

Cartesian coordinates of MPWB1K/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	3.09762500	-0.98910400	0.00040200
C	1.10958600	-0.10165100	0.00010200
C	-0.32060800	-0.12718800	-0.00004000
C	-2.68770500	-0.81549800	-0.00014200
C	2.01543800	0.90634300	0.00012200
C	3.30951800	0.34396800	0.00032500
C	-1.16509100	0.94263900	-0.00030000
C	-2.50909400	0.52424200	-0.00034800
O	1.78651400	-1.26884700	0.00027600
H	4.24867300	0.86299300	0.00039600
H	-0.84833400	1.97078200	-0.00044900
F	1.72134300	2.19423200	-0.00001900
F	-3.50794300	1.39432700	-0.00059300
S	-1.17838300	-1.61820800	0.00013900
H	3.75751600	-1.83408600	0.00054200
H	-3.61446000	-1.35711200	-0.00014700

CFOFS-2

0 1			
C	-5.28000600	-2.70930800	-0.00036600
C	-4.29587400	-0.76797000	-0.00009500
C	-3.17306700	0.11311600	0.00003400
C	-0.89842500	1.07342600	0.00006000
C	0.50645400	1.31696400	0.00002000
C	2.59597800	0.66666100	-0.00014800
C	-5.63549900	-0.55628200	-0.00019600
C	-6.28508900	-1.80766400	-0.00038800
C	-3.19703100	1.47927500	0.00034800
C	-1.89882500	1.99946700	0.00035300
C	2.57760300	2.02395200	-0.00006400
C	1.24362300	2.46189100	0.00001700
O	-4.08537900	-2.10064900	-0.00020800
O	1.31371400	0.23840400	-0.00009300
H	-7.34127800	-1.99689700	-0.00050900
H	-4.09255700	2.07555500	0.00057200
H	0.87707800	3.46961800	0.00008500
C	3.65215100	-0.29282300	-0.00009900
C	4.98383000	-2.36771400	0.00076300
C	5.73038000	-1.24034700	-0.00047700
C	4.99359200	-0.04192800	-0.00099900
H	5.43019700	0.94115600	-0.00197800
F	-6.21683100	0.62905600	-0.00013800
F	-1.65254900	3.30221200	0.00063700
F	3.65002600	2.79381900	-0.00008600
F	7.05497900	-1.24245000	-0.00121100
S	-1.56949700	-0.51116400	-0.00026800
S	3.31912300	-1.98091400	0.00139500
H	-5.25980800	-3.78122200	-0.00045700
H	5.32628400	-3.38503600	0.00127800

CFOFS-3

0 1

C	-4.87588500	4.69924300	0.00239900
C	-5.40162800	2.58759500	0.00056200
C	-5.12560700	1.18758200	0.00042800
C	-4.02614400	-1.02197000	-0.00031100
C	-3.11604800	-2.11821900	-0.00034200
C	-1.10208400	-2.97356600	-0.00002900
C	-6.55384300	3.30384300	-0.00221900
C	-6.22603600	4.67520200	-0.00095400
C	-6.03418100	0.16672100	0.00056500
C	-5.38886000	-1.07346900	0.00007400
C	-1.99527000	-3.99817200	0.00005300
C	-3.29454700	-3.46948600	-0.00018800
O	-4.37076200	3.45808400	0.00337900
O	-1.80349600	-1.81784700	-0.00032300
H	-6.90077600	5.50949700	-0.00238800
H	-7.10191700	0.29670200	0.00094000
H	-4.22706800	-3.99876200	-0.00012000
C	0.31954900	-2.92015500	0.00005600
C	2.67547400	-2.17832700	0.00015100
C	2.51257500	-3.53231900	0.00060100
C	3.89933400	-1.44816300	-0.00021100
C	5.04966200	0.41416200	-0.00061200
C	5.92628000	-0.62213400	-0.00109400
O	3.80141700	-0.10397500	-0.00003300
C	5.20757500	-1.82800700	-0.00105600
C	1.18772600	-3.97739600	0.00059600
H	5.59308600	-2.82857800	-0.00147400
H	0.89067100	-5.01138800	0.00092800
F	-7.76864900	2.78744000	-0.00542200
F	-6.04910100	-2.22296100	0.00017100
F	-1.67143900	-5.27707900	0.00034900
F	3.54498700	-4.36374200	0.00094100
F	7.24035400	-0.49642200	-0.00168400
C	5.21477700	1.83106800	-0.00013500
C	4.84380100	4.26784800	0.00344500
C	6.14888100	3.91500100	-0.00180700
C	6.38804200	2.52820500	-0.00392900
H	7.36442100	2.07590400	-0.00808000
F	7.14155400	4.79217700	-0.00495000
S	-3.50231600	0.61717500	-0.00009200
S	1.13753100	-1.40501300	-0.00015500
S	3.84938500	2.87824000	0.00618600
H	-4.15942600	5.49681400	0.00446900
H	4.42952400	5.25805500	0.00561100

CFOFS-4

0 1

C	2.13026700	5.58103200	-0.84019400
C	3.89984200	4.37122000	-0.46557700
C	4.61130500	3.15200600	-0.25474000
C	5.24108700	0.78279600	0.03823800
C	5.28476600	-0.63632500	0.15657100
C	4.34509100	-2.61205400	0.20352100
C	4.28901900	5.66956600	-0.53237800
C	3.14993000	6.46413100	-0.77427700
C	5.95362900	3.00349100	-0.04636600

C	6.28625300	1.65537500	0.11548000
C	5.68532800	-2.77920900	0.35576300
C	6.30666000	-1.52205500	0.32882100
O	2.56501300	4.32674700	-0.65676000
O	4.10811100	-1.28664000	0.08200900
H	3.10661700	7.53079000	-0.88261300
H	6.66229900	3.81161100	-0.01194900
H	7.35103000	-1.29801300	0.42057300
C	3.24797200	-3.51613100	0.15819700
C	0.99409400	-4.51844900	0.04862100
C	2.00909300	-5.42609300	0.13563200
C	-0.40187000	-4.78523300	-0.03693000
C	-2.49723400	-4.16525600	-0.15313900
C	-2.45741500	-5.52375700	-0.17810400
O	-1.22404100	-3.71895800	-0.06590800
C	-1.12071000	-5.94162600	-0.10341100
C	3.29464800	-4.88334900	0.20021500
H	-0.73855400	-6.94339000	-0.10111200
H	4.19754600	-5.46379200	0.27018900
F	5.52915300	6.09924900	-0.39252800
F	7.52919000	1.24872900	0.32884500
F	6.28516000	-3.94439300	0.50386800
F	1.78368600	-6.73215900	0.15357800
F	-3.51658000	-6.30612800	-0.25952800
C	-3.56157500	-3.22228900	-0.19315700
C	-4.92050800	-1.15884000	-0.18302200
C	-5.64320100	-2.30785800	-0.31747800
C	-4.89709900	-3.48882300	-0.32495100
H	-5.31833800	-4.47373800	-0.42062100
F	-6.96382200	-2.29921100	-0.43222900
C	-5.41713100	0.17627700	-0.13976900
C	-5.17332700	2.33869300	0.09507100
C	-6.48733400	2.08546900	-0.13378000
C	-4.44016800	3.53722600	0.34280600
C	-2.68587600	5.18634900	0.87365000
C	-3.90029200	5.73569800	0.64543000
O	-4.51994900	1.15479400	0.08885900
C	-6.66515500	0.70172900	-0.28785400
C	-4.91933600	4.81516200	0.33979700
H	-5.94019800	5.08396200	0.13263000
H	-7.57497200	0.16770800	-0.47964100
F	-7.43257900	3.00446600	-0.19575900
F	-4.13274800	7.03881800	0.69967200
S	3.77924300	1.64600400	-0.24772700
S	1.63644400	-2.92172100	0.04456800
S	-3.24507900	-1.53477700	-0.06100900
S	-2.76186100	3.48539200	0.71891600
H	-1.77312900	5.68967200	1.13033600
H	1.07701000	5.69167900	-1.00877200

CFOFS-5

0 1

C	-3.79892900	-2.49644600	1.26612600
C	-2.26502600	-4.31149200	0.60154700
C	-1.13714700	-5.12360700	0.28731200
C	1.01142900	-5.41326100	-0.02384400
C	2.36308700	-4.97795500	-0.10955000

C	4.41610400	-3.60621100	-0.18317700
C	5.38837000	-2.56592000	-0.17472100
C	5.98293600	-0.46125000	-0.08116900
C	-4.26922700	0.79542100	2.41717800
C	-5.58324100	0.54568400	2.22790900
C	-5.62299000	-0.77652700	1.74119200
C	-4.35283500	-1.24646400	1.67243600
C	0.39135400	-6.60660800	-0.22228500
C	-0.98820200	-6.44115300	-0.02726000
C	-3.58629300	-4.64551600	0.54447700
C	-4.47566600	-3.63064600	0.91423000
C	3.47923400	-5.74037300	-0.32097700
C	4.62630400	-4.94329500	-0.35744600
C	7.11028100	-1.21455400	-0.18599700
C	6.74969500	-2.56809000	-0.24714800
O	0.05930500	-4.50545400	0.28990200
O	4.92598900	-1.30503300	-0.07550800
O	-3.52262200	-0.26853100	2.09202000
H	-6.41061000	1.20838000	2.39431800
H	-5.54701200	-3.72630000	0.91272400
H	-1.75760800	-7.18373500	-0.10276300
H	3.48079600	-6.80890600	-0.44182000
H	7.39515800	-3.42004900	-0.32857000
C	5.75459500	0.94018300	0.00533500
C	4.73684000	3.18935000	0.12902800
C	6.10191900	3.18715800	0.13680200
C	3.87488000	4.32138800	0.19711100
C	1.90603500	5.27870400	0.18802700
C	2.84613600	6.24742600	0.35110500
O	2.55156800	4.09320500	0.09353200
C	4.11554100	5.65346200	0.35961600
C	6.70007000	1.92763500	0.06660500
H	5.06773800	6.13268600	0.47100400
H	7.76213400	1.76073100	0.06138600
H	-3.73235900	1.65564800	2.76582900
F	-6.69957900	-1.44977200	1.38244800
F	-3.99154700	-5.84856700	0.16476400
F	1.00208100	-7.72895500	-0.54789100
F	5.83777500	-5.44598100	-0.54627900
F	8.33765500	-0.73291000	-0.22291500
F	6.80763100	4.30685500	0.20842800
F	2.58811700	7.53477100	0.47715000
C	0.48673400	5.31131700	0.09131100
C	-1.89796100	4.74121800	-0.22758700
C	-1.66694800	6.05364400	0.06364700
C	-0.32637700	6.40051300	0.24827400
H	0.01400300	7.39280800	0.48338100
F	-2.65122600	6.93601500	0.16664000
C	-3.15466000	4.11200900	-0.46495800
C	-4.39630700	2.38619400	-0.99159900
C	-5.21847100	3.44147000	-0.76168200
C	-4.62379100	1.02636400	-1.35734800
C	-4.35044500	-1.35387000	-1.93516600
C	-5.64108300	-0.95433900	-1.86564000
O	-3.12592000	2.80837000	-0.80398400
C	-4.44064400	4.56055900	-0.42294300
C	-5.82393500	0.40251900	-1.54115200

H	-6.78334800	0.87875300	-1.44270800
H	-4.77737000	5.55036300	-0.18614900
F	-6.53608500	3.40401800	-0.84423000
F	-6.66803700	-1.76247400	-2.08171900
S	-2.09550700	-2.68304600	1.13535300
S	2.73613800	-3.30344800	0.03734900
S	4.15276300	1.57211100	0.03143500
S	-0.40418600	3.88496300	-0.27983900
S	-3.30254900	-0.05000100	-1.59004800
H	-3.97391300	-2.33493800	-2.15563800

CFOFS-6

0 1

C	3.97712400	-0.81665000	1.97214900
C	4.09181000	1.61311800	1.56972100
C	3.82513900	2.98886800	1.31359100
C	2.47279200	4.65718500	0.90928700
C	1.20555500	5.24819600	0.65723100
C	-1.19722000	5.64221800	0.23873600
C	-2.60748100	5.56570100	0.05415800
C	-4.51163400	4.49586700	-0.08983200
C	2.11409400	-3.69979400	2.76186000
C	3.24051600	-4.36731900	2.42994900
C	4.15158100	-3.35737400	2.06046800
C	3.53888900	-2.15597500	2.19958700
C	3.74288300	5.14195500	0.92967600
C	4.62631600	4.08593800	1.19356700
C	5.30625700	0.99456500	1.60417000
C	5.26664300	-0.38493500	1.83516900
C	0.93613500	6.57189400	0.44107300
C	-0.42691600	6.76917400	0.20949200
C	-4.75858200	5.82481100	-0.24303300
C	-3.55117100	6.52743200	-0.15482800
O	2.53385100	3.32979700	1.15229300
O	-3.17842500	4.34547600	0.09132600
O	2.27814200	-2.37696400	2.62800500
H	3.40273200	-5.42774600	2.43197500
H	6.13171000	-1.02238200	1.89227700
H	5.69504400	4.11958300	1.27490200
H	1.67558300	7.35288300	0.44979300
H	-3.39525500	7.58536000	-0.22914000
C	-5.36991300	3.36047500	-0.08833700
C	-6.34275200	1.08391600	-0.03860400
C	-7.25962000	2.09000400	-0.14716200
C	-6.62510800	-0.31189600	0.02465000
C	-6.08000800	-2.43129100	0.09919100
C	-7.43653000	-2.34097300	0.13810600
O	-5.58729500	-1.17199500	0.02872300
C	-7.80549300	-0.99226600	0.09168500
C	-6.73599500	3.38200000	-0.17851300
H	-8.79604900	-0.58497500	0.10880900
H	-7.33474700	4.27124400	-0.25884900
H	1.14876300	-4.02072100	3.10065700
F	5.38184500	-3.53348700	1.61345200
F	6.43891400	1.65961000	1.42817400
F	4.06757900	6.40399400	0.73372500
F	-0.94315400	7.96804000	-0.02025300

F	-5.94984800	6.35476100	-0.44191000
F	-8.56261900	1.85705600	-0.21426900
F	-8.26235000	-3.36722200	0.20644300
C	-5.20363800	-3.55291800	0.09718800
C	-3.26380500	-5.08334600	-0.03155900
C	-4.46129400	-5.70588800	0.16907600
C	-5.57058500	-4.86367800	0.24598500
H	-6.57750600	-5.20579400	0.40142800
F	-4.56119700	-7.02242600	0.28352000
C	-1.98765300	-5.70434300	-0.15683900
C	0.17450400	-5.67245000	-0.50134700
C	-0.20222800	-6.96329700	-0.30473600
C	1.42882700	-5.05746300	-0.76781400
C	3.23731500	-3.43963100	-1.21896000
C	3.65191700	-4.73651200	-1.15104400
O	-0.93413300	-4.90249100	-0.40636400
C	-1.58492800	-7.00565600	-0.08135900
C	2.64334400	-5.67329800	-0.90402600
H	2.80174000	-6.73488400	-0.83465300
H	-2.19483100	-7.86697000	0.10527800
F	0.61795300	-7.99741600	-0.32192700
F	4.92327600	-5.07738300	-1.30702300
S	2.83893800	0.46153900	1.81785800
S	-0.20951600	4.26919500	0.56546700
S	-4.75580400	1.75433400	0.02792300
S	-3.50555500	-3.37904700	-0.13295200
S	1.54213500	-3.34930500	-0.94323600
C	4.02727900	-2.27857200	-1.45627900
C	5.36597000	-2.07726100	-1.60202100
O	3.36072700	-1.11425900	-1.57326700
C	5.49264800	-0.69790300	-1.83165100
H	6.14046100	-2.81664800	-1.54865000
C	4.25828500	-0.13166600	-1.80701800
C	3.79408600	1.21034900	-1.94929900
C	4.55157300	2.34159200	-2.03652700
S	2.11072300	1.56273700	-2.00378500
C	3.73767600	3.48400900	-2.14621800
H	5.62666700	2.36256300	-2.00792800
C	2.40767100	3.23882400	-2.15086600
H	1.60444000	3.94887000	-2.21532600
F	6.62110500	-0.04128300	-2.02577200
F	4.25603900	4.70213600	-2.22127800

TOS-1

0 1

C	-2.61776500	0.84623200	0.00053000
C	-2.58965100	-0.50488100	0.00009200
C	-1.29945000	-1.06869800	-0.00031700
C	-0.34053900	-0.10189700	-0.00013600
C	1.07770200	-0.29497000	0.00002800
C	2.13697000	0.54981300	0.00003700
O	1.55418500	-1.55787100	0.00023100
C	3.32225800	-0.21538100	0.00021700
C	2.89338800	-1.49504000	0.00030000
H	3.40619900	-2.43671900	0.00042800
S	-1.02890500	1.47651300	-0.00063500
H	-3.47794700	1.48844000	0.00104800

F	2.05247500	1.86840900	-0.00009400
H	-1.09718800	-2.12540800	-0.00040100
H	4.33375700	0.14256000	0.00026400
F	-3.67839800	-1.25965100	0.00037000

TOS-2

0 1

C	6.26959600	-0.43462100	-0.00005900
C	5.49111200	-1.53952100	-0.00004000
C	4.10634000	-1.28730600	-0.00002800
C	3.85243400	0.05194500	-0.00003900
C	2.57080500	0.68092700	-0.00003200
C	2.15671700	1.97337000	-0.00004100
O	1.47245000	-0.10479400	-0.00001200
C	0.75378200	1.99867200	-0.00002600
C	0.38508100	0.68771700	-0.00000800
C	-0.89159600	0.04592300	0.00001200
C	-1.17881600	-1.28767100	0.00003100
C	-2.54548000	-1.60101500	0.00004600
C	-3.31483500	-0.47650400	0.00003900
C	-4.74122800	-0.41047900	0.00005000
C	-5.63235200	0.61153500	0.00004400
O	-5.43678000	-1.56768000	0.00007100
C	-6.93478800	0.07160200	0.00006300
C	-6.74219700	-1.26466800	0.00007700
H	-7.41643100	-2.09846700	0.00009200
S	-2.35655400	0.95479600	0.00001200
S	5.30563000	0.97676700	-0.00006300
H	7.34185000	-0.38358000	-0.00007000
F	-5.31168100	1.89217500	0.00002500
F	2.95789800	3.02257500	-0.00006100
F	-0.25183200	-2.22807300	0.00003500
F	5.97390600	-2.77309600	-0.00003300
H	-7.86562300	0.60520200	0.00006500
H	-2.93421200	-2.60411600	0.00006200
H	0.11610900	2.86240600	-0.00002800
H	3.34567400	-2.04835200	-0.00001300

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0 1

C	10.00295300	2.18798000	-0.00008100
C	10.41207100	0.90125400	-0.00005700
O	8.66533100	2.27329600	-0.00008300
C	9.21608300	0.15545200	-0.00004200
C	8.16927800	1.01789700	-0.00005900
C	6.75172600	0.84622600	-0.00005500
C	5.80492700	1.82673400	-0.00007300
C	4.51066700	1.28848700	-0.00006300
C	4.45175900	-0.07501900	-0.00003800
C	3.29386700	-0.91091600	-0.00002200
C	3.12731200	-2.26353900	0.00000400
O	2.09946700	-0.29211800	-0.00003500
C	1.73731800	-2.45045600	0.00000900
C	1.13257300	-1.23444500	-0.00001600
C	-0.22480300	-0.80506900	-0.00002300
C	-0.67436100	0.48286700	-0.00005600
C	-2.07422500	0.53466700	-0.00003900

C	-2.70008200	-0.67831000	0.00000300
S	6.04716000	-0.72610100	-0.00002300
S	-1.52307400	-1.93870200	0.00000100
C	-4.10058800	-0.95793800	0.00004000
C	-4.81003400	-2.12080500	0.00009300
O	-4.93402000	0.09818500	0.00002200
C	-6.15476900	-1.71648500	0.00010400
C	-6.20329800	-0.36100800	0.00005500
C	-7.26567700	0.59282300	0.00003300
C	-7.14435100	1.95017700	-0.00006500
S	-8.91641800	0.09997600	0.00002800
C	-8.40729600	2.57125800	0.00005600
C	-9.45839700	1.72134900	0.00023300
H	-10.50373300	1.96537100	0.00038200
F	9.10895700	-1.16060000	-0.00001700
F	1.10103600	-3.60631200	0.00003300
F	-7.21144600	-2.50774300	0.00015400
H	11.41788100	0.52774400	-0.00005000
H	3.88780200	-3.02118200	0.00002000
H	-4.42998300	-3.12485900	0.00012200
F	3.43747700	2.05783900	-0.00007800
F	-2.72486800	1.68388900	-0.00005400
F	-8.53456300	3.88994200	0.00006700
H	6.02055000	2.88064600	-0.00009300
H	-0.03362300	1.34733500	-0.00008200
H	-6.20434300	2.47399000	-0.00015000
H	10.53127700	3.12107600	-0.00009900

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0 1

C	-11.27973200	2.09466900	0.00014700
C	-12.46470200	1.43544100	0.00017500
C	-13.50644200	2.38502600	0.00017800
C	-12.87156500	3.57664300	0.00015300
O	-11.54053000	3.41890600	0.00013300
C	-9.91668400	1.66922500	0.00013100
C	-8.80748800	2.46161000	0.00010200
C	-7.63250800	1.69738700	0.00008800
C	-7.82188600	0.34593900	0.00010500
C	-6.83984800	-0.69069200	0.00009300
C	-6.93552200	-2.05027900	0.00011100
O	-5.54944000	-0.31130800	0.00005800
C	-5.60752100	-2.49968700	0.00008800
C	-4.78079700	-1.42197400	0.00005500
C	-3.36644700	-1.26133700	0.00002200
C	-2.67854300	-0.08287300	-0.00001500
C	-1.29508300	-0.29993400	-0.00003500
C	-0.91320700	-1.61095000	-0.00001300
C	0.40756700	-2.15250900	-0.00001900
C	0.88169100	-3.43090500	0.00000200
O	1.42702900	-1.27486100	-0.00005000
C	2.27756100	-3.29161300	-0.00001400
C	2.58464300	-1.96891600	-0.00004900
C	3.81039900	-1.24490400	-0.00008100
C	3.96625300	0.11033200	-0.00012300
C	5.32098200	0.46808500	-0.00013200
C	6.19711300	-0.57818900	-0.00009700

S	-9.50913600	-0.00439000	0.00015100
S	-2.30946400	-2.62271700	0.00002100
S	5.32644400	-2.06591700	-0.00008100
C	7.62487500	-0.54707400	-0.00008500
C	8.56618100	-1.53169500	-0.00005800
O	8.21316200	0.66309300	-0.00010300
C	9.79315200	-0.85012000	-0.00006700
C	9.55171500	0.48473000	-0.00010900
C	10.38809600	1.64129400	-0.00015500
C	9.98362900	2.94253100	-0.00028100
S	12.10554900	1.50604700	-0.00026700
C	11.08781400	3.81528500	-0.00007400
C	12.29402500	3.20556800	0.00018600
H	13.26455700	3.66413400	0.00044000
F	-12.59588500	0.12208300	0.00019400
F	-5.20487000	-3.75576100	0.00009600
F	3.16734500	-4.26638400	-0.00000100
F	10.99430000	-1.39821100	-0.00004500
H	-14.56316900	2.19945700	0.00019800
H	-7.82763700	-2.64748300	0.00013900
H	0.31598700	-4.34331100	0.00002800
H	8.40871300	-2.59365900	-0.00003600
F	-6.43825100	2.25973500	0.00005600
F	-0.43664800	0.70319900	-0.00006600
F	5.70861800	1.73071500	-0.00016000
F	10.93489000	5.13129100	0.00000200
H	-8.82801600	3.53716400	0.00008900
H	-3.14147400	0.88838100	-0.00002400
H	3.15148500	0.81319700	-0.00014000
H	8.95438200	3.25661500	-0.00038200
H	-13.22270600	4.58981900	0.00014500

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0 1

C	8.18385800	-1.13205800	-0.00007600
C	9.22103000	-2.00959800	-0.00009700
C	10.42300500	-1.28824400	-0.00010200
C	10.04011000	0.02017000	-0.00008700
O	8.69855400	0.11653000	-0.00006200
C	10.78158500	1.24038600	-0.00008500
C	10.31494600	2.52282900	-0.00011100
C	11.30505900	3.51493000	-0.00010600
C	12.55506600	2.97088000	-0.00007600
C	13.79956500	3.67130400	-0.00005600
C	15.09656000	3.27442700	-0.00003800
O	13.77805000	5.02084100	-0.00005900
C	15.91648300	4.42092500	-0.00002900
C	15.04635000	5.45336000	-0.00004500
C	6.76810600	-1.27885400	-0.00006800
C	5.84035800	-0.27809400	-0.00004700
C	4.53736500	-0.79161900	-0.00005000
C	4.45088500	-2.15452500	-0.00007300
C	3.27616500	-2.96524400	-0.00009500
C	3.07964600	-4.31450500	-0.00019100
O	2.09576600	-2.32077600	0.00000600
C	1.68576400	-4.47047600	-0.00016500
C	1.10818500	-3.24132000	-0.00004700

C	-0.23795200	-2.77972100	0.00002200
C	-0.65314900	-1.47993800	0.00013700
C	-2.05045100	-1.39151900	0.00016600
C	-2.70818900	-2.58813600	0.00007300
C	-4.11501200	-2.82977500	0.00007100
C	-4.85519200	-3.97475200	0.00007400
O	-4.92011100	-1.75239900	0.00007700
C	-6.18772900	-3.53633300	0.00005600
C	-6.20163800	-2.17865300	0.00006500
C	-7.23330500	-1.19751500	0.00006800
C	-7.06851000	0.15649500	0.00009700
C	-8.30168100	0.82085500	0.00009700
C	-9.39843000	0.00785500	0.00006500
S	12.50496500	1.24911100	-0.00006400
S	6.03347700	-2.83807200	-0.00007500
S	-1.56453300	-3.87958100	-0.00003100
S	-8.89847700	-1.64233600	0.00002100
C	-10.77779000	0.37893900	0.00006400
C	-11.93235300	-0.34431400	0.00005300
O	-11.05160800	1.69601000	0.00007000
C	-12.95487300	0.61802900	0.00004600
C	-12.39238000	1.85249100	0.00008300
C	-12.91381900	3.18088200	0.00011000
C	-12.19247600	4.33721300	0.00011000
S	-14.60892300	3.48450500	0.00011400
C	-13.03931000	5.46102900	0.00011600
C	-14.36079200	5.17660700	0.00010700
H	-15.18361400	5.86595500	0.00009200
F	15.50121500	2.01820100	-0.00002900
F	9.09350500	-3.32285100	-0.00011000
F	1.02245000	-5.61069100	-0.00024000
F	-7.26567600	-4.29742500	0.00004500
F	-14.25450400	0.38399500	0.00002500
H	16.98866800	4.46054700	-0.00001500
H	11.42165500	-1.68217500	-0.00012100
H	3.82326100	-5.08868500	-0.00028000
H	-4.50057500	-4.98803600	0.00008300
H	-12.04024800	-1.41243000	0.00004400
F	9.02937500	2.82335700	-0.00013700
F	3.47904000	-0.00220100	-0.00004100
F	-2.67201900	-0.22676900	0.00026600
F	-8.38054200	2.13927800	0.00012900
F	-12.55831700	6.69548500	0.00009800
H	11.10158500	4.57128700	-0.00012000
H	6.07997200	0.77078100	-0.00003500
H	0.01073100	-0.63312600	0.00019200
H	-6.11252200	0.65018800	0.00012300
H	-11.11713700	4.37851200	0.00009700
H	15.17773900	6.51759000	-0.00004600

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0 1

C	4.75530400	-3.80434000	0.00024100
C	5.57578500	-4.88688400	-0.00015500
C	6.90618800	-4.44545700	-0.00023600
C	6.81863800	-3.08478500	0.00012700
O	5.53045800	-2.69801800	0.00041600

C	7.80678800	-2.05501300	0.00023300
C	7.62650300	-0.70148900	0.00066700
C	8.80483000	0.05571400	0.00060100
C	9.90984400	-0.74512900	0.00010200
C	11.27058400	-0.32718600	-0.00015200
C	12.45665100	-0.98892300	-0.00061100
O	11.53529900	0.99703200	0.00008000
C	13.49771400	-0.04992400	-0.00067500
C	12.87022400	1.16048400	-0.00023600
C	3.34242600	-3.63478600	0.00046700
C	2.66365200	-2.45082400	0.00088000
C	1.27897900	-2.65737200	0.00089000
C	0.88678100	-3.96562300	0.00050100
C	13.36360900	2.50033000	-0.00007200
C	12.65931700	3.66903600	0.00039000
C	13.44017900	4.83317700	0.00042200
C	14.77155100	4.53901100	-0.00002900
C	15.86235400	5.46043700	-0.00015100
C	17.21024100	5.30769500	-0.00056000
O	15.59349900	6.78288300	0.00019300
C	17.80614700	6.58484600	-0.00047000
C	16.76141600	7.44028200	-0.00000300
H	16.69564900	8.51056500	0.00023100
C	-0.43882300	-4.49458500	0.00031900
C	-0.92729900	-5.76806400	0.00002700
O	-1.44820700	-3.60583800	0.00042800
C	-2.32153800	-5.61289300	-0.00004000
C	-2.61351800	-4.28697400	0.00020400
C	-3.82905300	-3.54698500	0.00023900
C	-3.96229100	-2.18904600	0.00049600
C	-5.31031500	-1.80937900	0.00038700
C	-6.20382300	-2.84172500	0.00005600
C	-7.62992800	-2.78322800	-0.00017200
C	-8.59249300	-3.74874400	-0.00046000
O	-8.19221500	-1.56136000	-0.00011800
C	-9.80398300	-3.04255400	-0.00058700
C	-9.53475000	-1.71173700	-0.00037900
C	-10.34112000	-0.53920800	-0.00039600
C	-9.90084600	0.75179100	-0.00017400
C	-10.97082100	1.65576200	-0.00019000
C	-12.21134100	1.08655700	-0.00042000
S	15.05291300	2.83963500	-0.00047500
S	9.49206700	-2.41707200	-0.00022100
S	2.27541100	-4.98835100	0.00023000
S	-5.35757600	-4.34397300	-0.00008000
S	-12.06225700	-0.63184200	-0.00078700
C	-13.48693300	1.72923000	-0.00042800
C	-14.76254900	1.25057500	-0.00065800
O	-13.49276100	3.07409000	-0.00016200
C	-15.57273800	2.39757300	-0.00052400
C	-14.77530000	3.49496100	-0.00021900
C	-15.02053100	4.90108800	0.00003400
C	-14.08274500	5.88991800	0.00028400
S	-16.62070700	5.53846100	-0.00006700
C	-14.68731400	7.16051700	0.00076200
C	-16.03911000	7.14666100	0.00081500
H	-16.70741400	7.98666000	0.00124600

F	17.83686300	4.14576400	-0.00097200
F	12.58252400	-2.30184600	-0.00094100
F	5.16495700	-6.14030500	-0.00042300
F	-3.22421100	-6.57544500	-0.00030500
F	-11.01687100	-3.56210300	-0.00087100
F	-16.89260200	2.42736800	-0.00066700
H	18.85282900	6.82060500	-0.00071700
H	14.55324800	-0.24549800	-0.00100000
H	7.79488000	-5.04771200	-0.00052400
H	-0.37150900	-6.68651000	-0.00012200
H	-8.45641500	-4.81361900	-0.00056900
H	-15.08112600	0.22533000	-0.00089300
F	11.33995200	3.71547600	0.00077600
F	6.43513100	-0.13314100	0.00108700
F	0.42813900	-1.64779300	0.00119000
F	-5.67747900	-0.54108600	0.00056300
F	-10.77574900	2.96184400	0.00007700
F	-13.96881400	8.27368800	0.00130000
H	13.03755900	5.83075900	0.00075300
H	8.83554900	1.13118200	0.00087700
H	3.13464600	-1.48344700	0.00110100
H	-3.13585300	-1.49999100	0.00072300
H	-8.86331000	1.03694400	0.00005400
H	-13.02074800	5.71613400	0.00034600