

Cartesian coordinates of B3LYP/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	2.57335100	-1.21266400	0.00009700
C	0.65617300	-0.10957900	0.00003700
C	1.64142100	0.84730300	0.00010800
C	2.86229500	0.11777400	0.00012000
O	1.21295900	-1.36006200	-0.00000100
C	-0.78033700	-0.03382800	-0.00003300
C	-3.24528300	-0.47122000	0.00007700
C	-2.96407500	0.86685700	0.00004500
C	-1.56459500	1.09624300	0.00002800
S	-1.80983000	-1.44926700	-0.00039200
H	3.16803600	-2.11078900	0.00010400
H	-4.21606900	-0.94740000	0.00018200
F	-1.03903400	2.33598200	0.00014600
F	4.08563700	0.65767100	0.00016800
H	-3.70041200	1.66117200	0.00015900
H	1.50892700	1.91758400	0.00013500

CFSFO-2

0 1			
C	-2.84389500	0.32675200	-0.00008200
C	-0.46688800	1.14937600	-0.00005500
C	0.95836700	1.25706600	-0.00006700
C	3.04267200	0.48062000	0.00001900
C	4.01466300	-0.57334700	0.00005100
C	5.25632800	-2.74591500	-0.00004100
C	-5.19328700	-2.33702900	-0.00016500
C	-6.09500200	-1.31634500	0.00015000
C	-5.38717100	-0.08381500	0.00025300
C	-4.05817700	-0.43771100	-0.00004000
C	3.15232800	1.85401400	-0.00015300
C	1.82249200	2.32872200	-0.00004900
C	-1.38424000	2.18332800	-0.00002600
C	-2.70632200	1.69823500	-0.00004000
C	5.38725500	-0.45256100	0.00014700
C	6.10543500	-1.67340300	0.00013300
O	1.72221400	0.11480400	0.00002300
O	-3.93369100	-1.80137200	-0.00031400
H	-5.27229100	-3.41122300	-0.00045400
S	-1.25727000	-0.41751600	-0.00016200
S	3.58625300	-2.27103900	-0.00003500
F	6.00160300	0.74499100	0.00025900
F	-3.77096200	2.52156100	0.00001500
H	7.18699800	-1.73142500	0.00020500
H	-1.12343400	3.23339100	0.00003200
F	1.44360800	3.61233600	-0.00004600
F	-7.42629700	-1.44330600	0.00036600
H	4.06228700	2.43300800	-0.00026500
H	-5.79648600	0.91404100	0.00051300
H	5.51209200	-3.79652200	-0.00011100

## CFSFO-3

0 1

C	5.13353800	0.69508500	0.00001900
C	3.77908000	-1.42458000	-0.00047600
C	2.72761300	-2.39104200	-0.00050600
C	0.60894400	-3.07276300	-0.00016500
C	-0.80179400	-2.84607000	0.00012400
C	-3.13270500	-1.90148100	0.00036800
C	-4.27409400	-1.04339800	0.00045200
C	-5.32691900	0.91581500	0.00009600
C	5.32843600	4.24172500	0.00173700
C	6.66846700	3.99836300	0.00088100
C	6.87552500	2.59231800	0.00005200
C	5.61270600	2.04735200	0.00046500
C	1.37617300	-4.22015000	-0.00062800
C	2.71226500	-3.76860200	-0.00082000
C	5.14062400	-1.66668700	-0.00113400
C	5.87641900	-0.46633000	-0.00082800
C	-1.81039800	-3.78967400	0.00052600
C	-3.12287000	-3.28526200	0.00065100
C	-6.31623300	-0.04359700	0.00091400
C	-5.63134300	-1.27750800	0.00108800
O	1.42020200	-1.96731100	-0.00006200
O	-4.09372800	0.31936000	-0.00008200
O	4.67068500	3.04126300	0.00148700
C	-5.36403400	2.34871600	-0.00046100
C	-4.87052000	4.80094800	-0.00145900
C	-6.21583300	4.55222800	-0.00120200
C	-6.47793500	3.16040600	-0.00059000
H	4.72559700	5.13429400	0.00249900
S	3.42734300	0.29503100	0.00049800
S	-1.50702200	-1.24053000	-0.00003800
S	-3.92476800	3.34536300	-0.00096800
F	-7.72788000	2.66185600	-0.00022900
F	-1.54864900	-5.10923800	0.00073600
F	7.22238300	-0.45133400	-0.00134900
H	-6.99184900	5.30778000	-0.00142400
H	-4.01012200	-3.90451200	0.00095800
H	5.58686500	-2.65231300	-0.00177800
F	-6.19438200	-2.49084900	0.00178100
F	3.80545600	-4.54071500	-0.00125100
F	7.63533600	4.92243400	0.00082800
H	-7.38170500	0.12299400	0.00130600
H	1.02187300	-5.23878700	-0.00078200
H	7.81425500	2.06144500	-0.00073500
H	-4.37207500	5.76051200	-0.00192400

## CFSFO-4

0 1

C	5.13980200	2.56822800	-0.20193500
C	5.40584300	0.08645000	0.11090300
C	5.19179700	-1.32113600	0.22142400
C	3.97299900	-3.18332000	0.25075800
C	2.73832700	-3.89869500	0.18313500

C	0.34000300	-4.64150900	0.03431400
C	-1.08131300	-4.69921900	-0.07452300
C	-3.13377100	-3.84967800	-0.20620700
C	3.10704900	5.40405600	-0.86894400
C	4.28698800	6.06980700	-0.73012700
C	5.31058700	5.12654100	-0.44321700
C	4.67478300	3.90703300	-0.42454700
C	5.28301500	-3.58497800	0.41866000
C	6.03778900	-2.39404000	0.39796300
C	6.60704100	0.76449700	0.21282200
C	6.43196600	2.15012300	0.03488000
C	2.55147900	-5.26719100	0.21277900
C	1.21913500	-5.70686500	0.12946300
C	-3.28605500	-5.22040000	-0.27306500
C	-1.97838500	-5.73963100	-0.18735200
O	3.91348900	-1.81867500	0.13190000
O	-1.80592500	-3.53100000	-0.08740900
O	3.33925400	4.06796900	-0.68115400
C	-4.06593100	-2.76759400	-0.22842600
C	-5.24745000	-0.54900300	-0.17170600
C	-6.11978100	-1.60780800	-0.35581800
C	-5.57363300	0.83851500	-0.08856200
C	-5.13641600	3.00097400	0.19265300
C	-6.49529600	2.91607000	-0.02208000
O	-4.57536400	1.75217700	0.15250800
C	-6.75399800	1.53987400	-0.19756900
C	-5.43704600	-2.83642000	-0.38283300
H	2.09621400	5.70227400	-1.09106700
C	-4.25874800	4.10595000	0.44453700
C	-2.33665100	5.63262900	0.92325200
C	-3.51297800	6.31972100	0.79572400
C	-4.59036700	5.44128200	0.52535400
S	4.06991600	1.18032900	-0.20603100
S	1.18219800	-3.10157400	0.04672500
S	-3.58446700	-1.09239200	-0.03756200
S	-2.53887900	3.92136900	0.71459000
F	-5.85238900	5.87709000	0.35978900
F	-6.07520600	-4.00925200	-0.54551300
F	3.58487200	-6.12234000	0.31622300
F	7.46162300	3.01536600	0.09141300
H	-3.62384900	7.39320300	0.88733700
H	-7.19186300	-1.50762300	-0.46217500
H	0.92144600	-6.74699300	0.14040700
H	7.56234200	0.29364400	0.40365700
F	-7.94855900	0.98662300	-0.43300700
F	-1.64052300	-7.03375800	-0.21138000
F	7.36660200	-2.30105800	0.52548700
F	4.46177200	7.39111700	-0.84300200
H	-7.20131000	3.73097200	-0.04720400
H	-4.21114400	-5.76654800	-0.36777700
H	5.64240300	-4.59450900	0.54045900
H	6.35886600	5.31688300	-0.27615300
H	-1.35347300	6.03154100	1.13183900

CFSFO-5

0 1

C	4.73942900	2.34708400	1.12947200
C	3.31326500	4.30356000	0.43852900
C	2.23786000	5.17534200	0.08856000
C	0.11440000	5.73154700	-0.27860400
C	-1.28624500	5.45983800	-0.35215200
C	-3.60569600	4.48229200	-0.35212800
C	-4.74838700	3.63287400	-0.26243800
C	-5.83186400	1.70532500	-0.01453600
C	5.07661100	-1.06054600	2.07427500
C	6.39103600	-0.72213500	2.18795400
C	6.53854000	0.65057600	1.85045200
C	5.26813700	1.07860600	1.54186500
C	0.84850000	6.88457900	-0.47529000
C	2.18677900	6.51268900	-0.23878300
C	4.65482700	4.62946600	0.52634400
C	5.43005800	3.52050600	0.91449000
C	-2.29958900	6.36516800	-0.60341500
C	-3.60339000	5.84349600	-0.60724300
C	-6.80718100	2.67535500	-0.13815500
C	-6.10350600	3.88495900	-0.29536500
O	0.94869500	4.69669700	0.05955700
O	-4.58799000	2.27801400	-0.08809900
O	4.37829200	0.04724900	1.67595300
C	-5.90210600	0.28934500	0.15747100
C	-5.48789700	-2.18182800	0.37977200
C	-6.83163600	-1.86000800	0.47166200
C	-4.90405800	-3.48052700	0.46273100
C	-3.24289800	-4.95902900	0.38231600
C	-4.38061300	-5.68343900	0.67863300
O	-3.55353400	-3.63026300	0.25345900
C	-5.41946800	-4.73219100	0.72390400
C	-7.03777500	-0.47650800	0.34229600
H	4.51638000	-1.96766500	2.22632200
C	-1.87863800	-5.33129000	0.18421100
C	0.58483800	-5.43821900	-0.30317000
C	0.05733100	-6.67533100	0.02458900
C	-1.32043000	-6.59043200	0.29138200
C	1.93817400	-5.12841800	-0.63372300
C	3.60891600	-3.78728700	-1.23211100
C	4.16559000	-5.03988500	-1.08262000
C	4.15619000	-2.51364800	-1.59539000
C	4.57821800	-0.11833500	-2.16845300
C	5.73165800	-0.85503100	-2.18091700
O	2.26710800	-3.83491000	-0.96279600
C	3.09290300	-5.87575700	-0.70418000
C	5.47524700	-2.20861900	-1.85490500
S	3.03081800	2.61667700	0.83721700
S	-1.97939900	3.86622500	-0.10824800
S	-4.49321800	-0.75500900	0.14004600
S	-0.63777400	-4.18013100	-0.27277300
S	3.18506300	-1.06742200	-1.76201100
F	6.44850600	-3.13540500	-1.79925400
F	-2.05474300	-7.66579100	0.62786100
F	-8.26478400	0.07284200	0.39042300
F	-2.04880000	7.66766900	-0.82884200
F	6.76522600	3.59970600	1.06841400
H	6.71858800	-0.46837700	-2.40266800

H	0.62915800	-7.59282300	0.06924800
H	-7.62555000	-2.58010100	0.61901200
H	-4.49179300	6.43394300	-0.78702300
H	5.05972800	5.61297300	0.32830100
F	3.16625500	-7.18649400	-0.44881000
F	-6.70795000	-4.98465800	0.97822700
F	-6.64701500	5.09748700	-0.45044100
F	3.25347800	7.31781900	-0.31329300
F	7.38446800	-1.53871700	2.55556300
H	5.19912600	-5.31190200	-1.22751600
H	-4.44984500	-6.74815900	0.83568800
H	-7.87507600	2.52702400	-0.12131400
H	0.46987300	7.85641300	-0.74892200
H	7.44441200	1.23585400	1.84084200
H	4.46201800	0.93813200	-2.36688000

CFSFO-6

0 1

C	4.38524500	0.37314600	-2.25986200
C	4.09586600	-2.08991000	-1.83733600
C	3.59146100	-3.39368000	-1.54441500
C	2.03582800	-4.89864300	-1.02813400
C	0.70221000	-5.30962800	-0.72118300
C	-1.76711700	-5.51913200	-0.26945100
C	-3.16322000	-5.29184300	-0.08548600
C	-5.02718700	-4.08216700	0.03432300
C	3.06128300	3.66416200	-2.45463100
C	4.33907600	3.97302800	-2.81105200
C	5.11257300	2.78097800	-2.81066400
C	4.23443200	1.78819200	-2.44239700
C	3.21563800	-5.60314200	-1.16129900
C	4.18616100	-4.63522200	-1.48753400
C	5.39803600	-1.75792000	-2.16626500
C	5.53401600	-0.37660100	-2.39787000
C	0.26208500	-6.59569700	-0.47238800
C	-1.11177100	-6.73831800	-0.21698700
C	-5.41603300	-5.39683600	0.20428000
C	-4.22582600	-6.14446200	0.12628200
O	2.25756200	-3.56510500	-1.25710000
O	-3.66831000	-4.01318300	-0.13898600
O	2.99054900	2.31667100	-2.22464200
C	-5.76741600	-2.86126900	0.00512300
C	-6.59232800	-0.48532200	-0.07294500
C	-7.62666400	-1.40361100	-0.00115900
C	-6.71480800	0.93362500	-0.14646000
C	-5.98261900	3.03390800	-0.19328900
C	-7.35658300	3.10870600	-0.31585800
O	-5.59078700	1.72387000	-0.09291700
C	-7.80061400	1.77255800	-0.28226300
C	-7.14206200	-2.72041400	0.04390800
H	2.15729500	4.23449000	-2.32368200
C	-4.96320300	4.03205400	-0.14006400
C	-2.84146100	5.36266400	0.08661600
C	-3.94165100	6.16189900	-0.17633700
C	-5.11375600	5.39699400	-0.29623800
C	-1.49191300	5.78348400	0.27282300

C	0.66932700	5.49969900	0.72312500
C	0.50661800	6.84974000	0.47885500
C	1.80477500	4.70643700	1.07022000
C	3.42883700	2.89456400	1.69477800
C	4.04045500	4.13030000	1.56726200
O	-0.53277300	4.85295400	0.59777900
C	-0.86521300	7.00904900	0.19805200
C	3.11322600	5.12634100	1.21772600
S	3.05379700	-0.67778500	-1.81816300
S	-0.65950800	-4.20456500	-0.63420700
S	-5.02374800	-1.27455500	-0.08905400
S	-3.27744800	3.66468100	0.17526800
S	1.70620000	2.98395400	1.38051700
C	4.04722100	1.65498400	2.03772400
C	5.34342500	1.29683100	2.33605900
O	3.27954100	0.51817700	2.11688000
C	5.39257400	-0.08696800	2.60701100
C	4.09431600	-0.52730000	2.45939500
C	3.48203700	-1.81609600	2.59408300
C	4.09384300	-3.00718200	2.92108700
S	1.77176400	-2.09416600	2.34749800
C	3.23759000	-4.13308200	2.98017400
C	1.94553200	-3.78535300	2.69185400
H	1.07687000	-4.42782200	2.65326600
F	5.41430400	-3.09104700	3.16563600
F	3.47024300	6.40998300	1.03694900
F	-6.31221900	5.95482500	-0.54409700
F	-7.96287500	-3.78333000	0.12128000
F	1.10242000	-7.64738000	-0.47657000
F	6.71258900	0.18000800	-2.73485900
H	3.57755700	-5.13252500	3.22194900
H	5.09739700	4.30853600	1.71374900
H	-3.90731300	7.23888500	-0.27363000
H	-8.67604100	-1.14184900	0.01998500
H	-1.59462300	-7.68443800	-0.01197900
H	6.21155400	-2.46733300	-2.23990500
F	6.37904100	2.14244900	2.36153300
F	-1.48070700	8.15892300	-0.09775700
F	-9.07065900	1.36155600	-0.36877900
F	-4.12270700	-7.47399800	0.23432600
F	5.48508600	-4.86812400	-1.71174300
F	4.79812800	5.19242400	-3.11361300
H	6.25403400	-0.67954500	2.87137200
H	1.27079600	7.61023800	0.50486400
H	-7.95211200	4.00281700	-0.40984100
H	-6.41800600	-5.76175900	0.36381500
H	3.35366800	-6.66613900	-1.04470800
H	6.15855500	2.67047900	-3.04901700

TFSFO-1

0 1

C	-3.16757300	-0.81781400	0.00004200
C	-3.05488600	0.54270500	-0.00003700
C	-1.69502200	0.95507400	-0.00004800
H	-3.88512200	1.23847800	-0.00000700
C	-0.77132400	-0.06629900	-0.00003400

C	0.66885700	0.00031000	0.00002600
C	1.64630800	-0.96555700	0.00005600
O	1.23930900	1.24372200	0.00017800
C	2.87501000	-0.25039900	0.00007200
H	1.51759700	-2.03806300	0.00002900
C	2.59654500	1.08206600	0.00007200
H	3.19803800	1.97575500	0.00008000
F	-1.35760600	2.25232500	-0.00002200
F	4.09251000	-0.80414800	0.00006800
S	-1.61736800	-1.60155500	-0.00018500
H	-4.06872100	-1.41517900	0.00012900

TFSSFO-2

0 1

C	6.81198400	-0.61668400	0.00000900
C	6.01372500	-1.72487300	0.00001200
C	4.63730500	-1.37702400	-0.00000500
H	6.36674300	-2.74888700	0.00002900
C	4.37336600	-0.02332000	-0.00002300
C	3.10692100	0.65545700	-0.00003900
C	2.75807800	1.98826400	-0.00005500
O	1.98091000	-0.12321500	-0.00003900
C	1.34569000	1.99987600	-0.00006700
H	3.41715300	2.84391700	-0.00005700
C	0.88505200	0.70409800	-0.00006000
C	-0.41325400	0.10395600	-0.00006900
C	-0.71522600	-1.24088800	-0.00007300
C	-2.10877600	-1.46842400	-0.00003500
H	0.02550100	-2.03025200	-0.00007400
C	-2.89777600	-0.33689400	-0.00001200
C	-4.33106300	-0.21795600	0.00006000
C	-5.17538500	0.86815200	0.00011700
O	-5.05964100	-1.37669300	0.00017400
C	-6.48600200	0.31912500	0.00014000
H	-4.90727900	1.91455200	0.00011200
C	-6.38378800	-1.03875100	0.00011300
H	-7.09716200	-1.84595700	0.00011700
F	3.67763600	-2.31225900	-0.00000100
F	0.56433200	3.08637400	-0.00008300
F	-2.61247900	-2.70996100	0.00000500
F	-7.62155700	1.02586100	0.00017000
S	-1.86983700	1.08583200	-0.00010800
S	5.89085100	0.85550600	-0.00002500
H	7.89216900	-0.57035300	0.00002100

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0 1

C	6.77166600	0.22003900	-0.00005600
C	6.76844300	1.59824700	-0.00008300
C	5.40483400	1.96356000	-0.00007800
C	4.63342200	0.82438900	-0.00005100
O	5.48665800	-0.25158800	-0.00003600
H	7.62098000	2.26132900	-0.00010300
C	3.22686500	0.57206300	-0.00003400
C	2.59346100	-0.65366900	-0.00000700

C	1.18981900	-0.52088700	0.00000300
H	3.11038300	-1.60470100	0.00000700
C	0.71235600	0.77591800	-0.00001700
C	-0.64057000	1.24614000	-0.00001500
C	-1.19169600	2.51128900	-0.00002800
O	-1.63480900	0.30343200	0.00000300
C	-2.58734700	2.30533700	-0.00001800
H	-0.67238600	3.45831700	-0.00004300
C	-2.84434200	0.95342400	0.00000100
C	7.82846600	-0.75313100	-0.00004600
C	7.74647400	-2.13010000	-0.00000200
C	8.99260800	-2.80985900	-0.00001100
C	10.04153100	-1.93500900	-0.00006800
H	9.07977000	-3.88946700	0.00001700
C	-4.03693000	0.16576700	0.00001600
C	-4.13749600	-1.20945900	0.00003300
C	-5.48211700	-1.63963300	0.00005300
H	-3.28864300	-1.88120200	0.00003500
C	-6.42957700	-0.63687800	0.00005000
C	-7.86436800	-0.73127200	0.00007500
C	-8.86009800	0.21809000	0.00009500
O	-8.41381200	-1.98504600	0.00012700
C	-10.07509800	-0.51854700	0.00009700
H	-8.74988300	1.29264100	0.00009300
C	-9.77355900	-1.84641200	0.00008900
H	-10.35986500	-2.75014700	0.00008800
F	6.58385200	-2.79577500	0.00004200
F	4.92006700	3.21048900	-0.00009600
F	0.38542600	-1.59209700	0.00002900
F	-3.52749900	3.25797700	-0.00002500
F	-5.79830700	-2.94180400	0.00007800
F	-11.30263200	0.01289400	0.00010300
S	-5.62313000	0.92211200	0.00001200
S	2.06798000	1.89262700	-0.00004900
S	9.51686700	-0.27995500	-0.00008200
H	11.09923400	-2.15928800	-0.00009300

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0 1

C	-3.12392400	-1.90674700	-0.00004200
C	-2.86504700	-3.26267400	-0.00006900
C	-1.45891800	-3.36917000	-0.00006100
C	-0.91001700	-2.10658100	-0.00003300
O	-1.94709300	-1.20602200	-0.00002000
H	-3.58066400	-4.07160100	-0.00009000
C	0.42502900	-1.60015500	-0.00001500
C	0.82198300	-0.27818900	0.00001500
C	2.22562600	-0.15015700	0.00002500
H	0.13858900	0.56123500	0.00002900
C	2.93445100	-1.33672200	0.00000400
C	4.35063900	-1.54887300	0.00000600
C	5.12631900	-2.69036700	-0.00001200
O	5.15347500	-0.43872900	0.00002900
C	6.45982400	-2.22986400	0.00000100
H	4.79054500	-3.71690400	-0.00003100
C	6.46262500	-0.85373900	0.00002500



C	-4.34009700	-1.15100900	-0.00003400
C	-4.52038600	0.21933200	0.00000700
C	-5.86018900	0.65768300	0.00000200
C	-6.74752700	-0.39908900	-0.00004600
H	-6.15553300	1.69903000	0.00002900
C	7.48727500	0.14263000	0.00004400
C	7.32683500	1.51219000	0.00006600
C	8.56610200	2.18818700	0.00008700
H	6.36638500	2.01145100	0.00007100
C	9.68582000	1.38228700	0.00007900
C	11.07723100	1.74512800	0.00010100
C	12.23383200	1.00007500	0.00011800
O	11.38108100	3.07987400	0.00015400
C	13.28857800	1.95219400	0.00011900
H	12.32747200	-0.07604000	0.00011500
C	12.74262200	3.19960500	0.00011200
H	13.14831700	4.19753700	0.00011100
F	-3.49970600	1.08660800	0.00004800
F	-0.75158400	-4.50483200	-0.00007900
F	2.81862200	1.05115100	0.00005300
F	7.55966000	-2.99257000	-0.00000900
F	8.63037400	3.52662700	0.00011600
F	14.59430400	1.66137000	0.00012000
C	-8.17489900	-0.33617800	-0.00006900
C	-9.17760800	-1.27826700	-0.00011700
O	-8.77087900	0.90089300	-0.00004200
C	-10.42765800	-0.62250800	-0.00011400
C	-10.12794300	0.72291400	-0.00007200
H	-11.40509400	-1.08194000	-0.00014300
C	-10.94471900	1.90470600	-0.00005200
C	-10.56096800	3.22976300	0.00000100
C	-11.62635900	4.16761900	0.00000600
C	-12.84235400	3.54551700	-0.00004700
H	-11.47334500	5.23987100	0.00004300
F	-8.97783100	-2.60101700	-0.00015600
F	-9.28031500	3.62259700	0.00004300
S	9.18748800	-0.30098600	0.00003900
S	1.80780600	-2.68459100	-0.00002900
S	-5.90823900	-1.94230100	-0.00007700
S	-12.69603300	1.81568400	-0.00008800
H	-13.82449000	3.99768100	-0.00005900

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0 1

C	0.62138300	-3.16309000	-0.00004100
C	1.14121900	-4.44231100	-0.00006900
C	2.54076900	-4.27105000	-0.00005800
C	2.83171500	-2.92545600	-0.00002700
O	1.63836100	-2.24535800	-0.00001500
H	0.59830800	-5.37596900	-0.00009200
C	4.04229000	-2.16858800	-0.00000600
C	4.17509600	-0.79459800	0.00002400
C	5.52721200	-0.39658200	0.00003500
H	3.34150500	-0.10411200	0.00003800
C	6.45293200	-1.42288900	0.00001300
C	7.88326200	-1.35559000	0.00001600

C	8.86620300	-2.32448800	-0.00000100
O	8.45493600	-0.11043200	0.00003800
C	10.08461600	-1.61341900	0.00001200
H	8.73679800	-3.39675200	-0.00001900
C	9.81979100	-0.26307100	0.00003500
C	-0.71904200	-2.66052800	-0.00003600
C	-1.16428600	-1.35179400	0.00001100
C	-2.56335300	-1.18365900	0.00000100
C	-3.22768800	-2.39388200	-0.00005500
H	-3.05664700	-0.22021200	0.00003400
C	10.63199500	0.91276800	0.00005500
C	10.21097400	2.22588000	0.00007800
C	11.29712500	3.12773400	0.00009300
H	9.17247900	2.53135900	0.00008500
C	12.55090300	2.55228300	0.00008100
C	13.84653200	3.17583400	0.00009000
C	15.12476900	2.66689600	0.00009100
O	13.88824600	4.54409100	0.00012400
C	15.97685600	3.80395400	0.00009600
H	15.42354600	1.62884100	0.00008000
C	15.20144700	4.92322600	0.00010300
H	15.40784000	5.98052900	0.00010800
F	-0.33273600	-0.30176800	0.00006200
F	3.45766300	-5.24557100	-0.00007600
F	5.87640500	0.89688700	0.00006400
F	11.31207000	-2.14727700	0.00000200
F	11.10321100	4.45374100	0.00011600
F	17.31418000	3.76938800	0.00009100
C	-4.63898800	-2.60929400	-0.00008100
C	-5.44028700	-3.72883200	-0.00014100
O	-5.46432400	-1.51132200	-0.00004600
C	-6.79281300	-3.33025900	-0.00014100
C	-6.76168600	-1.94994900	-0.00008400
H	-7.66202000	-3.97130400	-0.00017900
C	-7.79245600	-0.95619100	-0.00005800
C	-7.68131600	0.42153900	0.00000400
C	-8.89928200	1.13107600	0.00001400
C	-9.98849300	0.28364400	-0.00004200
H	-8.96986300	2.21118900	0.00006000
C	-11.37071800	0.64501000	-0.00005100
C	-12.54928000	-0.06484000	-0.00010300
O	-11.69299400	1.97984200	0.00000300
C	-13.63328900	0.83928000	-0.00008400
C	-13.05701200	2.09152700	-0.00001800
H	-14.68551000	0.59580300	-0.00011500
C	-13.60634800	3.41886000	0.00003100
C	-12.95081300	4.63265100	0.00010000
C	-13.79376100	5.77454200	0.00013600
C	-15.11381000	5.42365000	0.00009300
H	-13.41754000	6.79023300	0.00019000
H	-15.97786800	6.07358100	0.00010600
F	-4.98571200	-4.98690600	-0.00019000
F	-6.50151200	1.05532500	0.00005200
F	-12.63219100	-1.39981500	-0.00016200
F	-11.61595000	4.74508200	0.00013200
S	12.38606400	0.80471100	0.00005000
S	5.60962700	-2.96388000	-0.00002200

S	-2.10228800	-3.74343500	-0.00009500
S	-9.49150600	-1.40115300	-0.00010700
S	-15.33676400	3.70191500	0.00000800

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0 1

C	4.33996000	-3.87269300	-0.00010800
C	5.09994800	-5.02551000	-0.00014500
C	6.43899400	-4.58380600	-0.00014000
C	6.46128000	-3.20730100	-0.00010100
O	5.15768400	-2.77389200	-0.00008100
H	4.74961300	-6.04712800	-0.00017200
C	7.49931600	-2.22701200	-0.00007900
C	7.35772500	-0.85389700	-0.00003800
C	8.60434100	-0.19623400	-0.00002600
H	6.40400700	-0.34200300	-0.00001700
C	9.71492500	-1.01896700	-0.00005600
C	11.10395800	-0.67105200	-0.00005200
C	12.25827100	-1.42769500	-0.00008100
O	11.41953100	0.66219500	-0.00001300
C	13.31307000	-0.49087200	-0.00005800
H	12.34191100	-2.50448500	-0.00011500
C	12.78782200	0.78102700	-0.00001600
C	2.92719500	-3.64231000	-0.00009500
C	2.23380800	-2.44638300	-0.00006100
C	0.82891400	-2.55581500	-0.00005700
C	0.41483000	-3.87292300	-0.00008700
H	0.15637100	-1.70770700	-0.00003100
C	13.35264300	2.09378600	0.00002200
C	12.68048200	3.29780500	0.00006400
C	13.56701700	4.39643900	0.00009500
H	11.60208400	3.39160200	0.00007200
C	14.90980200	4.08015800	0.00007800
C	16.05638700	4.94789200	0.00010000
C	17.41005300	4.70221800	0.00008600
O	15.82624900	6.29736400	0.00014200
C	18.02012600	5.98549700	0.00012300
H	17.90828000	3.74382000	0.00005400
C	17.03842600	6.92903300	0.00015700
H	17.03143600	8.00625200	0.00019100
F	2.84315100	-1.25349900	-0.00003200
F	7.52842200	-5.36059700	-0.00016800
F	8.69013300	1.14074300	0.00001400
F	14.62159500	-0.77293500	-0.00007400
F	13.11485000	5.65791000	0.00013800
F	19.33787800	6.21636400	0.00012500
C	-0.92599400	-4.36249100	-0.00009100
C	-1.48972200	-5.61866400	-0.00011800
O	-1.95261500	-3.44967800	-0.00006500
C	-2.89414700	-5.49606500	-0.00010800
C	-3.13734500	-4.13677300	-0.00007500
H	-3.61926100	-6.29644700	-0.00012300
C	-4.34502700	-3.36846000	-0.00005300
C	-4.51139000	-1.99606200	-0.00002100
C	-5.84596700	-1.54365300	-0.00000600
C	-6.74488300	-2.59155700	-0.00002500

H	-6.13063200	-0.49936900	0.00001900
C	-8.17027800	-2.51384300	-0.00001700
C	-9.18261200	-3.44696000	-0.00003400
O	-8.75468900	-1.27086400	0.00001200
C	-10.42564200	-2.78153200	-0.00001300
C	-10.11416400	-1.43633700	0.00001400
H	-11.40721100	-3.23199000	-0.00001800
C	-10.92112800	-0.25364300	0.00004200
C	-10.53194300	1.07268900	0.00007100
C	-11.57990000	2.01532100	0.00009700
C	-12.81885300	1.40737300	0.00008700
H	-11.42925400	3.08719900	0.00011800
F	-0.79506700	-6.76201600	-0.00014900
F	-3.48126600	-1.14005100	-0.00000500
F	-8.99311300	-4.77119800	-0.00006400
F	-9.24797700	1.45320300	0.00007400
S	15.09337300	2.33425700	0.00002000
S	9.19276800	-2.69644500	-0.00010600
S	1.78303700	-4.97560400	-0.00012900
S	-5.92149800	-4.14372400	-0.00006600
S	-12.67540400	-0.34319700	0.00005300
C	-14.09850100	2.04274400	0.00010000
C	-15.39693700	1.58767600	0.00013300
O	-14.14232200	3.41529500	0.00008300
C	-16.27410700	2.69351600	0.00015300
C	-15.45494000	3.80220800	0.00010800
H	-17.35385000	2.66954700	0.00018500
C	-15.72327800	5.21344100	0.00009400
C	-14.83586800	6.26962300	0.00003600
S	-17.36071400	5.84068600	0.00016400
C	-15.43050400	7.55841800	0.00004200
C	-16.79423000	7.48173900	0.00009400
H	-14.85663900	8.47702400	0.00000200
H	-17.50915000	8.29287100	0.00010600
F	-13.50586700	6.11015100	-0.00001900
F	-15.74996100	0.29763000	0.00014800