

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

CFOFS-1

0 1			
C	3.14058200	-0.99752900	0.00005500
C	1.11807200	-0.10337700	0.00005400
C	2.03896400	0.91365300	-0.00008000
C	3.34432200	0.35023600	-0.00005200
O	1.80967800	-1.28872000	0.00022800
H	4.28612300	0.87876000	-0.00013600
C	-0.31912400	-0.12891400	0.00006300
C	-2.72645800	-0.81817500	-0.00024000
C	-2.53365200	0.53283400	0.00004300
C	-1.17686600	0.94900300	0.00024100
H	-0.85815200	1.98319300	0.00043800
F	1.74410800	2.22047600	-0.00021100
F	-3.54098900	1.42197000	0.00011000
S	-1.19950800	-1.64466900	-0.00008800
H	3.80512100	-1.84731400	0.00010800
H	-3.66149800	-1.35857300	-0.00042400

CFOFS-2

0 1			
C	5.36722700	-2.73286200	-0.00010500
C	4.35282300	-0.76849900	0.00000100
C	5.70987500	-0.55404700	-0.00004700
C	6.37196000	-1.81079100	-0.00010600
O	4.14803900	-2.12577600	-0.00006200
H	7.43686700	-1.99034000	-0.00014500
C	3.21992800	0.10931400	0.00005700
C	0.90182700	1.08250600	0.00004600
C	1.92063000	2.01286500	0.00021100
C	-0.50809400	1.32575200	0.00000100
C	-2.63349900	0.66740700	-0.00005800
C	-2.60408900	2.04258000	-0.00015300
O	-1.33126300	0.22934100	0.00003600
C	-1.26140300	2.48040700	-0.00007300
C	3.22833700	1.49047900	0.00021900
H	-0.89618800	3.49520200	-0.00010100
H	4.12343200	2.09855800	0.00034200
F	6.29827200	0.64844200	-0.00002800
F	1.67692200	3.33613400	0.00034900
F	-3.68795600	2.82826700	-0.00027500
C	-3.69785100	-0.29129700	-0.00006300
C	-5.06694900	-2.38903300	0.00054100
C	-5.80568900	-1.24070300	0.00003600
C	-5.05391400	-0.03861300	-0.00030800
H	-5.49047000	0.95149700	-0.00056800
F	-7.14897000	-1.22880500	0.00004600
S	1.58725900	-0.53102200	-0.00010300
S	-3.37051300	-2.01468200	-0.00003200
H	5.35209900	-3.81150500	-0.00013700
H	-5.41900200	-3.40981500	0.00096600

CFOFS-3

0 1

C	-5.14018900	4.75211400	-0.00152300
C	-5.59905200	2.58992500	-0.00033300
C	-6.78537100	3.28335800	-0.00043900
C	-6.50184800	4.67501800	-0.00117900
O	-4.58112200	3.51056000	-0.00107100
H	-7.21199600	5.48861100	-0.00138300
C	-5.27862500	1.19340700	0.00018100
C	-4.10172300	-1.02725600	0.00039800
C	-5.48019700	-1.10206100	0.00156600
C	-3.16842400	-2.11000100	0.00029600
C	-1.11175900	-2.95902700	-0.00000600
C	-2.01415800	-4.00048500	-0.00028000
O	-1.83548200	-1.79034900	0.00033000
C	-3.32507100	-3.48116700	0.00001400
C	-6.16080900	0.12985300	0.00142600
H	-4.25450000	-4.02812400	-0.00000800
H	-7.23857800	0.22640300	0.00225500
F	-8.00174500	2.72517600	0.00008500
F	-6.12894000	-2.28055400	0.00271200
F	-1.67926800	-5.29586900	-0.00067400
C	0.31438300	-2.90263800	-0.00005500
C	2.71946900	-2.16542500	-0.00017100
C	2.53170100	-3.53351500	-0.00044600
C	1.19526000	-3.97009500	-0.00039800
H	0.89671900	-5.01002000	-0.00062400
F	3.56719300	-4.39269500	-0.00081800
C	3.95870700	-1.45266000	-0.00025300
C	5.17631400	0.41018800	0.00006900
C	6.03047200	-0.66823900	-0.00064000
C	5.38510500	1.82710300	0.00038400
C	5.10050900	4.31614800	0.00024600
C	6.40197900	3.90330200	0.00101200
H	4.72083600	5.32700000	0.00008800
O	3.89365900	-0.08297500	0.00029100
C	5.27608400	-1.86140400	-0.00068900
C	6.59061300	2.49824800	0.00110500
H	7.55921700	2.01577700	0.00161800
H	5.64261600	-2.87573900	-0.00110900
F	7.36628300	-0.58259000	-0.00109400
F	7.44364800	4.75188500	0.00164300
S	-3.60971900	0.65528000	-0.00092200
S	1.15954500	-1.36422300	0.00036000
S	4.03329800	2.94546900	-0.00028900
H	-4.44551500	5.57746700	-0.00203300

CFOFS-4

0 1

C	2.62042100	5.72121500	-0.97091400
C	4.31771200	4.37166700	-0.54435200
C	4.94297800	3.10561200	-0.30215800
C	5.42870700	0.66636900	0.05517500
C	5.39249700	-0.75471600	0.20385400

C	4.34861600	-2.71843500	0.27506500
C	4.79693900	5.65730100	-0.62106900
C	3.71345900	6.53361600	-0.89518200
C	6.28559400	2.86284700	-0.08275600
C	6.53389700	1.49177200	0.11399900
C	5.69810400	-2.93419700	0.45334800
C	6.37710100	-1.69945800	0.41206100
O	2.96375000	4.42009400	-0.76271500
O	4.16766600	-1.36402800	0.12251200
H	3.75211700	7.60599400	-1.01671300
H	7.05173900	3.62672300	-0.06600700
H	7.43562500	-1.52165600	0.51617800
C	3.21777300	-3.58695100	0.22386700
C	0.90116800	-4.55474500	0.07761700
C	1.91283300	-5.48705800	0.20469300
C	-0.50135100	-4.79767400	-0.04013000
C	-2.62170600	-4.14299200	-0.20836800
C	-2.58586900	-5.52039500	-0.24052800
O	-1.32530900	-3.70288100	-0.08393600
C	-1.24910000	-5.95478700	-0.13363000
C	3.21690300	-4.96995700	0.29026900
H	-0.88040200	-6.96827800	-0.12902600
H	4.10527500	-5.57924900	0.39108400
F	6.07821800	6.00982500	-0.46212600
F	7.76928700	1.01141500	0.34231700
F	6.25781300	-4.13517700	0.63552000
F	1.66037500	-6.80780300	0.24053100
F	-3.66340900	-6.30524800	-0.35433300
C	-3.68363900	-3.19155900	-0.26344200
C	-5.07307600	-1.09478500	-0.24165100
C	-5.78606600	-2.26155900	-0.43537200
C	-5.03112000	-3.44747300	-0.45017800
H	-5.45310500	-4.43381200	-0.59043800
F	-7.12167700	-2.25875200	-0.59912200
C	-5.58221000	0.23945700	-0.17748600
C	-5.36729700	2.43448000	0.12035300
C	-6.68902300	2.15806500	-0.14277000
C	-4.65496800	3.64392900	0.40477000
C	-2.90938100	5.34579900	0.98235500
C	-4.15407400	5.86939900	0.78036100
H	-2.00089300	5.86697900	1.24487800
O	-4.68641800	1.24073900	0.09622000
C	-6.84629400	0.76851400	-0.33491400
C	-5.16075900	4.92683700	0.45166800
H	-6.19488200	5.18412600	0.26349800
H	-7.75333400	0.22920700	-0.55733200
F	-7.66247000	3.07473900	-0.20137400
F	-4.42583100	7.18157600	0.88070700
S	3.99807900	1.62938500	-0.26017300
S	1.59321000	-2.94336100	0.06090500
S	-3.37002500	-1.47538400	-0.06917200
S	-2.93858500	3.62178700	0.76849400
H	1.57412900	5.90375400	-1.16005500

0 1

C	4.89337100	1.92807400	1.27515500
C	3.63864700	3.98941600	0.57048200
C	2.67441000	4.97720900	0.20038300
C	0.60552200	5.68287200	-0.21429200
C	-0.81148100	5.56282900	-0.32849600
C	-3.19381800	4.75497800	-0.38061800
C	-4.42349700	4.03082200	-0.32199500
C	-5.64177900	2.18474600	-0.08049600
C	4.91062200	-1.51711900	2.17066000
C	6.25452600	-1.33683900	2.32011100
C	6.47361900	0.02866000	1.99937000
C	5.26896300	0.60530800	1.67501500
C	1.47072300	6.74350800	-0.37808600
C	2.78791300	6.31540900	-0.12007100
C	5.00251600	4.15790400	0.70558800
C	5.72582100	3.01710600	1.09886800
C	-1.70909700	6.57730300	-0.61707600
C	-3.03057200	6.10299900	-0.63834000
C	-6.49574400	3.25189400	-0.26034700
C	-5.74227000	4.43121800	-0.41669600
O	1.36045900	4.59028000	0.14297700
O	-4.35761900	2.67623700	-0.12084000
O	4.30268800	-0.36192600	1.78598700
H	6.99292000	-2.06806100	2.61360200
H	6.79782500	2.99914300	1.24450900
H	3.69380900	6.89909100	-0.15913000
H	-1.43141500	7.60691400	-0.79861700
H	-6.10688900	5.43417300	-0.57102900
C	-5.86474100	0.78816700	0.10549800
C	-5.63316700	-1.70409400	0.35785100
C	-6.93103600	-1.23279900	0.41080600
C	-5.19756600	-3.05949800	0.47062000
C	-3.65581000	-4.66379700	0.42833000
C	-4.87725200	-5.23892900	0.70515900
O	-3.86313400	-3.31171500	0.28529700
C	-5.86826200	-4.23755600	0.73513400
C	-7.08627300	0.15597400	0.26991000
H	-6.92298500	-4.35472100	0.92658900
H	-8.04090300	0.66453600	0.28875900
H	4.26070200	-2.36974800	2.28875400
F	7.65149100	0.66334000	2.00684500
F	5.59952600	5.34116900	0.47624200
F	1.09892300	7.98021800	-0.72675800
F	-4.07710300	6.90961700	-0.89009000
F	-7.83014400	3.16126200	-0.28148500
F	-7.97887700	-2.05763000	0.58783200
F	-5.07201000	-6.54676900	0.90782500
C	-2.34140100	-5.19250900	0.26161900
C	0.11356300	-5.50074700	-0.19003800
C	-0.56458000	-6.65674700	0.14209200
C	-1.93931300	-6.51041700	0.39814200
H	-2.59599300	-7.32716600	0.66724500
F	0.05671100	-7.84829800	0.21412000
C	1.50194100	-5.35546100	-0.49666400
C	3.28604300	-4.16336900	-1.09045200
C	3.67792600	-5.46817500	-0.89897400

C	3.98255300	-2.97114200	-1.47171900
C	4.60159500	-0.62654300	-2.09655400
C	5.65620400	-1.49398400	-2.07129100
H	4.60807200	0.42750200	-2.33062300
O	1.93646700	-4.10054900	-0.83803100
C	2.55837000	-6.24212500	-0.52209900
C	5.33246100	-2.82895100	-1.72085300
H	6.05397200	-3.63315300	-1.65938000
H	2.52599400	-7.29721400	-0.30085900
F	4.93041600	-5.91723200	-1.05067900
F	6.91828400	-1.12812500	-2.35199900
S	3.21741200	2.32916000	0.94740500
S	-1.62436400	4.02473000	-0.09294600
S	-4.53422600	-0.35660400	0.12323200
S	-1.00320700	-4.14869700	-0.18586700
S	3.13195600	-1.45180400	-1.67891500

CFOFS-6

0 1

C	-4.37315800	-1.13658500	-2.25714500
C	-4.46545600	1.32833100	-1.78243300
C	-4.21262500	2.70021100	-1.47206500
C	-2.89483900	4.41564000	-0.95862100
C	-1.66011200	5.07177900	-0.67831200
C	0.75224400	5.66783000	-0.27389300
C	2.17011800	5.72113800	-0.11182700
C	4.20929600	4.83538700	-0.02289000
C	-2.52219200	-4.16776000	-2.52160600
C	-3.72176700	-4.71516500	-2.87160900
C	-4.63966400	-3.63275300	-2.82774300
C	-3.96390900	-2.49445200	-2.45842500
C	-4.19293900	4.87237500	-1.04599400
C	-5.04355600	3.79861300	-1.37154300
C	-5.67971300	0.75371800	-2.10329100
C	-5.65221600	-0.62609500	-2.37361000
C	-1.48234200	6.42162600	-0.42232900
C	-0.13065300	6.72923800	-0.20186100
C	4.31596800	6.19903300	0.15106200
C	3.03451400	6.77816400	0.09969700
O	-2.91572800	3.06727600	-1.22446200
O	2.87339300	4.54601500	-0.18359400
O	-2.64849600	-2.83563400	-2.27083000
H	-3.93235400	-5.74356900	-3.12495500
H	-6.52342700	-1.21055800	-2.63808500
H	-6.11252400	3.82007600	-1.51137200
H	-2.28176400	7.14992300	-0.39922100
H	2.77418000	7.81982600	0.19742700
C	5.18220800	3.79297500	-0.05703100
C	6.40508400	1.59460200	-0.13451800
C	7.21738100	2.71033800	-0.05858800
C	6.82423200	0.23103800	-0.20047200
C	6.47761600	-1.96636900	-0.23372700
C	7.83340900	-1.73615400	-0.32990100
O	5.85810900	-0.74034000	-0.15461200
C	8.07349200	-0.34908300	-0.30933500
C	6.55829300	3.94856200	-0.01153400

H	9.02201700	0.16000400	-0.36878500
H	7.06500100	4.90231200	0.04893000
H	-1.53007800	-4.57315300	-2.40161700
F	-5.94923500	-3.69491200	-3.09858600
F	-6.81599300	1.47149500	-2.15475600
F	-4.56606200	6.14182700	-0.85295100
F	0.28408500	7.98177000	0.06035000
F	5.46736200	6.85334000	0.33872500
F	8.55878000	2.61209000	-0.03403100
F	8.76135200	-2.69485000	-0.42377900
C	5.69930300	-3.16019400	-0.18465800
C	3.85520300	-4.85656800	0.03346700
C	5.10909000	-5.38859600	-0.19834100
C	6.15627100	-4.46078300	-0.32258800
H	7.18799700	-4.73145800	-0.50307800
F	5.30917300	-6.71514300	-0.29848000
C	2.62682800	-5.56442200	0.20209300
C	0.44272900	-5.68100600	0.61704500
C	0.91456600	-6.95710700	0.39681300
C	-0.84578100	-5.15413600	0.93098500
C	-2.78689700	-3.66297200	1.50834900
C	-3.10424900	-4.99976900	1.36883400
O	1.51062000	-4.82343700	0.49333100
C	2.29820700	-6.90419500	0.13247100
C	-2.03473700	-5.85422200	1.04752300
H	-2.13142100	-6.92322000	0.91098500
H	2.96415900	-7.72551100	-0.07948100
F	0.15922600	-8.06168100	0.43242000
F	-4.36128600	-5.45225400	1.53017500
S	-3.21458400	0.10088000	-1.81147300
S	-0.13696800	4.19774000	-0.63507200
S	4.72437000	2.10047700	-0.15200900
S	3.96837000	-3.10692800	0.10081800
S	-1.07115800	-3.43915200	1.22789300
C	-3.66660800	-2.58246500	1.82827600
C	-5.02377300	-2.51457800	2.06462600
O	-3.10964000	-1.33456000	1.93666300
C	-5.28267000	-1.15164900	2.32629600
H	-5.72796800	-3.33131500	2.05024800
C	-4.10682300	-0.44177600	2.24668500
C	-3.78052300	0.94166600	2.42302600
C	-4.64852800	1.98235500	2.68417400
S	-2.12189900	1.50294900	2.32785800
C	-3.95836600	3.21508300	2.80024000
H	-5.72050800	1.87468300	2.78566300
C	-2.60394000	3.14145400	2.64014100
H	-1.88174800	3.94307800	2.68036000
F	-6.47747200	-0.61886500	2.61069600
F	-4.60946200	4.36441100	3.04769500

TFOFS-1

0 1

C	2.65331100	0.85418100	0.00007100
C	2.61764300	-0.50951700	-0.00000800
C	1.31746700	-1.07915000	-0.00007000
C	0.34015200	-0.11015200	-0.00002600

C	-1.08526200	-0.29913100	0.00002600
C	-2.16003100	0.55274900	0.00002700
O	-1.57414100	-1.58271600	0.00008100
C	-3.35678100	-0.21467700	0.00008900
C	-2.93446500	-1.51044400	0.00012000
H	-3.45216700	-2.45703100	0.00016600
S	1.04055900	1.49947500	-0.00015700
H	3.51850800	1.50035900	0.00015800
F	-2.07852900	1.88999700	-0.00001800
H	1.12166600	-2.14374600	-0.00008000
H	-4.37202200	0.15343100	0.00010600
F	3.72030600	-1.27733500	0.00003400

TFOFS-2

0 1

C	6.35042500	-0.44103500	-0.00005200
C	5.55793800	-1.55220600	-0.00003500
C	4.16224300	-1.29882800	-0.00002800
C	3.89410200	0.05262300	-0.00004000
C	2.60728400	0.68443600	-0.00003400
C	2.17832600	1.99009900	-0.00004400
O	1.49260300	-0.11651500	-0.00001300
C	0.76588900	2.01351700	-0.00003100
C	0.38430500	0.68886200	-0.00001100
C	-0.89600000	0.04317100	0.00000900
C	-1.19821900	-1.30371100	0.00002900
C	-2.57429400	-1.61938200	0.00004600
C	-3.36251500	-0.48953700	0.00004000
C	-4.79450800	-0.41729100	0.00005200
C	-5.69636700	0.61793800	0.00004500
O	-5.50994900	-1.58992100	0.00007100
C	-7.01211000	0.08227200	0.00008400
C	-6.83364800	-1.26942700	0.00006800
H	-7.51563500	-2.10547800	0.00007300
S	-2.38704900	0.97068200	0.00000900
S	5.37501800	0.99669300	-0.00006700
H	7.42905600	-0.38988400	-0.00005900
F	-5.36917500	1.91626600	0.00002600
F	2.98551600	3.05803500	-0.00006400
F	-0.26217800	-2.26253200	0.00003300
F	6.04493300	-2.80440900	-0.00002400
H	-7.94315900	0.62922600	0.00010000
H	-2.95798400	-2.63143900	0.00006300
H	0.12806900	2.88515700	-0.00003500
H	3.40195200	-2.06934500	-0.00001400

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C	-10.20281700	2.10839900	0.00015200
C	-10.57065400	0.79539400	0.00019700
O	-8.84732700	2.23939400	0.00011500
C	-9.34390900	0.07964100	0.00018700
C	-8.30490500	0.97746000	0.00013800
C	-6.87748300	0.84593000	0.00010800
C	-5.93651800	1.85267300	0.00006100

C	-4.61987900	1.34459200	0.00003600
C	-4.51264000	-0.03224100	0.00006400
C	-3.33873900	-0.85379500	0.00004500
C	-3.15508300	-2.22136500	0.00007400
O	-2.12521600	-0.21857500	-0.00001100
C	-1.75655300	-2.40506400	0.00003000
C	-1.13947100	-1.17477800	-0.00002400
C	0.22279700	-0.74498700	-0.00008300
C	0.69777300	0.55045300	-0.00014200
C	2.10734300	0.59462300	-0.00015700
C	2.74364300	-0.63170800	-0.00011900
S	-6.12039800	-0.73840400	0.00013700
S	1.53886800	-1.90954600	-0.00011500
C	4.14487100	-0.93164700	-0.00010200
C	4.84650100	-2.11882400	-0.00008500
O	5.01616800	0.12566800	-0.00009700
C	6.20744900	-1.74247700	-0.00008100
C	6.29617600	-0.37076400	-0.00009800
C	7.38448700	0.56179300	-0.00011500
C	7.30992400	1.93768100	-0.00022900
S	9.05338300	0.01393300	-0.00022400
C	8.59941800	2.52862800	0.00003600
C	9.64242200	1.64824300	0.00032400
H	10.70019000	1.86551300	0.00062900
F	-9.20239100	-1.25153900	0.00022000
F	-1.11249500	-3.57797200	0.00003800
F	7.25609200	-2.57476900	-0.00006300
H	-11.56970100	0.38555000	0.00023100
H	-3.91410800	-2.98972600	0.00012000
H	4.44709200	-3.12233600	-0.00007900
F	-3.55606600	2.15864100	-0.00001500
F	2.77104300	1.75869900	-0.00018500
F	8.76133900	3.86244300	0.00014600
H	-6.17270800	2.90893500	0.00004100
H	0.06591000	1.42936500	-0.00015200
H	6.38282000	2.49655300	-0.00034400
H	-10.76075700	3.03184100	0.00014100

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C	-11.45572500	2.07435200	0.00015000
C	-12.64790700	1.39285800	0.00020200
C	-13.71421800	2.33095000	0.00018100
C	-13.10086400	3.54882400	0.00011300
O	-11.74560400	3.41695700	0.00009200
C	-10.08012600	1.67168300	0.00014300
C	-8.96409100	2.48025500	0.00009300
C	-7.76914700	1.72985000	0.00008600
C	-7.92732200	0.35781700	0.00013200
C	-6.93067000	-0.67139600	0.00012900
C	-7.00840300	-2.04930300	0.00017700
O	-5.61948900	-0.27649900	0.00006800
C	-5.66963700	-2.49337000	0.00014500
C	-4.83150600	-1.40145900	0.00008100
C	-3.41344400	-1.23293800	0.00003000
C	-2.70952900	-0.04560400	-0.00003400

C	-1.31656200	-0.25988100	-0.00006700
C	-0.91502100	-1.58256600	-0.00002900
C	0.40815000	-2.12964600	-0.00004200
C	0.88554900	-3.42500600	-0.00000700
O	1.45485000	-1.24586700	-0.00009900
C	2.29027000	-3.29984800	-0.00004000
C	2.62517200	-1.96467900	-0.00009800
C	3.85972300	-1.24672100	-0.00014900
C	4.03561100	0.12202500	-0.00021600
C	5.39991600	0.47770900	-0.00021900
C	6.29274600	-0.57673700	-0.00015900
S	-9.64029600	-0.02811000	0.00022000
S	-2.33339400	-2.61883900	0.00004700
S	5.40160100	-2.09027100	-0.00015100
C	7.72546900	-0.55513500	-0.00012300
C	8.67710600	-1.55338400	-0.00007800
O	8.33598300	0.67153900	-0.00012600
C	9.91810500	-0.87948600	-0.00006400
C	9.69491400	0.47674800	-0.00010500
C	10.54395300	1.63128900	-0.00012700
C	10.15933200	2.95443800	-0.00026400
S	12.29371400	1.47621900	-0.00020300
C	11.28116600	3.82240000	-0.00002000
C	12.49669900	3.20162100	0.00027900
H	13.47758600	3.65320500	0.00056700
F	-12.76470000	0.05947800	0.00026500
F	-5.25786300	-3.76608800	0.00017400
F	3.17436800	-4.30435100	-0.00001900
F	11.12797000	-1.45305900	-0.00001900
H	-14.77339700	2.12075900	0.00021100
H	-7.89872000	-2.66071600	0.00023000
H	0.31211800	-4.34026500	0.00004100
H	8.51498600	-2.62122100	-0.00006100
F	-6.56935400	2.32518900	0.00002700
F	-0.45098900	0.76235200	-0.00012700
F	5.78872800	1.76005100	-0.00025600
F	11.13616500	5.15823400	0.00005100
H	-8.99395400	3.56216600	0.00005200
H	-3.17047400	0.93374800	-0.00005400
H	3.22419100	0.83844900	-0.00024300
H	9.12959600	3.28838200	-0.00039600
H	-13.47101200	4.56225800	0.00007500

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0 1

C	-8.33229700	-1.11272000	0.00012800
C	-9.36126300	-2.02713100	0.00018100
C	-10.59217200	-1.33875600	0.00018200
C	-10.25599800	-0.00006000	0.00012800
O	-8.89387300	0.14064600	0.00009200
C	-11.04105300	1.19834200	0.00010500
C	-10.62766000	2.51621300	0.00005400
C	-11.66002000	3.47802400	0.00003800
C	-12.90827500	2.89383500	0.00007500
C	-14.18335500	3.54851300	0.00006400
C	-15.48270800	3.10403200	0.00010000

O	-14.21488900	4.92172500	0.00000600
C	-16.35296200	4.22632400	0.00006500
C	-15.52091800	5.30666200	0.00001100
C	-6.90819900	-1.21641400	0.00010600
C	-5.99035300	-0.18531100	0.00005400
C	-4.66408300	-0.66204900	0.00003900
C	-4.52301500	-2.03718100	0.00008200
C	-3.32989900	-2.82823000	0.00007800
C	-3.11272700	-4.19179100	0.00012300
O	-2.13221700	-2.16379200	0.00002400
C	-1.71083600	-4.34118100	0.00009700
C	-1.12334400	-3.09600600	0.00003800
C	0.22709900	-2.63312300	-0.00000600
C	0.66856900	-1.32509600	-0.00006900
C	2.07565200	-1.24489800	-0.00009200
C	2.74383100	-2.45497000	-0.00004700
C	4.15142000	-2.71603600	-0.00004600
C	4.88551700	-3.88522300	0.00000100
O	4.99343700	-1.63558900	-0.00010100
C	6.23418700	-3.47338000	-0.00002300
C	6.28702500	-2.09781500	-0.00008800
C	7.34710000	-1.14088900	-0.00013900
C	7.23765700	0.23478600	-0.00021700
C	8.49965900	0.86354900	-0.00022000
C	9.59041500	0.01548400	-0.00014800
S	-12.79622800	1.14177500	0.00015300
S	-6.11336400	-2.78329000	0.00016000
S	1.57218700	-3.76398000	0.00001800
S	9.02943000	-1.64911600	-0.00012500
C	10.98829900	0.33018400	-0.00011100
C	12.12386500	-0.45250200	-0.00005200
O	11.33516700	1.65567800	-0.00013200
C	13.20094200	0.46081600	-0.00004800
C	12.70532900	1.74284300	-0.00011000
C	13.30029700	3.04669200	-0.00015100
C	12.65272600	4.26297300	-0.00031400
S	15.04464400	3.25349900	-0.00023100
C	13.57289300	5.34242900	-0.00007400
C	14.88986700	4.98397100	0.00024500
H	15.75740900	5.62696400	0.00053700
F	-15.84887700	1.81673600	0.00015700
F	-9.19628900	-3.35460400	0.00022600
F	-1.03804600	-5.49760400	0.00012800
F	7.30586500	-4.27474000	0.00001100
F	14.50246300	0.14647700	0.00000400
H	-17.43278600	4.21966100	0.00008000
H	-11.58180900	-1.77125300	0.00021900
H	-3.85298000	-4.97820200	0.00017000
H	4.51260400	-4.89883100	0.00004900
H	12.18300600	-1.53094200	-0.00002000
F	-9.33748400	2.87540600	0.00001600
F	-3.61855900	0.17508900	-0.00001600
F	2.70981200	-0.06492100	-0.00014700
F	8.61585600	2.19850000	-0.00026900
F	13.15728100	6.62023100	-0.00001900
H	-11.48618100	4.54629200	-0.00000500
H	-6.25572700	0.86405400	0.00002200

H	0.01396400	-0.46304700	-0.00009500
H	6.29632100	0.76917500	-0.00025400
H	11.57637000	4.37828600	-0.00045300
H	-15.69338300	6.37171000	-0.00003000

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C	4.82583500	-3.73645000	-0.00012800
C	5.64934000	-4.83980000	-0.00017000
C	6.99356000	-4.41452800	-0.00016800
C	6.93496200	-3.03489500	-0.00012200
O	5.62913000	-2.62215800	-0.00009800
C	7.94570700	-2.02123700	-0.00009800
C	7.80768100	-0.64579000	-0.00005200
C	9.01101700	0.08761400	-0.00003700
C	10.11723800	-0.73832400	-0.00007100
C	11.49114200	-0.34978900	-0.00006600
C	12.68361700	-1.03746900	-0.00009800
O	11.78796800	0.99117400	-0.00001900
C	13.75011600	-0.11467500	-0.00007200
C	13.15040600	1.12854000	-0.00002300
C	3.41064700	-3.54947600	-0.00011300
C	2.72224000	-2.35261000	-0.00007700
C	1.32690700	-2.54878700	-0.00006800
C	0.90784600	-3.86615300	-0.00009600
C	13.67626400	2.46111000	0.00002300
C	13.00301700	3.66708000	0.00007200
C	13.81780100	4.81898200	0.00011100
C	15.15883600	4.50099200	0.00009000
C	16.27419400	5.40105900	0.00011700
C	17.63664200	5.22886200	0.00010200
O	16.02665700	6.75207400	0.00016800
C	18.26152500	6.50409600	0.00014500
C	17.22770000	7.39339100	0.00018500
H	17.18070800	8.47129200	0.00022500
C	-0.42198400	-4.39571900	-0.00009200
C	-0.91550500	-5.68548800	-0.00011400
O	-1.45742500	-3.49898600	-0.00006200
C	-2.31812200	-5.54286000	-0.00009600
C	-2.63665300	-4.20348200	-0.00006500
C	-3.86243500	-3.47186200	-0.00003900
C	-4.02300500	-2.10061000	-0.00001300
C	-5.38276300	-1.73031300	0.00000700
C	-6.28754000	-2.77528700	-0.00000200
C	-7.71857400	-2.73734500	0.00001300
C	-8.68104100	-3.72721200	0.00000500
O	-8.31621700	-1.50457900	0.00004000
C	-9.91375400	-3.04236400	0.00003000
C	-9.67772000	-1.68625800	0.00005000
C	-10.51518100	-0.52958900	0.00007700
C	-10.12252100	0.79343200	0.00009800
C	-11.22666100	1.67040800	0.00011200
C	-12.46957500	1.06713400	0.00010400
S	15.40616600	2.76284600	0.00002100
S	9.65352500	-2.43280300	-0.00013200
S	2.31268900	-4.92124900	-0.00015000

S	-5.41295900	-4.29902800	-0.00004300
S	-12.26646800	-0.67761100	0.00009400
C	-13.77164400	1.66508000	0.00010900
C	-15.04494300	1.13514700	0.00012400
O	-13.83588900	3.03376400	0.00008900
C	-15.90891500	2.25215500	0.00012600
C	-15.15809200	3.40342400	0.00009900
C	-15.46992100	4.80226700	0.00008300
C	-14.58477800	5.85833900	0.00006500
S	-17.13381100	5.36543500	0.00010800
C	-15.26190900	7.10475300	0.00003100
C	-16.62448800	7.02654300	0.00002300
H	-17.34016300	7.83516400	-0.00000900
F	18.25544400	4.04203000	0.00005500
F	12.79021400	-2.37079800	-0.00014800
F	5.21958000	-6.10657200	-0.00020800
F	-3.21502200	-6.53570600	-0.00010700
F	-11.12979900	-3.60118500	0.00003200
F	-17.24733700	2.21471800	0.00014400
H	19.32027100	6.71641000	0.00014700
H	14.80667200	-0.33859300	-0.00008800
H	7.87542200	-5.03801400	-0.00019500
H	-0.35346000	-6.60774000	-0.00013900
H	-8.52883400	-4.79645000	-0.00001500
H	-15.32684100	0.09251600	0.00014000
F	11.66662100	3.75535200	0.00008500
F	6.61539800	-0.03563900	-0.00002100
F	0.47441000	-1.51571400	-0.00002800
F	-5.75854700	-0.44447000	0.00003600
F	-11.06393800	3.00061400	0.00012600
F	-14.59113900	8.26917300	-0.00000600
H	13.42992800	5.82939800	0.00015200
H	9.06023000	1.16887300	0.00000000
H	3.19615800	-1.37950900	-0.00005400
H	-3.20359300	-1.39340600	-0.00000800
H	-9.09080800	1.12094100	0.00009800
H	-13.50782800	5.74889700	0.00006400