C	6.40719700	-1.84548000	-0.00002700
C	6.40443400	-0.46978800	0.00002800
C	-4.42067400	-0.70982500	-0.00003600
C	-4.56450800	0.66546400	0.00001300
C	-5.91233000	1.08634700	0.00001700

C	-6.81294300	0.03723500	-0.00003100
C	7.43851000	0.51890800	0.00006900
C	7.29462400	1.89346400	0.00012200
C	8.52790900	2.58383400	0.00014800
C	9.62349700	1.74353800	0.00011400
C	11.01110500	2.10998000	0.00012400
C	12.18041100	1.39202700	0.00009900
O	11.33106700	3.44484800	0.00016700
C	13.25309700	2.32615000	0.00012800
C	12.69263300	3.56666400	0.00017000
H	13.09697800	4.56529300	0.00020300
C	-8.24159000	0.10958900	-0.00004300
C	-9.23942300	-0.83640100	-0.00008700
O	-8.83353500	1.35083900	-0.00000700
C	-10.47507200	-0.14969400	-0.00007600
C	-10.19900700	1.19651700	-0.00002600
C	-11.01700300	2.37451200	0.00000800
C	-10.60302100	3.69089500	0.00006400
C	-11.68547200	4.61310500	0.00007700
C	-12.90905500	3.99988800	0.00002600
S	9.13248100	0.06046100	0.00005600
S	1.73542100	-2.28625900	-0.00005700
S	-5.98360600	-1.50922200	-0.00007600
S	-12.76796600	2.27084500	-0.00000800
F	12.29092400	0.06057200	0.00005500
F	4.63066300	-3.53598000	-0.00009900
F	-3.82282300	-3.79964100	-0.00014600
F	-11.68913200	-0.70568100	-0.00010800
H	8.62068800	3.66337500	0.00018700
H	2.69390900	1.22649000	0.00008400
H	-3.71693400	1.34037400	0.00004500
H	-9.55731500	3.97483700	0.00009000
F	14.54992300	2.01905900	0.00011600
F	7.48675800	-2.63040800	-0.00005500
F	-0.84117500	-4.10130600	-0.00013700
F	-9.06855300	-2.16050200	-0.00013200
H	6.32605900	2.37894400	0.00014000
H	0.08054300	0.95728000	0.00006200
H	-6.22557700	2.12348800	0.00005100
H	-11.55746100	5.68995500	0.00011400
H	-13.88982400	4.45595900	0.00001700

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0 1

C	0.54201400	-2.76444100	-0.00005400
C	1.08149000	-4.03059600	-0.00010200
C	2.48665000	-3.89306200	-0.00009800
C	2.77048500	-2.54649400	-0.00004700
O	1.57861300	-1.86087000	-0.00002100
C	3.98800400	-1.79729700	-0.00002100
C	4.13666300	-0.42221000	0.00003100
C	5.48562600	-0.00620900	0.00004100
C	6.38278700	-1.05874100	-0.00000200
C	7.81096900	-0.99151800	-0.00000700
C	8.80494900	-1.94289000	-0.00004700
O	8.40824900	0.24706600	0.00003400

C	10.04298600	-1.26309800	-0.00003000
C	9.77355800	0.08599600	0.00002100
C	-0.79707900	-2.26412700	-0.00003600
C	-1.20722900	-0.94319200	0.00001600
C	-2.61082100	-0.79421000	0.00001700
C	-3.28924500	-1.99959400	-0.00003400
C	10.59683400	1.25596200	0.00005800
C	10.19052400	2.57694000	0.00011000
C	11.26756300	3.49217200	0.00013200
C	12.50466000	2.87896300	0.00009700
C	13.79560000	3.50612500	0.00010100
C	15.08128800	3.02676000	0.00007300
O	13.85256300	4.87766600	0.00014200
C	15.95402700	4.14987400	0.00009700
C	15.16521200	5.25927700	0.00014100
H	15.36976200	6.31708000	0.00017100
C	-4.70375200	-2.20659000	-0.00005200
C	-5.49838200	-3.33001800	-0.00010100
O	-5.52638700	-1.10454900	-0.00001500
C	-6.84303300	-2.89902300	-0.00009400
C	-6.83618200	-1.52291000	-0.00004000
C	-7.86686600	-0.53186700	-0.00001000
C	-7.71845500	0.84295100	0.00004600
C	-8.94765900	1.53768500	0.00005900
C	-10.04865100	0.70116500	0.00001300
C	-11.43009800	1.07245700	0.00000700
C	-12.60489200	0.35805600	-0.00003400
O	-11.74717100	2.41063300	0.00004800
C	-13.66807200	1.28973300	-0.00001400
C	-13.11448500	2.54754800	0.00003700
C	-13.66609300	3.87140800	0.00007900
C	-12.98368400	5.07078400	0.00014100
C	-13.84714600	6.20062300	0.00014900
C	-15.17256700	5.85929800	0.00008400
S	12.34753800	1.13285000	0.00004600
S	5.54779600	-2.60241000	-0.00005400
S	-2.17293200	-3.35402200	-0.00007900
S	-9.56269500	-0.98493800	-0.00003800
S	-15.39942100	4.13935100	0.00008500
F	15.44625300	1.74160600	0.00002900
F	8.62674700	-3.26570900	-0.00009500
F	0.39767000	-5.17677300	-0.00014500
F	-7.92513100	-3.68036200	-0.00013200
F	-14.97202000	1.00203300	-0.00004100
H	11.15062000	4.56935700	0.00016900
H	5.80240400	1.02986900	0.00007900
H	-0.50820900	-0.11540800	0.00005000
H	-6.74794900	1.32458200	0.00007300
H	-11.90161300	5.12716500	0.00016700
F	17.28568800	4.09797900	0.00008100
F	11.25462900	-1.82304800	-0.00005700
F	3.38022800	-4.88447400	-0.00013600
F	-5.07166400	-4.59458000	-0.00014800
F	-12.71720500	-0.97218800	-0.00008200
H	9.14658600	2.86690100	0.00012900
H	3.29142500	0.25559100	0.00005900
H	-3.12062200	0.16176200	0.00005200

H	-9.03581200	2.61750800	0.00009700
H	-13.49481900	7.22623100	0.00018300
H	-16.03502900	6.51201000	0.00006200

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0 1

C	4.26658900	-3.52059800	-0.00009400
C	5.04272800	-4.65704300	-0.00014300
C	6.39408200	-4.24816900	-0.00014200
C	6.40984100	-2.87203100	-0.00009200
O	5.10699700	-2.43219300	-0.00006300
C	7.45680700	-1.89852700	-0.00006800
C	7.33162400	-0.52110300	-0.00001300
C	8.57212600	0.15250100	-0.00000300
C	9.65912300	-0.70270500	-0.00004900
C	11.04591200	-0.35474900	-0.00005300
C	12.20875900	-1.09014500	-0.00009300
O	11.38591000	0.97767000	-0.00000800
C	13.28749800	-0.17844500	-0.00007200
C	12.75603000	1.09049700	-0.00002000
C	2.85554600	-3.29148600	-0.00007300
C	2.19541100	-2.07596300	-0.00003000
C	0.78974700	-2.20368900	-0.00002100
C	0.35973800	-3.51836000	-0.00005800
C	13.33082700	2.40058200	0.00002200
C	12.66959400	3.61416100	0.00007500
C	13.54269500	4.72558200	0.00010800
C	14.87710600	4.37092100	0.00008000
C	16.01762300	5.24205500	0.00009900
C	17.37279800	5.02705800	0.00008000
O	15.80134100	6.59756500	0.00014700
C	18.00552400	6.30093600	0.00011800
C	17.01231000	7.23185100	0.00015900
H	17.00311000	8.30919400	0.00019600
C	-0.98645700	-3.99906500	-0.00006200
C	-1.54370000	-5.25751800	-0.00008800
O	-2.01016900	-3.08091100	-0.00003600
C	-2.94670400	-5.10027000	-0.00007700
C	-3.21150700	-3.74973400	-0.00004500
C	-4.41860300	-2.98399300	-0.00002300
C	-4.54897400	-1.60698900	0.00000400
C	-5.89219200	-1.17309300	0.00001800
C	-6.80340300	-2.21368900	0.00000100
C	-8.23034600	-2.12757000	0.00000700
C	-9.23670200	-3.06612600	-0.00000400
O	-8.81155700	-0.88129900	0.00002600
C	-10.46564200	-2.37074500	0.00001000
C	-10.17897500	-1.02476500	0.00002800
C	-10.98712200	0.15471400	0.00004600
C	-10.56397300	1.47117800	0.00006200
C	-11.62752600	2.39995600	0.00007600
C	-12.87485900	1.80320600	0.00007000
S	15.07089500	2.62840800	0.00001300
S	9.14445600	-2.38050900	-0.00010700
S	1.71887800	-4.62890000	-0.00010400
S	-5.98896300	-3.76832200	-0.00003100

S	-12.73964400	0.05374100	0.00005100
C	-14.15312400	2.44539300	0.00007900
C	-15.44759000	1.98183800	0.00007700
O	-14.19478600	3.82002000	0.00009100
C	-16.30168400	3.10812300	0.00008900
C	-15.50665000	4.22907000	0.00009800
C	-15.78105800	5.63680100	0.00011100
C	-14.87220500	6.67521700	0.00012000
S	-17.42555900	6.24666400	0.00012100
C	-15.49193700	7.95512400	0.00012800
C	-16.85879300	7.88639600	0.00012400
H	-17.57298100	8.69868100	0.00012600
F	17.98472500	3.83938100	0.00003400
F	12.29665100	-2.42188700	-0.00014300
F	4.59529700	-5.91435000	-0.00018400
F	-3.85423200	-6.07887700	-0.00009400
F	-11.68441800	-2.91487200	0.00000600
F	-17.63671400	3.08774300	0.00009100
H	13.21335300	5.75784700	0.00015000
H	8.67838200	1.23070000	0.00003800
H	2.71961000	-1.12779900	-0.00000500
H	-3.69477900	-0.94049600	0.00001300
H	-9.51623900	1.74718200	0.00006300
H	-13.80067600	6.51431900	0.00011800
F	19.32098300	6.51440500	0.00011400
F	14.58602200	-0.48726000	-0.00009900
F	7.46319400	-5.04696100	-0.00018200
F	-0.87577200	-6.41297600	-0.00011800
F	-9.07517000	-4.39102200	-0.00002300
F	-15.82542800	0.70151600	0.00006500
H	11.58881300	3.68986000	0.00008900
H	6.36946300	-0.02303300	0.00001800
H	0.10327600	-1.36547700	0.00001000
H	-6.19521300	-0.13291300	0.00003900
H	-11.49586700	3.47534800	0.00008800
H	-14.94126500	8.88937600	0.00013400