

Cartesian coordinates of MPWB1K/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	-2.17847500	-1.44768800	0.00026500
C	-2.63204900	-0.17951100	-0.00001600
O	-0.83277100	-1.43323200	0.00020800
C	-1.49443100	0.65657800	-0.00003800
C	-0.40875300	-0.15438700	0.00006300
C	0.99820400	0.11034000	0.00007200
C	1.61230900	1.32848600	0.00018200
S	2.14536400	-1.16956500	-0.00023300
C	3.02003400	1.22365600	0.00023200
H	1.06947800	2.25820800	0.00036600
C	3.44654100	-0.06361300	-0.00008500
H	4.45806800	-0.42761300	-0.00012900
F	-1.49425200	1.97549400	-0.00019400
F	-3.88298000	0.22866200	-0.00013300
H	3.68571600	2.07060700	0.00041600
H	-2.66211300	-2.40289200	0.00031000

#### C2FOS-2

0 1

C	-5.00075504	-2.18717442	-0.00034026
C	-3.82734964	-0.33597085	-0.00046232
C	-5.13569706	0.02128689	0.00059252
C	-2.61643961	0.42252428	-0.00085011
C	-0.26894254	1.14961210	-0.00090869
C	-1.14580582	2.19924227	-0.00156377
O	-3.75353108	-1.68167391	-0.00107780
C	-5.88737482	-1.17286099	0.00054763
C	-2.48635528	1.78273190	-0.00152347
H	-3.33039378	2.45089626	-0.00186929
F	-5.61751130	1.24833709	0.00142671
S	-1.08696111	-0.36369446	-0.00068308
C	1.15504168	1.21113447	-0.00045088
C	2.03221785	2.24807398	0.00045578
O	1.86122923	0.06064736	-0.00074922
C	3.32371963	1.69584502	0.00067333
C	3.18054962	0.34547664	-0.00007986
C	4.12041964	-0.72934760	-0.00021103
C	5.48370386	-0.64508429	-0.00121639
S	3.59311978	-2.36569384	0.00126767
C	6.10111073	-1.91352326	-0.00084039
H	6.01325905	0.29257623	-0.00219218
C	5.20379060	-2.93089461	0.00041418
H	5.39988208	-3.98786177	0.00087703
F	4.45970675	2.36314975	0.00150689
F	-7.20041312	-1.25188743	0.00130456
F	1.72771157	3.52970190	0.00101788
H	-0.82597637	3.22762827	-0.00200044
H	7.16807256	-2.06180989	-0.00158261
H	-5.10141500	-3.25314485	-0.00069178

#### C2FOS-3

0 1

C	5.28035400	3.94636300	0.00036100
C	5.47669600	1.76381100	0.00024700
C	6.73193400	2.27638300	0.00049500
O	4.59882000	2.78580800	0.00016800
C	6.60135400	3.68178900	0.00056400
F	7.86062800	1.59555100	0.00064300
C	4.97937300	0.42460600	0.00008000
C	3.56558800	-1.58577000	-0.00017700
C	4.90173700	-1.88022800	-0.00015600
C	5.70808800	-0.73192400	-0.00001300
H	6.78457100	-0.74652600	0.00002500
C	2.47528000	-2.50320700	-0.00032200
C	0.34223800	-3.05483700	-0.00042400
C	1.05494300	-4.21235100	-0.00060000
C	-1.05607100	-2.78265500	-0.00037900
C	-3.27337200	-1.71942300	-0.00020900
C	-3.34283600	-3.08632800	-0.00043100
O	1.21338700	-2.02332100	-0.00025400
C	2.41367300	-3.86080800	-0.00053900
C	-2.07865200	-3.69237000	-0.00052800
H	-1.91749600	-4.75685800	-0.00070400
F	0.56347800	-5.43425000	-0.00079300
S	3.28878500	0.11189300	-0.00001300
S	-1.64476500	-1.16573500	-0.00011400
C	-4.35903400	-0.79641100	-0.00004200
C	-5.70741600	-0.96281900	0.00008000
O	-4.09738300	0.52819000	0.00005500
C	-6.28131700	0.31875700	0.00024500
C	-5.26004000	1.21380900	0.00023000
C	-5.22613400	2.64114900	0.00032200
C	-6.29195600	3.49587700	0.00087000
S	-3.73557000	3.49828100	-0.00035900
C	-5.89637000	4.84981400	0.00074100
H	-7.31440800	3.15787800	0.00135100
C	-4.54829600	4.99963100	0.00010700
H	-3.98250300	5.91373700	-0.00010100
F	-7.56855500	0.59904400	0.00038700
F	7.59497500	4.54359600	0.00078800
F	3.43570300	-4.69147800	-0.00066600
F	-6.35442900	-2.11002500	0.00004500
H	5.28048700	-2.88788200	-0.00024900
H	-4.27433000	-3.62627700	-0.00052400
H	-6.58617000	5.67717300	0.00111800
H	4.71125700	4.85324400	0.00032700

C2FOS-4

0 1

C	2.92140000	5.12934300	-0.78761200
C	4.48860400	3.64808200	-0.39605600
C	5.08675700	4.86496700	-0.41533300
C	4.07485000	5.81568100	-0.66785600
O	3.17125100	3.81740200	-0.62313300
C	4.98708700	2.32432200	-0.19468400
C	5.22271800	-0.10547300	0.08112700
C	6.41790100	0.55374500	0.17353000
C	4.99470200	-1.50822300	0.18098700

C	3.73820800	-3.31667700	0.20955200
C	5.02671500	-3.72362900	0.35592000
O	3.72923400	-1.97124900	0.10441500
C	5.82768200	-2.57078600	0.33761300
C	6.28229200	1.94185300	0.01628600
H	7.10078600	2.64025600	0.05532800
F	6.36784900	5.11576000	-0.23362700
F	5.44199600	-4.96611500	0.49055500
C	2.50091900	-4.01922400	0.15396700
C	0.12638500	-4.63789000	0.02252100
C	0.95076400	-5.72613200	0.12059900
C	2.30557700	-5.37336900	0.19625100
H	3.11525100	-6.07853200	0.27871100
C	-1.29433400	-4.62836600	-0.07661800
C	-3.26692800	-3.65622200	-0.20767100
C	-3.47926500	-4.99800000	-0.24530400
C	-4.14889700	-2.53840100	-0.23849900
C	-5.13976300	-0.28992700	-0.17497300
C	-6.07214100	-1.27271200	-0.36962900
O	-1.93844600	-3.44175400	-0.10535300
C	-2.22272900	-5.61770600	-0.16267100
C	-5.50728800	-2.55555700	-0.40553300
H	-6.06739400	-3.46448000	-0.54681200
F	-4.64574800	-5.60194600	-0.33870900
S	3.91747800	0.97843000	-0.20145900
S	1.01432200	-3.16472400	0.02089300
S	-3.55276700	-0.93777000	-0.03485500
C	-5.36476700	1.11440700	-0.08452100
C	-6.48231900	1.87857100	-0.19863800
O	-4.31974300	1.93076900	0.17151000
C	-6.09125000	3.21292200	-0.00225200
C	-4.75248500	3.20808800	0.22446200
C	-3.81412700	4.24904600	0.49776400
C	-4.06690500	5.58850600	0.59198200
S	-2.15260200	3.90339400	0.77101800
C	-2.90710400	6.33559600	0.88658900
H	-5.04906400	6.00875900	0.45599100
C	-1.80302400	5.55703500	1.01044400
H	-0.79810200	5.86348200	1.23892600
F	-6.87723300	4.26989000	-0.03007200
F	4.25098000	7.11569900	-0.76239300
F	7.13913200	-2.52497800	0.44872100
F	-1.98812600	-6.91336500	-0.16785800
F	-7.70306300	1.45098300	-0.44695000
H	7.35300200	0.04867900	0.34712300
H	0.58636200	-6.73891100	0.13756300
H	-7.12341600	-1.07069000	-0.48066500
H	-2.89568600	7.40634400	1.00387400
H	1.90947200	5.41789400	-0.98657700

2FOS-5

0 1

C	4.33839400	-0.15494100	-1.91377800
C	3.92889600	-2.24517400	-1.40803400
C	3.07636900	-3.35336200	-1.12001300
C	1.14888100	-4.78139500	-0.59117700
C	-0.16009200	-5.28499200	-0.33835300

C	-2.33381300	-5.07772500	-0.03923000
C	5.27372200	-2.08158900	-1.36074400
C	5.53296400	-0.73399500	-1.68375400
C	3.43494800	-4.64920600	-0.87852400
C	2.33261400	-5.46789900	-0.57976500
C	-2.04004900	-6.39865300	0.06880000
C	-0.65417300	-6.53205300	-0.12003100
O	3.36580200	-1.07042300	-1.75237500
O	-1.18689800	-4.41062300	-0.28780600
H	4.45741200	-4.98551200	-0.91335200
C	-3.54264900	-4.33428400	0.07200200
C	-5.21824400	-2.54347700	0.19483900
C	-5.76614400	-3.78752000	0.34853500
C	-5.88660900	-1.28637500	0.21094300
C	-5.97451200	0.91237300	0.12987400
C	-7.25206200	0.46613800	0.26117600
O	-5.15386100	-0.15897800	0.10092600
C	-7.19575400	-0.93578900	0.30980500
C	-4.80879100	-4.81059400	0.27773600
H	-5.03245600	-5.85956500	0.37560700
F	6.16736200	-2.99514800	-1.03690000
F	-2.89660800	-7.36843200	0.31400300
F	-8.33646300	1.21132100	0.32789200
C	-5.40499300	2.21364500	0.03156200
C	-3.87910300	4.13095700	-0.13632400
C	-5.19574500	4.50330700	-0.13247300
C	-6.06693000	3.40920500	-0.03787100
H	-7.14096200	3.48345100	-0.02103300
C	-2.74191800	4.98172500	-0.23715100
C	-0.58517600	5.43010500	-0.25367300
C	-1.24097500	6.60357400	-0.46098200
C	0.80076800	5.11506700	-0.14965100
C	2.97878500	4.03472700	0.21897200
C	3.09559600	5.34803800	-0.14741000
O	-1.50482000	4.45024800	-0.11871600
C	-2.61365500	6.31687400	-0.45273000
C	1.85410000	5.96482600	-0.35695300
H	1.72569300	6.99411700	-0.64686800
F	-0.69040500	7.78773000	-0.63448800
S	1.38043800	-3.12095300	-0.97393900
S	-3.51608900	-2.61832000	-0.03624700
S	-3.69797900	2.42458900	-0.01763900
S	1.33180900	3.54304400	0.30489100
C	4.03231400	3.11865900	0.50931200
C	5.38726800	3.21726300	0.45217900
O	3.71968600	1.87840100	0.94592000
C	5.91042600	1.98493800	0.87482700
C	4.85555800	1.18470900	1.17349400
C	4.76298700	-0.16670400	1.62059600
C	5.79004300	-1.04269800	1.83157100
S	3.24036700	-0.89888900	1.92762600
C	5.33576300	-2.31582500	2.23592000
H	6.82465800	-0.78036100	1.69005900
C	3.98289800	-2.38096500	2.32941400
H	3.37555500	-3.22667300	2.59824600
F	7.18580100	1.67113100	0.96330000
F	6.72128100	-0.16562500	-1.71763900

F	0.03722600	-7.65264400	-0.09206400
F	-8.21360800	-1.76214900	0.43032900
F	-3.59516800	7.17856200	-0.62043200
F	6.08374000	4.26925900	0.07337800
H	2.39435800	-6.52040300	-0.35920000
H	-6.81956300	-3.94609900	0.50598400
H	-5.51438000	5.52999500	-0.19856200
H	4.04327400	5.84611000	-0.25790900
H	5.98764300	-3.14648800	2.44824400
H	4.04293200	0.83935800	-2.18395200

2FOS-6

0 1

C	4.45136400	0.54216900	-1.75786400
C	4.30547200	-1.87692600	-1.36318800
C	3.86425500	-3.21182000	-1.13392700
C	2.36619700	-4.77360700	-0.73130300
C	1.05321000	-5.27233800	-0.49442000
C	-1.36966800	-5.56279400	-0.17096100
C	-2.78198300	-5.40507400	-0.05942100
C	-4.68618600	-4.29499600	-0.04979400
C	2.83090600	3.66307800	-2.07905500
C	4.08849500	4.14104400	-2.14567400
C	4.95086700	3.03058400	-2.03463000
C	4.16376600	1.93263400	-1.91250600
C	3.57435000	-5.39064700	-0.82103100
C	4.52817500	-4.39542500	-1.07615400
C	5.59730000	-1.43588900	-1.46000000
C	5.67998000	-0.05259600	-1.68505700
C	0.70257800	-6.57380400	-0.25752500
C	-0.67549600	-6.73956200	-0.07270600
C	-4.98623500	-5.60915400	0.12717400
C	-3.77681300	-6.31454700	0.11923300
O	2.55342600	-3.44987900	-0.91627000
O	-3.34344100	-4.17956200	-0.15895800
O	2.87570200	2.32640500	-1.94199700
H	6.60195700	0.49638100	-1.77218100
H	1.41739000	-7.37758400	-0.22290200
C	-5.51933000	-3.14109100	-0.12928400
C	-6.45945500	-0.86859700	-0.23144400
C	-7.42274200	-1.84104500	-0.22839500
C	-6.67920800	0.53793600	-0.29811500
C	-6.09186900	2.66079700	-0.25180600
C	-7.43556500	2.62215800	-0.45299900
O	-5.64116300	1.39071500	-0.15992800
C	-7.80936400	1.27135500	-0.48316100
C	-6.88845500	-3.13371300	-0.17031200
H	-7.48308900	-4.03074200	-0.16013800
H	1.86569300	4.12493300	-2.11434000
F	6.26825800	3.05820600	-2.05066700
F	3.80974700	-6.68093800	-0.69288700
F	-6.18587000	-6.13032900	0.27873500
F	-8.23842600	3.65627700	-0.59393400
C	-5.17477600	3.74350500	-0.12559700
C	-3.18848500	5.15699000	0.18941400
C	-4.32460900	5.88599600	-0.03539800
C	-5.45700600	5.08037400	-0.21439700

H	-6.44604400	5.46059000	-0.40273300
C	-1.87107600	5.65664700	0.39559200
C	0.29340800	5.46321100	0.75797100
C	0.02627400	6.78987200	0.63548400
C	1.49516000	4.73006400	0.97472500
C	3.16021200	2.96041900	1.33312100
C	3.72574700	4.20187800	1.22189900
O	-0.86461200	4.78389500	0.61213900
C	-1.35303800	6.91328800	0.40467300
C	2.77506200	5.21305400	1.01386900
H	3.01118700	6.25674600	0.89110100
F	0.89983000	7.77170400	0.71342700
S	3.17704200	-0.59410400	-1.56087900
S	-0.32039400	-4.23425200	-0.48743200
S	-4.87765500	-1.54448000	-0.16262100
S	-3.50538800	3.46573900	0.18218500
S	1.44843800	3.02517800	1.19516300
C	3.82886300	1.71542500	1.51624200
C	5.12961600	1.34799200	1.39388900
O	3.10708400	0.61855200	1.83596100
C	5.19303800	-0.03328200	1.63444200
C	3.92799200	-0.45043400	1.89756800
C	3.37675300	-1.73751700	2.17701900
C	4.05651500	-2.91767300	2.29443300
S	1.68601100	-1.96510600	2.37847300
C	3.20050600	-4.00754500	2.55747300
H	5.12638500	-2.98845500	2.19455000
C	1.89640900	-3.63866900	2.63456700
H	1.04128000	-4.26202000	2.82451200
F	6.27270700	-0.78640100	1.57239200
F	4.46596400	5.39648600	-2.26233100
F	5.82367100	-4.57498000	-1.23558900
F	-3.63787600	-7.61703800	0.25604100
F	-9.02837600	0.80603700	-0.66071500
F	-2.01920300	8.03481100	0.22478100
F	6.13305000	2.12751700	1.04638600
H	6.44846500	-2.08774300	-1.35966600
H	-1.14643500	-7.68787800	0.12041200
H	-8.47613300	-1.62347100	-0.26633000
H	-4.33161700	6.96203400	-0.07028600
H	4.78813300	4.36705100	1.28309800
H	3.54004800	-5.02096500	2.69237200

T2FOS-1

0 1

C	0.41694700	0.38482300	0.00000800
C	1.37565600	-0.57125400	-0.00004500
C	2.62166900	0.09232800	-0.00003900
C	2.35184900	1.41153300	0.00001800
O	1.01731000	1.59154600	0.00004600
C	-1.01408500	0.33228000	0.00003000
C	-1.87974800	1.38550500	0.00009400
C	-3.23124200	0.97575800	0.00010000
C	-3.36654100	-0.37279400	0.00004200
S	-1.85546200	-1.16829100	-0.00002700
F	1.17806400	-1.87515700	-0.00009200
H	-1.54799200	2.41022600	0.00013500

F	3.80219000	-0.48858100	-0.00008000
H	-4.06595200	1.65662200	0.00014700
H	2.96712900	2.28795000	0.00004300
H	-4.27359100	-0.94993800	0.00003400

T2FOS-2

0 1

C	-6.20989900	-1.43168200	-0.00006300
C	-6.33541400	-0.09036200	-0.00007900
O	-4.90344800	-1.75549500	-0.00004200
C	-5.02545000	0.43419600	-0.00006700
C	-4.17516000	-0.62096100	-0.00004400
C	-2.75032100	-0.73108700	-0.00002500
C	-2.01601600	-1.88162300	-0.00000200
C	-0.63214800	-1.64237000	0.00001200
C	-0.32638900	-0.31149700	0.00000000
C	0.97745600	0.26616700	0.00001000
C	1.43107800	1.54512500	0.00000200
O	2.04373900	-0.56404500	0.00003100
C	2.83447500	1.48411700	0.00002000
C	3.17586600	0.17099800	0.00003800
C	4.43288600	-0.50796000	0.00006000
C	4.64756700	-1.85592100	0.00007700
C	6.01987300	-2.18536400	0.00009300
C	6.81872600	-1.08997000	0.00008500
S	-1.74419600	0.66594700	-0.00002900
S	5.91905300	0.36055500	0.00007500
F	-4.68732100	1.70779500	-0.00007600
F	3.66669800	2.50519100	0.00002000
H	-2.46756000	-2.85916200	0.00000400
H	3.84411100	-2.57308100	0.00007500
F	-7.44549300	0.61494400	-0.00010200
F	0.68929800	2.63295600	-0.00001800
H	0.12065800	-2.41210400	0.00003100
H	6.39571500	-3.19487100	0.00010500
H	-6.91747100	-2.23541400	-0.00006400
H	7.89309200	-1.05188100	0.00009200

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C	-9.59854300	-2.19405100	-0.00011600
C	-9.90410800	-0.88212500	-0.00012700
O	-8.25980700	-2.33896700	-0.00009300
C	-8.67731300	-0.18554900	-0.00011200
C	-7.69230100	-1.11628600	-0.00009100
C	-6.26566800	-1.02442800	-0.00006900
C	-5.36899400	-2.05388500	-0.00004700
C	-4.03532800	-1.61260700	-0.00003000
C	-3.92926300	-0.25098800	-0.00004000
C	-2.73220800	0.52356000	-0.00002900
C	-2.49644500	1.86017600	-0.00003500
O	-1.54507200	-0.12021800	-0.00000800
C	-1.10310200	2.03239500	-0.00001700
C	-0.54910200	0.79237800	0.00000000
C	0.79859500	0.32733700	0.00002200
C	1.22534400	-0.97094900	0.00003900
C	2.62432100	-1.08320200	0.00005400

C	3.25285500	0.13000900	0.00004900
S	-5.47668200	0.50543800	-0.00006600
S	2.12255800	1.42952700	0.00003700
C	4.65826400	0.37135000	0.00005700
C	5.40637200	1.50368500	0.00005500
O	5.49294200	-0.69091000	0.00007000
C	6.75399600	1.10631200	0.00006800
C	6.76911800	-0.25000600	0.00007800
C	7.82197600	-1.21606000	0.00009400
C	7.69488600	-2.57469000	0.00011000
S	9.47721800	-0.74423100	0.00011700
C	8.94188000	-3.23543800	0.00010800
C	9.98821200	-2.37297300	0.00008300
H	11.03836000	-2.60307200	0.00006800
F	-8.51377800	1.12231600	-0.00011700
F	-0.45092500	3.17576600	-0.00001600
F	7.80786100	1.89591700	0.00007100
H	-5.67082500	-3.08760500	-0.00004400
H	0.54533000	-1.80595500	0.00003600
H	6.73882400	-3.07038100	0.00011400
F	-11.09924400	-0.33359700	-0.00014800
F	-3.41213000	2.80623800	-0.00005500
F	4.94873200	2.73828000	0.00004300
H	-3.17729400	-2.26323600	-0.00001300
H	3.16233100	-2.01598600	0.00006600
H	9.05484600	-4.30670000	0.00011000
H	-10.19090500	-3.08611600	-0.00012000

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C	10.85518500	2.11019200	-0.00009000
C	12.01489000	1.40958900	-0.00011800
C	13.06645000	2.35067400	-0.00011900
C	12.48938700	3.56796300	-0.00009000
O	11.15072700	3.42529700	-0.00007300
C	9.47921200	1.72384800	-0.00007500
C	8.39296400	2.55042100	-0.00003900
C	7.17700400	1.84827100	-0.00003300
C	7.34919400	0.49331200	-0.00006400
C	6.32475700	-0.49854400	-0.00006700
C	6.34069700	-1.85600800	-0.00009000
O	5.03796100	-0.08730500	-0.00004300
C	5.00334600	-2.28382400	-0.00007900
C	4.22862600	-1.16872300	-0.00005000
C	2.81869700	-0.95889000	-0.00002900
C	2.16579500	0.24177300	-0.00000200
C	0.76993200	0.10122100	0.00001200
C	0.36955700	-1.20548100	-0.00000400
C	-0.96998400	-1.69257300	0.00000300
C	-1.50592400	-2.94040500	-0.00000600
O	-1.97872100	-0.79418400	0.00002300
C	-2.90189200	-2.78807600	0.00000900
C	-3.15626400	-1.45461800	0.00002700
C	-4.36349600	-0.69683400	0.00004600
C	-4.48780900	0.66374000	0.00006200
C	-5.82592600	1.08768900	0.00007700
C	-6.71084700	0.04623500	0.00007300



S	9.01754300	0.06561000	-0.00010100
S	1.71492300	-2.28129500	-0.00003700
S	-5.90108000	-1.47385900	0.00005100
C	-8.13469200	0.12170900	0.00008400
C	-9.11151700	-0.82076000	0.00008300
O	-8.71758300	1.34039300	0.00010000
C	-10.33985500	-0.14029600	0.00009800
C	-10.05947500	1.18716900	0.00010800
C	-10.87726900	2.35816000	0.00012500
C	-10.45653400	3.65618400	0.00013500
S	-12.59531200	2.25750800	0.00013500
C	-11.52954800	4.57276400	0.00014900
C	-12.73844800	3.95901000	0.00014800
H	-13.71315900	4.41249100	0.00015600
F	12.13136800	0.09719500	-0.00014100
F	4.57475700	-3.52837800	-0.00009400
F	-3.80528700	-3.74581100	0.00000700
F	-11.54057000	-0.68090600	0.00010200
H	8.47911700	3.62377400	-0.00001800
H	2.68510700	1.18509600	0.00000600
H	-3.63815600	1.32532300	0.00006200
H	-9.41497400	3.93008600	0.00013300
F	14.35069000	2.06794000	-0.00014300
F	7.41294200	-2.61964600	-0.00011700
F	-0.83488000	-4.07257300	-0.00002500
F	-8.93139400	-2.12522000	0.00007000
H	6.20493900	2.31128600	-0.00000700
H	0.07341300	0.92242500	0.00003300
H	-6.14080700	2.11744600	0.00009000
H	-11.40665700	5.64292000	0.00015800
H	12.87903200	4.56536900	-0.00008000

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0 1

C	7.69998400	-0.99634100	-0.00005800
C	8.68099200	-1.93530600	-0.00005800
C	9.90617900	-1.25032600	-0.00005300
C	9.62012400	0.07690900	-0.00005000
O	8.27726300	0.22467300	-0.00005300
C	10.42958500	1.25036800	-0.00004500
C	9.99727800	2.54606200	-0.00004100
C	11.05376000	3.47103200	-0.00003600
C	12.28002900	2.87163200	-0.00003600
C	13.55495300	3.51801200	-0.00003000
C	14.82900900	3.05655500	-0.00002300
O	13.58916500	4.86540800	-0.00003000
C	15.67722900	4.18451500	-0.00001800
C	14.87416700	5.26621100	-0.00002300
C	6.27684800	-1.07599200	-0.00006000
C	5.39134000	-0.03481300	-0.00005200
C	4.05385200	-0.45928800	-0.00005500
C	3.93041400	-1.82013200	-0.00006600
C	2.72203600	-2.57582400	-0.00007000
C	2.46339100	-3.90845600	-0.00008200
O	1.54674700	-1.91152400	-0.00005900
C	1.06671400	-4.05612400	-0.00007800
C	0.53516800	-2.80639300	-0.00006300

C	-0.80206400	-2.31318300	-0.00005100
C	-1.19432300	-1.00405600	-0.00003400
C	-2.58909700	-0.85476800	-0.00002200
C	-3.24942300	-2.05149800	-0.00003000
C	-4.66062600	-2.25133100	-0.00002000
C	-5.44369300	-3.36067200	-0.00002600
O	-5.46187800	-1.16388300	0.00000100
C	-6.77769000	-2.92322000	-0.00000800
C	-6.75182400	-1.56554300	0.00000900
C	-7.76768900	-0.56587700	0.00003100
C	-7.58258800	0.78781600	0.00004700
C	-8.79057000	1.50153000	0.00006800
C	-9.88661800	0.68554100	0.00006900
S	12.14930000	1.15495500	-0.00004300
S	5.46808500	-2.59672900	-0.00007400
S	-2.15387300	-3.38082900	-0.00005500
S	-9.44002500	-0.97806800	0.00004000
C	-11.25451100	1.08689500	0.00008900
C	-12.42519900	0.40051100	0.00009300
O	-11.53442900	2.40813900	0.00010800
C	-13.45974700	1.35103900	0.00011600
C	-12.87410600	2.57517700	0.00012500
C	-13.39202200	3.90615300	0.00014700
C	-12.67538400	5.06757300	0.00015400
S	-15.08444400	4.21535800	0.00016500
C	-13.50043900	6.21219300	0.00017800
C	-14.82064500	5.90225100	0.00019000
H	-15.66020000	6.57371100	0.00021000
F	15.20052400	1.79228400	-0.00002000
F	8.50471600	-3.23998600	-0.00006100
F	0.39085400	-5.18532100	-0.00008600
F	-7.85544000	-3.67902800	-0.00000600
F	-14.75443800	1.10931900	0.00012800
H	10.92944200	4.54064100	-0.00003200
H	5.70574200	0.99509200	-0.00004300
H	-0.49287900	-0.18707800	-0.00002900
H	-6.60583700	1.24087700	0.00004400
H	-11.59858400	5.08623200	0.00014300
F	16.99186300	4.15685200	-0.00001100
F	11.10948300	-1.78368500	-0.00005000
F	3.36419700	-4.86846500	-0.00009400
F	-5.02388300	-4.60812200	-0.00004400
F	-12.55338700	-0.90970300	0.00007900
H	8.95345300	2.81056800	-0.00004200
H	3.20375600	0.20165900	-0.00004800
H	-3.10268800	0.09166200	-0.00000700
H	-8.86537800	2.57561500	0.00008400
H	-13.12752100	7.22275800	0.00018800
H	15.06188000	6.32046400	-0.00002300

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C	4.22569700	-3.59616400	-0.00009200
C	4.99300900	-4.71650900	-0.00014900
C	6.33319600	-4.29724100	-0.00014400
C	6.32578200	-2.93956600	-0.00008400

O	5.04180900	-2.52004400	-0.00005300
C	7.35543700	-1.95392800	-0.00005200
C	7.18925700	-0.59761300	0.00002400
C	8.40688900	0.09910700	0.00003600
C	9.49149200	-0.73223800	-0.00003000
C	10.86443700	-0.35025000	-0.00003700
C	12.02532000	-1.05463600	-0.00007700
O	11.16428200	0.96688800	0.00000500
C	13.07354500	-0.12117300	-0.00005800
C	12.50702400	1.11291600	-0.00000700
C	2.81766800	-3.37521600	-0.00007000
C	2.17695100	-2.16799200	-0.00001000
C	0.78002100	-2.29433100	-0.00000700
C	0.36663800	-3.59712800	-0.00006300
C	13.04871400	2.43192900	0.00002900
C	12.35664900	3.60984200	0.00008100
C	13.19801000	4.73456100	0.00010600
C	14.52234000	4.40317900	0.00007400
C	15.64123700	5.29299300	0.00008700
C	16.98082100	5.08977400	0.00007300
O	15.40987600	6.62042000	0.00012400
C	17.59146200	6.36231200	0.00010300
C	16.59147100	7.26519300	0.00013400
H	16.56898100	8.33577900	0.00016200
C	-0.97806900	-4.06939200	-0.00007500
C	-1.52849100	-5.31100900	-0.00010900
O	-1.97606000	-3.15943900	-0.00004600
C	-2.92256600	-5.14245300	-0.00009800
C	-3.16142900	-3.80602200	-0.00005900
C	-4.35707900	-3.03060700	-0.00003600
C	-4.45536600	-1.66775700	-0.00000400
C	-5.78477000	-1.21862700	0.00001200
C	-6.68919900	-2.24346300	-0.00000700
C	-8.11053700	-2.13781600	0.00000200
C	-9.10885000	-3.05861200	-0.00000100
O	-8.66551600	-0.90643600	0.00001800
C	-10.32108800	-2.35175300	0.00001400
C	-10.01105400	-1.02950400	0.00002500
C	-10.79964100	0.15739300	0.00004000
C	-10.34566700	1.44627800	0.00004800
C	-11.38539400	2.38873800	0.00006200
C	-12.62354300	1.81068300	0.00006700
S	14.75010900	2.69695800	0.00000900
S	9.02191300	-2.38947200	-0.00011100
S	1.70093500	-4.68664400	-0.00012300
S	-5.90847400	-3.77897400	-0.00004700
S	-12.52084000	0.09111100	0.00004900
C	-13.88403900	2.47734700	0.00008300
C	-15.16817500	2.03801900	0.00009200
O	-13.89563500	3.82771400	0.00009100
C	-15.99258200	3.17571300	0.00010700
C	-15.17499400	4.25869500	0.00010600
C	-15.41634000	5.66672400	0.00011600
C	-14.48247800	6.66180500	0.00011200
S	-17.01299800	6.30853500	0.00013000
C	-15.06202600	7.94824100	0.00012600
C	-16.41766700	7.90865700	0.00014000

H	-17.10620400	8.73425700	0.00015400
F	17.59036000	3.92145800	0.00003900
F	12.13579900	-2.36612100	-0.00012400
F	4.55487400	-5.95759900	-0.00019900
F	-3.83722700	-6.08917100	-0.00012100
F	-11.53327300	-2.86439000	0.00001800
F	-17.30918700	3.19529400	0.00012000
H	12.85414700	5.75508400	0.00014700
H	8.49682400	1.17207200	0.00009300
H	2.70570500	-1.22995500	0.00003000
H	-3.59328300	-1.02257300	0.00000700
H	-9.29750800	1.69309300	0.00004300
H	-13.42346000	6.46606600	0.00010100
F	18.88579800	6.59399500	0.00010100
F	14.36390900	-0.38257000	-0.00008300
F	7.40149400	-5.06606200	-0.00018900
F	-0.87041600	-6.45066400	-0.00014300
F	-8.95705600	-4.36640600	-0.00001500
F	-15.55761700	0.78039800	0.00008800
H	11.28059900	3.65153300	0.00010000
H	6.21908700	-0.13066900	0.00006900
H	0.09155900	-1.46636400	0.00003600
H	-6.07982000	-0.18306100	0.00003700
H	-11.24174500	3.45583500	0.00007100
H	-14.49450100	8.86380000	0.00012700