

Determining the stereochemical structures of aurantinin A and B with the assistance of biosynthetic investigations

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Dataset 1. Cartesian coordinates and energies of the low-energy conformers calculated at the B3LYP/6-311G(d,p) level for DFT NMR calculation

(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf A				C	-8.00078600	-1.34927400	-0.49637400
C	-0.15079400	-1.99603000	1.22086900	C	-5.56403100	0.53931900	-0.65620800
C	1.10065000	-1.95077200	0.74217300	O	-6.77050400	1.30013300	-0.50683500
C	-2.55273900	-2.46049400	0.89594900	C	-4.40926600	1.53049800	-1.02083700
C	-1.27031200	-2.51862300	0.47443400	C	-3.03826100	0.96927200	-0.67127600
C	-4.99057700	-2.72066000	0.33725500	O	-2.59837100	0.97737100	0.46233300
C	-5.52368900	-2.46021400	1.72283100	O	-2.35683800	0.49002400	-1.71379400
C	-3.67273000	-2.78120300	0.04398900	C	-4.51730200	2.10634300	-2.43593900
C	-5.99046700	-2.95374900	-0.77092000	C	-5.85239700	-0.52401600	-1.72148200
O	-1.21498000	1.98062800	2.91533100	H	-0.37118900	-1.54518800	2.18468700
C	-0.38622400	3.69680400	1.36577100	H	1.30365800	-2.39866700	-0.22867100
C	0.90135700	4.20664600	0.70946000	H	-2.74951800	-2.07171600	1.89065600
C	1.58001600	3.09666300	-0.09030400	H	-1.06314000	-2.90146600	-0.52361200
C	1.94789100	1.87380400	0.77923200	H	-6.27743000	-3.21209700	1.98095700
C	0.78495600	1.39007200	1.68050100	H	-4.74545600	-2.49398800	2.48490600
C	-0.04903000	2.53625800	2.31415200	H	-6.02235600	-1.48839500	1.79808000
C	2.57427300	0.80325900	-0.15741200	H	-3.40526600	-3.04658600	-0.97741000
C	3.12020200	-0.51888500	0.38469500	H	-5.45582700	-3.40911300	-1.61011600
C	2.31524800	-1.32289000	1.41274100	H	-6.73858800	-3.68782500	-0.44411300
C	2.00114300	-0.60950500	2.72303800	H	-1.74792200	1.59650800	2.20271900
C	1.30664300	0.52567100	2.81006400	H	-1.03736800	3.30025300	0.57518500
C	1.69370500	0.38057100	-1.33423000	H	0.67922900	5.05392100	0.05237200
O	2.42430200	-0.01132500	-2.42415100	H	1.58089700	4.58621100	1.48506700
C	3.57280600	0.71099900	-2.81568300	H	0.90199000	2.78984300	-0.89316000
C	4.88726800	0.26072900	-2.32255000	H	2.48704100	3.47554900	-0.57505100
C	5.13369400	-0.49172100	-1.21369200	H	0.52505300	2.95880100	3.14998900
C	4.24678400	-1.05220200	-0.16475400	H	2.95137000	-2.16733200	1.68201300
C	6.55030800	-0.98974000	-0.91842100	H	1.09397200	0.90081200	3.80798500
C	6.43526200	-1.85289700	0.34599800	H	6.93145300	-1.57192200	-1.76347700
C	4.96474200	-2.30836100	0.34899900	H	7.25480500	-0.17171000	-0.75003400
C	2.48254300	-1.33034100	3.95879800	H	7.12804300	-2.69531500	0.33708300
C	6.00599000	0.78279000	-3.20058700	H	4.69947500	-2.55692400	1.37527600
O	3.42626800	1.59779400	-3.60956100	H	2.18321800	-0.80860000	4.86949400
O	0.50066400	0.25834100	-1.34526200	H	2.07823000	-2.34893200	4.00074400
O	6.75822500	-1.12462900	1.52901200	H	3.57542000	-1.42389500	3.96451900
H	3.43291000	1.31307300	-0.60376500	H	6.96568700	0.32930700	-2.96711600
H	2.76213800	2.18580000	1.44603200	H	5.78117000	0.60640200	-4.25477600
C	-1.14061500	4.80845300	2.10166000	H	6.10238200	1.86684600	-3.08653700
H	0.09014700	0.81971400	1.05751900	H	6.10818600	-0.41951100	1.63153900
C	4.71241800	-3.53406000	-0.54453600	H	-2.02608300	4.41061700	2.59915400
C	-6.76745900	-1.71992600	-1.33494900	H	-0.50546600	5.26776500	2.86732200

H	-1.45177700	5.59648600	1.40945300	C	5.11542900	-0.51170100	-1.21324800
H	5.30455600	-4.38719900	-0.20166100	C	4.23379700	-1.05949500	-0.15590300
H	3.65910200	-3.82247400	-0.51894500	C	6.52528900	-1.03052300	-0.94881100
H	4.97160200	-3.33671400	-1.58837400	C	6.42578600	-1.88585600	0.32185500
H	-7.16379700	-2.08425800	-2.29092800	C	4.94762700	-2.31745700	0.36057100
H	-8.58354900	-0.56797400	-0.98695900	C	2.47109900	-1.30066800	3.97554500
H	-8.63909800	-2.22919500	-0.36946300	C	6.05658800	0.71335700	-3.17111400
H	-7.74494300	-0.97344700	0.49495500	O	3.43063500	1.65095000	-3.56460100
H	-5.30029000	0.06987000	0.29745700	O	0.50813000	0.24650300	-1.35637500
H	-6.67770700	1.86198000	0.26927700	O	6.78822000	-1.15632300	1.49262000
H	-4.52270300	2.34911500	-0.30165600	H	3.43614500	1.30981800	-0.59750400
H	-1.45634700	0.23535800	-1.43188000	H	2.75676100	2.19909400	1.43631300
H	-3.81100000	2.92813000	-2.57499200	C	-1.14082000	4.82913400	2.07539100
H	-4.30352500	1.35698500	-3.19806100	H	0.08449600	0.83107800	1.05577800
H	-5.52638900	2.49260800	-2.59154200	C	4.66067300	-3.55122500	-0.51139600
H	-4.90094600	-0.91539100	-2.09487900	C	-6.75681600	-1.73376100	-1.36005700
H	-6.32153200	0.00164600	-2.55857800	C	-8.02402700	-1.36199100	-0.57277900
B3LYP Energy = -2081.64656012 a.u.				C	-5.53346800	0.51407900	-0.64664300
(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf B				O	-6.70101800	1.26974200	-0.30773600
				C	-4.39141900	1.51948600	-1.01662600
C	-0.16154200	-1.98010200	1.24685300	C	-3.01369300	0.96469800	-0.68809000
C	1.08978000	-1.94496600	0.76684500	O	-2.55719500	0.96629600	0.43797400
C	-2.56544300	-2.44061900	0.92936700	O	-2.34230000	0.49383800	-1.74343800
C	-1.28301500	-2.51182400	0.50991700	C	-4.49927500	2.10754700	-2.42834700
C	-5.00370600	-2.69804300	0.36113800	C	-5.83579800	-0.53677900	-1.72776500
C	-5.55370300	-2.40050800	1.73193800	H	-0.38017700	-1.51420800	2.20383300
C	-3.68394700	-2.77377300	0.08026500	H	1.29127900	-2.40611800	-0.19812700
C	-5.99271100	-2.95505200	-0.75167100	H	-2.76247600	-2.03124700	1.91559200
O	-1.21852300	2.00604300	2.90740100	H	-1.07715000	-2.91405700	-0.48079700
C	-0.38938500	3.71151200	1.34560700	H	-6.26474400	-3.18135100	2.02494000
C	0.89868000	4.21424800	0.68448700	H	-4.77807200	-2.35385400	2.49581800
C	1.57562100	3.09762700	-0.10765900	H	-6.10677400	-1.45632500	1.75962200
C	1.94315700	1.88142200	0.77132700	H	-3.41148000	-3.06581100	-0.93264800
C	0.77965500	1.40510900	1.67496000	H	-5.45126800	-3.43658600	-1.57151900
C	-0.05336800	2.55654400	2.30093100	H	-6.74915900	-3.67557600	-0.41443900
C	2.57203500	0.80446600	-0.15656500	H	-1.75649700	1.62241000	2.19832100
C	3.11029500	-0.51789200	0.39267200	H	-1.04250800	3.31108800	0.55863100
C	2.30665700	-1.31167200	1.42934800	H	0.67735300	5.05721500	0.02163100
C	1.99312900	-0.58766600	2.73381600	H	1.57940700	4.59821800	1.45687600
C	1.29970900	0.54877300	2.81150000	H	0.89634000	2.78503800	-0.90722100
C	1.69966200	0.38140300	-1.33990200	H	2.48216000	3.47195400	-0.59683500
O	2.43991200	0.00054100	-2.42752800	H	0.52193600	2.98378300	3.13357700
C	3.58504300	0.73640600	-2.80411000	H	2.94330900	-2.15380500	1.70497100
C	4.89022100	0.25652400	-2.31710300	H	1.08586400	0.93118800	3.80637700

H	6.87922300	-1.61569200	-1.80484000	C	1.57934700	3.09834000	-0.08221500
H	7.24682400	-0.22131200	-0.80632000	C	1.94512300	1.87176300	0.78311400
H	7.10340700	-2.74029000	0.30258500	C	0.78100800	1.38859100	1.68339400
H	4.69963800	-2.54825900	1.39548900	C	-0.05040200	2.53454400	2.32081500
H	2.16977700	-0.77243000	4.88181800	C	2.56791600	0.80368300	-0.15874800
H	2.06570400	-2.31857300	4.02346600	C	3.11836300	-0.51692900	0.38054400
H	3.56387900	-1.39510000	3.98495900	C	2.31544400	-1.32224400	1.40882200
H	6.81497600	1.22718200	-2.57441300	C	1.99801700	-0.61264400	2.72017300
H	6.54724500	-0.14054200	-3.65043100	C	1.30071500	0.52022400	2.81063500
H	5.71480600	1.39294400	-3.94780000	C	1.68410200	0.38372000	-1.33278600
H	6.15404700	-0.43832900	1.60425300	O	2.41113500	-0.00666600	-2.42496500
H	-2.02746500	4.43642600	2.57470100	C	3.55993400	0.71720800	-2.81571300
H	-0.50421300	5.29138900	2.83805600	C	4.87405700	0.26495600	-2.32748200
H	-1.45043800	5.61379400	1.37862600	C	5.12673200	-0.48617100	-1.21816300
H	5.24739200	-4.40836800	-0.16913800	C	4.25017000	-1.04135200	-0.16176000
H	3.60423600	-3.82450800	-0.46201000	C	6.54513300	-0.98381100	-0.94176700
H	4.90259700	-3.37036700	-1.56241300	C	6.45329100	-1.85696800	0.30785100
H	-7.11422900	-2.11355500	-2.32555200	C	4.97448200	-2.28701600	0.36162300
H	-8.62348800	-0.62900400	-1.11988000	C	2.48275400	-1.33222200	3.95522200
H	-8.64300700	-2.25300600	-0.42973400	C	5.99022800	0.78880000	-3.20862300
H	-7.81268000	-0.92893600	0.40402600	O	3.41067200	1.60600700	-3.60742400
H	-5.24036700	0.03375800	0.28699000	O	0.49054400	0.25979200	-1.34072600
H	-7.11132000	1.56985300	-1.12538200	O	6.80228800	-1.02443100	1.41379900
H	-4.52583800	2.32077200	-0.28616400	H	3.42569600	1.31496600	-0.60471000
H	-1.43819400	0.24104800	-1.47088700	H	2.76137200	2.17837600	1.44938000
H	-3.77503100	2.91333200	-2.56676200	C	-1.13811900	4.80909000	2.11500200
H	-4.31248500	1.36188800	-3.20120600	H	0.08435600	0.82142200	1.05958100
H	-5.49299200	2.53644500	-2.58800600	C	4.69527300	-3.53289800	-0.49592600
H	-4.88833000	-0.93006000	-2.11138500	C	-6.76709700	-1.71953400	-1.33992100
H	-6.29806900	-0.00772000	-2.57161500	C	-8.00205200	-1.35199800	-0.50234500
B3LYP Energy = -2081.64600620 a.u.				C	-5.56522000	0.53769700	-0.65318600
(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf C				O	-6.77242700	1.29701700	-0.50114100
C	-0.15033800	-2.00031700	1.21734400	C	-4.41112200	1.53102100	-1.01331100
C	1.10098000	-1.95199300	0.73869900	C	-3.03958500	0.96986000	-0.66531300
C	-2.55214600	-2.46457500	0.89090500	O	-2.60166600	0.97325200	0.46908700
C	-1.26980500	-2.52043600	0.46899400	O	-2.35609900	0.49833400	-1.70969200
C	-4.99019100	-2.72407600	0.33103200	C	-4.51897000	2.11167900	-2.42654000
C	-5.52446600	-2.47085300	1.71745900	C	-5.85248300	-0.52185400	-1.72239700
C	-3.67226000	-2.78214200	0.03782200	H	-0.37125700	-1.55212500	2.18228900
C	-5.98988100	-2.95426800	-0.77801000	H	1.30363800	-2.39557300	-0.23426900
O	-1.21729600	1.97947500	2.92152000	H	-2.74881000	-2.07923800	1.88697200
C	-0.38588100	3.69812800	1.37588500	H	-1.06277300	-2.89811500	-0.53106000
C	0.90254200	4.20721000	0.72058600	H	-6.26687600	-3.23373900	1.97679000
				H	-4.74478500	-2.49311800	2.47844500

H	-6.03729000	-1.50653700	1.79313500				
H	-3.40471800	-3.04276600	-0.98482000		(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf D		
H	-5.45486100	-3.40782800	-1.61796900	C	-0.15344400	-2.00432000	1.21792400
H	-6.73796600	-3.68933900	-0.45315000	C	1.09626700	-1.95168600	0.73550000
H	-1.74950000	1.59496500	2.20856600	C	-2.55632400	-2.46632500	0.88912800
H	-1.03811500	3.30468400	0.58457200	C	-1.27369800	-2.52059000	0.46797200
H	0.68164200	5.05690300	0.06614200	C	-4.99368700	-2.72142900	0.32241900
H	1.58288700	4.58309800	1.49725900	C	-5.53170800	-2.46523700	1.70687800
H	0.90138600	2.79576500	-0.88683800	C	-3.67499600	-2.78175400	0.03324900
H	2.48747700	3.47712100	-0.56479500	C	-5.99033500	-2.95175000	-0.78941900
H	0.52479200	2.95350000	3.15762500	O	-1.23318100	1.93910700	2.93684700
H	2.95169700	-2.16711300	1.67733900	C	-0.40619600	3.67783200	1.41191400
H	1.08696800	0.89191000	3.80962800	C	0.88102400	4.20124800	0.76560600
H	6.92510900	-1.55329900	-1.79468400	C	1.56607400	3.10413400	-0.04621800
H	7.24181800	-0.16253100	-0.76066700	C	1.93746600	1.87230900	0.80910400
H	7.12351000	-2.72402000	0.25619700	C	0.77528400	1.37289100	1.70296800
H	4.71672200	-2.51139300	1.39758100	C	-0.06703800	2.50716400	2.34690300
H	2.17253900	-0.81835200	4.86677400	C	2.57061100	0.81656400	-0.14007700
H	2.09423800	-2.35719500	3.99199500	C	3.11241500	-0.51507000	0.38128800
H	3.57740300	-1.40605600	3.96500000	C	2.31384300	-1.32850400	1.40556200
H	6.94462500	0.31177400	-3.00109800	C	2.00515900	-0.62777700	2.72377800
H	5.74736500	0.64530600	-4.26347200	C	1.30393200	0.50176500	2.82415700
H	6.11096500	1.86721500	-3.06612500	C	1.69868400	0.41523500	-1.32989300
H	6.71135200	-1.53893200	2.22216700	O	2.43680100	0.07066700	-2.43095800
H	-2.02397400	4.41123700	2.61189800	C	3.58399200	0.81337800	-2.78448800
H	-0.50168800	5.26569600	2.88118900	C	4.88684600	0.31820900	-2.30861500
H	-1.44865700	5.59932900	1.42492600	C	5.11243000	-0.47585900	-1.22230600
H	5.29131300	-4.38336600	-0.15173500	C	4.23895700	-1.04026400	-0.17303800
H	3.64164200	-3.81499800	-0.44041100	C	6.52071900	-1.01132000	-0.98723600
H	4.93122600	-3.35751600	-1.54909700	C	6.43082900	-1.91092000	0.25325400
H	-7.16184500	-2.08175400	-2.29735900	C	4.95013800	-2.30486300	0.32648500
H	-8.58591300	-0.57145900	-0.99286100	C	2.51085100	-1.34899900	3.94907000
H	-8.63877200	-2.23338200	-0.37703100	C	6.05314000	0.79123600	-3.15474300
H	-7.74819800	-0.97650000	0.48956500	O	3.43354300	1.74577400	-3.52468800
H	-5.30131300	0.06429600	0.29851500	O	0.50824100	0.26673600	-1.34528400
H	-6.67825200	1.85887600	0.27480000	O	6.71650300	-1.19549800	1.45619900
H	-4.52575000	2.34675300	-0.29111800	H	3.43398300	1.33366600	-0.56839900
H	-1.45392200	0.24581400	-1.42988500	H	2.74983000	2.17825300	1.48037900
H	-3.81232300	2.93365100	-2.56275100	C	-1.16763900	4.77706100	2.15911300
H	-4.30514200	1.36466100	-3.19092400	H	0.08504800	0.80439000	1.07324100
H	-5.52786900	2.49894900	-2.58103300	C	4.62568600	-3.53755800	-0.53318700
H	-4.90061300	-0.91173500	-2.09624600	C	-6.76377100	-1.71697800	-1.35621000
H	-6.32131800	0.00619300	-2.55816000	C	-7.99968600	-1.34459700	-0.52219300
B3LYP Energy = -2081.64609877 a.u.				C	-5.55966000	0.54002500	-0.67290200

O	-6.76555800	1.30291900	-0.52782700	H	-8.58064900	-0.56375700	-1.01565900
C	-4.40175100	1.52915500	-1.03217300	H	-8.63871400	-2.22422000	-0.39621700
C	-3.03309100	0.96629600	-0.67534500	H	-7.74698200	-0.96762700	0.46947000
O	-2.60436200	0.96561700	0.46240800	H	-5.30031800	0.06909900	0.28123200
O	-2.34101000	0.49903300	-1.71615600	H	-6.67360100	1.86541300	0.24791000
C	-4.50228900	2.10476300	-2.44792900	H	-4.51766200	2.34796000	-0.31362000
C	-5.84572700	-0.52223600	-1.73968500	H	-1.44101600	0.24617500	-1.43011000
H	-0.37176500	-1.56368400	2.18691200	H	-3.79309000	2.92449200	-2.58431100
H	1.29455400	-2.38717100	-0.24201700	H	-4.28703600	1.35443500	-3.20867600
H	-2.75417900	-2.08454000	1.88630900	H	-5.50965100	2.49376300	-2.60808400
H	-1.06668700	-2.89457100	-0.53355000	H	-4.89346700	-0.91516200	-2.10934800
H	-6.27922800	-3.22390400	1.96385700	H	-6.31090200	0.00417100	-2.57853700
H	-4.75479100	-2.49153000	2.47055900	B3LYP Energy = -2081.64605982 a.u.			
H	-6.03929000	-1.49795100	1.78072900				
H	-3.40503600	-3.04319900	-0.98858700	(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf E			
H	-5.45352000	-3.40785000	-1.62687900	C	-0.22489800	-2.02774500	1.00289800
H	-6.74072700	-3.68494800	-0.46557300	C	1.00261200	-1.92131400	0.47203700
H	-1.76023000	1.55976100	2.21744200	C	-2.65368000	-2.41531500	0.74223200
H	-1.05337400	3.28819600	0.61468300	C	-1.39991900	-2.37308800	0.23663200
H	0.65693900	5.05609700	0.11893800	C	-5.12089200	-2.60858400	0.30924800
H	1.55701100	4.57336900	1.54793200	C	-5.55517900	-2.49219400	1.74938200
H	0.89073900	2.80507700	-0.85441200	C	-3.82592000	-2.61673600	-0.07752500
H	2.47224600	3.49259800	-0.52475700	C	-6.20153300	-2.75030000	-0.74027000
H	0.50140000	2.92192200	3.19034200	O	-1.07644300	1.55686000	3.29261600
H	2.95284600	-2.17415000	1.66450500	C	-0.33717000	3.45016000	1.90508300
H	1.09892700	0.87063000	3.82607000	C	0.92868100	4.07440000	1.30396500
H	6.86467200	-1.57030300	-1.86491200	C	1.63160000	3.09103000	0.37024200
H	7.23994000	-0.20005400	-0.83669000	C	2.02257800	1.76849100	1.06942900
H	7.07926300	-2.79166200	0.17134800	C	0.87472700	1.15569500	1.90957500
H	4.72665500	-2.52293600	1.36922500	C	0.05746700	2.20264800	2.70447000
H	2.21080600	-0.83919600	4.86641100	C	2.66484000	0.83918300	-0.00110400
H	2.12630000	-2.37545700	3.98767700	C	3.13426300	-0.58304900	0.31578700
H	3.60520100	-1.41845800	3.94004200	C	2.27789900	-1.50448600	1.19329500
H	6.55146100	-0.05347300	-3.64233800	C	2.05974200	-0.99375500	2.61387200
H	5.70889200	1.47717200	-3.92470500	C	1.41796300	0.14082400	2.89417100
H	6.80600000	1.30599800	-2.55117400	C	1.82900100	0.65048200	-1.26874600
H	7.64087200	-0.92859200	1.43783600	O	2.59464800	0.48327300	-2.38919800
H	-2.05254400	4.36899700	2.64940400	C	3.77820200	1.23138000	-2.57040300
H	-0.53650200	5.23018300	2.93175200	C	5.04356700	0.60521900	-2.14743300
H	-1.48100800	5.57202400	1.47571500	C	5.19209300	-0.37093000	-1.20766400
H	5.19652000	-4.40688300	-0.19446800	C	4.24778900	-1.06728400	-0.30150500
H	3.56420100	-3.78579400	-0.46858600	C	6.56721400	-0.99973100	-1.00487300
H	4.85728700	-3.36821000	-1.58874400	C	6.38006200	-2.07670900	0.07258600
H	-7.15730400	-2.08075200	-2.31358300	C	4.88557800	-2.43610700	-0.02391500

C	2.59182300	-1.89127400	3.70299200	H	2.15299900	-2.89378300	3.63336400
C	6.26078000	1.16161100	-2.85935800	H	3.67826200	-2.01640900	3.61924900
O	3.68895300	2.28605400	-3.13386000	H	7.00947100	1.52543400	-2.15053900
O	0.63933500	0.51692600	-1.33703000	H	6.74254900	0.38977300	-3.46901800
O	6.71893300	-1.60243900	1.37478500	H	5.97721700	1.98578800	-3.50925100
H	3.56190600	1.38112700	-0.31258500	H	6.11718900	-0.88167100	1.59514200
H	2.83356100	2.00179200	1.77121300	H	-1.98512500	3.97094900	3.22746800
C	-1.11529500	4.44554400	2.77111200	H	-0.48568900	4.83344100	3.57948300
H	0.17607600	0.67333500	1.21715100	H	-1.45589900	5.29733200	2.17559000
C	4.58160900	-3.45295500	-1.13684000	H	5.11918000	-4.38874200	-0.95984500
C	-7.04247700	-1.49645600	-1.13699500	H	3.51366300	-3.67927300	-1.17471800
C	-8.08374000	-1.08895100	-0.08388600	H	4.86962100	-3.07509100	-2.12162700
C	-5.52817700	0.62091700	-0.68251200	H	-7.61871900	-1.84676400	-2.00340700
O	-6.56290900	1.46691700	-0.15604800	H	-8.74080200	-0.30928100	-0.47624000
C	-4.41361500	1.52978100	-1.28432200	H	-8.70195600	-1.94985600	0.19062300
C	-3.13894600	0.75993200	-1.59610700	H	-7.63400300	-0.68713600	0.82347500
O	-3.03160200	-0.09488200	-2.44220600	H	-5.07898400	0.04214400	0.13225400
O	-2.10633900	1.16138500	-0.82362700	H	-6.18989400	1.98281700	0.56608200
C	-4.87557800	2.30826900	-2.52643000	H	-4.15797500	2.24767500	-0.49867400
C	-6.19237200	-0.32353500	-1.68884300	H	-1.29202100	0.70176100	-1.10602400
H	-0.37542600	-1.78065000	2.05110100	H	-4.14078100	3.06980200	-2.79927400
H	1.13669500	-2.17089800	-0.57799800	H	-5.00329200	1.64331000	-3.38159500
H	-2.78412100	-2.23906600	1.80716300	H	-5.82466600	2.80363400	-2.31557500
H	-1.26188600	-2.54181900	-0.82936000	H	-5.41560000	-0.73067900	-2.34119200
H	-6.37925400	-3.18210500	1.95560000	H	-6.83927500	0.29677500	-2.31787900
H	-4.74966400	-2.71702600	2.44894700	B3LYP Energy = -2081.64325501 a.u.			
H	-5.92800300	-1.48900100	1.98376500	(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf F			
H	-3.62309700	-2.72832300	-1.14012900	C	-0.16107300	-1.99337100	1.23434700
H	-5.73301500	-3.12297200	-1.65614300	C	1.08892200	-1.94963500	0.75158800
H	-6.91150300	-3.52342000	-0.41672600	C	-2.56538100	-2.45142400	0.91310500
H	-1.61162200	1.21034000	2.56872000	C	-1.28302600	-2.51787300	0.49282000
H	-0.98303000	3.12479800	1.07670300	C	-5.00361500	-2.70258100	0.34149400
H	0.67191900	4.98487200	0.75333900	C	-5.55368000	-2.41556200	1.71458900
H	1.60244000	4.38291800	2.11520100	C	-3.68379400	-2.77640300	0.06057200
H	0.95937500	2.88334000	-0.46712300	C	-5.99255200	-2.95039900	-0.77350500
H	2.53124700	3.54779000	-0.05718100	O	-1.22528700	1.97552800	2.92567300
H	0.65355100	2.53342300	3.56458400	C	-0.39875100	3.69588800	1.37863700
H	2.85217800	-2.42658800	1.29214200	C	0.88883400	4.20711900	0.72317900
H	1.27855700	0.39358300	3.94223900	C	1.56844800	3.09916100	-0.07869200
H	6.92754500	-1.42768500	-1.94694600	C	1.93764700	1.87493000	0.78843900
H	7.31765800	-0.27002900	-0.68832800	C	0.77415400	1.38916900	1.68760700
H	7.02343100	-2.94271300	-0.08721900	C	-0.06076200	2.53337800	2.32387000
H	4.58544600	-2.85786200	0.93392100	C	2.56708800	0.80810600	-0.15086900
H	2.37277100	-1.49223100	4.69495200				

C	3.10892600	-0.51729000	0.38594200	H	-1.05027200	3.30091500	0.58757300
C	2.30674100	-1.32022400	1.41643200	H	0.66629300	5.05584300	0.06800900
C	1.99386600	-0.60834000	2.72748400	H	1.56825400	4.58516300	1.49962100
C	1.29641600	0.52445700	2.81643300	H	0.89043900	2.79345900	-0.88212600
C	1.69403700	0.39469500	-1.33571400	H	2.47492700	3.47959000	-0.56299300
O	2.43072500	0.02963900	-2.42997800	H	0.51368500	2.95443100	3.16021300
C	3.57785500	0.76834700	-2.79830700	H	2.94287100	-2.16562600	1.68424900
C	4.88140300	0.28448100	-2.31477700	H	1.08492400	0.89905100	3.81482000
C	5.11045400	-0.49391800	-1.21778400	H	6.87435100	-1.58133100	-1.84297300
C	4.23756100	-1.04626600	-0.16019900	H	7.23586500	-0.20544300	-0.81156400
C	6.52106500	-1.01586300	-0.97468800	H	7.09621300	-2.76966800	0.20640200
C	6.44154300	-1.89189100	0.27321400	H	4.71425900	-2.51461200	1.39717900
C	4.95647200	-2.29893600	0.35546800	H	2.17399900	-0.80948300	4.87382600
C	2.48151900	-1.32561600	3.96264700	H	2.09202100	-2.35012000	4.00274000
C	6.04747900	0.75070700	-3.16479500	H	3.57611600	-1.40054900	3.96989600
O	3.42300900	1.68675000	-3.55461700	H	6.80225300	1.26492700	-2.56379100
O	0.50239600	0.25348700	-1.34971600	H	6.54281800	-0.09781600	-3.64897300
O	6.82576300	-1.06769300	1.37369400	H	5.70370400	1.43332300	-3.93790600
H	3.43081100	1.31905600	-0.58564700	H	6.74447400	-1.58316500	2.18245800
H	2.75176800	2.18562700	1.45547200	H	-2.03970400	4.40651800	2.61252200
C	-1.15335100	4.80538800	2.11751500	H	-0.51836400	5.26222900	2.88481300
H	0.07979600	0.81934800	1.06367900	H	-1.46393000	5.59561800	1.42744800
C	4.64517700	-3.54458800	-0.49140600	H	5.23486400	-4.40193200	-0.15338000
C	-6.75794200	-1.72464600	-1.37087800	H	3.58886800	-3.81185100	-0.41765100
C	-8.02205900	-1.35728800	-0.57669300	H	4.86643200	-3.37687300	-1.54907600
C	-5.53460700	0.51957000	-0.64667900	H	-7.11887800	-2.09758600	-2.33776800
O	-6.70226000	1.27486600	-0.30657800	H	-8.62301200	-0.62040400	-1.11677700
C	-4.39085300	1.52480300	-1.01056900	H	-8.64088500	-2.24895000	-0.43686900
C	-3.01421700	0.96690100	-0.68133700	H	-7.80684400	-0.93051200	0.40203400
O	-2.56494700	0.95519900	0.44754400	H	-5.24370800	0.03491000	0.28542600
O	-2.33669800	0.51064300	-1.73877500	H	-7.10772500	1.58298100	-1.12367600
C	-4.49564600	2.11910500	-2.41985700	H	-4.52543900	2.32326700	-0.27696100
C	-5.83667800	-0.52609500	-1.73294800	H	-1.43225100	0.25720200	-1.46662400
H	-0.37874300	-1.53852200	2.19683500	H	-3.76987400	2.92426500	-2.55360000
H	1.28792500	-2.39794600	-0.21994900	H	-4.30855400	1.37657700	-3.19565900
H	-2.76266300	-2.05186300	1.90330000	H	-5.48847900	2.55020200	-2.57948900
H	-1.07751900	-2.90876200	-0.50252100	H	-4.88923500	-0.91784100	-2.11824500
H	-6.27151000	-3.19361900	1.99827700	H	-6.29853300	0.00723800	-2.57432000
H	-4.77870700	-2.38336700	2.47989800	B3LYP Energy = -2081.64561385 a.u.			
H	-6.09885100	-1.46706600	1.75195200				
H	-3.41101700	-3.05942400	-0.95484300	(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf G			
H	-5.45075200	-3.42396600	-1.59779200	C	-0.22839900	-2.01877100	1.02104500
H	-6.74823900	-3.67478200	-0.44268500	C	0.99808400	-1.92568800	0.48561600
H	-1.76157700	1.59601400	2.21314000	C	-2.65868400	-2.40764200	0.76690500

C	-1.40391000	-2.38078400	0.26325600	C	-4.89363300	2.34241100	-2.46355900
C	-5.12526600	-2.59691800	0.32563800	C	-6.18590700	-0.32891200	-1.67007800
C	-5.57092100	-2.42990100	1.75709200	H	-0.37725200	-1.74938500	2.06390300
C	-3.82817200	-2.62651700	-0.05248500	H	1.12944300	-2.19775600	-0.55928400
C	-6.19811700	-2.75643500	-0.72923300	H	-2.79296500	-2.20229700	1.82601400
O	-1.01821200	1.61980700	3.33712900	H	-1.26440000	-2.57739800	-0.79785400
C	-0.32075900	3.47566500	1.87899600	H	-6.40337700	-3.10511700	1.97833900
C	0.92783800	4.08168000	1.22501400	H	-4.77333800	-2.64052700	2.47001500
C	1.60395700	3.07357600	0.29804300	H	-5.93319900	-1.41512500	1.95559100
C	2.01395300	1.76973900	1.02090300	H	-3.61998900	-2.77033500	-1.11035000
C	0.87970700	1.17470600	1.89165900	H	-5.72174100	-3.13787000	-1.63730800
C	0.09536900	2.24392200	2.69181700	H	-6.90804600	-3.52822900	-0.40241800
C	2.65380600	0.82301700	-0.03611500	H	-1.60613100	1.29696300	2.64382500
C	3.13226700	-0.59035000	0.30487400	H	-0.99343300	3.13519200	1.07834800
C	2.27656000	-1.50028100	1.19474500	H	0.65594900	4.97789000	0.65844800
C	2.06865000	-0.97040300	2.60972700	H	1.62451100	4.40986700	2.00864800
C	1.43179700	0.16920300	2.88104600	H	0.90876900	2.84274400	-0.51384700
C	1.81658900	0.60513400	-1.29717400	H	2.49126500	3.51899400	-0.16598100
O	2.58042600	0.40649300	-2.41462500	H	0.72594400	2.58990500	3.52094800
C	3.76426400	1.14607900	-2.62118600	H	2.84878200	-2.42254400	1.30225800
C	5.04003300	0.56343100	-2.16479400	H	1.30014600	0.43287800	3.92727300
C	5.20677500	-0.38227100	-1.19891900	H	6.98814500	-1.42840100	-1.85596000
C	4.25213700	-1.07667500	-0.29833900	H	7.31352900	-0.24223100	-0.59896500
C	6.58866900	-0.98621500	-0.93785900	H	7.04344400	-2.90777200	0.02325400
C	6.38001600	-2.05122900	0.14856000	H	4.57149400	-2.86013800	0.95288000
C	4.89664000	-2.43611400	0.00453800	H	2.39808200	-1.44213300	4.69459300
C	2.60820800	-1.85465000	3.70624800	H	2.16702200	-2.85717500	3.65354200
C	6.21537800	1.18666800	-2.88894200	H	3.69372500	-1.98284700	3.61502000
O	3.68170900	2.16729900	-3.24417800	H	7.14745300	0.65908200	-2.70341900
O	0.62652100	0.47576600	-1.36302500	H	6.03402700	1.21174800	-3.96565500
O	6.66359600	-1.55380800	1.45528300	H	6.34307000	2.22766300	-2.57657500
H	3.54640900	1.36381800	-0.36180400	H	6.03994900	-0.84269500	1.64413300
H	2.83200500	2.02423300	1.70725300	H	-1.92717200	4.03425700	3.23716800
C	-1.06796400	4.49321500	2.74639500	H	-0.41283600	4.89436500	3.52763600
H	0.15994700	0.69095900	1.22203400	H	-1.42159000	5.33388000	2.14276700
C	4.64374500	-3.46053000	-1.11412600	H	5.18735300	-4.38845300	-0.91542800
C	-7.04093000	-1.51073300	-1.14638500	H	3.58054600	-3.70097300	-1.18589500
C	-8.11513800	-1.11751100	-0.12015300	H	4.95899100	-3.08291600	-2.09058600
C	-5.50751500	0.59298400	-0.64500800	H	-7.58979100	-1.86437100	-2.02918600
O	-6.45457200	1.39606700	0.07193200	H	-8.79273700	-0.36819600	-0.54194400
C	-4.41762500	1.53384100	-1.24535800	H	-8.71909400	-1.98972900	0.14901100
C	-3.14671800	0.77823000	-1.60222300	H	-7.69798100	-0.68952200	0.78976700
O	-3.05681700	-0.06371400	-2.46455000	H	-5.02364300	-0.00495400	0.12778200
O	-2.09922900	1.16970400	-0.84791000	H	-7.07309600	1.76886100	-0.56466300

H	-4.17038400	2.22635600	-0.43918400	H	3.43527300	1.32851600	-0.57013600
H	-1.29230500	0.70620800	-1.14500500	H	2.74872900	2.18082200	1.47115400
H	-4.14688600	3.08988000	-2.74219400	C	-1.16483400	4.78065400	2.15398000
H	-5.06315000	1.69980400	-3.32863400	H	0.08341800	0.80493500	1.07270000
H	-5.81825700	2.87890700	-2.23351700	C	4.61670200	-3.54366900	-0.53870700
H	-5.41298400	-0.72476300	-2.33481800	C	-6.75935600	-1.71827100	-1.37883000
H	-6.83029400	0.29863400	-2.30152100	C	-8.02321900	-1.34953500	-0.58488700
B3LYP Energy = -2081.64275582 a.u.				C	-5.53418100	0.52430400	-0.65288900
(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf H				O	-6.70119100	1.28170500	-0.31505900
C	-0.16367300	-1.99678700	1.22985500	C	-4.38814400	1.52762200	-1.01484200
C	1.08395600	-1.94945300	0.74133200	C	-3.01289000	0.96793100	-0.68266600
C	-2.56981300	-2.45217300	0.90982400	O	-2.56750100	0.95248900	0.44754300
C	-1.28787200	-2.51610800	0.48799800	O	-2.33168600	0.51523900	-1.73949800
C	-5.00815500	-2.69953400	0.33499900	C	-4.48951500	2.12200100	-2.42432900
C	-5.55971600	-2.41405700	1.70786900	C	-5.83612200	-0.52082200	-1.73966400
C	-3.68805900	-2.77370600	0.05563400	H	-0.37686700	-1.54984200	2.19703300
C	-5.99579800	-2.94518200	-0.78168400	H	1.27687300	-2.39019100	-0.23495000
O	-1.22798900	1.94454400	2.93957100	H	-2.76683400	-2.05795500	1.90219900
C	-0.40653200	3.67931300	1.40672700	H	-1.08411500	-2.90163400	-0.50986600
C	0.87890900	4.20014400	0.75464500	H	-6.28087700	-3.19011500	1.98855900
C	1.56129100	3.10043900	-0.05614500	H	-4.78581900	-2.38659400	2.47446400
C	1.93560300	1.87164100	0.80220600	H	-6.10129100	-1.46351000	1.74685500
C	0.77534400	1.37451100	1.69950400	H	-3.41447000	-3.05469800	-0.96016800
C	-0.06469100	2.51074300	2.34324800	H	-5.45326700	-3.41828000	-1.60578800
C	2.56954600	0.81346800	-0.14413700	H	-6.75257800	-3.66934500	-0.45281300
C	3.10687500	-0.51951900	0.37885500	H	-1.76232700	1.56924600	2.22345500
C	2.30648000	-1.32897900	1.40486400	H	-1.05682500	3.28814700	0.61283100
C	2.00575200	-0.62420500	2.72268000	H	0.65304500	5.05317500	0.10616000
C	1.30688600	0.50680300	2.82194400	H	1.55756300	4.57439600	1.53363400
C	1.70136100	0.41220800	-1.33649100	H	0.88288300	2.79839100	-0.86062100
O	2.44185400	0.06954900	-2.43659600	H	2.46567600	3.48743700	-0.53935600
C	3.59143400	0.81052400	-2.78611000	H	0.50730700	2.92756900	3.18332600
C	4.89174400	0.31502600	-2.30374300	H	2.94249100	-2.17710100	1.66315200
C	5.11158500	-0.48210300	-1.21844500	H	1.10679200	0.87988700	3.82327700
C	4.23341400	-1.04705800	-0.17344600	H	6.86488500	-1.57740300	-1.85655200
C	6.51820800	-1.02009700	-0.97887600	H	7.23788600	-0.21016700	-0.82348400
C	6.42207500	-1.92264400	0.25899900	H	7.06932800	-2.80429800	0.17734900
C	4.94044100	-2.31408900	0.32566600	H	4.71267200	-2.53476500	1.36688500
C	2.51667000	-1.34214200	3.94766800	H	2.22211100	-0.82873300	4.86476800
C	6.06246400	0.78925300	-3.14310200	H	2.13066500	-2.36784700	3.99182100
O	3.44494300	1.74129800	-3.52922700	H	3.61087300	-1.41328700	3.93320700
O	0.51112300	0.26207200	-1.35497700	H	6.56025800	-0.05424300	-3.63341800
O	6.70435100	-1.21084100	1.46488800	H	5.72273700	1.48001100	-3.91074700
				H	6.81454100	1.29872200	-2.53413200

H	7.62877700	-0.94391100	1.45007600	O	2.59290200	0.50902600	-2.38377700
H	-2.04965000	4.37490400	2.64614100	C	3.78126400	1.25338700	-2.55610100
H	-0.53133300	5.23388100	2.92467000	C	5.04127300	0.61918100	-2.13385400
H	-1.47847500	5.57503600	1.47003100	C	5.18622000	-0.36687100	-1.20263500
H	5.18424100	-4.41525800	-0.20026000	C	4.24624700	-1.05879700	-0.29397100
H	3.55437800	-3.78955800	-0.47890400	C	6.55751700	-1.00563800	-1.02347100
H	4.85276700	-3.37183000	-1.59288700	C	6.38236300	-2.11167600	0.01489900
H	-7.12043500	-2.09012500	-2.34610700	C	4.87427100	-2.43057000	-0.02065500
H	-8.62314300	-0.61164700	-1.12477700	C	2.60094100	-1.87046500	3.70754800
H	-8.64320800	-2.24046700	-0.44551900	C	6.26213800	1.17697200	-2.83925500
H	-7.80761800	-0.92351500	0.39408800	O	3.69645900	2.30979600	-3.11778800
H	-5.24569700	0.03913000	0.27970200	O	0.64008000	0.52451300	-1.32891100
H	-7.10573300	1.58856400	-1.13306900	O	6.77529400	-1.55976800	1.27212100
H	-4.52297500	2.32638300	-0.28157800	H	3.56406600	1.38926500	-0.29929300
H	-1.42834800	0.26086200	-1.46495300	H	2.82946800	2.00182200	1.78465100
H	-3.76215700	2.92592700	-2.55689200	C	-1.13129200	4.44783200	2.76314100
H	-4.30227900	1.37912500	-3.19977400	H	0.17377500	0.67757000	1.21266200
H	-5.48139000	2.55467700	-2.58568300	C	4.51720300	-3.45735500	-1.10897000
H	-4.88866300	-0.91381900	-2.12363400	C	-7.03805400	-1.50037000	-1.14745900
H	-6.29606200	0.01324800	-2.58165200	C	-8.08243600	-1.09612900	-0.09617200
B3LYP Energy = -2081.64501986 a.u.				C	-5.52387600	0.61486500	-0.68153600
(2S, 3S, 5R, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a1, Conf I				O	-6.55975200	1.45853500	-0.15308500
C	-0.22734000	-2.02784800	1.00781100	C	-4.40861500	1.52638300	-1.27741100
C	0.99931000	-1.91373800	0.47650700	C	-3.13229500	0.75927700	-1.59019000
C	-2.65534900	-2.42152400	0.74246200	O	-3.02465100	-0.09678600	-2.43513600
C	-1.40094600	-2.37290900	0.23911700	O	-2.09987400	1.16578000	-0.82087800
C	-5.12130900	-2.61714200	0.30153200	C	-4.86838600	2.31000200	-2.51718100
C	-5.56021300	-2.50648000	1.74074000	C	-6.18631800	-0.32561500	-1.69285500
C	-3.82519400	-2.62187700	-0.08115800	H	-0.37863200	-1.78578400	2.05705600
C	-6.19847600	-2.75553200	-0.75202800	H	1.13219300	-2.15597200	-0.57537800
O	-1.09784200	1.55744300	3.27580400	H	-2.78840700	-2.25068900	1.80795400
C	-0.34522300	3.45518500	1.90110300	H	-1.26131400	-2.53510300	-0.82771600
C	0.92645600	4.08089200	1.31400900	H	-6.38456700	-3.19759400	1.94193300
C	1.63711600	3.10092500	0.38252700	H	-4.75657800	-2.73345200	2.44180100
C	2.02084300	1.77464700	1.07869600	H	-5.93413400	-1.50432700	1.97786400
C	0.86655600	1.16099300	1.91008100	H	-3.61912500	-2.72825700	-1.14368400
C	0.04180400	2.20525400	2.70023600	H	-5.72680400	-3.12506800	-1.66758400
C	2.66494000	0.84795900	0.00686100	H	-6.90958300	-3.52977200	-0.43358300
C	3.13194200	-0.57548600	0.31937000	H	-1.62352700	1.20972300	2.54554500
C	2.27445600	-1.49499300	1.19729400	H	-0.98339100	3.13261900	1.06574500
C	2.05486000	-0.98357100	2.61715700	H	0.67520000	4.99392000	0.76495700
C	1.40741800	0.14748900	2.89680300	H	1.59322200	4.38554100	2.13245000
C	1.82995300	0.66413100	-1.26110700	H	0.97246300	2.89841700	-0.46230300
				H	2.54121600	3.55860200	-0.03414700

H	0.62951900	2.53368700	3.56698000	O	-1.74278900	1.11918900	2.79654600
H	2.84724700	-2.41807500	1.29801500	C	-0.58062200	3.20147900	2.20824900
H	1.26968100	0.40269800	3.94455300	C	0.82437200	3.78931200	2.03503500
H	6.92135200	-1.40116300	-1.97705500	C	1.61708500	3.00263600	0.99369500
H	7.30260900	-0.28655700	-0.67353200	C	1.77072700	1.50931300	1.36093700
H	6.98643600	-2.99712400	-0.21799800	C	0.44360100	0.84108800	1.79815700
H	4.58453600	-2.83462900	0.95025100	C	-0.46709600	1.74274200	2.67349000
H	2.37193200	-1.47591900	4.69907700	C	2.52166700	0.81707300	0.19211400
H	2.18548100	-2.88293300	3.63766900	C	2.92365300	-0.65640500	0.25186300
H	3.69073600	-1.96595100	3.62525800	C	1.94331400	-1.71292200	0.77083300
H	7.01863100	1.51433400	-2.12586100	C	1.39240400	-1.50734900	2.17804500
H	6.73121100	0.41527000	-3.47163400	C	0.71515900	-0.42960200	2.57517000
H	5.98447500	2.01968200	-3.46756200	C	1.84519400	0.94923900	-1.17009300
H	6.66457200	-2.23602300	1.94803400	O	2.73145800	0.94607600	-2.20929800
H	-2.00571100	3.97194100	3.20934800	C	3.95230500	1.65345300	-2.11586600
H	-0.50927300	4.83242300	3.57896600	C	5.14864900	0.93219100	-1.64526800
H	-1.46568100	5.30204800	2.16751400	C	5.17988400	-0.20469900	-0.89480400
H	5.04564400	-4.40070300	-0.94225000	C	4.11171500	-1.04178500	-0.29277000
H	3.44528100	-3.66662400	-1.11037900	C	6.51212600	-0.89861000	-0.60334900
H	4.77908000	-3.09324500	-2.10615900	C	6.15950100	-2.16386700	0.19148000
H	-7.61170800	-1.84781600	-2.01678600	C	4.70296600	-2.45660400	-0.21073900
H	-8.73869700	-0.31561500	-0.48824800	C	1.60562200	-2.68078500	3.10424900
H	-8.70110800	-1.95799500	0.17435200	C	6.41567500	1.64820900	-2.06658000
H	-7.63520900	-0.69646600	0.81335900	O	3.96754300	2.78298800	-2.51695300
H	-5.07606100	0.03280500	0.13160500	O	0.66623400	0.93542300	-1.39584200
H	-6.18714800	1.97281400	0.57042800	O	6.28311700	-1.97063700	1.59899800
H	-4.15487900	2.24139900	-0.48850900	H	3.46011100	1.37286100	0.11138400
H	-1.28283000	0.71062000	-1.10375300	H	2.45381400	1.45758500	2.21844200
H	-4.13302700	3.07259900	-2.78547800	C	-1.43732800	4.02386200	3.17564500
H	-4.99465200	1.64864300	-3.37537800	H	-0.13097400	0.61293300	0.89555600
H	-5.81785200	2.80452000	-2.30596600	C	4.58719100	-3.21868500	-1.54147800
H	-5.40801900	-0.73040300	-2.34483800	C	-6.28731000	-1.37321300	-0.82746800
H	-6.83161400	0.29725100	-2.32106500	C	-7.51736000	-1.40556200	-1.74425500
B3LYP Energy = -2081.64300720 a.u.				C	-5.43142800	1.04683300	-1.18034400
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf A				O	-5.61443000	1.37422400	0.19307300
C	-0.42906900	-2.25945700	-0.03073900	C	-4.31047200	1.90007500	-1.82998500
C	0.87168000	-2.03380100	-0.26785500	O	-2.95455800	1.55826200	-1.23539900
C	-2.68713700	-2.91336700	-0.89122000	O	-2.75553400	1.42807300	-0.03652300
C	-1.37031100	-2.64661800	-1.06212200	O	-2.00267600	1.43816600	-2.15336800
C	-4.74932800	-2.91752800	0.53138400	C	-4.57181800	3.40927100	-1.66930600
C	-5.34421800	-2.95756200	1.91533200	C	-5.18138300	-0.45621700	-1.37733600
C	-3.40849900	-2.93059400	0.36705300	H	-0.80441100	-2.12379500	0.97815600
C	-5.75002500	-2.81514800	-0.59670500	H	1.24783800	-2.15137600	-1.28268100
				H	-3.25831200	-3.13443700	-1.78746100

H	-0.97187200	-2.70092000	-2.07232600	H	-4.24052500	-0.70022900	-0.87821900
H	-5.99223300	-2.09298000	2.09638800	H	-5.03373700	-0.65975400	-2.44658100
H	-5.97106900	-3.84894900	2.04108100	B3LYP Energy = -2081.66054321 a.u.			
H	-4.57452400	-2.96955600	2.68903300	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf B			
H	-2.80455300	-2.94792200	1.27021500	C	-0.42318700	-2.26445700	-0.02311500
H	-5.33033500	-3.18557300	-1.53723200	C	0.87727100	-2.03553000	-0.25881600
H	-6.60435600	-3.46219900	-0.36447600	C	-2.67894600	-2.92106000	-0.88901400
H	-2.12756800	1.09640500	1.90850900	C	-1.36173900	-2.65399500	-1.05618800
H	-1.07361600	3.19773400	1.22687700	C	-4.74495900	-2.92416600	0.52869100
H	0.75816800	4.83981100	1.73370900	C	-5.34292300	-2.96160900	1.91144200
H	1.34828800	3.77629700	3.00070000	C	-3.40380500	-2.93686400	0.36736100
H	1.10441100	3.09861500	0.03095800	C	-5.74321300	-2.82433900	-0.60179100
H	2.61299600	3.44059400	0.86102400	O	-1.74302300	1.13105700	2.80349400
H	-0.06129700	1.75690700	3.69396100	C	-0.57978600	3.21084600	2.20896600
H	2.52762400	-2.63272100	0.82499400	C	0.82540100	3.79667700	2.03086400
H	0.31876400	-0.43902800	3.58737200	C	1.61461400	3.00724700	0.98901400
H	7.02317600	-1.14722000	-1.53888100	C	1.76804600	1.51428200	1.35777000
H	7.19243000	-0.26975300	-0.02412700	C	0.44053000	0.84890800	1.79906300
H	6.82606800	-2.99626100	-0.03748400	C	-0.46645300	1.75272300	2.67586200
H	4.25726700	-3.05737100	0.58046200	C	2.51460200	0.82121600	0.18651200
H	1.13568800	-2.51522700	4.07522200	C	2.92412200	-0.64903800	0.25354200
H	1.18842500	-3.59985000	2.67538400	C	1.94762700	-1.70562100	0.77888400
H	2.67361200	-2.86673500	3.27133100	C	1.39227500	-1.49734500	2.18370700
H	7.30692400	1.04666800	-1.90786200	C	0.71094700	-0.42112700	2.57718000
H	6.36517000	1.93091500	-3.12004600	C	1.82932700	0.94527700	-1.17079000
H	6.52854700	2.58073800	-1.50495000	O	2.70769300	0.94064400	-2.21569200
H	5.63429900	-1.30909600	1.86669200	C	3.92913400	1.64931900	-2.13058500
H	-2.41430900	3.56014000	3.31715700	C	5.12801800	0.93086300	-1.66677500
H	-0.95579800	4.09691800	4.15727100	C	5.17043700	-0.20026900	-0.90624200
H	-1.58548900	5.04051200	2.79992200	C	4.11671100	-1.03130600	-0.27916500
H	5.09938500	-4.18288200	-1.47723000	C	6.51032600	-0.88443600	-0.63882300
H	3.54078400	-3.40966500	-1.78964300	C	6.19191000	-2.14616200	0.15960000
H	5.02262900	-2.65648400	-2.37215000	C	4.71497100	-2.43906200	-0.16870600
H	-6.59296300	-0.96391100	0.14047500	C	1.60675600	-2.66616100	3.11526000
H	-7.91922200	-0.40315900	-1.91465300	C	6.39060700	1.64607100	-2.10482200
H	-7.26789200	-1.83530500	-2.72093300	O	3.93968700	2.77734600	-2.53728100
H	-8.31889800	-2.00926300	-1.30897700	O	0.64837900	0.92593200	-1.38932300
H	-6.36872800	1.33517600	-1.66720500	O	6.37127200	-1.81367300	1.53614700
H	-4.74476800	1.29905600	0.61122400	H	3.45098200	1.37935300	0.10029800
H	-4.26634300	1.65773900	-2.89470900	H	2.45426800	1.46172700	2.21222300
H	-1.13668500	1.23241200	-1.74547900	C	-1.43292200	4.03548600	3.17757600
H	-3.77232600	3.99921300	-2.12362900	H	-0.13700200	0.62076300	0.89834600
H	-5.51167100	3.67491300	-2.15956400	C	4.55210900	-3.25206000	-1.46422800
H	-4.65446900	3.67150000	-0.61435500				

C	-6.28465000	-1.38406400	-0.83283800	H	3.49842500	-3.45664800	-1.66568700
C	-7.51171100	-1.41937800	-1.75353400	H	4.95190600	-2.71596600	-2.32932300
C	-5.43503200	1.03908900	-1.17605200	H	-6.59478300	-0.97680700	0.13452200
O	-5.61950200	1.36079800	0.19859200	H	-7.91569400	-0.41793200	-1.92474600
C	-4.31682200	1.89847100	-1.82228700	H	-7.25803100	-1.84789000	-2.72967800
C	-2.95987100	1.55785400	-1.22894500	H	-8.31305000	-2.02546100	-1.32114400
O	-2.76109300	1.42628500	-0.03010900	H	-6.37325200	1.32589500	-1.66213900
O	-2.00876000	1.43995500	-2.14742400	H	-4.74896900	1.28946600	0.61579800
C	-4.58275700	3.40609300	-1.65549000	H	-4.27208200	1.66048300	-2.88797300
C	-5.18017200	-0.46253500	-1.37804900	H	-1.14159100	1.23277300	-1.74171300
H	-0.80068400	-2.12738000	0.98476200	H	-3.78564000	4.00022300	-2.10854000
H	1.25398000	-2.15213900	-1.27357900	H	-5.52413500	3.67080600	-2.14337400
H	-3.24751000	-3.14303400	-1.78669000	H	-4.66464100	3.66416800	-0.59944800
H	-0.96066200	-2.70844900	-2.06537300	H	-4.23941700	-0.70564100	-0.87826000
H	-5.98866800	-2.09494100	2.09065200	H	-5.03035700	-0.66211700	-2.44774200
H	-5.97259600	-3.85109600	2.03678400	B3LYP Energy = -2081.66020715 a.u.			
H	-4.57475200	-2.97505000	2.68666700	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf C			
H	-2.80194400	-2.95226100	1.27197600	C	-0.43343400	-2.26072300	-0.01642000
H	-5.31991600	-3.19259700	-1.54154600	C	0.86546900	-2.02835200	-0.25730900
H	-6.59600400	-3.47445100	-0.37219300	C	-2.69174600	-2.91612300	-0.87780100
H	-2.12842800	1.10439800	1.91586600	C	-1.37481900	-2.64932800	-1.04728600
H	-1.07558200	3.20610500	1.22898400	C	-4.75626000	-2.91300600	0.54144000
H	0.75952100	4.84683500	1.72804700	C	-5.35384400	-2.94619400	1.92449200
H	1.35189900	3.78456100	2.99510800	C	-3.41526400	-2.92852600	0.37939600
H	1.09998500	3.10245000	0.02708900	C	-5.75491300	-2.81411600	-0.58894400
H	2.61069400	3.44370100	0.85363500	O	-1.76196400	1.10386100	2.78932900
H	-0.05781600	1.76780800	3.69516000	C	-0.60320200	3.19212100	2.21564200
H	2.53402500	-2.62415000	0.83727800	C	0.80082000	3.78545600	2.05400800
H	0.31181900	-0.43022200	3.58832000	C	1.60239300	3.00576600	1.01421000
H	7.01114900	-1.12828700	-1.58004200	C	1.75982900	1.51164500	1.37663400
H	7.18775800	-0.25090700	-0.06246000	C	0.43310500	0.83657700	1.80532000
H	6.84059600	-2.98615900	-0.11808000	C	-0.48720800	1.73213700	2.67651700
H	4.28410500	-3.00839100	0.65614000	C	2.51919300	0.82731100	0.20805700
H	1.12468000	-2.50305400	4.08070600	C	2.91701900	-0.64721800	0.25514100
H	1.20536800	-3.59173200	2.68512500	C	1.94148600	-1.70590600	0.77650000
H	2.67536200	-2.83660800	3.29619300	C	1.39577200	-1.50433600	2.18608400
H	7.28177000	1.03734900	-1.97539500	C	0.71094400	-0.43197900	2.58364000
H	6.31904900	1.94672800	-3.15183800	C	1.85309400	0.97460100	-1.15697500
H	6.52264800	2.56779800	-1.52944700	O	2.74802500	1.01284600	-2.18780100
H	6.14162900	-2.58273000	2.06744700	C	3.96506400	1.72045600	-2.05777500
H	-2.41002900	3.57298600	3.32248600	C	5.14920700	0.96210400	-1.62165100
H	-0.94847800	4.10939400	4.15773000	C	5.16008600	-0.19867900	-0.90411400
H	-1.58094400	5.05183400	2.80089000	C	4.10504500	-1.03090100	-0.28863900
H	5.07307200	-4.21126900	-1.38928900				

C	6.49175800	-0.90991000	-0.68994200	H	6.79628700	-3.03362600	-0.22075800
C	6.16820100	-2.19040600	0.09112200	H	4.28440000	-3.01626000	0.62926900
C	4.68659100	-2.44921200	-0.20840600	H	1.15997700	-2.51010600	4.08642600
C	1.63150400	-2.67050200	3.11522400	H	1.23107500	-3.59903800	2.69050400
C	6.45829200	1.60632100	-2.03635500	H	2.70364100	-2.83172800	3.27956200
O	3.97278900	2.86971700	-2.40092800	H	7.01480500	0.95832000	-2.72185400
O	0.67650900	0.93780100	-1.39514000	H	6.27358800	2.55461600	-2.53478600
O	6.26457700	-1.99608200	1.50295900	H	7.10372900	1.79464300	-1.17383000
H	3.46028000	1.38065400	0.14255800	H	7.18577500	-1.82623000	1.72341200
H	2.43979200	1.45790100	2.23598100	H	-2.44544300	3.53958900	3.31395100
C	-1.46941900	4.00771000	3.18037400	H	-0.99442100	4.07900000	4.16535400
H	-0.13504300	0.60559300	0.89932100	H	-1.61909500	5.02523800	2.80746600
C	4.47796500	-3.24454500	-1.50759000	H	4.97314000	-4.21804800	-1.44869200
C	-6.28693000	-1.37192800	-0.82992100	H	3.41536800	-3.41890200	-1.68867000
C	-7.51650600	-1.40596200	-1.74731300	H	4.87443400	-2.71298600	-2.37749400
C	-5.42352400	1.04275300	-1.20509200	H	-6.59175200	-0.95486900	0.13500500
O	-5.61221500	1.38542600	0.16384600	H	-7.91538600	-0.40341000	-1.92376400
C	-4.29659100	1.88538300	-1.85798400	H	-7.26761200	-1.84207600	-2.72134500
C	-2.94449500	1.54792700	-1.25166300	H	-8.32005700	-2.00490400	-1.30911000
O	-2.75494500	1.42319200	-0.05074000	H	-6.35751600	1.32886300	-1.69966500
O	-1.98571900	1.42671000	-2.16197300	H	-4.74445600	1.31240600	0.58653400
C	-4.55483400	3.39708300	-1.71647200	H	-4.24678000	1.63091000	-2.91965400
C	-5.17715600	-0.46299100	-1.38525500	H	-1.12112000	1.22582800	-1.74792400
H	-0.80639700	-2.12949800	0.99390300	H	-3.75109500	3.97942100	-2.17308000
H	1.23610500	-2.13925600	-1.27488700	H	-5.49128700	3.65956300	-2.21495500
H	-3.26174000	-3.13905100	-1.77436100	H	-4.64257200	3.67180500	-0.66508800
H	-0.97577100	-2.70448000	-2.05729200	H	-4.23865500	-0.70447800	-0.88067500
H	-6.00194000	-2.08053500	2.10027100	H	-5.02663900	-0.67790000	-2.45191900
H	-5.98118900	-3.83683000	2.05361500	B3LYP Energy = -2081.66017200 a.u.			
H	-4.58551300	-2.95447600	2.69960800				
H	-2.81265800	-2.94227600	1.28352700	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf D			
H	-5.33491100	-3.19203600	-1.52639400	C	0.42026500	-3.20421200	-0.16631900
H	-6.61185500	-3.45685600	-0.35415300	C	0.57661000	-1.93624800	0.23756300
H	-2.13866500	1.07946900	1.89797900	C	-2.04243400	-3.60502700	-0.57379500
H	-1.08969900	3.19021300	1.23102400	C	-0.73473600	-3.75390800	-0.88106000
H	0.73299500	4.83717400	1.75701600	C	-3.88453300	-2.72131200	0.88825600
H	1.31867800	3.76959200	3.02291500	C	-4.26026000	-2.06133500	2.19064900
H	1.09404600	3.10395800	0.04926300	C	-2.58365000	-2.94401400	0.59879400
H	2.59710000	3.44806100	0.88797100	C	-5.03855400	-3.06355200	-0.02639300
H	-0.08860300	1.74485100	3.69980500	O	-1.95651000	1.67297900	2.62060300
H	2.52885000	-2.62409400	0.82711400	C	-0.72554900	3.64268700	1.82835900
H	0.32071300	-0.44072800	3.59828800	C	0.69725900	4.17420700	1.62276100
H	6.95850600	-1.13672900	-1.65525600	C	1.49309500	3.25210700	0.70169900
H	7.20196900	-0.28106800	-0.14382200	C	1.59985100	1.80888600	1.24368800

C	0.25310200	1.22982500	1.74057800	H	-4.69793900	-3.64620100	-0.88660500
C	-0.66086600	2.25022100	2.47108600	H	-5.73957300	-3.70515800	0.52413000
C	2.33612900	0.96520400	0.16796900	H	-2.30765000	1.54827000	1.72743100
C	2.69941900	-0.50468600	0.37702900	H	-1.19320700	3.52833200	0.84112700
C	1.75047500	-1.47201400	1.09039400	H	0.66367900	5.18229900	1.19710200
C	1.19230300	-1.04756100	2.45309300	H	1.19923000	4.26597000	2.59576100
C	0.49534700	0.06729600	2.68006600	H	1.00484700	3.24792700	-0.27894000
C	1.65520700	0.95784800	-1.19840600	H	2.50254000	3.64790400	0.54306800
O	2.51695100	0.92212800	-2.24599300	H	-0.28992000	2.37850300	3.49652300
C	3.75379700	1.61431500	-2.20185400	H	2.33358500	-2.36899100	1.28193700
C	4.92528500	0.88020000	-1.69710800	H	0.07049400	0.18879200	3.67315400
C	4.91688000	-0.21800500	-0.88760000	H	6.70088500	-1.24212400	-1.55660600
C	3.84954100	-0.97385700	-0.18859200	H	6.95962300	-0.29377900	-0.10445800
C	6.23545100	-0.93587700	-0.61351400	H	6.50624800	-3.01206300	0.04780100
C	5.88388300	-2.14349900	0.26654900	H	3.96845200	-2.94150700	0.79562700
C	4.39831300	-2.39946100	-0.04477500	H	0.89610100	-1.78502200	4.46486100
C	1.38263800	-2.08298500	3.53458800	H	0.96878000	-3.05093700	3.22856500
C	6.24452000	1.46005000	-2.16963400	H	2.44717900	-2.24472500	3.74332300
O	3.77689500	2.71768600	-2.66866800	H	6.91116500	1.67687300	-1.33098400
O	0.47133800	0.86611600	-1.39710800	H	6.76787200	0.75499400	-2.82427100
O	6.09376500	-1.88174000	1.65270700	H	6.07858300	2.38130300	-2.72241500
H	3.28804100	1.48470400	0.02760600	H	5.49136800	-1.17666200	1.91739100
H	2.27503800	1.83721000	2.10786000	H	-2.57805500	4.17675300	2.83099000
C	-1.58530400	4.59632800	2.66348800	H	-1.12806800	4.77652600	3.64287000
H	-0.31695700	0.90743800	0.86479400	H	-1.69591600	5.56298700	2.16350100
C	4.19403900	-3.22144100	-1.32938600	H	4.63471100	-4.21656200	-1.22094400
C	-5.82996000	-1.83230500	-0.54396000	H	3.13151100	-3.33772800	-1.54934800
C	-7.02815200	-2.28473700	-1.38808600	H	4.65476300	-2.73889700	-2.19575500
C	-5.39634900	0.59423600	-1.32465100	H	-6.21583200	-1.28806100	0.32229700
O	-5.60983100	1.08931900	-0.00564500	H	-7.61399500	-1.43199200	-1.74265900
C	-4.43220800	1.50778500	-2.12698500	H	-6.69959300	-2.85161000	-2.26629600
C	-3.03787800	1.44684400	-1.52700100	H	-7.70050000	-2.92525200	-0.80973100
O	-2.81355800	1.57112000	-0.33092200	H	-6.37467500	0.65483700	-1.81266200
O	-2.08927600	1.24519500	-2.43244800	H	-4.73346900	1.25686900	0.36960100
C	-4.91999700	2.96692300	-2.17267800	H	-4.36257200	1.12119900	-3.14655200
C	-4.91145300	-0.86483000	-1.31209700	H	-1.20648900	1.17561800	-2.01108000
H	1.23354700	-3.90827800	0.01793600	H	-4.23040500	3.59538400	-2.74138300
H	-0.18456000	-1.20184800	0.00447100	H	-5.89917000	3.01328400	-2.65566300
H	-2.75009100	-4.08499800	-1.24261100	H	-5.02026400	3.37112100	-1.16520800
H	-0.49256600	-4.39349700	-1.72751900	H	-3.91817300	-0.88443100	-0.85366300
H	-4.75057000	-1.09677200	2.02131700	H	-4.78344300	-1.21241400	-2.34570500
H	-4.97325600	-2.67849000	2.75067700	B3LYP Energy = -2081.65557390 a.u.			
H	-3.38665500	-1.88430100	2.81969900				
H	-1.85202500	-2.61980900	1.33314500	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf E			

C	0.41940300	-3.22182100	-0.14780500	C	-3.01684500	1.44241700	-1.55239800
C	0.58041700	-1.94968300	0.24125500	O	-2.80606100	1.57253000	-0.35439300
C	-2.04482600	-3.61653800	-0.55094500	O	-2.05859800	1.24254300	-2.44743500
C	-0.73766800	-3.77673100	-0.85517900	C	-4.89051800	2.95465200	-2.23816300
C	-3.88204600	-2.69887900	0.89678100	C	-4.89810600	-0.86492300	-1.32537600
C	-4.25325500	-2.01697000	2.18912500	H	1.23053700	-3.92644800	0.04463200
C	-2.58260100	-2.93459800	0.61119700	H	-0.17738300	-1.21486300	-0.00183700
C	-5.03798300	-3.04713900	-0.01321300	H	-2.75480400	-4.10257300	-1.21293700
O	-1.98192600	1.63283500	2.61167100	H	-0.49858300	-4.42975400	-1.69227200
C	-0.74714800	3.61719500	1.86213700	H	-4.74343300	-1.05500500	2.00547600
C	0.67650700	4.15600000	1.68232000	H	-4.96493900	-2.62426100	2.76160700
C	1.48654200	3.24964300	0.75810700	H	-3.37753400	-1.82933800	2.81204900
C	1.59234000	1.79941800	1.28125300	H	-1.84920400	-2.60365000	1.34069600
C	0.24272900	1.20991600	1.75926300	H	-4.70038400	-3.64326200	-0.86535700
C	-0.68606000	2.21710200	2.48857800	H	-5.74270000	-3.67729700	0.54584800
C	2.33626800	0.97174400	0.19841200	H	-2.31867300	1.51820300	1.71166000
C	2.69519100	-0.50261900	0.37899000	H	-1.20098700	3.51347300	0.86726600
C	1.75370600	-1.47834400	1.09019100	H	0.64488600	5.17013500	1.27099000
C	1.19296900	-1.06558000	2.45556400	H	1.16592300	4.23497900	2.66279900
C	0.48683000	0.04154300	2.69010800	H	1.00947900	3.25800500	-0.22811200
C	1.66086000	0.98667400	-1.16987400	H	2.49634600	3.65079900	0.61689000
O	2.52036100	0.99372200	-2.21800700	H	-0.33138900	2.33451700	3.52098200
C	3.76141100	1.67895200	-2.15056600	H	2.34418100	-2.37094800	1.28041500
C	4.92444300	0.92970700	-1.65239800	H	0.06306300	0.15442100	3.68477800
C	4.90654700	-0.19634800	-0.88118300	H	6.70446900	-1.17339900	-1.58903200
C	3.83828700	-0.96377600	-0.20355300	H	6.92763100	-0.32025500	-0.06945400
C	6.22061800	-0.92973900	-0.63830200	H	6.46423800	-3.05338100	-0.15881800
C	5.87183200	-2.18616900	0.15784900	H	3.93678200	-2.96029500	0.71161100
C	4.37012200	-2.39697700	-0.11526100	H	0.90040200	-1.81866600	4.46216800
C	1.39540400	-2.10343000	3.53219200	H	0.99991700	-3.07726100	3.22016300
C	6.24982900	1.52129200	-2.09291000	H	2.46244200	-2.24375500	3.74454300
O	3.79172800	2.78905700	-2.60157300	H	6.92290300	1.67180600	-1.24541200
O	0.47782600	0.87807800	-1.37198400	H	6.76007800	0.85607800	-2.79834600
O	6.12553700	-1.88561000	1.53041700	H	6.09264800	2.47896800	-2.58283800
H	3.29044900	1.49107900	0.07432900	H	5.89251900	-2.65611900	2.05807000
H	2.26173900	1.81652200	2.14972800	H	-2.61444700	4.13144400	2.84769300
C	-1.62162400	4.55737600	2.69725700	H	-1.17728100	4.72849400	3.68420900
H	-0.31559600	0.89102000	0.87483900	H	-1.73056400	5.52920500	2.20696900
C	4.12246700	-3.17440000	-1.42055800	H	4.54799400	-4.18042300	-1.35809500
C	-5.82266200	-1.81886400	-0.54773000	H	3.05358900	-3.26416100	-1.62003700
C	-7.02102700	-2.27655000	-1.38875900	H	4.57322400	-2.66979600	-2.27954500
C	-5.37911800	0.59511100	-1.36143200	H	-6.20795500	-1.26215400	0.31081100
O	-5.60306500	1.10822700	-0.05100900	H	-7.60277800	-1.42580900	-1.75465200
C	-4.40556200	1.49550900	-2.16684300	H	-6.69304500	-2.85526500	-2.25946400

H	-7.69708100	-2.90742900	-0.80410700	O	3.80589700	2.81098000	-2.57840200
H	-6.35294400	0.65139300	-1.85893000	O	0.48481300	0.88710000	-1.37658300
H	-4.72927500	1.28037200	0.32847200	O	5.97757600	-2.00675000	1.56036300
H	-4.32614600	1.09479100	-3.18027700	H	3.29167000	1.49339200	0.08357700
H	-1.17857400	1.17937500	-2.01777900	H	2.25838700	1.81093100	2.15572800
H	-4.19367000	3.57407500	-2.80788600	C	-1.63381600	4.53565200	2.71255100
H	-5.86442800	2.99588400	-2.73219900	H	-0.31408900	0.87846000	0.87747600
H	-5.00087900	3.37256500	-1.23736000	C	4.11207000	-3.16584500	-1.44278700
H	-3.90714100	-0.88055000	-0.86189500	C	-5.82380800	-1.81239100	-0.54478500
H	-4.76606000	-1.22758000	-2.35332300	C	-7.02450700	-2.26927000	-1.38292400
B3LYP Energy = -2081.65538199 a.u.				C	-5.37823400	0.59909600	-1.36560300
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf F				O	-5.60326600	1.11602300	-0.05687400
C	0.41693300	-3.22077300	-0.15849500	C	-4.40253200	1.49621400	-2.17202500
C	0.57973100	-1.94978400	0.23376400	C	-3.01455900	1.44360500	-1.55581200
C	-2.04903400	-3.61173700	-0.55604600	O	-2.80507900	1.57252500	-0.35755600
C	-0.74275500	-3.77299900	-0.86355100	O	-2.05488200	1.24640500	-2.45013100
C	-3.88165300	-2.69368200	0.89730900	C	-4.88567700	2.95578600	-2.24775300
C	-4.24905000	-2.01234500	2.19107600	C	-4.89892800	-0.86136500	-1.32549700
C	-2.58317100	-2.93023200	0.60810200	H	1.22800100	-3.92628500	0.03013700
C	-5.04020600	-3.04114500	-0.00974100	H	-0.17858100	-1.21411600	-0.00528000
O	-1.98573600	1.61097100	2.61240500	H	-2.76116900	-4.09645500	-1.21672000
C	-0.75580900	3.60195600	1.87386100	H	-0.50668500	-4.42580100	-1.70171500
C	0.66619100	4.14622800	1.69744000	H	-4.74288600	-1.05184400	2.00945400
C	1.47916400	3.24663300	0.76925000	H	-4.95636300	-2.62155400	2.76700100
C	1.58950800	1.79479800	1.28682300	H	-3.37110200	-1.82183600	2.80995000
C	0.24237500	1.19783800	1.76292600	H	-1.84752200	-2.60062600	1.33591800
C	-0.69116000	2.19913600	2.49419500	H	-4.70545500	-3.63931600	-0.86158200
C	2.33709700	0.97314100	0.20181200	H	-5.74501500	-3.66909200	0.55170600
C	2.69440300	-0.50286100	0.37294200	H	-2.31991700	1.49819200	1.71126300
C	1.75583600	-1.48295000	1.08094300	H	-1.20859100	3.50136700	0.87820900
C	1.20228400	-1.07580200	2.45089800	H	0.63153100	5.16228200	1.29101900
C	0.49425300	0.02880900	2.69141000	H	1.15491200	4.22189500	2.67856300
C	1.66627300	0.99683000	-1.16838500	H	1.00173400	3.25773800	-0.21673900
O	2.53035300	1.01482400	-2.21422800	H	2.48766100	3.65180000	0.62940900
C	3.77049000	1.69707900	-2.13645900	H	-0.33892400	2.31326000	3.52777500
C	4.93154900	0.94215400	-1.64028800	H	2.34875000	-2.37484600	1.26495000
C	4.90806300	-0.19050700	-0.87914100	H	0.07822200	0.14055200	3.68950800
C	3.83729900	-0.96155200	-0.21225700	H	6.69590900	-1.17779100	-1.59649900
C	6.21928200	-0.93382000	-0.64079200	H	6.93366300	-0.31595800	-0.08737900
C	5.85553100	-2.19948600	0.15017600	H	6.44658300	-3.06674900	-0.16800200
C	4.36252700	-2.39852400	-0.13298600	H	3.94266400	-2.96125700	0.69788100
C	1.42067100	-2.11388000	3.52383100	H	0.93827800	-1.82969500	4.46070700
C	6.25863800	1.53550900	-2.07354800	H	1.02075200	-3.08734100	3.21629500
				H	2.49067400	-2.25467200	3.71750100

H	6.92876700	1.68509900	-1.22319000	C	1.16510200	-0.65185600	1.90199300
H	6.77218500	0.87331300	-2.77934800	C	0.65231600	0.57891600	1.87697000
H	6.10285900	2.49495600	-2.56045000	C	2.87342600	0.73929400	-1.70551400
H	6.90806800	-1.87799200	1.76928800	O	4.02982000	0.38238100	-2.36741700
H	-2.62527400	4.10569100	2.86047600	C	5.26011800	0.94715400	-1.99954800
H	-1.19066100	4.70378000	3.70057300	C	6.10237600	0.16667400	-1.07188700
H	-1.74572300	5.50932600	2.22655100	C	5.66496300	-0.75970500	-0.17403000
H	4.51997600	-4.17877900	-1.37981300	C	4.31818800	-1.24950900	0.21066600
H	3.04264500	-3.23745700	-1.64660200	C	6.68864500	-1.57488800	0.61133800
H	4.57429100	-2.66655100	-2.29919900	C	5.87414000	-2.54957600	1.47312300
H	-6.20661400	-1.25361300	0.31352800	C	4.53995800	-2.68221400	0.71561400
H	-7.60583200	-1.41815800	-1.74867900	C	1.10311900	-1.51292600	3.13806800
H	-6.69907800	-2.84953400	-2.25357400	C	7.57906100	0.49102800	-1.17310800
H	-7.70027200	-2.89852900	-0.79617500	O	5.58943300	1.98037300	-2.51483400
H	-6.35137500	0.65539700	-1.86445100	O	1.83324700	0.77248600	-2.28909400
H	-4.72966300	1.28547600	0.32425000	O	5.67323500	-2.06027900	2.79907800
H	-4.32217600	1.09290300	-3.18437500	H	4.10995400	1.27043900	-0.07488400
H	-1.17553500	1.18421600	-2.01922700	H	2.66026400	2.13412600	1.46794600
H	-4.18694900	3.57316300	-2.81740200	C	-0.85560400	5.19946100	0.72089300
H	-5.85853800	2.99697800	-2.74387100	H	0.31159000	1.15097200	-0.17859500
H	-4.99767300	3.37589200	-1.24804400	C	4.59885000	-3.69692000	-0.43854300
H	-3.90781600	-0.87696200	-0.86238600	C	-6.57884200	-2.03124300	-0.97473700
H	-4.76773400	-1.22697200	-2.35253100	C	-7.66517500	-2.11936400	-2.05442800
B3LYP Energy = -2081.65487922 a.u.				C	-6.63961900	0.39912000	-0.13394300
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf G				O	-6.74448200	-0.00027500	1.23171600
C	-0.38350100	-1.86422800	-0.35757400	C	-6.01436400	1.80879800	-0.26421700
C	0.92507400	-1.59173300	-0.47232300	C	-4.58879000	1.83054300	0.26330600
C	-2.50691800	-2.68754100	-1.39167300	O	-4.20970000	1.18683600	1.23096800
C	-1.23394100	-2.23239700	-1.47315400	O	-3.79119900	2.64608800	-0.41864300
C	-4.53996200	-3.26494800	-0.02911800	C	-6.84346400	2.87560700	0.47715200
C	-5.09775800	-3.61024700	1.32836700	C	-5.88904200	-0.65279300	-0.96645400
C	-3.22138600	-3.00823900	-0.17092000	H	-0.85156900	-1.78051600	0.61886800
C	-5.55304800	-3.18384700	-1.14643900	H	1.39483100	-1.67663300	-1.44742500
O	-1.54818300	2.42833400	1.02817000	H	-3.02626900	-2.85637600	-2.32942600
C	0.02806700	4.04002700	0.24616500	H	-0.80068800	-2.10464200	-2.46177100
C	1.51396700	4.41705200	0.24304000	H	-5.76113500	-2.81960300	1.69566000
C	2.36362000	3.27879600	-0.31660100	H	-5.69554700	-4.52840100	1.28541500
C	2.20543800	1.96681900	0.48286100	H	-4.30400600	-3.75321300	2.06410400
C	0.72527400	1.57991000	0.73949400	H	-2.61806300	-3.06776800	0.73119300
C	-0.16061300	2.79368700	1.11126100	H	-5.06304300	-3.07455200	-2.11783200
C	3.09405300	0.88544200	-0.19668500	H	-6.11098200	-4.12897400	-1.18280200
C	3.14180200	-0.56605900	0.28114300	H	-1.76567200	1.66952200	1.58402700
C	1.85887700	-1.28941900	0.69906500	H	-0.25942000	3.77558200	-0.78025300
				H	1.66268200	5.31960200	-0.35731300

H	1.83121200	4.66794100	1.26440700	C	-5.34820400	-3.08219000	1.93208500
H	2.07086200	3.11452900	-1.35719900	C	-3.39307700	-3.03057900	0.40735800
H	3.42136900	3.56363900	-0.32919300	C	-5.71478800	-2.87086700	-0.58400500
H	0.05797700	3.07895400	2.15233900	O	-1.75492700	1.40604200	2.76688000
H	2.18254600	-2.27359600	1.03885700	C	-0.55557900	3.41024100	2.01211100
H	0.19551300	0.94132000	2.79822600	C	0.85529300	3.94687400	1.75004000
H	7.35795900	-2.10447100	-0.07553700	C	1.59578400	3.06500500	0.74745400
H	7.32514700	-0.94844200	1.24249000	C	1.73051600	1.60286200	1.22708000
H	6.37256300	-3.51099100	1.60196500	C	0.39037800	0.99638400	1.70838500
H	3.78540100	-3.00435900	1.43117600	C	-0.46780300	1.97732900	2.55764400
H	0.58511000	-1.01072800	3.95729100	C	2.48865800	0.82284100	0.11894800
H	0.58525400	-2.45706200	2.93229900	C	2.89413200	-0.63739200	0.30152400
H	2.10985500	-1.77745900	3.48328900	C	1.90666500	-1.65306000	0.88091400
H	8.00896700	0.72580500	-0.19606200	C	1.30312300	-1.34529300	2.24714300
H	8.13851400	-0.36048100	-1.57597100	C	0.62208900	-0.23956100	2.55194000
H	7.73418500	1.34331300	-1.83039500	C	1.83180300	0.84726800	-1.26058400
H	5.18573700	-1.23045700	2.73828600	O	2.74402400	0.77823500	-2.27949000
H	-1.91187500	4.92857900	0.71394400	C	3.95181600	1.50604800	-2.20833900
H	-0.59154800	5.49761000	1.74142800	C	5.14033700	0.80009000	-1.69782900
H	-0.72321100	6.07128500	0.07440100	C	5.15403900	-0.28336900	-0.86936800
H	4.83590800	-4.69559200	-0.06099300	C	4.09209700	-1.06274000	-0.19066400
H	3.63817300	-3.74970700	-0.95578800	C	6.48698600	-0.95737900	-0.56079000
H	5.35439700	-3.42432000	-1.18040500	C	6.15580200	-2.13945500	0.35916500
H	-7.06004700	-2.15439000	-0.00028900	C	4.68622800	-2.46254300	0.02848500
H	-8.39981000	-1.31574600	-1.95005100	C	1.45972800	-2.46228300	3.25264000
H	-7.23015800	-2.04317800	-3.05714500	C	6.44807300	1.40688400	-2.16765300
H	-8.20721800	-3.06795900	-1.99659500	O	3.95382500	2.62180000	-2.64819800
H	-7.67315100	0.47417700	-0.48952400	O	0.66008400	0.79536800	-1.50930000
H	-5.85882800	0.12371700	1.60801300	O	6.32243500	-1.81325300	1.73747100
H	-5.96871400	2.07422000	-1.32397700	H	3.42735300	1.37293000	0.00788100
H	-2.89492700	2.62735500	0.00339500	H	2.40882600	1.60757800	2.09053400
H	-6.38031800	3.86134000	0.39492800	C	-1.34896600	4.31237900	2.96254900
H	-7.84575800	2.93195400	0.04495500	H	-0.21015700	0.74935700	0.82828900
H	-6.94392500	2.61448100	1.53132100	C	4.53538100	-3.36574200	-1.20696800
H	-4.88180500	-0.74957200	-0.55171800	C	-6.24143400	-1.42116200	-0.79017600
H	-5.77208500	-0.29090000	-1.99636100	C	-7.43113700	-1.42580800	-1.76011200
B3LYP Energy = -2081.65861015 a.u.				C	-5.40124300	1.01752300	-1.13361800
				O	-5.55793000	1.41706900	0.22750900
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26R, 27R)-a2,Conf H				C	-4.28452100	1.88195300	-1.76004300
C	-0.43444500	-2.27851000	0.04776200	C	-2.89480100	1.50896100	-1.25828000
C	0.87023100	-2.05448300	-0.16554500	O	-2.52741000	1.58777200	-0.10513500
C	-2.65689100	-3.00376300	-0.84293200	O	-2.09240100	1.11137300	-2.25320100
C	-1.34367500	-2.71313300	-0.99338100	C	-4.52695500	3.38226900	-1.52598800
C	-4.73436100	-3.01047200	0.55764700	C	-5.11027700	-0.48445600	-1.25310500

H	-0.84039400	-2.09269800	1.03651500	H	-3.76830100	3.98302100	-2.03390000
H	1.27415500	-2.22166000	-1.16241900	H	-5.50575700	3.66986300	-1.91911000
H	-3.20938900	-3.24412300	-1.74588100	H	-4.50371700	3.60579700	-0.46040600
H	-0.92449000	-2.77577900	-1.99456500	H	-4.21888500	-0.68573500	-0.65593800
H	-5.99250700	-2.21853600	2.13218200	H	-4.86148200	-0.71774700	-2.29622000
H	-5.98246600	-3.97220600	2.02772800	B3LYP Energy = -2081.65159460 a.u.			
H	-4.58819100	-3.11949300	2.71427700	(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf A			
H	-2.79845400	-3.07005900	1.31596600	C	-0.01198900	-2.08308100	1.49135200
H	-5.27903600	-3.21290100	-1.52751100	C	1.13746500	-1.62596800	0.95842200
H	-6.57769400	-3.51884100	-0.38881900	C	-2.42441200	-2.53936800	1.61221500
H	-2.20131300	1.38747600	1.90671500	C	-1.35537300	-2.03092000	0.95587100
H	-1.08701900	3.36459300	1.05354200	C	-4.88875600	-2.95207400	1.74913500
H	0.80183200	4.97319900	1.37196000	C	-4.87702100	-3.57682100	3.12127900
H	1.41319700	3.99443600	2.69569600	C	-3.78089500	-2.51325600	1.11335900
H	1.05341400	3.09281000	-0.20369900	C	-6.27641200	-2.88942700	1.14107500
H	2.59474900	3.47009800	0.54912000	O	5.62293000	-3.82846600	-0.93903000
H	-0.02035900	2.03766100	3.55963600	C	7.02729500	-1.85824000	-0.51973400
H	2.49207500	-2.56313300	1.02481700	C	7.06925000	-0.34266700	-0.74470000
H	0.18043500	-0.19567800	3.54419000	C	5.87148500	0.34576800	-0.09484300
H	6.96471000	-1.28861100	-1.48965600	C	4.51274400	-0.19124000	-0.60181200
H	7.19355700	-0.28123200	-0.07193800	C	4.43137400	-1.73399800	-0.54853600
H	6.81219200	-2.99425900	0.19154200	C	5.71821600	-2.41023700	-1.09671900
H	4.25898400	-2.96882400	0.89314500	C	3.40558400	0.61052100	0.13663400
H	0.94741900	-2.23283400	4.18858200	C	1.93285600	0.44740400	-0.21702800
H	1.05355100	-3.40355800	2.86280700	C	1.31138000	-0.94317900	-0.39276700
H	2.51669800	-2.64577800	3.48158000	C	1.97982300	-1.94721200	-1.33621500
H	7.01116400	0.69411300	-2.77931600	C	3.26928700	-2.29082700	-1.34269700
H	6.26246800	2.29885500	-2.76079200	C	3.46875200	0.53842000	1.66355900
H	7.08798400	1.68355600	-1.32515300	O	3.01086500	1.69985300	2.24407900
H	5.68518000	-1.12430000	1.95974600	C	3.38406300	2.93473300	1.68699600
H	-2.33486900	3.89063600	3.16163900	C	2.40157800	3.58224600	0.79893100
H	-0.83042600	4.42110700	3.92203200	C	1.43922300	2.96316300	0.05071100
H	-1.47721800	5.31217300	2.53697800	C	1.12593300	1.54963700	-0.26257800
H	5.05100200	-4.31772600	-1.05196900	C	0.34483500	3.81487800	-0.58026900
H	3.48313600	-3.58157700	-1.40486600	C	-0.87894700	2.90206200	-0.53990500
H	4.94755100	-2.89698700	-2.10485200	C	-0.31006300	1.50915000	-0.83475400
H	-6.60099100	-1.07197100	0.18732800	C	0.99687600	-2.68680300	-2.21389000
H	-7.83968300	-0.42323800	-1.91322400	C	2.54710500	5.09328400	0.77425000
H	-7.13118600	-1.81238800	-2.73986800	O	4.42044800	3.42679000	2.04243100
H	-8.24219200	-2.05749100	-1.38687900	O	3.74614500	-0.40691100	2.33894600
H	-6.31531800	1.26766800	-1.69383600	O	-1.52965800	2.97798400	0.74568500
H	-6.33647500	0.97887600	0.58154900	H	3.64127900	1.64810500	-0.11684700
H	-4.29505200	1.67804100	-2.83340400	H	4.41800200	0.09142200	-1.65837100
H	-1.19621000	0.93626600	-1.90300100				

C	8.24847400	-2.56345700	-1.11788400	H	8.32043800	-2.36922800	-2.19361100
H	4.34696000	-2.02966100	0.50625800	H	9.17093400	-2.20569500	-0.65178700
C	-0.33851300	1.25095700	-2.35530200	H	-1.37350300	1.20989700	-2.70157900
C	-6.52343900	-2.03027200	-0.11218100	H	0.17843500	2.04570000	-2.90074400
C	-7.91702700	-2.33397200	-0.68239000	H	0.15065900	0.31331600	-2.61842300
C	-6.49123200	0.39361300	-1.03506100	H	-5.79502300	-2.30409200	-0.88106000
O	-5.82713700	-0.11130600	-2.18840000	H	-8.07953400	-1.81628700	-1.62955900
C	-6.04736900	1.84252000	-0.71074400	H	-8.03650200	-3.40491500	-0.87028500
C	-4.55513500	1.90485200	-0.42748300	H	-8.70603800	-2.02926300	0.01487100
O	-3.71927400	1.27405700	-1.05886000	H	-7.54823500	0.44204900	-1.31450300
O	-4.23650600	2.74465500	0.55089300	H	-4.88377900	0.07345100	-2.06030100
C	-6.37895300	2.81207900	-1.86192200	H	-6.56502400	2.17446400	0.19317000
C	-6.34366000	-0.53080400	0.18928500	H	-3.25186700	2.77071300	0.66128900
H	0.07254200	-2.57750500	2.45772100	H	-6.03244200	3.82422300	-1.64060200
H	2.04765400	-1.79251800	1.51913600	H	-5.91690900	2.46987500	-2.78880900
H	-2.24428700	-2.99086600	2.58380500	H	-7.46039700	2.84866800	-2.01462200
H	-1.51710500	-1.57127600	-0.01591000	H	-7.08319600	-0.22245100	0.94096600
H	-5.41825300	-4.52980400	3.11004300	H	-5.36167300	-0.37653300	0.64596600
H	-3.87732200	-3.76655300	3.50865300	B3LYP Energy = -2081.65705421 a.u.			
H	-5.39895600	-2.93226000	3.83869200	(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf B			
H	-3.89531100	-2.07662000	0.12557800	C	0.03270900	-2.13120700	1.41380100
H	-6.57465300	-3.92427500	0.91599700	C	1.17396800	-1.63659500	0.89679400
H	-6.97525300	-2.56878400	1.92809500	C	-2.37136000	-2.65112900	1.49385500
H	5.50707600	-4.01100500	0.00052300	C	-1.30758900	-2.09376300	0.86974400
H	7.01645500	-2.04053300	0.56572400	C	-4.82774100	-3.12527200	1.57517300
H	7.99834900	0.07073300	-0.33955700	C	-4.81552700	-3.84595600	2.89905600
H	7.08442800	-0.13898700	-1.82393900	C	-3.72295500	-2.62398000	0.98214800
H	5.93753800	0.20407500	0.98876600	C	-6.21010700	-3.04311800	0.95721600
H	5.91800200	1.42591100	-0.27020200	O	5.62402200	-3.83465400	-0.56900000
H	5.74375500	-2.26482000	-2.18427900	C	6.99696100	-1.90164300	-0.35655800
H	0.31657800	-0.78221400	-0.79267300	C	7.08334200	-0.40500900	-0.67502100
H	3.54608300	-3.10799800	-2.00201300	C	5.88625200	0.34833100	-0.09857500
H	0.15730400	4.74635600	-0.04943600	C	4.53167100	-0.17935400	-0.62369600
H	0.59466500	4.06495800	-1.61856500	C	4.41402700	-1.71838800	-0.53337000
H	-1.65028100	3.18730600	-1.25247400	C	5.70832900	-2.46133900	-0.95643200
H	-0.93799700	0.76959300	-0.33602400	C	3.41358200	0.64529700	0.07487000
H	1.49142600	-3.46347600	-2.79924700	C	1.93947300	0.46862100	-0.27347300
H	0.21690200	-3.16190800	-1.60830100	C	1.32681200	-0.92958200	-0.44349500
H	0.48978400	-2.00901000	-2.91043200	C	1.99943300	-1.89925000	-1.42085500
H	1.84817000	5.57003100	1.47149400	C	3.29030900	-2.23714800	-1.40744100
H	3.55407400	5.36599600	1.08429500	C	3.46256300	0.61239100	1.60559300
H	2.36393400	5.50718000	-0.21763500	O	3.03687800	1.80045000	2.15588400
H	-0.98204000	2.54585300	1.41193700	C	3.41020700	3.01103800	1.55122500
H	8.18524000	-3.64338300	-0.97911500				

C	2.41031400	3.63197700	0.66358900	H	3.58997800	-2.97104800	-2.15592700
C	1.43227300	2.98824600	-0.04132500	H	0.13581400	4.76016400	-0.13667500
C	1.12273100	1.56435300	-0.31799000	H	0.51497100	4.04361900	-1.70556700
C	0.30941300	3.81756800	-0.65232900	H	-1.71206800	3.16025300	-1.21626300
C	-0.90224800	2.89461500	-0.54013500	H	-0.93266100	0.76200900	-0.32178800
C	-0.33027400	1.50546000	-0.84588300	H	1.54604600	-3.32280500	-2.98586500
C	1.04162700	-2.57365400	-2.37288400	H	0.23673600	-3.07241400	-1.82153600
C	2.55172500	5.14157200	0.59386600	H	0.56545600	-1.85217700	-3.04620400
O	4.45462500	3.51020200	1.87067300	H	1.88216500	5.63632300	1.30725600
O	3.70277900	-0.32374000	2.30632500	H	3.57039400	5.42163900	0.85621000
O	-1.48826300	2.97899500	0.77505000	H	2.32856100	5.53029500	-0.39988700
H	3.64884600	1.67555600	-0.20733300	H	-0.88998800	2.58834800	1.42318600
H	4.46623600	0.08426600	-1.68716900	H	8.13969900	-3.73321400	-0.61643500
C	8.22643200	-2.67164800	-0.84937700	H	8.34118500	-2.57098900	-1.93451900
H	4.24345900	-1.99301700	0.51255900	H	9.13676500	-2.28658000	-0.38085400
C	-0.40926200	1.24332000	-2.36386100	H	-1.45531900	1.19818700	-2.67491800
C	-6.47324900	-2.06272500	-0.20087500	H	0.08549700	2.03829000	-2.92877100
C	-7.86491600	-2.32488800	-0.79598600	H	0.07313900	0.30714800	-2.64243600
C	-6.54636300	0.45131000	-0.84706200	H	-5.74512700	-2.24625900	-0.99673400
O	-5.96057400	0.08916100	-2.09309600	H	-8.03107800	-1.71647500	-1.68649000
C	-6.09248300	1.86076400	-0.39301100	H	-7.97290600	-3.37344700	-1.08831200
C	-4.58332100	1.92526400	-0.21911000	H	-8.65607200	-2.09941600	-0.07154600
O	-3.78885600	1.34924500	-0.94853800	H	-7.62043900	0.51364400	-1.04706300
O	-4.20218100	2.71047000	0.78204100	H	-5.01021700	0.25962500	-2.00341500
C	-6.52460300	2.95089300	-1.39392900	H	-6.54043900	2.07820600	0.58048200
C	-6.31020300	-0.60052900	0.25482000	H	-3.21279500	2.75125200	0.81473900
H	0.12232700	-2.64298800	2.37046700	H	-6.16573000	3.93573100	-1.08665200
H	2.08524400	-1.78665200	1.46000800	H	-6.14028700	2.72370100	-2.38929400
H	-2.19253300	-3.14086100	2.44700600	H	-7.61519000	2.98855500	-1.45150900
H	-1.47339000	-1.59989900	-0.08442200	H	-7.01483000	-0.39760600	1.07302000
H	-5.34231900	-4.80337000	2.81492600	H	-5.30916900	-0.47053300	0.67583900
H	-3.81532600	-4.04948100	3.27814800	B3LYP Energy = -2081.65541305 a.u.			
H	-5.35179400	-3.26274700	3.65721900	(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf C			
H	-3.83758400	-2.12542200	0.02392200	C	0.09508000	3.43810900	-0.71630600
H	-6.47359400	-4.05686300	0.62017000	C	1.39800500	3.14739300	-0.89422600
H	-6.92697000	-2.82818700	1.76348800	C	-2.31920700	2.99575900	-0.64292000
H	4.78945300	-4.19291200	-0.88732000	C	-1.06589400	2.62001800	-0.98782800
H	6.92582500	-2.02112300	0.73254000	C	-4.76029300	2.44249500	-0.49164400
H	8.01049800	0.00815800	-0.26566400	C	-5.17480500	3.67844600	0.26496300
H	7.13501400	-0.26386800	-1.76314400	C	-3.49125200	2.18406400	-0.87636600
H	5.91789200	0.25712500	0.99175300	C	-5.87360300	1.47429800	-0.81868700
H	5.96494200	1.41729500	-0.32454600	O	-1.23986700	-1.78571200	-2.24024000
H	5.79686000	-2.39413300	-2.05507300	C	0.25747600	-3.38241100	-1.13862600
H	0.32567600	-0.77500700	-0.82879300				

C	1.73190200	-3.74639800	-0.91468900	H	-4.38216600	4.42146900	0.34067900
C	2.58855500	-2.53699300	-0.52383100	H	-6.03467500	4.15225500	-0.22159100
C	2.51081100	-1.45946400	-1.61610500	H	-3.30792900	1.25939000	-1.41923000
C	1.03369100	-1.02407300	-1.79943600	H	-6.67111300	2.02617100	-1.33401800
C	0.11497300	-2.21867800	-2.13821400	H	-5.51744300	0.72286000	-1.52944700
C	3.40754100	-0.19539800	-1.40662300	H	-1.51281400	-1.48460300	-1.35818400
C	2.72673900	0.90129200	-0.58245400	H	-0.14352200	-3.01798900	-0.18274600
C	2.05702400	1.93045800	-1.52086600	H	1.80290900	-4.51967100	-0.14235200
C	1.29192800	1.34124300	-2.71589300	H	2.14000800	-4.19322800	-1.83122400
C	0.87707400	0.07410600	-2.82332200	H	2.23052600	-2.12593400	0.42697000
C	4.82483000	-0.51659100	-1.02168800	H	3.62125600	-2.85061100	-0.37464300
O	5.51597700	0.62279000	-0.56861400	H	0.37619300	-2.58135100	-3.14142300
C	5.84928100	0.65215000	0.76306600	H	2.95510800	2.36258000	-1.99940800
C	4.94785100	-0.10159800	1.69091400	H	0.37065500	-0.21159300	-3.74144900
C	3.60679400	0.06397600	1.66510900	H	2.34134500	-1.36953100	2.73010600
C	2.79440200	0.94249700	0.76550200	H	3.20238200	-0.25557200	3.78355100
C	2.69590800	-0.33879100	2.82011600	H	1.23463700	1.03933800	3.71312200
C	1.48829100	0.62615900	2.73649800	H	1.02652100	2.13455300	1.26502300
C	1.91285900	1.73058900	1.74191100	H	2.04687100	2.70227200	-4.21610300
C	1.08734100	2.31001900	-3.85781700	H	0.58473300	1.82497900	-4.69586700
C	5.69436000	-0.86567700	2.75325200	H	0.48860200	3.17220400	-3.55229400
O	6.78759600	1.29683800	1.13453700	H	6.28541300	-1.66438400	2.29236900
O	5.40366600	-1.54990100	-1.16594400	H	6.39851500	-0.20555500	3.26589000
O	0.29325400	-0.04601800	2.30381400	H	5.02984500	-1.32165700	3.48499700
H	3.54117500	0.22854800	-2.41120400	H	0.27728600	-0.14693900	1.34236600
H	2.85459200	-1.91984600	-2.55103800	H	-1.60491600	-4.30956300	-1.76974400
C	-0.56966800	-4.59551200	-1.57634300	H	-0.16611300	-5.02894500	-2.49794800
H	0.69238800	-0.64773700	-0.82740300	H	-0.56006600	-5.37647400	-0.81024500
C	2.66647700	2.86844100	2.45080000	H	2.01792400	3.35930200	3.18213700
C	-6.52181000	0.76659000	0.39972900	H	3.55602600	2.50574100	2.97254700
C	-7.81807300	0.05739300	-0.02283300	H	2.99384700	3.62004200	1.73005500
C	-4.85599600	-1.27396100	0.42358000	H	-6.81467200	1.54918800	1.11075900
O	-5.86230400	-2.19915300	0.00418200	H	-8.27815900	-0.45555000	0.82611600
C	-3.78810300	-2.04047300	1.27000100	H	-8.53910500	0.78531000	-0.40758500
C	-2.52229700	-1.21466500	1.42443900	H	-7.63432100	-0.69238900	-0.79224700
O	-1.78514000	-0.95674800	0.48180400	H	-4.33762900	-0.87048500	-0.45299500
O	-2.26485300	-0.80749600	2.65972100	H	-5.46550500	-2.81152000	-0.62414500
C	-4.33829200	-2.61761200	2.57644500	H	-3.47120000	-2.86974300	0.62529800
C	-5.54162200	-0.13841300	1.18597400	H	-1.37530500	-0.37314400	2.66827100
H	-0.12255500	4.40706500	-0.26849200	H	-3.61899500	-3.30111600	3.03231800
H	2.10724800	3.90467300	-0.57132800	H	-4.55685000	-1.83745200	3.30558200
H	-2.44669400	3.95712800	-0.15173800	H	-5.25548800	-3.17018400	2.36602500
H	-0.92076000	1.65682600	-1.46457600	H	-4.75488600	0.49193500	1.61479800
H	-5.49186500	3.43085600	1.28426600	H	-6.08758000	-0.57143500	2.02983500

B3LYP Energy = -2081.65347045 a.u.

(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf D

C	0.10337800	-3.49821400	0.79731200	C	-4.71599200	1.17256500	-0.23189200
C	1.39312100	-3.15948500	0.98353100	O	-5.72584800	1.93928600	0.43018700
C	-2.31567000	-3.09927500	0.61757900	C	-3.70502600	2.14602400	-0.91711200
C	-1.08785600	-2.71207000	1.03563600	C	-2.48606000	1.42990500	-1.46683000
C	-4.74571200	-2.55098000	0.30381000	O	-2.05024100	1.55916400	-2.59096700
C	-5.09259000	-3.74847500	-0.54282700	O	-1.88840400	0.64039800	-0.54840400
C	-3.51304700	-2.31102600	0.80202200	C	-4.33580000	3.06946300	-1.96007500
C	-5.88954800	-1.60385400	0.59081000	C	-5.39141200	0.20746500	-1.20770700
O	-1.22953300	1.88293200	2.10965100	H	-0.07605800	-4.47989000	0.36065200
C	0.31359000	3.41121300	0.96803900	H	2.13079700	-3.89800200	0.68142100
C	1.79866000	3.74544500	0.76482000	H	-2.39941200	-4.04942100	0.09603700
C	2.64392000	2.51017000	0.43623200	H	-0.98183300	-1.75744200	1.54068600
C	2.53011600	1.47407100	1.56511700	H	-5.39995200	-3.44567800	-1.54992000
C	1.03980100	1.06868600	1.72905800	H	-4.26893900	-4.45281100	-0.64982500
C	0.13913300	2.28996600	2.00864400	H	-5.94261000	-4.28624500	-0.10771200
C	3.40574900	0.18563300	1.40539000	H	-3.38131400	-1.41455700	1.40343800
C	2.69841900	-0.91719300	0.61492800	H	-6.73224100	-2.19136200	0.97862800
C	2.01345100	-1.90840100	1.58045200	H	-5.61119700	-0.91001400	1.38911200
C	1.22013900	-1.27186900	2.72983100	H	-1.45156500	1.41058900	1.29458700
C	0.83500400	0.00822500	2.78484000	H	-0.06844700	3.01764700	0.01518900
C	4.82729000	0.46455000	1.00272700	H	1.89794600	4.48968300	-0.03246600
O	5.48455800	-0.70003400	0.56476900	H	2.19076700	4.21934000	1.67471100
C	5.80067400	-0.77107800	-0.76998600	H	2.29287600	2.06681800	-0.50113700
C	4.90378400	-0.02837600	-1.70985000	H	3.68359800	2.80401200	0.29568100
C	3.55814700	-0.15551300	-1.66600900	H	0.38599700	2.68963200	3.00081400
C	2.72583300	-0.97429900	-0.73279000	H	2.90205400	-2.31211300	2.10044600
C	2.65737700	0.24398100	-2.83404200	H	0.31727600	0.33660400	3.68234100
C	1.36014000	-0.56964500	-2.63212000	H	2.43607200	1.31490200	-2.83826400
C	1.74631600	-1.70026100	-1.65978000	H	3.12391200	0.00578900	-3.79302400
C	0.96893800	-2.19456600	3.90045600	H	0.97192000	-0.96945300	-3.57356600
C	5.65354800	0.67435100	-2.81221200	H	0.85758800	-2.03471200	-1.13755500
O	6.72461300	-1.44139900	-1.13288400	H	0.46589700	-1.66697300	4.71229700
O	5.43259700	1.48598000	1.12041600	H	0.35239000	-3.05118000	3.61542600
O	0.33904600	0.22868400	-2.00738900	H	1.91104600	-2.59977100	4.28907700
H	3.53282800	-0.20515900	2.42405500	H	6.27804500	1.47009200	-2.39218100
H	2.86648700	1.95688500	2.49149700	H	6.32698900	-0.02533100	-3.31366400
C	-0.50190400	4.65302200	1.34264000	H	4.98939700	1.12369800	-3.54847300
H	0.72851900	0.67063800	0.75609900	H	-0.13665200	0.76084400	-2.66490900
C	2.37341300	-2.88771100	-2.40885500	H	-1.54587200	4.39534200	1.52918400
C	-6.41892200	-0.79673800	-0.62505800	H	-0.10567300	5.11550200	2.25309500
C	-7.77244700	-0.15083300	-0.28789700	H	-0.46559100	5.40241600	0.54669400
				H	1.65590500	-3.32330200	-3.11058100
				H	3.26376500	-2.59392500	-2.97121300
				H	2.67345600	-3.66702800	-1.70655500

H	-6.61021100	-1.51240500	-1.43428900	C	1.63013700	-1.53323500	-1.85906400
H	-8.15828100	0.41221700	-1.14262200	C	0.93917900	-2.58913200	3.64260400
H	-8.50881500	-0.92010700	-0.03548800	C	5.57866100	0.83938200	-2.82755800
H	-7.68693500	0.54132700	0.54928200	O	6.55754500	-1.55207300	-1.47927200
H	-4.15637900	0.59368100	0.50751400	O	5.52492700	1.15783400	1.16109900
H	-5.31385500	2.40933300	1.16295000	O	0.15364600	0.42991900	-2.16466100
H	-3.30917100	2.75861900	-0.09452400	H	3.56995500	-0.57549100	2.31836700
H	-1.08510500	0.23429900	-0.95809000	H	3.04284200	1.57990600	2.68958100
H	-3.64384100	3.86561000	-2.23938800	C	-0.09916700	4.64106800	2.18668800
H	-4.59147600	2.52807700	-2.87175200	H	0.73015100	0.70333600	0.91334600
H	-5.24081600	3.51756700	-1.54853600	C	2.23308700	-2.65248900	-2.72553400
H	-4.59250100	-0.35796400	-1.70040500	C	-6.28603800	-0.51704300	0.00332600
H	-5.89283200	0.78438800	-1.99076600	C	-7.57719400	0.19778400	0.42308100
B3LYP Energy = -2081.65196723 a.u.				C	-5.14211500	1.51607100	-1.14518200
(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf E				O	-5.30729000	0.95806200	-2.44466300
C	-0.02706500	-3.55933500	0.48465800	C	-3.92347200	2.48116200	-1.06359200
C	1.27216200	-3.23587500	0.62500500	C	-2.60496000	1.73802000	-1.17423300
C	-2.45662600	-3.20634300	0.57547700	O	-1.76228900	1.68089100	-0.29616000
C	-1.20113400	-2.83709300	0.92063300	O	-2.43543800	1.13558900	-2.35771300
C	-4.90192400	-2.63262500	0.51805700	C	-4.01438700	3.59752400	-2.11798000
C	-5.32716800	-3.68473000	-0.47144000	C	-5.08186500	0.43787000	-0.05526500
C	-3.63722700	-2.46985800	0.96390800	H	-0.23324200	-4.47569600	-0.06705700
C	-5.99463000	-1.69515700	0.97773200	H	1.98579400	-3.91955900	0.17320000
O	-1.02879100	1.85302000	2.54770100	H	-2.57833100	-4.08925000	-0.04726700
C	0.57967900	3.41662000	1.56350100	H	-1.06408900	-1.94345700	1.52118800
C	2.07295400	3.66198500	1.30669300	H	-5.82608300	-3.22770900	-1.33329000
C	2.78985800	2.42788200	0.74799100	H	-4.50107900	-4.28764700	-0.84674000
C	2.64408900	1.24869100	1.72236700	H	-6.05848100	-4.36126600	-0.01349200
C	1.13731500	0.92655700	1.90764200	H	-3.46043100	-1.66761000	1.67778800
C	0.35735500	2.15848500	2.42453100	H	-6.92307200	-2.26307900	1.11148100
C	3.43290200	-0.05302800	1.36190700	H	-5.73798200	-1.27678300	1.95736000
C	2.64082500	-1.01563400	0.47478200	H	-1.38903300	1.77577200	1.65094500
C	1.94293300	-2.08085100	1.34512800	H	0.10296500	3.21684700	0.59471200
C	1.20794700	-1.54548700	2.58127800	H	2.18988500	4.50598500	0.61856000
C	0.89446000	-0.26378200	2.80747600	H	2.56030900	3.96341600	2.24355900
C	4.85653000	0.19400900	0.94386500	H	2.35806900	2.16172800	-0.22405700
O	5.43238700	-0.94395400	0.34674000	H	3.84194000	2.65735600	0.58378900
C	5.69622100	-0.87296600	-0.99873400	H	0.69501900	2.36756300	3.44864800
C	4.81943800	0.03482800	-1.80489900	H	2.82970600	-2.57098800	1.78975300
C	3.47177300	-0.03054700	-1.72813500	H	0.40770800	-0.03295900	3.75113600
C	2.63330200	-0.92587100	-0.87224300	H	2.30066900	1.60161100	-2.59996400
C	2.54708200	0.55318000	-2.79157900	H	2.99403000	0.50824500	-3.78658100
C	1.25931600	-0.30258900	-2.71995200	H	0.91351000	-0.59679400	-3.71094800
				H	0.73618500	-1.90142500	-1.36631200

H	0.48672600	-2.13775300	4.52681300	C	1.24345800	0.61410300	-0.08363000
H	0.27294500	-3.37666900	3.28174300	C	1.74447600	-0.82696700	-0.20294500
H	1.87024600	-3.08030800	3.95013800	C	1.80741000	-1.22469800	-1.69245300
H	6.25766800	1.53637400	-2.32487300	C	3.23926200	-0.95359100	-2.20084600
H	6.19787800	0.17966700	-3.44060900	C	3.93516100	0.13911700	-1.84772800
H	4.92223400	1.41967500	-3.47336600	C	1.15703400	0.96241400	1.37116500
H	0.29762100	0.62195600	-1.22853700	O	0.09809900	0.22748800	1.90392600
H	-1.15270800	4.44082000	2.38688700	C	0.27864500	-0.44458400	3.07368900
H	0.37762600	4.90779300	3.13619900	C	1.62268100	-1.00812100	3.28457400
H	-0.02956200	5.50875800	1.52399900	C	2.41540000	-1.43581800	2.26774400
H	1.50040300	-3.00863300	-3.45563800	C	2.20797100	-1.62379300	0.78920200
H	3.11911900	-2.31395000	-3.26946300	C	3.74595800	-2.09886400	2.60494200
H	2.53381600	-3.50007500	-2.10760000	C	4.22498700	-2.78606300	1.31409100
H	-6.43338000	-0.92233300	-1.00331100	C	2.92784200	-2.95481500	0.50417400
H	-7.84447700	0.99658000	-0.27282500	C	3.85632200	-1.94599700	-3.15951900
H	-8.41785600	-0.50110200	0.45392400	C	2.02905000	-1.15372300	4.73291200
H	-7.47505600	0.63958900	1.42058100	O	-0.66473000	-0.57848200	3.82137900
H	-6.02886900	2.13962600	-0.99821900	O	1.82212600	1.69461900	2.03838500
H	-4.46512900	0.56322900	-2.70465500	O	5.19764400	-2.01896200	0.61058200
H	-3.92259500	2.92273300	-0.06425600	H	0.20005800	0.60407600	-0.42339800
H	-1.52507400	0.74249600	-2.38566000	H	1.62922000	1.46657300	-2.00921100
H	-3.15181000	4.26632400	-2.06500000	C	4.64533600	5.04896000	-2.07312500
H	-4.07358200	3.17625100	-3.12094300	H	3.92723000	1.32910600	-0.03737400
H	-4.91415200	4.19280700	-1.94380000	C	2.11149300	-4.17927800	0.94893500
H	-4.96493200	0.93026700	0.91955200	C	-5.92846500	0.39894700	-1.58619900
H	-4.17500000	-0.15517200	-0.21097600	C	-7.16982900	1.25954200	-1.86858900
B3LYP Energy = -2081.65798860 a.u.				C	-5.46391100	1.65374600	0.63401700
(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf F				O	-4.63986200	2.55574300	-0.09901300
C	-0.07034600	-2.86435900	-2.22139400	C	-4.97245900	1.49527400	2.09263300
C	1.23404100	-2.58572200	-2.03408200	O	-3.53884000	0.98432100	2.15148200
C	-2.48148500	-2.39798400	-2.28707600	O	-2.71987100	1.14555500	1.26378400
C	-1.20699200	-1.97549200	-2.11828300	O	-3.26552300	0.37324300	3.30173400
C	-4.93867100	-1.94653700	-2.31641100	C	-5.06207100	2.82423500	2.86981700
C	-5.35978700	-3.36078300	-2.62628800	C	-5.62846000	0.29698500	-0.07751900
C	-3.65237200	-1.55771400	-2.17892800	H	-0.31696100	-3.89405000	-2.47407200
C	-6.11320300	-0.99311900	-2.21717300	H	1.92710800	-3.40897800	-2.14947100
O	5.71183900	2.36697600	-1.60947400	H	-2.62925900	-3.45142000	-2.50852600
C	3.87299900	3.96683700	-1.31153900	H	-1.03402300	-0.92930600	-1.87967200
C	2.35603100	4.10865400	-1.48392300	H	-6.04688300	-3.37342900	-3.47997800
C	1.61965400	3.07939100	-0.63049100	H	-4.53025200	-4.02707300	-2.85676700
C	2.00733400	1.62991600	-0.99371000	H	-5.90992700	-3.78755600	-1.77926400
C	3.53649300	1.38643100	-1.06558200	H	-3.45266300	-0.51431400	-1.95278900
C	4.30218400	2.56152400	-1.75273600	H	-6.49912200	-0.86211800	-3.23940600
				H	-6.92411000	-1.51096000	-1.68417100

H	5.92053800	2.41477200	-0.66923100	C	2.28371600	3.01559100	0.52420100
H	4.10106400	4.06524500	-0.23894800	C	1.02407100	2.65841000	0.86547300
H	2.04162000	5.11776800	-1.19971200	C	4.72545100	2.45663000	0.44381000
H	2.09812000	3.99096200	-2.54522000	C	5.15910900	3.68083400	-0.32197500
H	1.84817100	3.27743000	0.41688700	C	3.44754500	2.20633100	0.80330700
H	0.53536700	3.19008800	-0.74460000	C	5.82920100	1.49320600	0.81466400
H	4.13200000	2.48644700	-2.83336600	O	1.23606800	-1.60070200	2.37672100
H	1.16329900	-0.51343500	-2.21640300	C	-0.21780700	-3.27655000	1.33293200
H	4.94402500	0.21741300	-2.24244700	C	-1.68300900	-3.68047100	1.11767600
H	4.48168800	-1.35934400	2.93579600	C	-2.56018100	-2.50991400	0.65832600
H	3.63131300	-2.81774000	3.42159100	C	-2.51033600	-1.37356300	1.69104300
H	4.70450500	-3.74445900	1.52352200	C	-1.04253800	-0.90458300	1.86634200
H	3.19057600	-3.06352800	-0.54383700	C	-0.10764400	-2.06376900	2.27578900
H	4.81858600	-1.58096200	-3.52002000	C	-3.42506000	-0.13680300	1.40670500
H	4.02523400	-2.92555900	-2.70086400	C	-2.75339800	0.92114400	0.52704700
H	3.20478300	-2.11075200	-4.02418500	C	-2.10127400	2.00941100	1.40986300
H	2.95219600	-0.60331200	4.93604700	C	-1.35091300	1.49982700	2.65006700
H	1.24681900	-0.77097200	5.38584300	C	-0.91875400	0.24764800	2.83331900
H	2.20536000	-2.20021800	5.00155900	C	-4.83445200	-0.49877800	1.03070700
H	4.74452900	-1.36383000	0.06333200	O	-5.53904900	0.60755400	0.51824300
H	5.72236800	4.91319800	-1.96735200	C	-5.86756700	0.56411500	-0.81384200
H	4.40866100	5.01479400	-3.14201000	C	-4.95357700	-0.22553500	-1.69825400
H	4.38208100	6.04438100	-1.70476800	C	-3.61448200	-0.04401200	-1.67665300
H	2.67556300	-5.09901100	0.76850200	C	-2.81396300	0.88804600	-0.82166900
H	1.86516900	-4.13866800	2.01323500	C	-2.69689300	-0.49701900	-2.80836800
H	1.17313900	-4.23610600	0.39511100	C	-1.48546400	0.46332000	-2.75193300
H	-5.07908500	0.89892800	-2.06138200	C	-1.92650500	1.62414500	-1.83267200
H	-7.02253000	2.28530300	-1.52703800	C	-1.17866600	2.53512000	3.73739600
H	-7.38192100	1.29706600	-2.94117600	C	-5.68626900	-1.05181600	-2.72278100
H	-8.05749100	0.85417700	-1.36910500	O	-6.81211300	1.17720100	-1.22159500
H	-6.44283900	2.14014100	0.68308200	O	-5.39959200	-1.53190000	1.22202200
H	-3.73400100	2.22896100	0.01906300	O	-0.30727700	-0.19008900	-2.24745500
H	-5.59790900	0.75356700	2.59908100	H	-3.57099400	0.34015500	2.38544300
H	-2.31975900	0.09891000	3.34659600	H	-2.85545100	-1.78911900	2.64621300
H	-4.67289500	2.71459200	3.88364900	C	0.63137700	-4.44985800	1.83259700
H	-4.49832500	3.60160500	2.35125900	H	-0.69362500	-0.57279100	0.88033700
H	-6.10399600	3.14796000	2.93467500	C	-2.67588800	2.71437500	-2.61669300
H	-6.44558100	-0.24845200	0.41481800	C	6.51577600	0.78028700	-0.37945100
H	-4.72464000	-0.30161900	0.06642700	C	7.80936500	0.09147800	0.08502000
B3LYP Energy = -2081.64930590 a.u.				C	4.92920700	-1.32671600	-0.42530900
				O	5.90071700	-2.25816700	0.05311800
(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf G				C	3.85677100	-2.09978000	-1.25775300
C	-0.13012400	3.46765600	0.54343700	C	2.57367500	-1.29458700	-1.37648900
C	-1.43565100	3.18981600	0.72301000	O	1.87836800	-1.00959200	-0.41206300

O	2.25236600	-0.93912300	-2.61486700	H	6.51534000	-2.45007800	-0.66250100
C	4.37358800	-2.65081200	-2.59010700	H	3.58799600	-2.94029400	-0.60973100
C	5.55967200	-0.14348600	-1.17355600	H	1.35504500	-0.52085900	-2.60052800
H	0.09562800	4.41249800	0.05037400	H	3.62493900	-3.29091200	-3.06002400
H	-2.13987000	3.93070200	0.35445600	H	4.61648700	-1.85860900	-3.29881000
H	2.42286300	3.95677800	-0.00173700	H	5.26508800	-3.26149100	-2.42383800
H	0.86957200	1.71658000	1.38018400	H	4.74727800	0.46923000	-1.58039400
H	5.47307700	3.42371000	-1.34011000	H	6.10717700	-0.52861800	-2.04343700
H	4.37708900	4.43457000	-0.40260500	B3LYP Energy = -2081.65257913 a.u.			
H	6.02456100	4.14655400	0.16239600	(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf H			
H	3.24920200	1.29238100	1.35856000	C	0.01585100	-2.10203900	1.47438800
H	6.60896800	2.05117700	1.35020100	C	1.16363000	-1.62672800	0.95382300
H	5.45203400	0.74621800	1.51890600	C	-2.39143800	-2.61001500	1.54465500
H	1.54406700	-1.39780500	1.47908400	C	-1.31952100	-2.07203900	0.91756500
H	0.18243800	-2.95022000	0.36297500	C	-4.84920400	-3.08147400	1.60947800
H	-1.73276600	-4.49326200	0.38528300	C	-4.85259300	-3.76942100	2.95082000
H	-2.08944900	-4.08842000	2.05298000	C	-3.73749700	-2.59459200	1.01755100
H	-2.20365500	-2.14536000	-0.31192700	C	-6.22406100	-3.01728800	0.97258300
H	-3.58589000	-2.85075300	0.52071300	O	5.59514500	-3.78890700	-0.70940400
H	-0.37799900	-2.38119300	3.29191100	C	7.04210500	-1.82466100	-0.41739800
H	-3.00889600	2.46451000	1.84712100	C	7.09037700	-0.32160200	-0.71046400
H	-0.42283500	0.01944800	3.77294400	C	5.87954800	0.38446200	-0.10488800
H	-2.35153000	-1.52659600	-2.67953900	C	4.52999700	-0.18186100	-0.60527000
H	-3.19629800	-0.44373000	-3.77790000	C	4.45406200	-1.72300900	-0.51174100
H	-1.20271900	0.81704600	-3.74384200	C	5.75093900	-2.39914000	-1.01334200
H	-1.04762300	2.06059100	-1.37068500	C	3.41131400	0.63092800	0.10316400
H	-0.68520100	2.10589400	4.61054700	C	1.94019000	0.44534900	-0.24584200
H	-0.58419200	3.38529500	3.39231900	C	1.33579300	-0.95463100	-0.40268200
H	-2.14877700	2.93546400	4.05595300	C	2.01986900	-1.95950500	-1.33481200
H	-6.27526600	-1.82860800	-2.22348200	C	3.31125100	-2.29377800	-1.32323400
H	-6.39126000	-0.42616700	-3.27604900	C	3.46895100	0.60177000	1.63259700
H	-5.01282300	-1.54186600	-3.42364100	O	3.01863700	1.78307100	2.18007400
H	-0.32255500	-0.23259500	-1.28207500	C	3.38356700	2.99881400	1.58000800
H	1.66191000	-4.13741700	2.00793600	C	2.38759100	3.61232100	0.68333900
H	0.23613900	-4.84138300	2.77638600	C	1.41995200	2.96235800	-0.03084300
H	0.63413500	-5.26987700	1.10829200	C	1.11936100	1.53717800	-0.30379100
H	-2.02089700	3.16276800	-3.36935400	C	0.30144400	3.78397600	-0.65979100
H	-3.55942400	2.31952100	-3.12519600	C	-0.90823900	2.85697500	-0.55920200
H	-3.01254600	3.50716900	-1.94593500	C	-0.32771700	1.46720300	-0.84570100
H	6.81704800	1.55815600	-1.09176000	C	1.05119900	-2.71078900	-2.21811800
H	8.30956800	-0.41159800	-0.74934800	C	2.52115300	5.12277300	0.61118900
H	8.50884400	0.83101700	0.48590600	O	4.42126500	3.50697000	1.90878900
H	7.61542100	-0.65351200	0.85736400	O	3.73619600	-0.32573400	2.33485400
H	4.42604700	-0.97178000	0.47532700				

O	-1.51244800	2.94906900	0.74768900	H	2.31143800	5.50689900	-0.38736300
H	3.63834800	1.66297600	-0.17949200	H	-0.92724800	2.55311800	1.40446900
H	4.44092300	0.07344400	-1.66937400	H	8.28536700	-3.60826700	-0.65908500
C	8.28665200	-2.55127300	-0.93894600	H	8.35773000	-2.48366600	-2.03076800
H	4.35108800	-2.01082400	0.54051200	H	9.19625600	-2.11111600	-0.52172900
C	-0.38881000	1.18647900	-2.36132500	H	-1.43105300	1.13546200	-2.68411100
C	-6.47761300	-2.05912000	-0.20620800	H	0.11067200	1.97616900	-2.92967700
C	-7.86265100	-2.33598800	-0.81000700	H	0.09902100	0.24779400	-2.62292500
C	-6.56056500	0.44392900	-0.89479200	H	-5.74105900	-2.25501200	-0.99132200
O	-5.97086200	0.06396600	-2.13353600	H	-8.02120600	-1.74548400	-1.71385300
C	-6.11234200	1.86219800	-0.46196900	H	-7.96532700	-3.39039200	-1.08260200
C	-4.60414200	1.92934800	-0.28151100	H	-8.66145700	-2.09840000	-0.09789200
O	-3.80700800	1.36075700	-1.01378100	H	-7.63450700	0.49937700	-1.09789600
O	-4.22715700	2.70446300	0.72889900	H	-5.02201100	0.24508200	-2.04783900
C	-6.54077400	2.93407000	-1.48353100	H	-6.56597200	2.09406700	0.50543300
C	-6.32274500	-0.58868500	0.22477200	H	-3.23761600	2.74088700	0.76820600
H	0.09528900	-2.59308900	2.44276900	H	-6.18619400	3.92498500	-1.19080000
H	2.07130100	-1.77420200	1.52406900	H	-6.14963000	2.69144500	-2.47253300
H	-2.22380500	-3.07523000	2.51199300	H	-7.63111000	2.96816700	-1.54843100
H	-1.47325400	-1.60357400	-0.05130700	H	-7.03055500	-0.37525200	1.03760900
H	-5.37615500	-4.73002700	2.88360000	H	-5.32356200	-0.44743700	0.64666400
H	-3.85689100	-3.96110400	3.34754700	B3LYP Energy = -2081.65549083 a.u.			
H	-5.39981500	-3.16917900	3.68763600	(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf I			
H	-3.84070200	-2.12101700	0.04538200	C	0.63332600	2.64246700	-1.10179700
H	-6.47905300	-4.03815800	0.65072800	C	1.77927700	2.22441200	-0.53192300
H	-6.95216700	-2.79056300	1.76543800	C	-1.80839100	2.97044600	-1.24791800
H	6.25275300	-4.28289700	-1.20668100	C	-0.71912100	2.46377500	-0.62569100
H	6.99007500	-1.96603300	0.66985800	C	-4.29911600	3.24918000	-1.31758900
H	8.01070000	0.11133000	-0.30550900	C	-4.34047700	4.12275100	-2.54550200
H	7.12306200	-0.16006800	-1.79658400	C	-3.16088600	2.76630600	-0.77605700
H	5.93544700	0.28596700	0.98391500	C	-5.66976900	3.01104100	-0.71212600
H	5.92028700	1.45701400	-0.32282500	O	6.99627600	2.23442200	-0.02707900
H	5.80007200	-2.26676000	-2.10838800	C	7.23076100	-0.10846900	-0.72198300
H	0.34102300	-0.81045800	-0.80823800	C	6.68581900	-1.51119800	-0.43045900
H	3.60119000	-3.11277200	-1.97433500	C	5.17703500	-1.57314800	-0.65227200
H	0.11700900	4.72856900	-0.15155500	C	4.39366600	-0.55081600	0.20311700
H	0.52038200	4.00519100	-1.71144300	C	4.96554100	0.88258400	0.08227400
H	-1.70956000	3.11449000	-1.24836000	C	6.51552300	0.90318900	0.18188400
H	-0.93174000	0.72635800	-0.31961900	C	2.88491900	-0.75611900	-0.11243800
H	1.55735000	-3.48686900	-2.79457400	C	1.82947200	0.00834800	0.67298700
H	0.26975400	-3.18974900	-1.61748200	C	1.94036100	1.52977200	0.82166900
H	0.54521000	-2.04128200	-2.92352700	C	3.18514100	2.09193500	1.50706100
H	1.83680800	5.61563300	1.31173600	C	4.44295600	1.82841000	1.14687100
H	3.53364800	5.41026300	0.88872100				

C	2.49800900	-0.63166600	-1.58460300	H	4.80574400	-2.57997800	-0.43299700
O	1.37852100	-1.39400600	-1.85917600	H	6.79349600	0.68042300	1.22004700
C	1.30840500	-2.69760800	-1.34508200	H	1.09391400	1.83815300	1.42925600
C	0.47074300	-2.90200400	-0.14700000	H	5.22282200	2.38191600	1.66126200
C	0.23323900	-2.00275000	0.85412100	H	-1.59002900	-3.02259400	1.54404400
C	0.72404100	-0.63771300	1.14354600	H	-0.36786300	-2.78554700	2.78914800
C	-0.82557400	-2.33344600	1.90108400	H	-1.92146300	-0.96017100	3.22057000
C	-1.40980500	-0.96678800	2.25457000	H	-0.52872600	0.96205700	2.01427700
C	-0.18512700	-0.04621600	2.24209800	H	3.81049700	3.55715000	2.97127700
C	2.89296300	3.11938500	2.57449600	H	2.27501800	3.92957500	2.16961300
C	-0.13964300	-4.29186300	-0.09228100	H	2.33341300	2.68650500	3.41165100
O	1.85095500	-3.57862800	-1.95737400	H	-1.19540600	-4.25889400	-0.38332100
O	2.96836200	0.08505800	-2.41405600	H	0.38259400	-4.95024600	-0.78321300
O	-2.34690000	-0.52399900	1.25996400	H	-0.08063800	-4.72743700	0.90669900
H	2.72122100	-1.80670200	0.14250100	H	-2.44532900	-1.19948800	0.57039800
H	4.50783400	-0.84298000	1.25531900	H	9.11747800	0.97681100	-0.73936500
C	8.75179400	-0.03433300	-0.55669200	H	9.04617500	-0.31632600	0.46008700
H	4.70984400	1.25782500	-0.91860300	H	9.25164400	-0.71647700	-1.25023100
C	0.52476900	-0.03072600	3.60918200	H	-0.13671400	0.37145400	4.38228400
C	-5.87394800	1.86389600	0.29692400	H	0.83041400	-1.03541100	3.91472600
C	-7.24495800	2.01308200	0.97393700	H	1.42603800	0.58252900	3.57786500
C	-5.92711200	-0.72332900	0.52064000	H	-5.11621000	1.93930200	1.08265800
O	-5.14935800	-0.68241200	1.69930500	H	-7.37777500	1.28192600	1.77352300
C	-5.80572100	-2.08391200	-0.25257400	H	-7.34982700	3.00627300	1.41955500
C	-4.52066400	-2.18141300	-1.04281900	H	-8.06103300	1.88571200	0.25334100
O	-3.40688700	-2.33835700	-0.57874400	H	-6.96238800	-0.71702100	0.87550400
O	-4.71241900	-2.07473400	-2.36940400	H	-4.20780200	-0.53025400	1.50039200
C	-5.93368800	-3.27507600	0.70750300	H	-6.62266900	-2.10303900	-0.97845200
C	-5.71210600	0.49337500	-0.39188200	H	-3.83826400	-2.11935600	-2.78918100
H	0.72774500	3.16507200	-2.05199100	H	-5.89094400	-4.22611800	0.17086400
H	2.70142000	2.41288900	-1.06700800	H	-5.13731000	-3.24854000	1.44971600
H	-1.65405800	3.55662700	-2.14981000	H	-6.88939000	-3.22301600	1.23419800
H	-0.87999800	1.86063400	0.26049600	H	-6.42381500	0.42659700	-1.22540800
H	-4.90373000	5.04101400	-2.34173600	H	-4.71395300	0.44305900	-0.83964500
H	-3.35551000	4.41103400	-2.90923400	B3LYP Energy = -2081.65016716 a.u.			
H	-4.86562300	3.61216200	-3.36167600	(2R, 3R, 5S, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a3,Conf J			
H	-3.23653800	2.14769000	0.11375100	C	-0.11283000	-2.28166200	-1.20011600
H	-5.97561200	3.95269300	-0.23241800	C	-1.26938000	-1.74563500	-0.76562200
H	-6.38751300	2.87658700	-1.53447600	C	2.28881200	-2.81455100	-1.14671700
H	6.71101000	2.51277500	-0.90497400	C	1.19025300	-2.27189600	-0.57152900
H	6.98104600	0.14231400	-1.76448700	C	4.75706400	-3.26157800	-1.10352700
H	7.18496000	-2.24682500	-1.06929700	C	4.83455800	-3.93031900	-2.45206200
H	6.92955800	-1.78425200	0.60536000	C	3.60619700	-2.81192600	-0.55357800
H	4.97392500	-1.39139300	-1.71200300				

C	6.07226700	-3.13353200	-0.35679200	H	2.16870800	-3.26910200	-2.12616800
O	-6.04018200	-3.53765700	0.90079800	H	1.29620800	-1.81109300	0.40741000
C	-7.26061100	-1.49158900	0.30828800	H	5.20338400	-4.95672100	-2.33711900
C	-7.20378300	0.03179000	0.46593600	H	3.87800400	-3.97704000	-2.97078300
C	-5.91653200	0.60071700	-0.12570800	H	5.54653600	-3.41846300	-3.10612200
C	-4.63808400	-0.01073200	0.49393100	H	3.66023200	-2.38408500	0.44544500
C	-4.66985400	-1.55623300	0.50772100	H	5.90153700	-3.30938000	0.71081900
C	-6.03682700	-2.11040600	0.99458700	H	6.74758700	-3.92681200	-0.69608900
C	-3.43021100	0.67399400	-0.20207200	H	-5.88151500	-3.76986300	-0.02142100
C	-1.99920500	0.42727200	0.25676200	H	-7.19430800	-1.72535600	-0.76542900
C	-1.49382400	-0.99274800	0.54000500	H	-8.06967600	0.49161000	-0.02093700
C	-2.29762700	-1.90486700	1.47102200	H	-7.27625700	0.28692300	1.53193100
C	-3.60601400	-2.15828200	1.40045600	H	-5.92080100	0.41666000	-1.20503700
C	-3.40106400	0.52716200	-1.72450400	H	-5.89253300	1.68810300	0.00324100
O	-2.83513300	1.62515200	-2.33031500	H	-6.12125300	-1.91423200	2.07117300
C	-3.14893600	2.90981800	-1.85305700	H	-0.52255700	-0.87919900	1.00829300
C	-2.17792600	3.52975900	-0.93348700	H	-3.98397600	-2.92493000	2.07013700
C	-1.30800500	2.88415700	-0.09896300	H	0.08810000	4.57915700	0.00372600
C	-1.11710800	1.47037900	0.30029900	H	-0.49240300	4.00517800	1.56927100
C	-0.19641400	3.68879100	0.56149200	H	1.70392700	2.95508700	1.39584600
C	0.96156000	2.69659500	0.64546100	H	0.87359400	0.55568800	0.52793800
C	0.27679700	1.36044200	0.96163800	H	-2.02224300	-3.38228500	3.02655600
C	-1.43357700	-2.66914800	2.44739900	H	-0.64878000	-3.22486700	1.92172000
C	-2.21601500	5.04686600	-0.98365700	H	-0.93011000	-1.99560200	3.15071700
O	-4.12186300	3.45577000	-2.29803100	H	-1.43753600	5.44130900	-1.64722800
O	-3.69522300	-0.43464100	-2.36957700	H	-3.17689200	5.37344100	-1.37666900
O	1.70281800	2.66208300	-0.59149400	H	-2.07229100	5.49319900	0.00074200
H	-3.60464300	1.73693700	-0.01297600	H	1.16575000	2.25638900	-1.28215500
H	-4.58908900	0.31099800	1.54230300	H	-8.57506600	-3.16547400	0.76417000
C	-8.56704700	-2.07842600	0.85185400	H	-8.69355500	-1.82853800	1.91087200
H	-4.53935300	-1.90491000	-0.52582600	H	-9.42823900	-1.67824000	0.30931500
C	0.20255900	1.17144500	2.49101500	H	1.21201000	1.08855600	2.89994400
C	6.82702900	-1.77646700	-0.49658100	H	-0.29236200	2.02234900	2.96778800
C	7.07899800	-1.37594200	-1.95571600	H	-0.36079100	0.27994500	2.76662400
C	6.77735700	0.70301900	0.25408900	H	7.80511500	-1.92991600	-0.02997900
O	8.17085800	0.53723400	0.53279600	H	7.75659900	-0.52140400	-2.00575700
C	6.14878900	1.73066000	1.24667600	H	7.54861500	-2.19325000	-2.51073500
C	4.66221600	1.90324500	0.97104200	H	6.15226100	-1.10479600	-2.47093200
O	3.78449600	1.66196000	1.77222100	H	6.64960000	1.11037200	-0.75469800
O	4.42428000	2.35113900	-0.26886800	H	8.61376300	1.37461000	0.36226100
C	6.41336100	1.41001500	2.71871500	H	6.60947200	2.69706000	1.00161000
C	6.11863900	-0.67475200	0.31428800	H	3.44913300	2.42541300	-0.40720200
H	-0.15479000	-2.80531400	-2.15369500	H	6.11615100	2.24773300	3.35261200
H	-2.14748000	-1.88391200	-1.38249200	H	5.84314700	0.54032100	3.04652900

H	7.47466800	1.21126800	2.87051600	C	0.20848700	0.63595100	2.63902300
H	5.08991700	-0.56232800	-0.04183700	C	6.88944500	-2.07577800	0.01296600
H	6.06059600	-1.00213300	1.35762500	C	8.16983300	-2.43085000	0.78104200
B3LYP Energy = -2081.64983779 a.u.				C	6.92431300	0.49939100	0.01710400
(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4.Conf A				O	6.77649300	0.61412700	-1.39668500
C	-0.13760600	-2.16765900	-1.37764400	C	6.45425900	1.77308100	0.76855400
C	-1.31934700	-1.67245700	-0.96198300	C	4.94259400	1.93496100	0.76638300
C	2.25745800	-2.73235200	-1.16111800	O	4.26889500	2.09595500	1.75839400
C	1.07949500	-2.35103100	-0.61567200	O	4.41922700	1.89652700	-0.47620700
C	4.71779400	-3.14300900	-0.87823700	C	7.12965400	3.04148500	0.21717200
C	5.05093400	-3.26272100	-2.34257500	C	6.25008800	-0.77777200	0.54068200
C	3.47515500	-2.90799400	-0.40254400	H	-0.08101000	-2.47842700	-2.41940000
C	5.88855400	-3.26101000	0.06900600	H	-2.13460800	-1.63667100	-1.67337000
O	-6.37234800	-3.43823200	0.22408700	H	2.29009200	-2.89992900	-2.23433700
C	-7.44467800	-1.23787400	0.03899200	H	1.05053900	-2.17605500	0.45687200
C	-7.28769500	0.21882300	0.48838600	H	5.69112500	-4.13352200	-2.52009200
C	-5.95747300	0.80293100	0.01871100	H	4.17034200	-3.35814000	-2.97695400
C	-4.73052300	-0.00260500	0.50706400	H	5.61172900	-2.38525600	-2.68418300
C	-4.86884600	-1.51533900	0.22301400	H	3.36422300	-2.81870500	0.67694700
C	-6.27560200	-2.06016800	0.59401400	H	5.52485500	-3.36807800	1.09721200
C	-3.47420200	0.71189800	-0.06065000	H	6.44000500	-4.18087900	-0.16640000
C	-2.06615500	0.31177800	0.35589200	H	-6.22213300	-3.49674500	-0.72652800
C	-1.64533900	-1.16154600	0.43785900	H	-7.37774700	-1.26387100	-1.05959300
C	-2.54269600	-2.19122400	1.12691000	H	-8.11441600	0.82194800	0.09992100
C	-3.85928500	-2.34991200	0.97793200	H	-7.35675000	0.26765000	1.58357700
C	-3.43168200	0.79530100	-1.58864900	H	-5.96043400	0.83314400	-1.07642500
O	-2.83637000	1.95354500	-2.02431200	H	-5.86258200	1.84053200	0.35571100
C	-3.07240000	3.15575200	-1.33251600	H	-6.36223300	-2.07190100	1.68804900
C	-2.03692700	3.56531300	-0.36808700	H	-0.71732600	-1.17595400	0.99786900
C	-1.19552300	2.74380200	0.32997100	H	-4.29408500	-3.21903700	1.46230500
C	-1.11336900	1.27766700	0.52948400	H	0.35001400	4.28618800	0.56638900
C	0.00954900	3.36185400	1.02945600	H	-0.21053600	3.57723100	2.08193200
C	1.07208500	2.26947000	0.92903900	H	1.88868000	2.38384900	1.63882700
C	0.27690300	0.97478900	1.13515400	H	0.78582100	0.16998200	0.60214700
C	-1.75667800	-3.19289400	1.94315900	H	-2.40420100	-3.96934200	2.35309000
C	-1.95921900	5.07238300	-0.20393600	H	-0.98883300	-3.67968800	1.33165500
O	-4.02558500	3.81369200	-1.64878800	H	-1.23908000	-2.70760600	2.77942100
O	-3.73767800	-0.05613200	-2.37008900	H	-2.91041300	5.51771900	-0.49019900
O	1.72192900	2.30494100	-0.35962500	H	-1.73322100	5.36276600	0.82223500
H	-3.58786300	1.74083300	0.29272900	H	-1.18713100	5.50249800	-0.85269400
H	-4.66728300	0.11225500	1.59689200	H	1.09640200	2.05527000	-1.05005100
C	-8.79588700	-1.82671700	0.45605000	H	-8.87564000	-2.87371800	0.16120000
H	-4.74949100	-1.66465500	-0.85833000	H	-8.92211100	-1.77604500	1.54307100
				H	-9.61980000	-1.27189100	-0.00169300

H	1.21160000	0.44002500	3.02656500	C	-1.23993800	1.31153800	0.85364900
H	-0.21746900	1.46467500	3.21081400	C	-0.32124900	3.40352900	1.64062100
H	-0.41256900	-0.23896700	2.83378500	C	0.80318000	2.36869100	1.65801600
H	7.15652000	-1.90324800	-1.03427500	C	0.06112600	1.02442300	1.64047400
H	8.88992900	-1.60829300	0.76820200	C	-1.88914500	-3.17174400	2.07858400
H	7.94692300	-2.66133400	1.82871900	C	-2.10363100	5.10643800	0.14404600
H	8.66308200	-3.30416200	0.34472700	O	-3.87623300	3.85155500	-1.64419300
H	8.00565600	0.43375900	0.17634900	O	-3.47676900	0.03791000	-2.42131700
H	5.85725700	0.86383300	-1.56143500	O	1.67730100	2.54210200	0.53099700
H	6.72323200	1.65513200	1.82121300	H	-3.66355700	1.72398900	0.29963300
H	3.43902300	2.02724300	-0.43086000	H	-4.85457000	0.05906500	1.42023400
H	6.79986200	3.92942600	0.76196100	C	-8.75447300	-1.98138400	-0.19835300
H	8.21436100	2.96030000	0.32535800	H	-4.58581600	-1.70658200	-1.03003400
H	6.90514900	3.17174600	-0.84126600	C	-0.21664700	0.56512000	3.08725600
H	5.19654100	-0.74319700	0.24324500	C	6.96607200	-2.07934900	0.20106900
H	6.26668700	-0.78238700	1.63844200	C	8.22237500	-2.32046700	1.04801400
B3LYP Energy = -2081.65805605 a.u.				C	7.00950800	0.43442400	-0.35886800
(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf B				O	6.83221000	0.21322900	-1.75591500
C	-0.05688600	-2.11549300	-1.15589600	C	6.50888300	1.83878800	0.06374000
C	-1.26274900	-1.62856700	-0.80573500	C	5.00897400	1.95561200	-0.15178000
C	2.31013100	-2.71770800	-0.83616700	O	4.43459700	1.54866100	-1.14630100
C	1.12842500	-2.28019800	-0.34301500	O	4.37625600	2.56569700	0.84989000
C	4.75108200	-3.17332900	-0.50428100	C	7.22713100	2.95971600	-0.71034400
C	5.07732100	-3.43963500	-1.95086700	C	6.35777700	-0.68819700	0.46440300
C	3.51518000	-2.86361900	-0.05361600	H	0.05067700	-2.43605400	-2.19056900
C	5.92613100	-3.20600700	0.44403200	H	-2.03659600	-1.60663900	-1.56170700
O	-6.27897700	-3.52514400	-0.13927600	H	2.35855000	-2.94910800	-1.89660500
C	-7.38067500	-1.35427300	-0.45534600	H	1.07368200	-2.03935900	0.71586400
C	-7.31815400	0.10548000	0.00747200	H	5.74516000	-4.30289600	-2.04047400
C	-5.95766200	0.72570700	-0.30143200	H	4.19580800	-3.63315700	-2.56119000
C	-4.77692600	-0.04780000	0.33048700	H	5.60539000	-2.58473500	-2.38827100
C	-4.83603600	-1.56269500	0.03000300	H	3.40597300	-2.66941200	1.01226700
C	-6.26203900	-2.14476700	0.23419200	H	5.57101500	-3.14725200	1.47934700
C	-3.48072400	0.70987800	-0.06654400	H	6.44101800	-4.17054500	0.34093200
C	-2.12360300	0.32743000	0.50844600	H	-6.02378100	-3.58022500	-1.06750000
C	-1.67714600	-1.13790500	0.57676000	H	-7.18468300	-1.37608200	-1.53839100
C	-2.61016900	-2.18761100	1.18597400	H	-8.10841800	0.68672500	-0.47808400
C	-3.90075500	-2.37250700	0.90120000	H	-7.51916700	0.15019500	1.08646400
C	-3.25797200	0.85088800	-1.57402700	H	-5.83115700	0.75795500	-1.38862200
O	-2.60716500	2.02295200	-1.88311400	H	-5.93156700	1.76464200	0.04419200
C	-2.96515900	3.20208600	-1.20837800	H	-6.47492600	-2.15787300	1.31084800
C	-2.10166800	3.60547300	-0.08302800	H	-0.78448100	-1.15267400	1.19209200
C	-1.35528900	2.78147000	0.71169500	H	-4.36899000	-3.24715800	1.34240600
				H	0.04482900	4.36997200	1.29994900

H	-0.73131300	3.53610200	2.64926100	C	4.31343500	-0.60629700	0.00087200
H	1.45437700	2.46909700	2.52656900	C	4.98795700	0.77804300	-0.16524400
H	0.68833800	0.28653900	1.13552200	C	6.54013900	0.67846800	-0.13603500
H	-2.55783300	-3.96263000	2.42157300	C	2.77698400	-0.68121100	-0.23344800
H	-1.05402100	-3.64085200	1.54624100	C	1.88601600	0.10683100	0.71683100
H	-1.46747800	-2.67884000	2.96274000	C	2.05911400	1.61751000	0.85999100
H	-1.23682900	5.57907400	-0.33241600	C	3.39935100	2.14834100	1.36245000
H	-2.99766900	5.54027500	-0.29963500	C	4.59834100	1.79731200	0.89056200
H	-2.08293300	5.36209700	1.20398000	C	2.32249800	-0.44272200	-1.64866600
H	1.26594200	2.22027700	-0.27996100	O	0.99998200	-0.83099600	-1.91482500
H	-8.77116600	-3.02842100	-0.50307900	C	0.23965000	-1.88358000	-1.47387600
H	-9.00661300	-1.94068200	0.86686800	C	0.31884300	-2.54381600	-0.13939800
H	-9.53470700	-1.44606800	-0.74675100	C	0.44112400	-1.91141600	1.06260100
H	0.72136600	0.35572200	3.60910900	C	0.88860200	-0.54561900	1.36310400
H	-0.75048500	1.33694400	3.64826900	C	-0.14482400	-2.47876400	2.34086200
H	-0.83094400	-0.33439000	3.11951200	C	-0.78206300	-1.23754400	3.01227600
H	7.25621400	-2.11024000	-0.85346500	C	0.18882400	-0.07944100	2.65110100
H	8.96587000	-1.53292200	0.89597100	C	3.27668700	3.26841700	2.36924300
H	7.97709200	-2.34417100	2.11565400	C	-0.15146000	-3.98584500	-0.20075300
H	8.69668400	-3.27272000	0.79303500	O	-0.59865900	-2.26502000	-2.26648800
H	8.09360100	0.42129800	-0.20083100	O	2.92081300	0.06708500	-2.54563000
H	5.91125600	0.45254600	-1.94756900	O	-2.11603700	-1.01186000	2.60066200
H	6.69890500	1.96750800	1.13249800	H	2.53389600	-1.73155800	-0.05060900
H	3.40906200	2.58970300	0.64684100	H	4.45072400	-0.89763300	1.05042900
H	6.85530200	3.94364800	-0.41482900	C	8.66079800	-0.44390500	-0.95422400
H	8.29996300	2.92457300	-0.50421700	H	4.72208300	1.15642700	-1.16241300
H	7.08391200	2.83352800	-1.78391400	C	1.18631700	0.15539900	3.80115800
H	5.29248000	-0.70407600	0.21484700	C	-6.66101100	1.51066000	-0.71472300
H	6.42986600	-0.45201300	1.53450700	C	-8.01110800	1.51895200	0.01985600
B3LYP Energy = -2081.65707625 a.u.				C	-5.46955500	-0.55983300	0.39452200
				O	-6.52690300	-0.73475100	1.34253700
(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf C				C	-4.79920200	-1.94231200	0.11661200
C	0.52928700	2.66269600	-0.93045400	C	-3.46068800	-1.75342200	-0.57734900
C	1.74111200	2.29676000	-0.47289300	O	-2.57945300	-1.04256600	-0.12184700
C	-1.92533600	2.80055000	-0.89955700	O	-3.30354200	-2.44504800	-1.70127300
C	-0.75596400	2.48357600	-0.29784500	C	-5.73118200	-2.96688300	-0.53323900
C	-4.43176600	2.83067200	-0.85765200	C	-6.04691100	0.09647300	-0.86044800
C	-4.62260900	3.40456200	-2.23840000	H	0.50222700	3.12850700	-1.91368600
C	-3.22335500	2.58946300	-0.30345700	H	2.59878600	2.48564300	-1.10766700
C	-5.69939400	2.54999300	-0.08354900	H	-1.88028100	3.21731300	-1.90206200
O	7.11400900	1.96257700	-0.39719100	H	-0.78968200	2.04331200	0.69394700
C	7.13255900	-0.39973700	-1.05184000	H	-5.34922200	4.22418100	-2.21278700
C	6.49464400	-1.75072100	-0.71302900	H	-3.70055700	3.78834000	-2.67286700
C	4.97696600	-1.69738500	-0.87098700	H	-5.02348700	2.65416600	-2.92907100

H	-3.20754400	2.17623100	0.70284200	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf D			
H	-5.45163500	2.24473100	0.93741900	C	-0.20833000	-2.25072900	-1.24890300
H	-6.26054100	3.49046900	0.00752900	C	-1.37627800	-1.72778700	-0.82846700
H	6.81912500	2.24190200	-1.27169900	C	2.19333800	-2.80021300	-1.07470100
H	6.85677800	-0.14435600	-2.08665600	C	1.03113200	-2.39343600	-0.51431600
H	6.90841300	-2.53210200	-1.35869500	C	4.66154500	-3.19675500	-0.84928400
H	6.76022300	-2.02667100	0.31658200	C	4.94972100	-3.38400500	-2.31609200
H	4.74233200	-1.51484800	-1.92340200	C	3.43411800	-2.93903700	-0.34640500
H	4.54009400	-2.66855400	-0.61160500	C	5.86113600	-3.27877900	0.06525700
H	6.84867400	0.45371500	0.89292800	O	-6.28866600	-3.42713800	-0.03408400
H	1.30117800	1.93849000	1.57431300	C	-7.37004800	-1.31002500	-0.15402100
H	5.44717900	2.35087600	1.28007900	C	-7.29323700	0.14709600	0.31356400
H	-0.88497000	-3.26223000	2.18790400	C	-5.95718200	0.77868000	-0.07222000
H	0.64989500	-2.88125500	2.98152000	C	-4.73883900	0.01873100	0.50049900
H	-0.83856700	-1.36592200	4.09497000	C	-4.81543000	-1.50654700	0.25763500
H	-0.40800900	0.82390400	2.49975200	C	-6.23029500	-2.09812600	0.48910400
H	4.25258300	3.68128500	2.62945800	C	-3.46498000	0.73660000	-0.02817900
H	2.65874300	4.07937900	1.96608400	C	-2.06175900	0.34228700	0.41760400
H	2.79149100	2.93483900	3.29348400	C	-1.64932600	-1.13284100	0.54747100
H	-1.24342300	-4.06192600	-0.18660000	C	-2.54728200	-2.08756000	1.33762500
H	0.18193500	-4.45856100	-1.12542800	C	-3.85997200	-2.25225700	1.16531000
H	0.24113100	-4.55918900	0.63922100	C	-3.38212900	0.81013500	-1.55720500
H	-2.16883400	-0.92678300	1.63098700	O	-2.80542400	1.97973400	-1.98910700
H	9.09654700	0.53262200	-1.16843500	C	-3.06085600	3.17773100	-1.30005800
H	8.97699900	-0.73604800	0.05302600	C	-2.03353100	3.59395800	-0.32950300
H	9.07429100	-1.17182100	-1.65810000	C	-1.18935600	2.77568400	0.36783300
H	0.66094300	0.50664500	4.69373800	C	-1.10743100	1.30936700	0.57774200
H	1.70674600	-0.77185400	4.05979600	C	0.02145300	3.39764300	1.05445000
H	1.94820900	0.88967600	3.54298500	C	1.08148600	2.30393300	0.94453900
H	-6.86483600	1.83976700	-1.74122200	C	0.28719900	1.01344800	1.17805600
H	-8.70138500	0.79666200	-0.42506200	C	-1.79125200	-2.96297400	2.30885200
H	-7.89675300	1.25453100	1.07094900	C	-1.96309600	5.10119100	-0.16797700
H	-8.47346100	2.50891900	-0.04618800	O	-4.01552400	3.82954600	-1.62381000
H	-4.69603300	0.08634100	0.81957000	O	-3.64510200	-0.05421500	-2.33871600
H	-6.13084100	-0.97282200	2.18749600	O	1.70663700	2.32603000	-0.35611800
H	-4.51057700	-2.30991300	1.11113200	H	-3.59073400	1.76680700	0.31773400
H	-2.37324300	-2.33436200	-2.01000500	H	-4.73493800	0.17234700	1.58706100
H	-5.28794200	-3.96412500	-0.51478900	C	-8.73128100	-1.94469600	0.14928000
H	-6.67286900	-2.99426500	0.01772700	H	-4.57786800	-1.70270100	-0.79272400
H	-5.94106400	-2.72306300	-1.57506400	C	0.23526400	0.70091000	2.68804600
H	-6.81501100	-0.56096200	-1.27951400	C	6.85578600	-2.09306800	-0.05764500
H	-5.23903600	0.14120000	-1.59965400	C	8.16641700	-2.43044900	0.66649200
B3LYP Energy = -2081.64827396 a.u.				C	6.90242200	0.48302900	-0.08030500
				O	6.72643700	0.58658700	-1.49140700

C	6.45424300	1.76497500	0.67064600	H	7.98559600	-2.63759900	1.72711400
C	4.94378400	1.93366900	0.69972800	H	8.64216000	-3.31356100	0.23044800
O	4.29169100	2.10318400	1.70480300	H	7.98642800	0.41412300	0.05729400
O	4.39445800	1.89065900	-0.53130200	H	5.80492900	0.83769100	-1.64032100
C	7.12265000	3.02559400	0.09349600	H	6.74587800	1.65457600	1.71806900
C	6.23365900	-0.78652200	0.46842900	H	3.41656500	2.02962300	-0.46587900
H	-0.18259900	-2.61870700	-2.27298000	H	6.81022200	3.91945900	0.63884000
H	-2.20970400	-1.72435900	-1.51883200	H	8.20920600	2.93970800	0.17649900
H	2.19360200	-3.02162100	-2.13855700	H	6.87350800	3.14854100	-0.96027200
H	1.03341800	-2.16423000	0.54847900	H	5.17453000	-0.75094100	0.19139600
H	5.56178400	-4.27849300	-2.47460900	H	6.27224300	-0.78062300	1.56570800
H	4.05020600	-3.47994100	-2.92305200	B3LYP Energy = -2081.65611338 a.u.			
H	5.52415100	-2.53697200	-2.70794300	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf E			
H	3.35660600	-2.80089800	0.73087800	C	-0.02784900	-1.98628100	-1.42577900
H	5.52951300	-3.35404400	1.10708900	C	-1.22701100	-1.59566000	-0.95207400
H	6.40862400	-4.20410000	-0.15713700	C	2.40861200	-2.35274700	-1.36115800
H	-5.54560700	-3.92836200	0.31618700	C	1.26001200	-1.95453400	-0.76703200
H	-7.20899600	-1.33566500	-1.23983700	C	4.87976100	-2.75504200	-1.22388300
H	-8.11297000	0.72201200	-0.12837900	C	5.05398400	-3.26801900	-2.63025600
H	-7.43572000	0.19115900	1.40201700	C	3.69698500	-2.35588600	-0.70637900
H	-5.89404600	0.80264900	-1.16500800	C	6.13208900	-2.75560400	-0.37660200
H	-5.91817200	1.82042800	0.26370400	O	-5.97476200	-3.76701500	0.56932400
H	-6.41640200	-2.12286200	1.57730500	C	-7.27617100	-1.70687400	0.27202900
H	-0.70349000	-1.13143300	1.07588700	C	-7.25964500	-0.21391300	0.61810400
H	-4.32306800	-3.00801100	1.80039400	C	-6.01344700	0.46849100	0.05912900
H	0.35601300	4.32027200	0.58377700	C	-4.69478100	-0.16972400	0.55437700
H	-0.18595500	3.61644100	2.10862200	C	-4.68034100	-1.70573400	0.38220800
H	1.91151300	2.42258700	1.63777800	C	-6.01142900	-2.36298200	0.83964700
H	0.78995300	0.19961500	0.65261600	C	-3.53647900	0.62918700	-0.10204200
H	-2.44966200	-3.68558600	2.79404900	C	-2.08467900	0.39748100	0.29144900
H	-0.99904700	-3.51917400	1.79514300	C	-1.51344700	-1.01844700	0.42999900
H	-1.30736900	-2.36799000	3.09203400	C	-2.26847900	-2.07677400	1.23663100
H	-1.20798300	5.53671700	-0.83300700	C	-3.56710900	-2.37438800	1.15835800
H	-2.92324800	5.53840700	-0.43704100	C	-3.54802300	0.62597600	-1.63208000
H	-1.71952500	5.39452800	0.85313700	O	-3.06211700	1.80321300	-2.14933400
H	1.06324100	2.08966600	-1.03478100	C	-3.40081400	3.01982700	-1.53091600
H	-8.75983800	-2.98173000	-0.18586700	C	-2.39971500	3.58797100	-0.61114100
H	-8.93728500	-1.93046300	1.22548800	C	-1.47335000	2.89860800	0.12144600
H	-9.53387400	-1.39521100	-0.35104200	C	-1.23484600	1.46330700	0.39770700
H	1.24311600	0.51540400	3.06844600	C	-0.33772900	3.67660500	0.77513500
H	-0.18822400	1.53735600	3.25014300	C	0.83334700	2.69746000	0.72418000
H	-0.37977800	-0.17266700	2.90471500	C	0.18567300	1.33620100	0.99529800
H	7.08088900	-1.94130700	-1.11789100	C	-1.35289300	-2.92753200	2.08741800
H	8.88537000	-1.60909100	0.60677100				

C	-2.47341000	5.10245700	-0.53497600	H	-0.86371800	-2.33122600	2.86670400
O	-4.41655100	3.56393300	-1.86937700	H	-1.74769500	5.56926800	-1.21134800
O	-3.80906500	-0.28882800	-2.35542300	H	-3.46435400	5.43321200	-0.84055400
O	1.48923700	2.74517100	-0.55937600	H	-2.27797500	5.47314600	0.47164100
H	-3.74463900	1.66146300	0.19395400	H	0.91363200	2.35454300	-1.22783400
H	-4.61366900	0.02876300	1.63098700	H	-8.52410400	-3.46839300	0.55108500
C	-8.54557300	-2.40119800	0.77482100	H	-8.64452400	-2.29025700	1.86020100
H	-4.57723200	-1.92246800	-0.68959000	H	-9.43592400	-1.96594500	0.31225500
C	0.17810500	1.05068300	2.51098200	H	1.20541900	0.94087200	2.86551400
C	7.21105000	-1.70797400	-0.76078200	H	-0.29754300	1.86459000	3.06573900
C	8.57044300	-2.09664400	-0.15863800	H	-0.36918900	0.13867200	2.75136200
C	6.53545400	0.13429100	0.99788800	H	7.33007500	-1.74919900	-1.85040000
O	7.78791200	0.07430100	1.69006400	H	9.33362800	-1.35079300	-0.39471300
C	5.92408100	1.55835500	1.17059000	H	8.52168600	-2.17193100	0.92804700
C	4.45577600	1.55578100	0.76228100	H	8.89979600	-3.05981000	-0.56106400
O	3.61745600	0.89452800	1.34364100	H	5.82743000	-0.56791900	1.45223200
O	4.17821700	2.35094600	-0.27239300	H	7.61477400	0.18339500	2.63080500
C	6.77099000	2.67159300	0.54935400	H	5.88410700	1.71295300	2.25679500
C	6.78673200	-0.24950600	-0.46209000	H	3.20434800	2.35604700	-0.44042500
H	-0.01706500	-2.39254800	-2.43579200	H	6.74401700	2.64258600	-0.53990600
H	-2.08955200	-1.72145200	-1.59381900	H	6.40792700	3.65385100	0.85850700
H	2.35113000	-2.70275600	-2.38831600	H	7.80616400	2.56443600	0.87859100
H	1.31420100	-1.60607200	0.26078700	H	7.56096400	0.41543000	-0.85764200
H	5.44794300	-4.29117100	-2.61415200	H	5.87278400	-0.03519500	-1.02697200
H	4.12978900	-3.27388800	-3.20592700	B3LYP Energy = -2081.64996225 a.u.			
H	5.78208900	-2.66473600	-3.18285800	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf F			
H	3.69104700	-2.00566500	0.32368700	C	-0.11804400	-2.19551200	-1.05044100
H	5.86626100	-2.63498900	0.67766600	C	-1.31313300	-1.68665500	-0.69501600
H	6.59727100	-3.74669000	-0.46020600	C	2.25829000	-2.77517800	-0.77078400
H	-5.84509200	-3.87836200	-0.37959200	C	1.08828700	-2.32434400	-0.26216800
H	-7.23739700	-1.80204900	-0.82393000	C	4.70908200	-3.20901300	-0.49631500
H	-8.15687600	0.27299800	0.22296400	C	4.99538500	-3.50165800	-1.94632600
H	-7.29878300	-0.09740800	1.70953500	C	3.48493800	-2.89404700	-0.01784300
H	-6.05366000	0.41968100	-1.03436400	C	5.90981400	-3.22214100	0.41934700
H	-6.01721000	1.53187700	0.32119100	O	-6.19462900	-3.50210700	-0.34577800
H	-6.06507500	-2.30405600	1.93430400	C	-7.29903600	-1.40933800	-0.59206900
H	-0.55614700	-0.90849200	0.92615300	C	-7.29021500	0.05700400	-0.14645000
H	-3.89518500	-3.24038900	1.72537300	C	-5.93157400	0.70298600	-0.40829400
H	-0.09702300	4.60577500	0.26167000	C	-4.77124800	-0.02405800	0.30811500
H	-0.57819000	3.92163100	1.81684000	C	-4.79076700	-1.55156200	0.07033700
H	1.61774900	2.93010000	1.44171100	C	-6.21161800	-2.16805800	0.16741800
H	0.78139700	0.57389600	0.49332100	C	-3.46062800	0.72571800	-0.06276800
H	-1.89911300	-3.73690900	2.57404600	C	-2.11529900	0.35238900	0.55019600
H	-0.55657300	-3.37128000	1.47949600				

C	-1.68175300	-1.11684000	0.66844400	H	-8.07024300	0.61043600	-0.67852400
C	-2.62771000	-2.09679700	1.36838600	H	-7.54078800	0.11763500	0.92148900
C	-3.91531500	-2.28012000	1.06971800	H	-5.75332400	0.70257100	-1.48808800
C	-3.19644300	0.83914600	-1.56756200	H	-5.94421600	1.75243400	-0.09452900
O	-2.54530300	2.01118500	-1.88168600	H	-6.50234100	-2.18749600	1.23257900
C	-2.92232900	3.19786600	-1.23502300	H	-0.77317100	-1.11712900	1.26006800
C	-2.08050700	3.62123000	-0.10010000	H	-4.42344300	-3.04960800	1.65144500
C	-1.34649600	2.81029100	0.71835300	H	0.04469800	4.40923000	1.29784800
C	-1.23413500	1.34158800	0.88770400	H	-0.74688900	3.59780500	2.65169000
C	-0.32505800	3.44844900	1.65035400	H	1.44105900	2.53093500	2.57166100
C	0.79928500	2.41460000	1.69808500	H	0.68958100	0.32114600	1.22015700
C	0.05591600	1.07090800	1.69902200	H	-2.63606000	-3.71693800	2.80384300
C	-1.94827400	-2.97756100	2.38961600	H	-1.10710700	-3.51429400	1.93652100
C	-2.08871600	5.12528900	0.10279100	H	-1.54099500	-2.39341300	3.22257400
O	-3.82689800	3.83805000	-1.69715100	H	-1.22061500	5.59334900	-0.37588500
O	-3.38435500	0.00945500	-2.40446400	H	-2.98117300	5.54817200	-0.35463400
O	1.68557400	2.56644300	0.57833300	H	-2.07634900	5.39827900	1.15844000
H	-3.65166800	1.74627300	0.28066900	H	1.27891100	2.24281100	-0.23441200
H	-4.90169800	0.13283200	1.38660700	H	-8.65228400	-3.10614400	-0.72050100
C	-8.67218600	-2.06282800	-0.40480800	H	-8.97863500	-2.03218200	0.64687700
H	-4.44992000	-1.74956600	-0.95121000	H	-9.43300300	-1.53732700	-0.98905600
C	-0.24157100	0.64766000	3.15250000	H	0.68859400	0.44314600	3.69013800
C	6.93858500	-2.09555700	0.13261300	H	-0.77570200	1.43622200	3.68935800
C	8.22262500	-2.32809000	0.93940500	H	-0.86349800	-0.24530900	3.19793300
C	6.96435400	0.41565000	-0.43821700	H	7.19334300	-2.13335600	-0.93090700
O	6.73696000	0.19623200	-1.82804400	H	8.95905300	-1.54017200	0.75796100
C	6.48743700	1.82251800	0.00299800	H	8.01220000	-2.34510600	2.01458200
C	4.98213800	1.95072000	-0.16109000	H	8.69047600	-3.28104200	0.67539800
O	4.36989600	1.54260800	-1.13246400	H	8.05320000	0.39651800	-0.31822400
O	4.38945900	2.57327500	0.85721300	H	5.81057900	0.43893800	-1.98619700
C	7.18651000	2.93999600	-0.79353900	H	6.71470800	1.94857600	1.06482100
C	6.33617300	-0.70411900	0.40691100	H	3.41679600	2.60613900	0.68364000
H	-0.03810600	-2.56558200	-2.07092500	H	6.82969500	3.92580200	-0.48605800
H	-2.10351300	-1.69576600	-1.43353600	H	8.26516100	2.89899600	-0.62174600
H	2.27851900	-3.04275000	-1.82360700	H	7.00843900	2.81480800	-1.86201400
H	1.06007000	-2.04399400	0.78813900	H	5.26431500	-0.72138000	0.18684700
H	5.67831100	-4.35250400	-2.03881500	H	6.43787300	-0.46428900	1.47386500
H	4.09929300	-3.72651800	-2.52388400	B3LYP Energy = -2081.65512117 a.u.			
H	5.49017900	-2.64573700	-2.41911700				
H	3.40448200	-2.67563700	1.04585200	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf G			
H	5.58316100	-3.14978300	1.46314300	C	-0.01219200	-1.97281500	-1.43049200
H	6.42511300	-4.18635600	0.31577800	C	-1.21078700	-1.58105000	-0.95614500
H	-5.48162600	-3.98753000	0.08092300	C	2.42206000	-2.35506400	-1.35920500
H	-7.03765700	-1.45046000	-1.65765000	C	1.27630000	-1.93666000	-0.77358900

C	4.88955500	-2.77417400	-1.20361800	C	6.77229200	-0.25393000	-0.46363700
C	5.06512300	-3.32622000	-2.59502400	H	-0.00314200	-2.38522700	-2.43803200
C	3.70861300	-2.35254900	-0.70049800	H	-2.07438600	-1.71055600	-1.59567300
C	6.13905200	-2.76072200	-0.35155100	H	2.36347400	-2.72667100	-2.37874900
O	-5.92379800	-3.79952100	0.56757400	H	1.33435500	-1.56737700	0.24655800
C	-7.24875500	-1.75456000	0.26893300	H	5.42421100	-4.36142600	-2.54974900
C	-7.24962800	-0.26157200	0.61545300	H	4.14864100	-3.31541500	-3.18292500
C	-6.01095600	0.43540600	0.05769200	H	5.81994700	-2.76105000	-3.15227300
C	-4.68551300	-0.18767400	0.55410800	H	3.70184000	-1.97516400	0.31962800
C	-4.65322400	-1.72340000	0.38191600	H	5.87106700	-2.62778500	0.70028800
C	-5.97711700	-2.39602100	0.83775400	H	6.60972500	-3.75004800	-0.42230700
C	-3.53535900	0.62477500	-0.10028700	H	-5.79124200	-3.90948500	-0.38110200
C	-2.08075800	0.40677100	0.29128200	H	-7.20770900	-1.84897500	-0.82700900
C	-1.49542200	-1.00355900	0.42609300	H	-8.15209100	0.21505200	0.21966900
C	-2.23797100	-2.06751800	1.23730000	H	-7.29113400	-0.14581200	1.70687200
C	-3.53348700	-2.37861600	1.16028600	H	-6.04974900	0.38628600	-1.03580200
C	-3.54730900	0.62643100	-1.63030600	H	-6.02720200	1.49863500	0.31999500
O	-3.07372300	1.81038900	-2.14388800	H	-6.03255000	-2.33767800	1.93234600
C	-3.42581700	3.02138700	-1.52196600	H	-0.53679100	-0.88503500	0.91759600
C	-2.43219100	3.59680900	-0.59862800	H	-3.85276900	-3.24574700	1.73057300
C	-1.49776900	2.91487800	0.13062000	H	-0.14214400	4.63781600	0.27911000
C	-1.24219900	1.48120000	0.40009900	H	-0.61243500	3.93847700	1.83101200
C	-0.37096500	3.70284800	0.78738900	H	1.59493300	2.97910900	1.44409400
C	0.81147200	2.73791400	0.72781800	H	0.78526000	0.61457000	0.48807900
C	0.18108400	1.36753600	0.99418900	H	-1.85081700	-3.71844900	2.58087200
C	-1.31319200	-2.90549800	2.09063100	H	-0.51277700	-3.34350000	1.48396000
C	-2.52407600	5.10990400	-0.51488100	H	-0.82943400	-2.30143300	2.86723400
O	-4.44663400	3.55607000	-1.86018900	H	-1.80511400	5.58883700	-1.18998900
O	-3.79921500	-0.28858100	-2.35660200	H	-3.51937500	5.43009600	-0.81755300
O	1.46224200	2.80047700	-0.55766500	H	-2.33180200	5.47793400	0.49330000
H	-3.75418000	1.65392500	0.19890800	H	0.89263500	2.39815900	-1.22431700
H	-4.60810000	0.01144100	1.63087300	H	-8.47710700	-3.53021200	0.54561000
C	-8.51064600	-2.46350000	0.77021200	H	-8.61166000	-2.35466500	1.85560200
H	-4.54614400	-1.93897700	-0.68974000	H	-9.40550400	-2.03788800	0.30734700
C	0.18067000	1.07504600	2.50858000	H	1.20964700	0.96860600	2.85953800
C	7.21142100	-1.71107900	-0.74761600	H	-0.29750700	1.88338500	3.06922500
C	8.57270900	-2.08072800	-0.13641600	H	-0.35989800	0.15855800	2.74669400
C	6.51652800	0.14335100	0.99780900	H	7.33350900	-1.76544500	-1.83628800
O	7.69114700	0.05117700	1.80909400	H	9.34028100	-1.35060000	-0.41382600
C	5.89293400	1.56233600	1.15731400	H	8.52833300	-2.11834500	0.95255700
C	4.43312600	1.55008600	0.72073800	H	8.90141200	-3.05701900	-0.50515900
O	3.60457900	0.81433700	1.21928800	H	5.81266800	-0.55215600	1.45674200
O	4.14815600	2.43306200	-0.24011200	H	8.41073500	0.49452000	1.34831200
C	6.72989300	2.69203700	0.54976700	H	5.84888300	1.70565600	2.24241700

H	3.17789700	2.42636100	-0.42704400	H	4.47183200	-0.88806800	1.10280800
H	6.77562400	2.63351500	-0.53825100	C	8.59333600	-1.06672400	-1.14359900
H	6.30749000	3.66522800	0.80446100	H	4.77921600	0.81680900	-1.38396600
H	7.74850500	2.66448300	0.94740400	C	1.36063700	0.69376200	3.85486000
H	7.53641800	0.41585100	-0.87932800	C	-6.32387600	1.64227600	-0.29071700
H	5.85825500	-0.05446300	-1.03449400	C	-7.67696300	1.78828000	0.41932100
B3LYP Energy = -2081.64982959 a.u.				C	-6.19934500	-0.92988100	-0.47340600
(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf H				O	-6.12671400	-0.93282000	-1.89533100
C	0.72714300	2.63726400	-1.18397500	C	-5.59354000	-2.21691000	0.15576700
C	1.94440300	2.28969600	-0.72485800	C	-4.07930700	-2.23879300	0.05631800
C	-1.72123700	2.87828800	-1.06084300	O	-3.33041500	-2.29851600	1.01356500
C	-0.53586300	2.56598400	-0.48793800	O	-3.64561300	-2.19334000	-1.20817500
C	-4.21905700	3.03107100	-0.87838600	C	-6.20289400	-3.48931300	-0.45826500
C	-4.48581300	3.44870900	-2.30068800	C	-5.59472000	0.35067200	0.11991100
C	-2.98893900	2.78806600	-0.37391700	H	0.67606500	2.99373500	-2.21099700
C	-5.44354100	2.88894200	-0.00385100	H	2.78618600	2.38052500	-1.40203400
O	7.26267100	1.51278400	-0.87055900	H	-1.71496700	3.20724300	-2.09647500
C	7.06937700	-0.91378100	-1.17065600	H	-0.54315100	2.21236100	0.53749300
C	6.35632500	-2.14563300	-0.60281400	H	-5.03942500	4.39467300	-2.32256900
C	4.84049500	-1.99456100	-0.69847100	H	-3.57981800	3.57678200	-2.89147500
C	4.30761600	-0.73792000	0.02783100	H	-5.11197100	2.70949800	-2.81223600
C	5.07632700	0.55054900	-0.35989100	H	-2.92769600	2.47503400	0.66657800
C	6.61489700	0.32906400	-0.39536100	H	-5.14371600	2.86867000	1.04979400
C	2.76045900	-0.71475500	-0.13525000	H	-6.06994600	3.78097100	-0.13433700
C	1.98252400	0.26367800	0.73585400	H	6.92907300	1.69131600	-1.75738900
C	2.28339500	1.75880000	0.67020400	H	6.74989900	-0.78899800	-2.21664300
C	3.68604300	2.22892400	1.04677600	H	6.67509800	-3.04399400	-1.14129000
C	4.82726600	1.72438300	0.57107100	H	6.65948500	-2.28725100	0.44344000
C	2.26631300	-0.64048900	-1.55535300	H	4.56171100	-1.95148100	-1.75498900
O	0.90344200	-0.95015100	-1.73472600	H	4.34930200	-2.87861200	-0.27605400
C	0.04115900	-1.77635100	-1.07381700	H	6.97017100	0.22838300	0.63812900
C	0.19373700	-2.33190500	0.30115900	H	1.59421400	2.23138000	1.37045100
C	0.41173800	-1.56644000	1.40394500	H	5.73725900	2.24419400	0.85532000
C	0.96844600	-0.21033600	1.49799900	H	-0.97257700	-2.66201100	2.71354200
C	-0.20376900	-1.89073900	2.75009100	H	0.55255600	-2.19996600	3.48102800
C	-0.77277600	-0.50996500	3.14236300	H	-0.98745300	-0.45002100	4.21679000
C	0.34083000	0.47300000	2.72401700	H	-0.13312400	1.42521600	2.47569800
C	3.70411600	3.45795900	1.92508500	H	4.72125200	3.81401200	2.09623500
C	-0.35383800	-3.74133500	0.42565100	H	3.13039200	4.26965800	1.46239900
O	-0.96639700	-2.05451800	-1.69573200	H	3.24273400	3.26438500	2.90028100
O	2.86501500	-0.32329700	-2.53610500	H	-1.42743500	-3.73480300	0.63006800
O	-1.92909400	-0.17722900	2.38819900	H	-0.19490800	-4.30153500	-0.49674700
H	2.44586300	-1.70745900	0.19902200	H	0.14662000	-4.27255500	1.23714100
				H	-2.41899300	-0.97367900	2.13728400

H	9.08475500	-0.16938900	-1.52128400	C	0.19386800	-1.82102700	-1.42645400
H	8.94808100	-1.23532800	-0.12099100	C	0.28706600	-2.49382300	-0.10027000
H	8.90941100	-1.91924800	-1.75148700	C	0.44741500	-1.87254700	1.10307900
H	0.88158400	1.17237600	4.71381600	C	0.92888600	-0.51810100	1.40135400
H	1.79282400	-0.25232400	4.19344100	C	-0.11618900	-2.43932600	2.39080000
H	2.18743700	1.32587600	3.53071400	C	-0.70939000	-1.19237400	3.09140200
H	-6.50803700	1.58456300	-1.36830700	C	0.26755400	-0.04600900	2.70665700
H	-8.33271000	0.93449400	0.23039500	C	3.40126300	3.24856900	2.37204300
H	-7.54253100	1.87313900	1.50347400	C	-0.20587500	-3.92829300	-0.16148400
H	-8.20359700	2.68410600	0.07815600	O	-0.66925300	-2.17723700	-2.20522000
H	-7.27075200	-0.96630100	-0.25336400	O	2.89665300	0.06509500	-2.54876100
H	-5.20197000	-1.07590500	-2.13633300	O	-2.05262100	-0.94305000	2.73567900
H	-5.80969000	-2.19286000	1.22660900	H	2.52444100	-1.72936700	-0.05140200
H	-2.65783900	-2.19295900	-1.25748300	H	4.47516000	-0.93235200	1.01872500
H	-5.77800500	-4.38919000	-0.00648300	C	8.65449700	-0.54390800	-1.06962200
H	-7.28196600	-3.50059000	-0.28478900	H	4.74031900	1.12397400	-1.19250000
H	-6.03249300	-3.51885800	-1.53385700	C	1.29632600	0.17322200	3.83199500
H	-4.54864200	0.41395900	-0.19983700	C	-6.62154600	1.56582500	-0.75037200
H	-5.57940200	0.27552600	1.21525800	C	-7.99320500	1.60707800	-0.05706000
B3LYP Energy = -2081.65549364 a.u.				C	-5.64359200	-0.61666500	0.36412400
(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf I				O	-6.73897200	-0.81691400	1.25985100
C	0.58486900	2.66516900	-0.90328000	C	-4.95455200	-1.98935900	0.08673700
C	1.80152000	2.31414900	-0.44739600	C	-3.56882700	-1.78149700	-0.50162300
C	-1.86881800	2.78844100	-0.86815100	O	-2.72047100	-1.08477900	0.02955300
C	-0.69904600	2.44908300	-0.27954000	O	-3.34106900	-2.44130500	-1.63366300
C	-4.37154100	2.85121000	-0.81962300	C	-5.82373100	-2.98854000	-0.68286600
C	-4.55206000	3.51630800	-2.16106900	C	-6.04359300	0.13814900	-0.91138100
C	-3.16788400	2.55281200	-0.28350000	H	0.55256000	3.15003400	-1.87708800
C	-5.64455000	2.55281600	-0.06163200	H	2.65774800	2.52928400	-1.07589200
O	7.16000800	1.88639100	-0.47510000	H	-1.82253400	3.25238800	-1.84964800
C	7.12551400	-0.47434800	-1.13523900	H	-0.73096400	1.96560700	0.69172400
C	6.47212100	-1.81510900	-0.78543400	H	-5.27783000	4.33361700	-2.08618700
C	4.95275800	-1.73618300	-0.91356400	H	-3.62678200	3.92769000	-2.56211300
C	4.32441900	-0.63574100	-0.02747100	H	-4.94716600	2.81483300	-2.90460300
C	5.01979200	0.73726300	-0.20219800	H	-3.15665900	2.07421000	0.69326900
C	6.57016700	0.61128600	-0.20513800	H	-5.40482600	2.19102300	0.94231300
C	2.78284800	-0.68254100	-0.23393400	H	-6.18773900	3.49809200	0.07624300
C	1.92508500	0.11732100	0.73650000	H	6.85069200	2.17345400	-1.34207600
C	2.12798900	1.62406900	0.87872100	H	6.83256900	-0.21228800	-2.16366700
C	3.48564200	2.12942400	1.36043100	H	6.86003300	-2.60239000	-1.43994600
C	4.66919300	1.75893600	0.86508300	H	6.75327600	-2.09680400	0.23846000
C	2.30565000	-0.42923800	-1.63874400	H	4.70083000	-1.54809300	-1.96096300
O	0.96594800	-0.78142900	-1.87523600	H	4.50462600	-2.70027400	-0.64695700
				H	6.89595100	0.37869200	0.81672200

H	1.38686000	1.95742000	1.60521300	C	-7.25641200	0.11763200	-0.87093400
H	5.53513200	2.29532600	1.24076000	C	-6.73771500	1.49018400	-0.42781200
H	-0.87684800	-3.20558000	2.25108000	C	-5.22493900	1.58978100	-0.60281700
H	0.68714700	-2.86516200	3.00514500	C	-4.45114000	0.49813600	0.17123500
H	-0.72661700	-1.32685800	4.17478600	C	-4.99503100	-0.92137800	-0.11621000
H	-0.32252900	0.86457200	2.57277800	C	-6.54705400	-0.97397600	-0.05985800
H	4.38913500	3.64196900	2.61685000	C	-2.93820600	0.75700900	-0.06936500
H	2.79242400	4.07235500	1.98110400	C	-1.89504700	-0.04730300	0.69306800
H	2.92496900	2.92222200	3.30333500	C	-1.96882000	-1.58071800	0.70786000
H	-1.29761800	-3.99121700	-0.11447400	C	-3.23755300	-2.24640000	1.24178200
H	0.09433400	-4.39680800	-1.09959500	C	-4.48377000	-1.97422100	0.84783400
H	0.20345600	-4.51447000	0.66155200	C	-2.49149500	0.76523000	-1.53003400
H	-2.16558000	-0.91920600	1.76981700	O	-1.37407500	1.55457000	-1.69357400
H	9.10163600	0.42589200	-1.29085600	C	-1.34996500	2.81826200	-1.08400700
H	8.98691100	-0.84357400	-0.06982500	C	-0.58720500	2.95344900	0.17360300
H	9.04108300	-1.27685300	-1.78351400	C	-0.38941900	1.99357100	1.12465400
H	0.79684300	0.52711800	4.73822300	C	-0.83052800	0.58701800	1.26273000
H	1.81123000	-0.76148600	4.07465800	C	0.54854300	2.28710600	2.28930500
H	2.06082700	0.89910100	3.55861500	C	1.19827500	0.93481000	2.59602200
H	-6.78035400	1.92648200	-1.77388800	C	0.06476800	-0.07560100	2.33028400
H	-8.69502300	0.91255900	-0.53087800	C	-2.97284300	-3.39892100	2.18216500
H	-7.91788600	1.34127800	0.99779200	C	-0.01883800	4.34881300	0.35735300
H	-8.42593300	2.60925400	-0.13092400	O	-1.88508600	3.73038900	-1.65504100
H	-4.92899200	-0.02346200	0.93504700	O	-2.92069600	0.11431800	-2.43503300
H	-7.47916100	-1.17233100	0.75758600	O	2.34516200	0.69043500	1.78971800
H	-4.76352600	-2.38937600	1.08938800	H	-2.80754200	1.78548600	0.27727800
H	-2.39829700	-2.31107000	-1.89822000	H	-4.60539900	0.67974800	1.24315700
H	-5.34177900	-3.96606500	-0.72888200	C	-8.77951500	0.00947600	-0.74822000
H	-6.78337000	-3.12168700	-0.17629200	H	-4.71249900	-1.18340600	-1.14564800
H	-6.00898600	-2.66984900	-1.70945800	C	-0.71933700	-0.36149100	3.62615500
H	-6.77771000	-0.46109100	-1.46540100	C	6.40753600	-1.77345100	-0.14757100
H	-5.15753200	0.19610500	-1.55404800	C	7.60730500	-1.81783000	0.81021800
B3LYP Energy = -2081.64713208 a.u.				C	6.15878100	0.81253500	0.08782700
				O	6.84107000	1.08824100	-1.16187600
(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf J				C	5.15821500	1.96171300	0.31118100
C	-0.54584800	-2.63103100	-1.16755200	C	4.08557500	2.06683100	-0.77989300
C	-1.70169900	-2.13387600	-0.68945500	O	2.91167200	2.23690900	-0.53073400
C	1.88705000	-3.05889700	-1.10137700	O	4.50943600	2.02083300	-2.04715500
C	0.72503400	-2.73723400	-0.48947000	C	5.86870900	3.32213800	0.45869500
C	4.39400700	-3.21149300	-0.92975000	C	5.48554900	-0.56117600	0.09306300
C	4.68247700	-3.45378500	-2.38770300	H	-0.55146100	-2.96416300	-2.20355500
C	3.15638300	-3.06781700	-0.41027100	H	-2.54673300	-2.10647800	-1.36489600
C	5.60124900	-3.09799200	-0.02709700	H	1.86798200	-3.27250800	-2.16649800
O	-7.00100500	-2.28131700	-0.42509400	H	0.76144600	-2.50593900	0.57076800

H	5.29104600	-4.35719500	-2.51235200	H	4.98515600	-0.67532200	1.06180200
H	3.78126700	-3.57155500	-2.98795500	B3LYP Energy = -2081.64600924 a.u.			
H	5.25873000	-2.62774100	-2.82158100	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf K			
H	3.08906200	-2.88716100	0.66108700	C	0.37960200	2.48387500	-1.26199400
H	5.28468900	-3.20209800	1.01638300	C	1.60952700	2.14102300	-0.83183700
H	6.29046900	-3.92736300	-0.23178600	C	-2.07806700	2.65342500	-1.06546100
H	-6.68912400	-2.45695600	-1.32031000	C	-0.86117100	2.40921600	-0.52653600
H	-6.98146600	-0.02300200	-1.92747800	C	-4.57451000	2.70979700	-0.76327000
H	-7.23147800	2.27998600	-1.00302900	C	-4.92367800	3.13028500	-2.16683500
H	-7.00996900	1.65584500	0.62349700	C	-3.31037900	2.52649800	-0.32314400
H	-4.99028700	1.51277500	-1.66915800	C	-5.73628400	2.53443400	0.18860800
H	-4.87289200	2.57472500	-0.27812800	O	7.22476400	2.02815300	-0.05180700
H	-6.85489400	-0.86905300	0.98834600	C	7.38546100	-0.39745300	-0.34138300
H	-1.15633700	-1.91603700	1.34601600	C	6.69934800	-1.71212300	0.04203300
H	-5.26638600	-2.61351300	1.24528400	C	5.24375600	-1.72864300	-0.41795000
H	1.29824500	3.04381200	2.06529300	C	4.41665500	-0.55623000	0.15712600
H	-0.02521500	2.63834400	3.15630100	C	5.09810000	0.81573000	-0.06643400
H	1.54151700	0.86782100	3.63148800	C	6.61671400	0.77610600	0.27931400
H	0.52723500	-0.99545200	1.97192000	C	2.94870300	-0.70499300	-0.34459800
H	-3.89748800	-3.90427700	2.46571400	C	1.91431600	0.06870100	0.46864800
H	-2.31226800	-4.13622400	1.71068500	C	1.97371900	1.58954100	0.54636500
H	-2.47194500	-3.06757500	3.09893100	C	3.24261800	2.28254600	1.03016800
H	1.05122400	4.34850900	0.12266000	C	4.50428600	1.96285800	0.72818400
H	-0.51376500	5.04162400	-0.31962000	C	2.78676200	-0.58647400	-1.84437000
H	-0.14537400	4.71562900	1.37722400	O	1.56033500	-1.02732300	-2.35955100
H	2.28594200	1.18686900	0.95571300	C	0.42827900	-1.43527200	-1.70226100
H	-9.12722900	-0.98338700	-1.03615100	C	0.42463800	-2.42250200	-0.55788500
H	-9.09932200	0.18800300	0.28432000	C	0.53724800	-1.99630100	0.71683500
H	-9.27400800	0.75003200	-1.38326400	C	0.92042100	-0.62069700	1.08012200
H	-0.07614700	-0.84918100	4.36484100	C	-0.00421600	-2.66088200	1.95944700
H	-1.09770100	0.56465100	4.06918600	C	-0.75437400	-1.48199100	2.63983500
H	-1.58148600	-1.00393500	3.44691600	C	0.10436100	-0.21833900	2.31625000
H	6.79399700	-1.72042900	-1.17596900	C	2.95660500	3.53758800	1.82502500
H	8.27613100	-0.96112600	0.68666000	C	0.00625900	-3.80749700	-0.98707800
H	7.27317600	-1.82760100	1.85278600	O	-0.61860800	-1.08672800	-2.18928800
H	8.20202500	-2.72000500	0.64403700	O	3.58416200	-0.19927900	-2.64293500
H	6.89759200	0.86981800	0.89560600	O	-2.09668500	-1.36861600	2.19649600
H	7.38277700	0.33016600	-1.40175100	H	2.71511100	-1.75765400	-0.16264200
H	4.61337700	1.74215600	1.23131100	H	4.35364600	-0.70502200	1.24291900
H	5.45727500	1.77312400	-2.05246800	C	8.86228200	-0.37994300	0.06579900
H	5.14338400	4.11906500	0.63467800	H	5.03661000	1.04392300	-1.13937700
H	6.55449600	3.29384600	1.30944900	C	0.99412800	0.16479200	3.51237700
H	6.44577100	3.56857400	-0.43375200	C	-6.82694400	1.51723500	-0.22990700
H	4.69010500	-0.57156400	-0.65749300				

C	-8.00598800	1.57746900	0.75418800	H	1.65632100	0.99909600	3.27959400
C	-5.41603400	-0.53640600	0.63005500	H	-7.21591200	1.83906000	-1.20405300
O	-6.14654700	-0.57180200	1.86032800	H	-8.80479800	0.89796600	0.44337600
C	-4.92598500	-1.97867200	0.28008700	H	-7.69799200	1.28610200	1.75830000
C	-3.94283800	-1.95370600	-0.87775800	H	-8.42423400	2.58831200	0.79220500
O	-4.10009800	-2.46231700	-1.95771800	H	-4.52386300	0.08308500	0.75681900
O	-2.81476300	-1.26935100	-0.55358700	H	-5.52789000	-0.81403000	2.55814000
C	-6.05710300	-2.97931900	0.04379500	H	-4.33966400	-2.29212700	1.15302800
C	-6.30145700	0.07760400	-0.45522200	H	-2.18683600	-1.24988900	-1.31118500
H	0.29759200	2.83713000	-2.28783500	H	-5.67150800	-4.00102400	0.02991800
H	2.44021700	2.24173100	-1.52244500	H	-6.79253300	-2.89595600	0.84547900
H	-2.12718800	2.93300100	-2.11413600	H	-6.55059200	-2.80752200	-0.91329600
H	-0.82094400	2.11576500	0.51826100	H	-7.16647400	-0.57234200	-0.61850700
H	-5.61231400	3.98249300	-2.14760500	H	-5.72307900	0.05443700	-1.38555600
H	-4.05295400	3.41593800	-2.75573100	B3LYP Energy = -2081.64657521 a.u.			
H	-5.43759000	2.32710700	-2.70623500	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf L			
H	-3.18713600	2.23619700	0.71872500	C	0.57863900	2.67384700	-0.85916600
H	-5.36173400	2.26991300	1.18201300	C	1.78303300	2.29422400	-0.39314000
H	-6.23521700	3.50783900	0.29949500	C	-1.87549800	2.82417100	-0.85545100
H	7.11439500	2.16441100	-1.00003800	C	-0.71555000	2.48208100	-0.24905900
H	7.32425400	-0.29015300	-1.43529300	C	-4.38178700	2.86719000	-0.84370100
H	7.23875700	-2.55725200	-0.39774800	C	-4.55167500	3.47511800	-2.21271400
H	6.75377200	-1.84265800	1.13136700	C	-3.18180300	2.60452600	-0.28099600
H	5.22059600	-1.69098000	-1.51081000	C	-5.66081200	2.57762300	-0.09202900
H	4.77012300	-2.67151800	-0.12144900	O	7.00907700	1.97973500	-0.69323300
H	6.71874900	0.71038900	1.36982900	C	7.08197100	-0.34895800	-1.15614700
H	1.17938500	1.88370800	1.23238200	C	6.50089400	-1.71117800	-0.76592000
H	5.26347900	2.65369900	1.08215200	C	4.97761400	-1.70599800	-0.87245600
H	-0.67657500	-3.49902900	1.77978000	C	4.31469300	-0.63032700	0.01723700
H	0.81094900	-3.00434600	2.60732600	C	4.96170500	0.76809200	-0.14586600
H	-0.82621600	-1.63242100	3.71820100	C	6.51251800	0.72231300	-0.22707600
H	-0.59084300	0.59957800	2.10852200	C	2.77525000	-0.70555000	-0.20267200
H	3.87343000	4.07729600	2.06621500	C	1.88905100	0.07392800	0.76058900
H	2.29954100	4.21119200	1.26317700	C	2.07316300	1.58369500	0.92880900
H	2.44136400	3.30631000	2.76503200	C	3.41325700	2.07807000	1.46912500
H	-0.95367400	-3.78667600	-1.51194200	C	4.60514200	1.72285300	0.98184500
H	0.73994400	-4.23421600	-1.67973700	C	2.30945600	-0.44721900	-1.61238900
H	-0.07275900	-4.47763200	-0.13196100	O	0.97757900	-0.81923400	-1.86589200
H	-2.12991200	-1.27028600	1.23052300	C	0.23382000	-1.89325400	-1.45474600
H	9.32755200	0.57403400	-0.18466300	C	0.30705800	-2.56409300	-0.12624400
H	8.96839400	-0.52926100	1.14584800	C	0.42819900	-1.93997300	1.08032200
H	9.41387400	-1.17929200	-0.43725000	C	0.88492800	-0.57997700	1.39583100
H	0.37727000	0.44814500	4.36983500	C	-0.17323200	-2.51342800	2.34904700
H	1.62605800	-0.67614800	3.81347700				

C	-0.80697300	-1.27242400	3.02323800	H	-0.39572900	0.79213400	2.54932400
C	0.18396900	-0.12436300	2.68738000	H	4.28538600	3.50547300	2.84424800
C	3.30432800	3.13250100	2.54432700	H	2.71332700	3.98181400	2.18213500
C	-0.16814500	-4.00359200	-0.19817300	H	2.79634000	2.75712700	3.43890400
O	-0.59036300	-2.27851200	-2.26082200	H	-1.26049400	-4.07545000	-0.18917700
O	2.90056800	0.06756300	-2.50962200	H	0.16697600	-4.47082900	-1.12490900
O	-2.13168200	-1.02644700	2.59486700	H	0.21875400	-4.58405200	0.63954400
H	2.53222800	-1.75796700	-0.03069300	H	-2.17409900	-0.94514100	1.62440700
H	4.46584200	-0.93363200	1.06121800	H	9.00520100	0.63230500	-1.41576800
C	8.61417900	-0.34740700	-1.14048500	H	8.99462000	-0.59675700	-0.14345100
H	4.63408500	1.18366200	-1.10506100	H	9.00831000	-1.08825200	-1.84221000
C	1.17785800	0.06912000	3.84813300	H	0.65469200	0.41958700	4.74231700
C	-6.61989800	1.55704900	-0.75674900	H	1.67406600	-0.87398900	4.09655800
C	-7.98448600	1.56931300	-0.04945600	H	1.95948100	0.78770900	3.60640400
C	-5.47403300	-0.54143800	0.34864200	H	-6.79930300	1.90191700	-1.78260100
O	-6.55190900	-0.71353900	1.27381400	H	-8.67202400	0.85845900	-0.51644200
C	-4.81729300	-1.92949900	0.06606100	H	-7.89355200	1.29180600	1.00049500
C	-3.46641200	-1.75063600	-0.60616400	H	-8.43654700	2.56415200	-0.11327400
O	-2.58286000	-1.05589500	-0.13051600	H	-4.70023800	0.08842200	0.79708600
O	-3.30248900	-2.43216800	-1.73498800	H	-6.17580000	-0.96801000	2.12306700
C	-5.75240600	-2.93469800	-0.60921300	H	-4.54863400	-2.31172800	1.06068000
C	-6.01689300	0.13871400	-0.90908500	H	-2.36698300	-2.32989600	-2.03083000
H	0.56696800	3.16341900	-1.83097300	H	-5.32214400	-3.93766800	-0.59536000
H	2.65003700	2.49390700	-1.01152400	H	-6.70270900	-2.95603700	-0.07300700
H	-1.81554300	3.27100400	-1.84410000	H	-5.94314900	-2.67668800	-1.65130800
H	-0.76503100	2.01067000	0.72764500	H	-6.78197000	-0.50450600	-1.35477800
H	-5.28184600	4.29114000	-2.17896900	H	-5.19201700	0.18561600	-1.62916300
H	-3.62399200	3.87287400	-2.62201200	B3LYP Energy = -2081.64619560 a.u.			
H	-4.93742100	2.74078400	-2.92875800				
H	-3.18036700	2.16616300	0.71472900	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf M			
H	-5.42836600	2.25039900	0.92571800	C	-0.48076100	-2.51012400	-1.21384400
H	-6.21746900	3.51954800	0.01046500	C	-1.72169100	-2.26317800	-0.75713600
H	6.64486000	2.67941500	-0.14258400	C	1.96952700	-2.63363600	-1.11816300
H	6.74480200	-0.10631300	-2.17243200	C	0.78247300	-2.34752200	-0.53404000
H	6.91478100	-2.48954100	-1.41488900	C	4.46918000	-2.59515500	-1.05044600
H	6.81090600	-1.96350900	0.25747600	C	4.68471300	-3.26875900	-2.38221800
H	4.70507400	-1.53650300	-1.91756600	C	3.25181000	-2.36988400	-0.50919900
H	4.57678300	-2.68713900	-0.59252500	C	5.71888200	-2.15795900	-0.32357000
H	6.90217900	0.52598900	0.78701000	O	-6.70798400	-1.64348900	-1.66003900
H	1.30922600	1.89920700	1.63910400	C	-6.55249800	0.80352500	-1.80718300
H	5.46100000	2.19188200	1.46812900	C	-6.03301600	2.02306800	-1.03722700
H	-0.91777300	-3.28967000	2.18181800	C	-4.52978500	1.91862000	-0.79134700
H	0.61155800	-2.92768300	2.99429500	C	-4.12951000	0.64218900	-0.01614900
H	-0.88064900	-1.41013800	4.10380300	C	-4.73331800	-0.64005100	-0.63583900

C	-6.23131800	-0.46388500	-1.00623500	H	6.34956500	-3.03849700	-0.13779200
C	-2.58887600	0.69185300	0.19292100	H	-6.18525000	-1.76401600	-2.46103600
C	-1.86815800	-0.39641100	0.97828600	H	-6.00393100	0.74502700	-2.75985500
C	-2.14269600	-1.87302000	0.66391000	H	-6.25495800	2.93942200	-1.59333400
C	-3.57375900	-2.36791500	0.88197600	H	-6.57012800	2.10197200	-0.08234900
C	-4.64517900	-1.84274100	0.28462300	H	-4.01909900	1.93170600	-1.75867000
C	-1.75725400	0.89481200	-1.06960800	H	-4.17659400	2.79702500	-0.24021400
O	-0.56516900	1.55082100	-0.76665300	H	-6.80909900	-0.42529800	-0.07395400
C	-0.62283500	2.68016400	0.09598500	H	-1.50967800	-2.44555700	1.33861600
C	-0.27455300	2.45431500	1.50369600	H	-5.59188900	-2.35184400	0.43854200
C	-0.32694900	1.26969100	2.18570400	H	1.25089600	1.83826800	3.60053400
C	-0.90045400	-0.05800200	1.88141400	H	-0.27113200	1.36034800	4.35303500
C	0.40623600	1.15590000	3.51481100	H	1.05136700	-0.65843400	4.56253600
C	0.86640300	-0.30778800	3.54485800	H	0.05296300	-1.96499100	2.45182600
C	-0.32509800	-1.05109600	2.91261400	H	-4.72681600	-3.98407100	1.73559200
C	-3.69563300	-3.62823200	1.70380400	H	-3.07350300	-4.42422300	1.27743500
C	0.23559600	3.71115000	2.18505400	H	-3.35559800	-3.48406400	2.73470900
O	-0.84412800	3.74691400	-0.40843400	H	1.33109500	3.75061700	2.16773900
O	-1.95663800	0.48823800	-2.17063100	H	-0.13317300	4.58966200	1.65872100
O	2.08438400	-0.51048900	2.84766900	H	-0.08333700	3.76901500	3.22617100
H	-2.45051600	1.60378700	0.78010100	H	2.11738600	0.02678400	2.04131700
H	-4.55199300	0.72482600	0.99389000	H	-8.40807500	0.01839600	-2.63132400
C	-8.04914600	0.91002700	-2.11585700	H	-8.62939200	1.01731600	-1.19293200
H	-4.19758800	-0.84050900	-1.57503200	H	-8.25545200	1.78193000	-2.74300700
C	-1.36636400	-1.42018500	3.98723200	H	-0.94335000	-2.13558100	4.69839200
C	6.58975100	-1.12580800	-1.08900400	H	-1.68862700	-0.53837900	4.54853200
C	7.91155500	-0.88894700	-0.34510600	H	-2.25993600	-1.86288100	3.54886800
C	5.49319300	1.12500800	-0.29473900	H	6.84894100	-1.58035200	-2.05292200
O	6.70063300	1.82498900	0.02846300	H	8.53934300	-0.16726700	-0.87216600
C	4.38298500	2.16448700	-0.64460500	H	7.74486200	-0.49433800	0.65923400
C	3.00329300	1.53086600	-0.54307500	H	8.46733900	-1.82739500	-0.25440100
O	2.60733900	0.98141800	0.46667900	H	5.14311000	0.56289500	0.57768900
O	2.25163600	1.66090400	-1.63760600	H	6.57562200	2.26805200	0.87385200
C	4.65219500	2.94765400	-1.93102300	H	4.39027200	2.86959800	0.19753500
C	5.82408500	0.17075600	-1.44515800	H	1.35550700	1.31571200	-1.45624500
H	-0.40762300	-2.83544400	-2.25012700	H	3.95304200	3.77906400	-2.03524200
H	-2.53986800	-2.39089800	-1.45517800	H	5.66725500	3.34750700	-1.89889900
H	1.95135300	-3.04239500	-2.12528600	H	4.55033000	2.32164800	-2.81804800
H	0.79031000	-1.92372300	0.46407300	H	6.41420800	0.73547200	-2.17377300
H	5.47968100	-4.01848200	-2.30252400	H	4.89127400	-0.10872200	-1.94608400
H	3.79226900	-3.77042300	-2.75442700	B3LYP Energy = -2081.64637550 a.u.			
H	5.00705100	-2.55388400	-3.14811600				
H	3.21192100	-1.90239800	0.47173300	(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf N			
H	5.45088900	-1.75915200	0.65995900	C	-0.06918800	-2.03952900	-1.32826700

C	-1.25761600	-1.62709100	-0.84632400	O	3.60826600	0.90661100	1.30018300
C	2.36757000	-2.40743400	-1.30056900	O	4.15502400	2.35587400	-0.32711200
C	1.23321100	-1.97732300	-0.70129100	C	6.76105000	2.66170700	0.45065800
C	4.84060400	-2.80782700	-1.19723600	C	6.74808900	-0.27453800	-0.51912300
C	4.98782800	-3.37065600	-2.58742300	H	-0.08158500	-2.49371000	-2.31753100
C	3.66885900	-2.38667700	-0.67229200	H	-2.13383400	-1.78063700	-1.46236100
C	6.10864300	-2.78233200	-0.37399100	H	2.28721300	-2.80594200	-2.30833100
O	-5.88863900	-3.78388400	0.34399100	H	1.31219400	-1.57807500	0.30629200
C	-7.19796400	-1.80655000	0.14387600	H	5.34971600	-4.40479900	-2.54145600
C	-7.25505600	-0.31887800	0.50669100	H	4.05993900	-3.36481900	-3.15714700
C	-6.01608400	0.41790900	0.00190200	H	5.73087300	-2.80826400	-3.16276200
C	-4.69718700	-0.16504500	0.55867400	H	3.68349700	-1.99840300	0.34394600
C	-4.61916400	-1.70346800	0.42099300	H	5.86227500	-2.64066700	0.68233700
C	-5.94868500	-2.42135700	0.77233400	H	6.57866300	-3.77199600	-0.44517900
C	-3.53353300	0.64687100	-0.07655200	H	-5.07560600	-4.17562200	0.67813000
C	-2.08180700	0.43248600	0.33392400	H	-7.08921300	-1.89470900	-0.94512400
C	-1.50434600	-0.97986000	0.51041000	H	-8.15366700	0.13367400	0.07584700
C	-2.24883000	-1.97590400	1.40284900	H	-7.34544300	-0.21055400	1.59612900
C	-3.54398600	-2.28486700	1.31604300	H	-6.00784200	0.36507700	-1.09162800
C	-3.51972000	0.63391700	-1.60851300	H	-6.07412500	1.48061800	0.26114900
O	-3.05924200	1.82130600	-2.12775600	H	-6.07639600	-2.38574300	1.86867700
C	-3.41790000	3.03139600	-1.51178200	H	-0.53387700	-0.85057600	0.97421400
C	-2.41912000	3.61515800	-0.59888400	H	-3.89027500	-3.04531800	2.01647800
C	-1.48378400	2.93686700	0.13158900	H	-0.11386200	4.65102300	0.23886900
C	-1.23726900	1.50439900	0.42261200	H	-0.57475300	3.98323100	1.80714800
C	-0.34516500	3.72698300	0.76581100	H	1.62204400	2.99716500	1.41600300
C	0.82850100	2.75111900	0.71299200	H	0.78285900	0.62283900	0.52449200
C	0.18744400	1.39333200	1.01437600	H	-1.89604500	-3.47310900	2.92655100
C	-1.35054100	-2.70852900	2.37034400	H	-0.52739000	-3.19805600	1.83792700
C	-2.50464900	5.12913300	-0.53417300	H	-0.89640700	-2.02321600	3.09504900
O	-4.44262500	3.56039700	-1.84659100	H	-1.79800000	5.59656200	-1.23009700
O	-3.74191600	-0.29187300	-2.32926800	H	-3.50486600	5.44738500	-0.82289700
O	1.46684300	2.78028200	-0.57950200	H	-2.29241600	5.51091000	0.46473300
H	-3.75817400	1.67808300	0.21137700	H	0.87570100	2.39520700	-1.23764600
H	-4.66254300	0.06370000	1.63155800	H	-8.40002900	-3.61146200	0.30284800
C	-8.46567900	-2.55572800	0.56702600	H	-8.61695000	-2.48633500	1.65015600
H	-4.41819600	-1.94800100	-0.62703700	H	-9.34722900	-2.12977300	0.07926700
C	0.19165800	1.14007700	2.53564500	H	1.22150400	1.03377000	2.88398900
C	7.17296000	-1.73622500	-0.80118200	H	-0.27666400	1.96653800	3.07774000
C	8.54776400	-2.10732500	-0.22336700	H	-0.35645700	0.23547100	2.79945700
C	6.51710300	0.13222000	0.93801500	H	7.26706300	-1.79630300	-1.89237700
O	7.77734300	0.07546700	1.61610600	H	9.30103900	-1.36123900	-0.48880700
C	5.91528400	1.56189300	1.09690800	H	8.52326200	-2.16481600	0.86513400
C	4.44204000	1.56260800	0.70624600	H	8.87386600	-3.07506700	-0.61734200

H	5.81092600	-0.55934000	1.41111400	O	-3.69613200	-0.05584000	-2.36733000
H	7.61640200	0.20163800	2.55687700	O	1.71917900	2.31124500	-0.34751800
H	5.88883700	1.73224700	2.18127500	H	-3.58513400	1.74862900	0.29243100
H	3.17919000	2.36730000	-0.48223400	H	-4.69241600	0.14244300	1.58384500
H	6.72111100	2.61814600	-0.63773000	C	-8.77506600	-1.85189400	0.28665700
H	6.40714200	3.65012300	0.75049000	H	-4.69317200	-1.70810300	-0.82727900
H	7.79944000	2.55305100	0.76909200	C	0.21160500	0.66174000	2.66623600
H	7.51386200	0.38607900	-0.93763000	C	6.87410900	-2.08298800	-0.02947300
H	5.82478500	-0.07232000	-1.07313700	C	8.16956200	-2.43474100	0.71474700
B3LYP Energy = -2081.64812851 a.u.				C	6.91722900	0.49286900	-0.01783800
(2S, 3S, 5R, 13S, 16R, 17S, 18R, 21R, 22R, 26R, 27R)-a4,Conf O				O	6.75967900	0.61326600	-1.42990400
C	-0.17403300	-2.20719900	-1.32753800	C	6.45627200	1.76498000	0.74199000
C	-1.34889500	-1.70192400	-0.90481500	C	4.94511500	1.93117500	0.75262900
C	2.22677300	-2.75878300	-1.13641200	O	4.28038900	2.09393800	1.75047500
C	1.05649100	-2.36756600	-0.58179500	O	4.41143600	1.89492500	-0.48538800
C	4.69152400	-3.16398800	-0.88098600	C	7.13024700	3.03361200	0.18937800
C	5.00383000	-3.31522200	-2.34705300	C	6.24363200	-0.78434500	0.50646300
C	3.45611000	-2.91739800	-0.39262500	H	-0.13562500	-2.54781900	-2.36067700
C	5.87549600	-3.26880200	0.05152100	H	-2.17712300	-1.68844900	-1.60170500
O	-6.25617100	-3.41622800	0.13819700	H	2.24297900	-2.95142600	-2.20576100
C	-7.40598600	-1.25363600	-0.05523900	H	1.04367600	-2.16807700	0.48683400
C	-7.29058900	0.20601900	0.39435500	H	5.62136700	-4.20381800	-2.51737900
C	-5.94961900	0.79858900	-0.03290300	H	4.11388300	-3.39986500	-2.96967600
C	-4.73074100	0.00517400	0.49538500	H	5.58102500	-2.45718900	-2.70998000
C	-4.84711700	-1.51496800	0.24003300	H	3.36085400	-2.80645900	0.68641900
C	-6.25766200	-2.05274700	0.57284300	H	5.52607500	-3.36557200	1.08573000
C	-3.46554400	0.71843600	-0.05573200	H	6.42514500	-4.19039100	-0.18126900
C	-2.06143300	0.32215700	0.37899200	H	-7.01707800	-3.85764100	0.52549700
C	-1.64684200	-1.15149200	0.48537900	H	-7.27378000	-1.29497300	-1.14423600
C	-2.54519800	-2.14875800	1.21991800	H	-8.10726100	0.79696000	-0.03239200
C	-3.85940500	-2.31279800	1.06129600	H	-7.40312700	0.26387300	1.48571800
C	-3.40370300	0.79738700	-1.58432400	H	-5.92097100	0.82421900	-1.12729100
O	-2.80880500	1.95953400	-2.01520000	H	-5.87257300	1.83794000	0.30317500
C	-3.05693300	3.16014100	-1.32795100	H	-6.38480300	-2.01758100	1.66911500
C	-2.02979600	3.57436400	-0.35683100	H	-0.70955000	-1.15886900	1.02934700
C	-1.19002600	2.75481500	0.34510400	H	-4.30364900	-3.15442200	1.58382000
C	-1.10887500	1.28903200	0.55000900	H	0.35421000	4.29855300	0.57933200
C	0.01421700	3.37503100	1.04439900	H	-0.20519300	3.59193200	2.09665100
C	1.07608500	2.28198300	0.94471400	H	1.89626400	2.39864100	1.65000000
C	0.28041200	0.98926100	1.16002500	H	0.78901300	0.18019300	0.63307300
C	-1.76768700	-3.10708700	2.09336900	H	-2.41955500	-3.86241000	2.53510300
C	-1.95671300	5.08162900	-0.19408400	H	-0.99502100	-3.62518500	1.51414200
O	-4.01049800	3.81458600	-1.65149900	H	-1.25688100	-2.58163700	2.90929500
				H	-1.18823100	5.51423300	-0.84552500

H	-2.91042200	5.52285700	-0.47869600	H	5.83898800	0.86224200	-1.58743600
H	-1.72920300	5.37396500	0.83117700	H	6.73360100	1.64280400	1.79201200
H	1.08906900	2.06118900	-1.03369600	H	3.43184400	2.02844100	-0.43174600
H	-8.88341700	-2.86671400	-0.10597800	H	6.80755900	3.92043400	0.74023400
H	-8.93596500	-1.88225800	1.37060700	H	8.21566600	2.94917400	0.28765000
H	-9.57955800	-1.25322300	-0.14880100	H	6.89672600	3.16815700	-0.86657300
H	1.21467200	0.46931900	3.05578200	H	5.18789600	-0.74636300	0.21724600
H	-0.21541400	1.49417900	3.23180600	H	6.26894200	-0.79249900	1.60410000
H	-0.40879800	-0.21217700	2.86671500	B3LYP Energy = -2081.65641190 a.u.			
H	7.12054300	-1.91334500	-1.08224000				
H	8.88968400	-1.61270900	0.68456700				
H	7.96715300	-2.66104500	1.76752300				
H	8.65387700	-3.31005600	0.27242400				
H	7.99950900	0.42413100	0.13325200				

Dataset 2. Cartesian coordinates and energies of the low-energy enantiomers calculated at the B3LYP/6-311G(d,p) level in methanol for ECD calculation

(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf A	C	6.85677200	0.47403200	-0.16541400			
C	-0.13457700	-2.13588000	-1.36021400	O	6.60777400	0.43507900	-1.57438000
C	-1.32440600	-1.65370000	-0.95745500	C	6.43534600	1.81958400	0.46966400
C	2.25126600	-2.69084000	-1.06999300	C	4.92849100	1.95760200	0.57362200
C	1.05330400	-2.32913100	-0.55780300	O	4.33484700	2.21711700	1.59922100
C	4.69135400	-3.10510000	-0.71658300	O	4.31015600	1.77462300	-0.60377900
C	5.06188000	-3.17030200	-2.17318300	C	7.03105300	3.02147500	-0.27916800
C	3.43789100	-2.87875500	-0.26915500	C	6.21180100	-0.72581700	0.53172900
C	5.83884500	-3.22647000	0.25180700	H	-0.04340200	-2.42183100	-2.40607000
O	-6.32029300	-3.43285000	-0.02421000	H	-2.13354000	-1.59431300	-1.67299600
C	-7.38471700	-1.22389600	-0.14120500	H	2.32622200	-2.83108200	-2.14462400
C	-7.26142900	0.19527200	0.41751000	H	0.98492100	-2.18073100	0.51592000
C	-5.91980300	0.81219200	0.04215900	H	5.80027600	-3.95867000	-2.34749800
C	-4.71295000	-0.01985100	0.52346500	H	4.20827700	-3.35179000	-2.82495700
C	-4.83313400	-1.51294300	0.15788500	H	5.52530300	-2.22732700	-2.48453600
C	-6.24934400	-2.07503800	0.42850800	H	3.29385800	-2.80393200	0.80699900
C	-3.45187400	0.71730900	0.01864500	H	5.46075200	-3.27615300	1.27841800
C	-2.05240900	0.28816200	0.40838300	H	6.37218200	-4.16592500	0.05837900
C	-1.64804600	-1.18182400	0.45005400	H	-6.16760400	-3.42688700	-0.97684500
C	-2.54889300	-2.21710900	1.11058000	H	-7.25144000	-1.17454800	-1.23173900
C	-3.86005500	-2.37040700	0.92892200	H	-8.07653300	0.81834000	0.03821500
C	-3.38969000	0.87137500	-1.49614200	H	-7.37083700	0.16308400	1.50900800
O	-2.83424600	2.05926400	-1.88563300	H	-5.88150700	0.91086900	-1.04820700
C	-3.05621100	3.22621900	-1.12191500	H	-5.83760100	1.82369900	0.45134900
C	-2.04341300	3.55953600	-0.12218800	H	-6.39191800	-2.14335200	1.51366900
C	-1.16696200	2.69765900	0.47644600	H	-0.72201400	-1.21811400	1.00794200
C	-1.08177300	1.23129500	0.58207800	H	-4.31308600	-3.23589800	1.40223300
C	0.06135000	3.27136700	1.16481000	H	0.38104200	4.22325900	0.74650900
C	1.11287800	2.18610700	0.95257700	H	-0.11923300	3.41717200	2.23517100
C	0.32349800	0.88431900	1.11154700	H	1.95553300	2.25882800	1.63497200
C	-1.77105100	-3.21786200	1.92932800	H	0.80053300	0.10864300	0.51149400
C	-1.98405200	5.04196100	0.18358800	H	-2.41769100	-4.00314300	2.32316900
O	-3.98566200	3.92068700	-1.44467200	H	-0.98914000	-3.68853500	1.32317200
O	-3.66081500	0.04682700	-2.32394000	H	-1.26742100	-2.73174700	2.77230700
O	1.70878600	2.30169900	-0.35685000	H	-2.96223700	5.48849100	0.01502400
H	-3.56148800	1.72747800	0.42334000	H	-1.68627200	5.23056900	1.21384000
H	-4.67783900	0.04158500	1.61693200	H	-1.27242200	5.55156600	-0.47549100
C	-8.75286600	-1.83766300	0.15852100	H	1.06541300	2.07387000	-1.03914200
H	-4.65762200	-1.61168300	-0.91976400	H	-8.82434800	-2.85181800	-0.23628100
C	0.31017900	0.46680800	2.59422000	H	-8.92488900	-1.88341200	1.23917800
C	6.85501100	-2.06615300	0.14289700	H	-9.55121800	-1.23570900	-0.28358300
C	8.09768100	-2.35565900	0.98921000	H	1.32179400	0.21478100	2.92038600

H	-0.05898100	1.27953700	3.22369900	C	-0.30417600	3.35693200	1.67348600
H	-0.33110500	-0.39558000	2.77276900	C	0.85263600	2.37922400	1.48396900
H	7.16423000	-1.99068900	-0.90360400	C	0.16645000	1.00927500	1.45991500
H	8.81778400	-1.53469500	0.93409800	C	-1.70706200	-3.24447400	1.87028600
H	7.82580100	-2.49049300	2.04136300	C	-2.33848600	5.05519300	0.54311500
H	8.60203700	-3.26494500	0.65103500	O	-4.03476700	3.93198100	-1.38503400
H	7.94517000	0.41502100	-0.07392100	O	-3.47573200	0.12596600	-2.36658200
H	5.66836300	0.63288700	-1.69167900	O	1.55655100	2.66375600	0.26024800
H	6.79958300	1.82204100	1.49903900	H	-3.67391200	1.66166700	0.45220200
H	3.32962900	1.92105400	-0.50532700	H	-4.77988100	-0.11476200	1.48565000
H	6.74917800	3.96052300	0.20206800	C	-8.64379700	-2.14285000	-0.20895200
H	8.12131100	2.95104900	-0.27902300	H	-4.51354000	-1.68749200	-1.09171600
H	6.68927600	3.04025600	-1.31371600	C	0.04545100	0.47078000	2.89840600
H	5.15013600	-0.73211100	0.26557300	C	6.96590700	-1.97936400	0.40942800
H	6.26273200	-0.59629800	1.61924100	C	8.16842500	-2.13875400	1.34325600
B3LYP Energy = -2081.91058472 a.u.				C	6.92020200	0.46132900	-0.38083200
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf B				O	6.75654600	0.08913300	-1.75413800
C	0.04886200	-1.98890600	-1.24665400	C	6.33974600	1.86526600	-0.11163600
C	-1.17397900	-1.53983300	-0.90871600	C	4.84015200	1.88356200	-0.34394700
C	2.40024300	-2.59394800	-0.82335400	O	4.28065200	1.25486500	-1.22991900
C	1.19462800	-2.16717100	-0.38285100	O	4.19100800	2.68257100	0.49318300
C	4.80609000	-3.08380200	-0.35359100	C	6.99714600	2.94297000	-0.99125000
C	5.20550000	-3.34501800	-1.78016300	C	6.31557600	-0.59344200	0.54988500
C	3.55344500	-2.75566200	0.02942700	H	0.20442700	-2.26350200	-2.28798600
C	5.93060100	-3.10541200	0.64891000	H	-1.93951000	-1.48914800	-1.67116900
O	-6.13016600	-3.61253700	-0.31624400	H	2.51023400	-2.80542700	-1.88309600
C	-7.29646800	-1.45838800	-0.44232100	H	1.08735200	-1.95316500	0.67660500
C	-7.26919600	-0.04138000	0.13581200	H	5.90319300	-4.18637700	-1.83368300
C	-5.93894100	0.63891000	-0.15815000	H	4.35864600	-3.56263300	-2.42947500
C	-4.72786400	-0.14211400	0.39118800	H	5.72893300	-2.47306500	-2.18796500
C	-4.74668400	-1.62708900	-0.02156800	H	3.38690300	-2.55460900	1.08609000
C	-6.14627600	-2.26296400	0.16581200	H	5.53039400	-3.01383800	1.66419400
C	-3.47604000	0.67958800	0.01458400	H	6.45284400	-4.06870100	0.59126400
C	-2.08974200	0.30722600	0.49860200	H	-5.94350800	-3.57816300	-1.26219800
C	-1.60252500	-1.13592200	0.49162700	H	-7.11909500	-1.38887600	-1.52547200
C	-2.48537500	-2.24695200	1.04808600	H	-8.09042200	0.54806900	-0.28208600
C	-3.77238500	-2.46061100	0.77478200	H	-7.43611600	-0.09156200	1.21929700
C	-3.30177700	0.91322600	-1.47926700	H	-5.83894000	0.74593100	-1.24365800
O	-2.75974200	2.13978200	-1.76044000	H	-5.92873000	1.64999400	0.26008700
C	-3.11851300	3.26180700	-0.98283400	H	-6.33614900	-2.36175700	1.24132800
C	-2.25353500	3.59490500	0.14942900	H	-0.70952700	-1.15089300	1.10187500
C	-1.39347000	2.75560200	0.80036200	H	-4.20294300	-3.37148000	1.17873200
C	-1.20606600	1.29499900	0.81861200	H	-0.02212200	4.36528000	1.37987800
				H	-0.61195700	3.38233800	2.72413700

H	1.60759500	2.45443900	2.26442400	C	5.07176400	0.68396500	0.00244000
H	0.76208200	0.32434700	0.85414400	C	6.59715100	0.49589100	0.20741500
H	-2.33082100	-4.08580900	2.17509300	C	2.82164000	-0.62811800	-0.37376700
H	-0.85713500	-3.63501400	1.30016200	C	1.87710500	0.10465700	0.56814500
H	-1.29529700	-2.77775000	2.77194900	C	2.08118300	1.59014600	0.80520800
H	-1.59571300	5.65192000	0.00226800	C	3.39072500	2.06256300	1.41306600
H	-3.32097900	5.44591300	0.28540600	C	4.61531300	1.69460000	1.03255100
H	-2.17534200	5.19643100	1.61018700	C	2.59542700	-0.25658200	-1.81224100
H	1.03253200	2.39803700	-0.50503400	O	1.29504100	-0.44872900	-2.30586400
H	-8.64526900	-3.15541300	-0.61401900	C	0.20107600	-1.07597800	-1.78729700
H	-8.86061800	-2.20705800	0.86268500	C	0.22399200	-2.15714100	-0.75370700
H	-9.45124000	-1.57771300	-0.68196200	C	0.39417200	-1.87781600	0.55089500
H	1.03740700	0.27012800	3.30939900	C	0.82340100	-0.56822800	1.07410900
H	-0.45166800	1.19794400	3.54403600	C	-0.07076500	-2.72152200	1.70406200
H	-0.53442200	-0.44982900	2.94649000	C	-0.49906400	-1.68721200	2.78372000
H	7.32107800	-2.07123800	-0.62059100	C	-0.07870800	-0.26896400	2.26581500
H	8.89906300	-1.33968700	1.18833400	C	3.20811600	3.13097700	2.46277500
H	7.85298400	-2.10355900	2.39137100	C	-0.28248500	-3.48012200	-1.27468300
H	8.67659200	-3.09263800	1.17565700	O	-0.84626900	-0.77831900	-2.32481000
H	8.00147800	0.51762400	-0.22301500	O	3.37728400	0.18379400	-2.60209800
H	5.81260000	0.21942700	-1.93983400	O	-1.88024600	-1.74532800	3.10524100
H	6.51237000	2.11428100	0.93779700	H	2.51180200	-1.67514300	-0.33848400
H	3.21663800	2.66051500	0.29070600	H	4.29237800	-0.97436000	1.10406600
H	6.56901200	3.92720600	-0.79162700	C	8.72664500	-0.72489800	-0.40032100
H	8.06839200	2.98503700	-0.78210800	H	4.94861000	1.10015200	-1.00516200
H	6.86280700	2.70650100	-2.04740100	C	0.46355700	0.58280400	3.41518800
H	5.25010400	-0.66506300	0.31802800	C	-6.67667800	1.47139200	-0.45462200
H	6.39217000	-0.25135800	1.58865700	C	-7.92703200	1.54523100	0.42844400
B3LYP Energy = -2081.91002275 a.u.				C	-5.77064900	-0.76383500	0.53605200
				O	-6.96607100	-1.21200900	1.17869000
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf C				C	-4.87294300	-1.99428900	0.20272800
C	0.60494700	2.60433800	-1.00266700	C	-3.51547900	-1.49133000	-0.23316200
C	1.82385700	2.31350300	-0.51201400	O	-2.71246900	-1.00512900	0.54763500
C	-1.86255400	2.55353600	-0.94667700	O	-3.27902500	-1.58395100	-1.53533300
C	-0.66200500	2.33343100	-0.36392100	C	-5.53461800	-2.97636600	-0.76232500
C	-4.35960700	2.57784200	-0.76873300	C	-6.17419800	0.03598900	-0.70127200
C	-4.62969100	3.09012200	-2.15687500	H	0.55391300	3.08009000	-1.97945400
C	-3.12444300	2.32915400	-0.28183300	H	2.70024300	2.56337100	-1.09894400
C	-5.57418900	2.39615200	0.10763200	H	-1.87306900	2.93408900	-1.96380200
O	7.26540700	1.75273100	0.03544400	H	-0.65214900	1.93474100	0.64454100
C	7.22537400	-0.59540600	-0.66121700	H	-5.32019400	3.93923500	-2.12085500
C	6.48753000	-1.91231200	-0.41335600	H	-3.72877300	3.40480500	-2.68070600
C	5.00806800	-1.77618500	-0.74900900	H	-5.11507200	2.32030800	-2.76648800
C	4.31072900	-0.65980300	0.05393300	H	-3.05402200	1.94564400	0.73322900

H	-5.26615400	2.04582600	1.09707300	C	-0.19620700	-2.20249700	-1.27516500
H	-6.02875500	3.38468300	0.26025700	C	-1.37682800	-1.70467800	-0.86431000
H	7.11043100	2.03792300	-0.87316500	C	2.19933800	-2.73375500	-1.02262000
H	7.07399300	-0.31124100	-1.71277300	C	1.01076100	-2.36476400	-0.49413700
H	6.93531100	-2.70962300	-1.01401700	C	4.64903400	-3.12727800	-0.71134200
H	6.61279200	-2.20143500	0.63807100	C	4.99150600	-3.21693400	-2.17346600
H	4.91079400	-1.57235500	-1.81845600	C	3.40384100	-2.89717800	-0.24312500
H	4.48725600	-2.71931500	-0.55551300	C	5.81533000	-3.23427200	0.23625100
H	6.77395300	0.23634700	1.25813600	O	-6.26201600	-3.38974500	-0.26334000
H	1.29419400	1.89691600	1.48593000	C	-7.33154000	-1.25724200	-0.28030200
H	5.43891000	2.21128900	1.51528900	C	-7.26100400	0.16102500	0.29098900
H	-0.90410200	-3.37743900	1.45363000	C	-5.91830400	0.80633800	-0.02806600
H	0.74638500	-3.34592900	2.07940500	C	-4.72081300	0.00407000	0.51906600
H	0.02220200	-1.89728500	3.71885200	C	-4.79939600	-1.49984600	0.18629200
H	-0.99954100	0.18399500	1.88679900	C	-6.21867600	-2.09136600	0.34318900
H	4.16484800	3.53576300	2.79616500	C	-3.44490800	0.73552600	0.04132400
H	2.60118600	3.95521400	2.07066800	C	-2.05075900	0.30235300	0.45184000
H	2.67761300	2.73809900	3.33641000	C	-1.65923800	-1.17178800	0.52867000
H	-1.33078100	-3.41604500	-1.57875300	C	-2.56470800	-2.14842800	1.26888300
H	0.29209000	-3.79576200	-2.14986100	C	-3.87392400	-2.29904600	1.07379600
H	-0.18815600	-4.25251500	-0.51365400	C	-3.35509500	0.88107400	-1.47423200
H	-2.36082100	-1.48596800	2.29950300	O	-2.81040600	2.07357900	-1.86339100
H	9.23766700	0.22442400	-0.56473800	C	-3.03959400	3.23922000	-1.10078200
H	8.91113100	-1.03310100	0.63442700	C	-2.03041200	3.57255100	-0.09740900
H	9.16953200	-1.47698900	-1.05867100	C	-1.15566100	2.70980400	0.50177600
H	-0.17445600	0.43791100	4.29076300	C	-1.07565300	1.24272700	0.61609900
H	1.48173600	0.28475900	3.67917400	C	0.07750500	3.28272400	1.18228100
H	0.46477600	1.65070100	3.19835800	C	1.12340000	2.19304400	0.96539000
H	-6.95744900	1.86018200	-1.43951500	C	0.33063600	0.89586500	1.14383200
H	-8.71995200	0.90179300	0.03940700	C	-1.81543900	-3.05754200	2.20870200
H	-7.71434900	1.22072800	1.44846600	C	-1.96999700	5.05512900	0.20634700
H	-8.30513300	2.57114600	0.46356300	O	-3.96745400	3.93337300	-1.42832600
H	-5.19938300	-0.12938000	1.22164100	O	-3.60065700	0.04773600	-2.30095300
H	-6.72660900	-1.56330800	2.04343300	O	1.70278600	2.29756500	-0.35206500
H	-4.69057900	-2.49388200	1.16019400	H	-3.55787400	1.74761400	0.44049000
H	-2.37420700	-1.23564300	-1.74645600	H	-4.72899100	0.09666300	1.61049200
H	-4.93676400	-3.88417900	-0.86324800	C	-8.70365600	-1.89453000	-0.05371500
H	-6.51689000	-3.25000600	-0.37550200	H	-4.53335100	-1.63523300	-0.86567200
H	-5.65924300	-2.54294000	-1.75448500	C	0.32584000	0.49810500	2.63179800
H	-6.95090300	-0.52786500	-1.22641300	C	6.83176900	-2.07839700	0.09130300
H	-5.31542100	0.08597400	-1.37645400	C	8.09165700	-2.36270600	0.91374700
B3LYP Energy = -2081.90662631 a.u.				C	6.84318900	0.46088900	-0.22849000
				O	6.57584000	0.41923500	-1.63395400
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf D				C	6.43771900	1.81042500	0.40859700

C	4.93319100	1.95544800	0.53264100	H	8.58583000	-3.27705500	0.57421300
O	4.35433200	2.21935500	1.56558900	H	7.93227100	0.39596700	-0.15094000
O	4.29859400	1.77218900	-0.63591800	H	5.63592500	0.62117300	-1.73975200
C	7.02931900	3.00733500	-0.35125900	H	6.81610400	1.81347200	1.43286700
C	6.20007500	-0.73306200	0.48045200	H	3.31970500	1.91998000	-0.52390300
H	-0.12872200	-2.52764500	-2.31131400	H	6.75818300	3.94902400	0.13100600
H	-2.20023900	-1.66982800	-1.56447700	H	8.11914200	2.93170400	-0.36500300
H	2.25128300	-2.90313100	-2.09439100	H	6.67434200	3.02503200	-1.38137000
H	0.96561100	-2.18653900	0.57627800	H	5.13550900	-0.73544200	0.22581300
H	5.71871300	-4.01521900	-2.35008100	H	6.26346500	-0.59957600	1.56687600
H	4.12450200	-3.39813900	-2.80733800	B3LYP Energy = -2081.90914482 a.u.			
H	5.45897600	-2.28343000	-2.50661400	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a-2,Conf E			
H	3.28113100	-2.80273500	0.83414800	C	0.01285800	-1.92893300	-1.42251600
H	5.45728200	-3.26802100	1.27068600	C	-1.18638300	-1.56532900	-0.93233600
H	6.34283900	-4.17781900	0.04667700	C	2.44723100	-2.25421400	-1.37961400
H	-5.58781300	-3.93932100	0.15019300	C	1.30301100	-1.86357300	-0.77271300
H	-7.13981300	-1.20440500	-1.36017300	C	4.90904600	-2.66684800	-1.28750000
H	-8.07229600	0.76708800	-0.12216300	C	5.05988700	-3.12587500	-2.71213800
H	-7.41605200	0.12391400	1.37676000	C	3.74088600	-2.26883400	-0.73881600
H	-5.83428400	0.89424300	-1.11632900	C	6.17524200	-2.69999100	-0.46955600
H	-5.87547500	1.82330500	0.37371600	O	-5.77097600	-3.84792300	0.56994400
H	-6.43714600	-2.18408600	1.41896200	C	-7.13386800	-1.83347500	0.24235500
H	-0.71934200	-1.19909800	1.06258500	C	-7.18025400	-0.34715700	0.60412800
H	-4.35339100	-3.07546800	1.66836900	C	-5.95496500	0.38143500	0.06674100
H	0.39691700	4.23230300	0.75861100	C	-4.62622900	-0.21264500	0.57766900
H	-0.09530700	3.43218800	2.25331000	C	-4.55375300	-1.74395700	0.40983200
H	1.97463900	2.26744400	1.63684000	C	-5.86551000	-2.44376600	0.84007400
H	0.80075900	0.11075500	0.55034200	C	-3.49770800	0.61689200	-0.07568200
H	-2.47375900	-3.80237100	2.65800100	C	-2.04200200	0.41818800	0.29589900
H	-1.01413300	-3.58366900	1.67809600	C	-1.44130800	-0.97509200	0.44339900
H	-1.34019100	-2.48756300	3.01433300	C	-2.15044300	-2.02445800	1.28939800
H	-1.26503700	5.56518300	-0.45952000	C	-3.43783100	-2.36153700	1.21856700
H	-2.95038400	5.49984900	0.04523700	C	-3.51486200	0.61283400	-1.59801900
H	-1.66410200	5.24527700	1.23385500	O	-3.08790100	1.80221200	-2.12784200
H	1.04905600	2.07190800	-1.02516300	C	-3.44190700	3.01402100	-1.49620800
H	-8.74130200	-2.90332200	-0.46582500	C	-2.46372100	3.58783500	-0.57343900
H	-8.92580900	-1.95652200	1.01704400	C	-1.48680700	2.91744400	0.10885600
H	-9.48834700	-1.29671600	-0.52518000	C	-1.20868900	1.49488100	0.36627500
H	1.33953000	0.25108600	2.95533500	C	-0.35200800	3.71790100	0.72679700
H	-0.04037800	1.31850300	3.25286800	C	0.83418000	2.76247600	0.64234500
H	-0.31320100	-0.36214800	2.82559700	C	0.22223500	1.39062200	0.92660300
H	7.11832100	-2.01469600	-0.96241000	C	-1.20159500	-2.80355200	2.16560100
H	8.81302600	-1.54483000	0.83506100	C	-2.58340400	5.09297100	-0.44526100
H	7.84174000	-2.48599900	1.97273900				

O	-4.46176200	3.54158800	-1.86027200	H	-1.89610100	5.60087300	-1.13075100
O	-3.74303600	-0.31178000	-2.32604700	H	-3.59385100	5.40391000	-0.70229800
O	1.45092100	2.81626600	-0.66155300	H	-2.36113200	5.43175900	0.56598800
H	-3.72777700	1.64331200	0.22365800	H	0.86646700	2.40759700	-1.31214300
H	-4.56058000	-0.00566100	1.65197600	H	-8.33584300	-3.63352400	0.45655900
C	-8.38779100	-2.57378100	0.70903000	H	-8.50101000	-2.49080900	1.79524600
H	-4.41779600	-1.96219000	-0.65633700	H	-9.28197400	-2.14955400	0.24468800
C	0.24106600	1.11078000	2.43967200	H	1.27450500	1.01465300	2.77703000
C	7.19711900	-1.58781900	-0.80679100	H	-0.23540100	1.92292800	2.99410500
C	8.56950700	-1.93257400	-0.21530600	H	-0.29076000	0.19314800	2.69006100
C	6.34820900	0.06606400	1.03705500	H	7.31682100	-1.57129300	-1.89600600
O	7.55505500	-0.00239200	1.80364200	H	9.29373800	-1.13928900	-0.41915700
C	5.66319800	1.43988500	1.27861200	H	8.51339800	-2.05519200	0.86633400
C	4.25213500	1.41676700	0.71603400	H	8.94776000	-2.86007900	-0.65530600
O	3.39588300	0.65391300	1.12324100	H	5.64990400	-0.70066400	1.38462400
O	4.03791900	2.30824700	-0.25133000	H	7.31399100	0.01687300	2.73636100
C	6.51529100	2.62911500	0.83758100	H	5.51185600	1.49782500	2.36316400
C	6.69407700	-0.17914100	-0.42936900	H	3.07764100	2.32149800	-0.50225800
H	0.02461200	-2.34641500	-2.42757700	H	6.61152200	2.67870700	-0.24705600
H	-2.06162800	-1.71921000	-1.54853300	H	6.07445800	3.56803800	1.17651000
H	2.37897500	-2.60423500	-2.40572800	H	7.51156300	2.53680800	1.27239100
H	1.36119100	-1.50744600	0.25132800	H	7.45098600	0.54935800	-0.73424300
H	5.40289600	-4.16644600	-2.73851600	H	5.79805300	0.03480400	-1.02106300
H	4.14087600	-3.05594000	-3.29094400	B3LYP Energy = -2081.90512134 a.u.			
H	5.82358100	-2.53562400	-3.22844600	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf F			
H	3.75134600	-1.94013800	0.29718100	C	0.00455000	-2.04834900	-1.12294000
H	5.93517900	-2.66085900	0.59628700	C	-1.20390800	-1.56899900	-0.77507600
H	6.66971900	-3.66410200	-0.64022300	C	2.36380400	-2.64727900	-0.73559200
H	-5.66453000	-3.95116200	-0.38334800	C	1.17425100	-2.18786800	-0.28482200
H	-7.06139900	-1.91742300	-0.85178700	C	4.78018200	-3.12020100	-0.30780700
H	-8.09012500	0.10728800	0.20138200	C	5.14180200	-3.43617700	-1.73351600
H	-7.23284900	-0.24442500	1.69543200	C	3.53818600	-2.77470300	0.09352800
H	-5.97896000	0.33295600	-1.02700000	C	5.92934400	-3.10145200	0.66561500
H	-5.99388100	1.44164300	0.33511400	O	-5.85658500	-3.66722700	-0.55045200
H	-5.94505200	-2.38271400	1.93213500	C	-7.11476300	-1.63996600	-0.64763700
H	-0.47349300	-0.83732700	0.90672800	C	-7.23516200	-0.23864700	-0.04460200
H	-3.74822700	-3.20737900	1.82398700	C	-5.93855000	0.54225100	-0.22531800
H	-0.15028300	4.65171500	0.20640700	C	-4.72089700	-0.16055200	0.40860400
H	-0.56847700	3.95599800	1.77392100	C	-4.62818300	-1.65785500	0.04968600
H	1.63113900	3.01639800	1.33760000	C	-5.99253900	-2.38148800	0.06823200
H	0.81868300	0.63857200	0.41295200	C	-3.48007100	0.69517300	0.06069400
H	-1.71078100	-3.61612300	2.68568200	C	-2.08696500	0.36140400	0.56375700
H	-0.38959900	-3.23182800	1.56732800	C	-1.57676300	-1.07668800	0.61101500
H	-0.73301900	-2.15600100	2.91472900				

C	-2.43866700	-2.13296300	1.29532100	H	-7.48365500	-0.32142000	1.02104600
C	-3.71483100	-2.38555700	1.00899500	H	-5.77015100	0.67359600	-1.29904000
C	-3.28431100	0.91727500	-1.43469900	H	-6.03044700	1.54480400	0.20378400
O	-2.80104100	2.16372100	-1.72801800	H	-6.29926600	-2.51226700	1.11830900
C	-3.19262500	3.27548700	-0.95246200	H	-0.65817500	-1.04631900	1.18013700
C	-2.31946000	3.64333500	0.16197300	H	-4.17681700	-3.19679100	1.56999100
C	-1.43065000	2.83093200	0.80765700	H	-0.07303000	4.47381400	1.31765200
C	-1.21906700	1.37305100	0.85327200	H	-0.62162200	3.52006800	2.69977900
C	-0.33394500	3.46991600	1.64448800	H	1.60072300	2.61120900	2.22487400
C	0.83341900	2.50388100	1.46031800	H	0.76245300	0.42748800	0.90014100
C	0.16463300	1.12588100	1.48848800	H	-2.30971700	-3.78225600	2.68456300
C	-1.68453500	-2.98289400	2.28430600	H	-0.80753100	-3.43748900	1.81057700
C	-2.42869300	5.10703600	0.53541700	H	-1.31485400	-2.38404100	3.12343800
O	-4.13615000	3.91158900	-1.34621800	H	-1.71675700	5.71282200	-0.03607300
O	-3.40161600	0.10913600	-2.31257200	H	-3.42761400	5.46918900	0.29932200
O	1.51238900	2.76244900	0.21671100	H	-2.23938300	5.26974200	1.59501400
H	-3.71094300	1.67549300	0.48663600	H	0.97728000	2.46864100	-0.53052700
H	-4.83113000	-0.09558000	1.49654800	H	-8.33466800	-3.40478400	-1.00670200
C	-8.43446200	-2.41009500	-0.57134400	H	-8.75264500	-2.52624200	0.47030600
H	-4.25719500	-1.74675300	-0.97511200	H	-9.22397900	-1.87475900	-1.10563700
C	0.06575500	0.63627200	2.94575700	H	1.06449600	0.46482400	3.35344500
C	6.94680700	-1.97304200	0.36617300	H	-0.43697700	1.37683400	3.57140900
C	8.17843300	-2.09979000	1.26626900	H	-0.49881900	-0.29050500	3.02913100
C	6.85209600	0.44413900	-0.48691300	H	7.27058200	-2.08814100	-0.67190800
O	6.64117000	0.03535100	-1.84338800	H	8.89679600	-1.29865500	1.07012600
C	6.27697300	1.85287300	-0.23410400	H	7.89424700	-2.04225500	2.32227300
C	4.77099400	1.87050300	-0.42221600	H	8.68969500	-3.05325700	1.10588600
O	4.17903600	1.20138400	-1.25575500	H	7.93817800	0.50830800	-0.37000000
O	4.15515800	2.72132400	0.38908900	H	5.68961600	0.15126300	-1.99620800
C	6.90810700	2.90938800	-1.15816400	H	6.48036000	2.12766000	0.80343700
C	6.28846600	-0.58921500	0.49209600	H	3.17569000	2.70786400	0.21228000
H	0.12632700	-2.38327200	-2.15100000	H	6.48437000	3.89787500	-0.97114700
H	-1.98825000	-1.55095400	-1.51878100	H	7.98475200	2.95709600	-0.98034900
H	2.44317800	-2.91477500	-1.78537300	H	6.74457200	2.64620200	-2.20388400
H	1.10036100	-1.91521200	0.76393700	H	5.21640800	-0.67510200	0.29917300
H	5.86132100	-4.25944100	-1.77254200	H	6.39815000	-0.21849300	1.51798200
H	4.28080100	-3.70605200	-2.34370500	B3LYP Energy = -2081.90857767 a.u.			
H	5.62533800	-2.56931600	-2.19751900				
H	3.39878900	-2.52939900	1.14472500	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf G			
H	5.55420000	-2.98256900	1.68765600	C	0.01492600	-1.93181800	-1.42148800
H	6.45940400	-4.06118800	0.62361000	C	-1.18509200	-1.55992500	-0.93946300
H	-5.15975700	-4.14939400	-0.09231000	C	2.44662500	-2.27932600	-1.35352100
H	-6.82527200	-1.53927700	-1.70215300	C	1.29924500	-1.87916200	-0.75923400
H	-8.06086000	0.29923300	-0.51909400	C	4.90643900	-2.69975300	-1.23250700

C	5.07198800	-3.16807000	-2.65253000	H	0.03226100	-2.34444600	-2.42843900
C	3.73326200	-2.29665200	-0.69869600	H	-2.05697400	-1.70185900	-1.56329000
C	6.16449900	-2.72095400	-0.40168500	H	2.38744400	-2.63006000	-2.37991700
O	-5.77491000	-3.85253400	0.53311900	H	1.35032400	-1.52276700	0.26505700
C	-7.13734500	-1.83493200	0.22302000	H	5.48832600	-4.18141700	-2.66907900
C	-7.18459900	-0.35237000	0.59976500	H	4.14267400	-3.17256600	-3.21887500
C	-5.95840800	0.38196000	0.07236000	H	5.78386900	-2.53209400	-3.18883900
C	-4.63042400	-0.21756500	0.57892200	H	3.73411600	-1.95935100	0.33455700
C	-4.55766200	-1.74698200	0.39510400	H	5.91486000	-2.64601700	0.65996700
C	-5.86986800	-2.45107100	0.81663000	H	6.65179900	-3.69407500	-0.53820300
C	-3.50128700	0.61855400	-0.06475100	H	-5.66751300	-3.94667600	-0.42100400
C	-2.04491200	0.41590200	0.30171100	H	-7.06303400	-1.90788500	-0.87180800
C	-1.44476000	-0.97840800	0.43909200	H	-8.09373300	0.10604100	0.19986500
C	-2.15556900	-2.03475300	1.27524000	H	-7.23938100	-0.26072700	1.69196500
C	-3.44269500	-2.37176800	1.19944300	H	-5.98068500	0.34541300	-1.02190100
C	-3.51878700	0.62995000	-1.58717200	H	-5.99781300	1.43923800	0.35201800
O	-3.10090800	1.82694200	-2.10609500	H	-5.95094200	-2.40050600	1.90911700
C	-3.45453400	3.03033500	-1.45812500	H	-0.47849700	-0.84388800	0.90638500
C	-2.47305700	3.59414000	-0.53276000	H	-3.75369000	-3.22276700	1.79730800
C	-1.49083800	2.91679300	0.13485800	H	-0.15552200	4.65135300	0.24193000
C	-1.21039600	1.49157300	0.37560400	H	-0.55736300	3.93479400	1.80458000
C	-0.35131500	3.71078100	0.75226200	H	1.63939700	3.00419400	1.33183200
C	0.83439700	2.75718200	0.64346700	H	0.81671300	0.63471300	0.39406000
C	0.22609100	1.38222800	0.92126600	H	-1.71855800	-3.63682000	2.66022400
C	-1.20815300	-2.82083700	2.14674700	H	-0.39563600	-3.24537200	1.54656900
C	-2.59471700	5.09727700	-0.38500500	H	-0.74020700	-2.17895700	2.90113000
O	-4.47643600	3.56080400	-1.81198500	H	-1.91586000	5.61529100	-1.07134500
O	-3.74056900	-0.28946300	-2.32387300	H	-3.60851400	5.40877700	-0.62798300
O	1.43492800	2.82542800	-0.66727700	H	-2.36306700	5.42430100	0.62796400
H	-3.73095200	1.64171300	0.24582600	H	0.84455100	2.42034700	-1.31470800
H	-4.56616200	-0.02188000	1.65541500	H	-8.33962600	-3.63709900	0.41642700
C	-8.39197700	-2.58007600	0.67998000	H	-8.50687100	-2.50861700	1.76683000
H	-4.41999800	-1.95414300	-0.67305900	H	-9.28543300	-2.15095700	0.21873800
C	0.26257700	1.08966500	2.43173000	H	1.30023400	0.99535800	2.75654500
C	7.19796400	-1.62829100	-0.76430200	H	-0.21084100	1.89528400	2.99812600
C	8.56112600	-1.95862400	-0.14271800	H	-0.26196200	0.16764500	2.68127100
C	6.35569200	0.09891200	1.01893800	H	7.33338000	-1.65074900	-1.85122400
O	7.49226000	0.00125400	1.88368800	H	9.29429900	-1.17813800	-0.36745800
C	5.68195500	1.48475900	1.21180900	H	8.49213300	-2.05003900	0.94167300
C	4.26619800	1.44847600	0.66141900	H	8.94165700	-2.90093200	-0.54698200
O	3.42163700	0.67590000	1.07418000	H	5.65382500	-0.64289100	1.40021600
O	4.03238000	2.34231300	-0.29945600	H	8.22925800	0.45776400	1.46384100
C	6.52737600	2.66008200	0.72081000	H	5.54980000	1.57572900	2.29487100
C	6.69397500	-0.20617000	-0.44283400	H	3.06857900	2.34838400	-0.53677800

H	6.65497600	2.64935900	-0.36177500	C	8.44533700	-1.32569400	-1.20826300
H	6.06098500	3.60826300	0.99131700	H	4.71961600	0.71092300	-1.36365700
H	7.51465100	2.63277500	1.18812000	C	1.31940400	0.98653400	3.79818300
H	7.44726100	0.51086600	-0.78843100	C	-6.20585700	1.60108100	-0.42077500
H	5.79674600	-0.01543700	-1.04135600	C	-7.55083400	1.80507600	0.28331700
B3LYP Energy = -2081.90554218 a.u.				C	-6.13637600	-0.97079700	-0.43036400
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf H				O	-6.06083200	-1.08287200	-1.85228600
C	0.86504800	2.51582800	-1.34319300	C	-5.54421300	-2.21190000	0.29038500
C	2.07737400	2.26830800	-0.81579600	C	-4.03566000	-2.19422800	0.19060100
C	-1.59154600	2.67662100	-1.26065100	O	-3.28705000	-2.00749800	1.13269400
C	-0.40596700	2.40229800	-0.66988400	O	-3.60008000	-2.37675800	-1.05833800
C	-4.07766700	2.88519000	-1.07531400	C	-6.14147300	-3.52204500	-0.23689600
C	-4.33768400	3.23970400	-2.51308200	C	-5.49657400	0.32944700	0.05921100
C	-2.85561300	2.61754600	-0.56581500	H	0.82584600	2.82686300	-2.38496200
C	-5.29996300	2.83539900	-0.19475300	H	2.95092400	2.37712700	-1.44731500
O	7.23353200	1.31127000	-0.95591600	H	-1.58533700	2.98183100	-2.30318800
C	6.93122800	-1.11251500	-1.18142500	H	-0.41567500	2.07420800	0.36210000
C	6.19947200	-2.29398200	-0.54117500	H	-4.85422000	4.20358100	-2.57878700
C	4.69082300	-2.09099200	-0.59961400	H	-3.43378900	3.29470100	-3.11719800
C	4.22995300	-0.79295100	0.09375000	H	-5.00105600	2.50007400	-2.97405500
C	5.03810600	0.44880200	-0.34675500	H	-2.79488800	2.34046600	0.48461200
C	6.55837300	0.16352300	-0.42566800	H	-5.00176800	2.85781800	0.85871500
C	2.69152400	-0.70635900	-0.05735200	H	-5.89833000	3.73610000	-0.37690300
C	1.96194400	0.35037600	0.75190900	H	6.90183300	1.45135600	-1.85099300
C	2.34565400	1.81473400	0.61672200	H	6.57182100	-1.00674400	-2.21546200
C	3.75382900	2.21810400	1.02410800	H	6.47061000	-3.22241200	-1.05235900
C	4.86765900	1.64075200	0.57315700	H	6.52920700	-2.39967200	0.50037800
C	2.18783500	-0.65515000	-1.46790400	H	4.38630000	-2.07263000	-1.64907500
O	0.80875400	-0.89991300	-1.61262900	H	4.17489500	-2.93595800	-0.13296400
C	-0.02997600	-1.75311900	-0.95073100	H	6.94274800	0.07204600	0.59720700
C	0.07801100	-2.19425800	0.45469000	H	1.66024400	2.36479900	1.26075800
C	0.28511000	-1.34109300	1.49448900	H	5.80510000	2.09507200	0.87835400
C	0.90186400	-0.01597100	1.50467000	H	-1.18940600	-2.26397000	2.82879400
C	-0.38233800	-1.53405600	2.83855000	H	0.33785500	-1.82988500	3.60801800
C	-0.87934200	-0.10141800	3.11566000	H	-1.12769700	0.04878100	4.17126300
C	0.30019300	0.78075700	2.66797900	H	-0.09434300	1.75008800	2.35720300
C	3.81663000	3.44699500	1.89439200	H	4.84687500	3.74465000	2.09493400
C	-0.48151800	-3.57995300	0.69185900	H	3.30354700	4.28439800	1.40724400
O	-0.98793200	-2.11854600	-1.61437900	H	3.31196100	3.28816600	2.85304700
O	2.77812900	-0.39207200	-2.47181900	H	-1.55731800	-3.55344000	0.87384500
O	-1.99809100	0.23442300	2.29519100	H	-0.29999000	-4.21979500	-0.17180500
H	2.32895800	-1.66582500	0.32121500	H	-0.00059900	-4.03114500	1.56034300
H	4.40158000	-0.91695100	1.16934500	H	-2.47795700	-0.56859700	2.04271700
				H	8.95585700	-0.47046900	-1.65267000

H	8.83216300	-1.45915300	-0.19226000	C	0.22823900	-2.17011200	-0.74179400
H	8.69916700	-2.21967800	-1.78410300	C	0.39777900	-1.88178700	0.56139900
H	0.87161400	1.55199700	4.61911500	C	0.82298000	-0.56980100	1.08147500
H	1.66924200	0.02950800	4.19316900	C	-0.06376400	-2.72301400	1.71768900
H	2.19455700	1.52988900	3.44429100	C	-0.50527400	-1.68686000	2.78991000
H	-6.38925300	1.49460300	-1.49437700	C	-0.07754400	-0.26971600	2.27458000
H	-8.22194300	0.95536500	0.13693900	C	3.20820100	3.12572600	2.47331400
H	-7.40526200	1.93482700	1.36100000	C	-0.27229900	-3.50076300	-1.25009000
H	-8.05752100	2.69579800	-0.09753400	O	-0.85205700	-0.82939000	-2.33765800
H	-7.20599400	-0.97104100	-0.20798100	O	3.35835300	0.19101900	-2.60003700
H	-5.13340000	-1.23388600	-2.07845700	O	-1.89055300	-1.74364000	3.09324700
H	-5.77005700	-2.10482900	1.35291900	H	2.51000400	-1.67435000	-0.33424700
H	-2.61189200	-2.31735500	-1.11550500	H	4.29604600	-0.97391300	1.09992900
H	-5.71980000	-4.38423100	0.28423900	C	8.72288300	-0.71223400	-0.42174300
H	-7.22193100	-3.52112100	-0.07561700	H	4.93876400	1.10756500	-1.00661000
H	-5.95379500	-3.63033100	-1.30432700	C	0.47117300	0.57644100	3.42531100
H	-4.45670100	0.34796100	-0.28499000	C	-6.66825800	1.47181400	-0.47273100
H	-5.46065500	0.32826600	1.15530300	C	-7.93313800	1.53990200	0.39057700
B3LYP Energy = -2081.91154822 a.u.				C	-5.74205900	-0.74867700	0.54664300
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf I				O	-6.86526800	-1.15606400	1.32980800
C	0.60384000	2.60458700	-0.99712700	C	-4.86322500	-1.99476100	0.22187100
C	1.82225200	2.31447700	-0.50503500	C	-3.50715800	-1.51052200	-0.23742900
C	-1.86338100	2.55780400	-0.94388300	O	-2.69701500	-1.00815300	0.52550800
C	-0.66400800	2.33149900	-0.36103200	O	-3.28023900	-1.63557800	-1.53877800
C	-4.35998700	2.59320700	-0.77090700	C	-5.53560200	-2.99142600	-0.72146900
C	-4.62330200	3.11558200	-2.15677000	C	-6.14719300	0.04048900	-0.70203200
C	-3.12744600	2.33532800	-0.28211600	H	0.55395400	3.08275100	-1.97278900
C	-5.57966500	2.40787000	0.09787900	H	2.69906200	2.56701300	-1.09012700
O	7.25876400	1.76176400	0.02617400	H	-1.87132700	2.94372100	-1.95900800
C	7.22038900	-0.58469100	-0.67649800	H	-0.65565900	1.92850600	0.64571800
C	6.48594300	-1.90361400	-0.42924800	H	-5.31463500	3.96383200	-2.11798700
C	5.00488500	-1.76924800	-0.75853100	H	-3.71997200	3.43505600	-2.67340800
C	4.30894100	-0.65646100	0.05057100	H	-5.10447400	2.35000000	-2.77503600
C	5.06709600	0.68889800	-0.00064700	H	-3.06105600	1.94507900	0.73064700
C	6.59365200	0.50318700	0.19747100	H	-5.27805200	2.06310500	1.09116100
C	2.81802400	-0.62684200	-0.37023400	H	-6.04334700	3.39312800	0.24233700
C	1.87527300	0.10439000	0.57453200	H	7.09969600	2.04902400	-0.88107500
C	2.07900500	1.58996700	0.81165400	H	7.06435700	-0.29804200	-1.72668200
C	3.38914200	2.06133800	1.41932200	H	6.93275700	-2.69846100	-1.03387700
C	4.61302100	1.69552000	1.03450700	H	6.61595400	-2.19537600	0.62086800
C	2.58298300	-0.25357000	-1.80628700	H	4.90291300	-1.56241700	-1.82698100
O	1.27896000	-0.44619500	-2.29196300	H	4.48656000	-2.71388600	-0.56571500
C	0.19541200	-1.09896600	-1.78451000	H	6.77518200	0.24120700	1.24677900
				H	1.29205700	1.89672800	1.49246800

H	5.43755900	2.21067200	1.51727500	C	-6.42854300	1.70441400	-0.60204500
H	-0.88952500	-3.38894700	1.46890700	C	-4.90560000	1.72641400	-0.64216100
H	0.75891200	-3.33634400	2.09938500	C	-4.26572600	0.56784500	0.14928200
H	0.00329100	-1.89598100	3.73212300	C	-4.86359400	-0.80552000	-0.22201500
H	-0.99640500	0.18968000	1.89844100	C	-6.40878500	-0.76570800	-0.30835500
H	4.16546600	3.52998400	2.80581800	C	-2.73271300	0.73137700	0.02632500
H	2.59977900	3.95092600	2.08557400	C	-1.80392400	-0.18143100	0.80376100
H	2.68015500	2.72943000	3.34685300	C	-1.98442200	-1.69512200	0.73708900
H	-1.32727300	-3.45184900	-1.53292700	C	-3.30989800	-2.27184500	1.21644300
H	0.28848400	-3.81100800	-2.13593100	C	-4.50679300	-1.89748600	0.76383300
H	-0.15244200	-4.27011200	-0.48958000	C	-2.18376100	0.75763000	-1.38531200
H	-2.36076400	-1.48232400	2.28201600	O	-0.97499300	1.41804800	-1.45530100
H	9.23169900	0.23834900	-0.58570800	C	-0.80415000	2.67827100	-0.84746800
H	8.91183200	-1.02277100	0.61150100	C	-0.38929700	2.76129100	0.55589400
H	9.16451400	-1.46191600	-1.08367900	C	-0.27070400	1.74106600	1.45572200
H	-0.16723400	0.43465900	4.30108400	C	-0.73438600	0.34721000	1.45453100
H	1.48740800	0.27084700	3.68816300	C	0.60541600	1.92202600	2.68536900
H	0.47983000	1.64460000	3.21035100	C	1.23119300	0.53483900	2.86193100
H	-6.93834900	1.85121400	-1.46407600	C	0.07506000	-0.41610200	2.51431100
H	-8.71735600	0.89196500	-0.01127100	C	-3.17013200	-3.43986900	2.15838600
H	-7.73568100	1.22253700	1.41556000	C	0.09298300	4.14930800	0.91859100
H	-8.32067700	2.56234800	0.41338700	O	-0.90339400	3.63381400	-1.57768100
H	-5.15183000	-0.11715500	1.21284500	O	-2.61533800	0.21381800	-2.36109400
H	-7.54706600	-1.48167100	0.73216900	O	2.35495300	0.35341800	2.00286300
H	-4.68588100	-2.47292900	1.18906400	H	-2.54777600	1.73313100	0.42298100
H	-2.37595300	-1.29305500	-1.76290200	H	-4.48715700	0.73085700	1.21071900
H	-4.92075100	-3.88517800	-0.84127700	C	-8.49688800	0.36017100	-1.18491300
H	-6.49639700	-3.30442800	-0.30722600	H	-4.50428200	-1.06575900	-1.22586400
H	-5.70462000	-2.56497000	-1.71010400	C	-0.78062500	-0.71711400	3.75591300
H	-6.91057800	-0.53119700	-1.24304300	C	6.30120000	-1.52413000	-0.26176600
H	-5.28332700	0.09450900	-1.37111100	C	7.52141900	-1.45887700	0.66120800
B3LYP Energy = -2081.90678428 a.u.				C	5.79028100	1.02431000	-0.08567800
				O	6.31297800	1.33093100	-1.40126100
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf J				C	4.65405500	2.02609300	0.17547200
C	-0.55538700	-2.60029600	-1.18893400	C	3.50215400	1.83729600	-0.80641300
C	-1.72888700	-2.18206100	-0.68267000	O	2.33833200	1.74835100	-0.46456600
C	1.88417600	-2.95498800	-1.13101700	O	3.82136100	1.80273000	-2.10272200
C	0.71534600	-2.67746300	-0.50977700	C	5.13487600	3.48668700	0.14366900
C	4.38421300	-3.05732700	-0.99466200	C	5.28397300	-0.41064500	0.01945700
C	4.64689500	-3.21385600	-2.46605900	H	-0.54698800	-2.89643600	-2.23594700
C	3.15466800	-2.96292400	-0.44601000	H	-2.58646600	-2.16430700	-1.34133800
C	5.60661000	-2.90495900	-0.12517600	H	1.86735100	-3.13843600	-2.20157200
O	-6.89747500	-2.03827500	-0.75149500	H	0.74197200	-2.47547900	0.55525800
C	-6.96818000	0.38163000	-1.15076100	H	5.35847300	-4.02757300	-2.64058900

H	3.74732500	-3.41770600	-3.04476300	B3LYP Energy = -2081.90738069 a.u.			
H	5.10581400	-2.30572600	-2.87402900				
H	3.09867700	-2.81669100	0.63081200	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf K			
H	5.33191300	-3.04252900	0.92552600	C	0.46970800	2.45892000	-1.30260400
H	6.34011400	-3.68023000	-0.37408000	C	1.70814300	2.20803700	-0.83834000
H	-6.53629000	-2.19424600	-1.63239700	C	-1.99161900	2.49250400	-1.11136300
H	-6.59100700	0.25813600	-2.17638400	C	-0.76539600	2.31133700	-0.57045100
H	-6.82953000	2.54040500	-1.18266100	C	-4.47731700	2.53933000	-0.80209000
H	-6.78246100	1.83754300	0.42825200	C	-4.82614900	2.91475800	-2.21596000
H	-4.58666500	1.67148600	-1.68707500	C	-3.21548300	2.35319800	-0.35966800
H	-4.52787400	2.67379900	-0.24471000	C	-5.64083900	2.40877500	0.14895800
H	-6.80627100	-0.66187700	0.70841400	O	7.28156200	1.76046400	-0.06477600
H	-1.21233400	-2.12279900	1.36970600	C	7.26956100	-0.66949300	-0.35210900
H	-5.36073200	-2.46127400	1.12595800	C	6.50189900	-1.93025700	0.04744700
H	1.36664000	2.68987100	2.56782900	C	5.05164100	-1.84996500	-0.41101400
H	-0.00199700	2.17944000	3.55977200	C	4.31318800	-0.62428800	0.16186800
H	1.59686000	0.36653700	3.87542800	C	5.08256300	0.69553300	-0.06304800
H	0.50103300	-1.34295300	2.13259600	C	6.59109800	0.55049500	0.27437200
H	-4.13981700	-3.87779200	2.39965200	C	2.84895200	-0.67105100	-0.34702700
H	-2.54284500	-4.21757600	1.70742200	C	1.87688300	0.16217900	0.47121800
H	-2.68226500	-3.14990600	3.09455600	C	2.03531400	1.66758200	0.54998200
H	1.13602500	4.28343100	0.61020200	C	3.33648900	2.27388800	1.04086800
H	-0.49816300	4.89743500	0.39343300	C	4.57289800	1.87231300	0.74011800
H	0.02212500	4.33759300	1.98777600	C	2.70109400	-0.51547300	-1.83610800
H	2.18459300	0.78894800	1.14807900	O	1.43952700	-0.83168900	-2.35535400
H	-8.86891500	-0.59401200	-1.56001000	C	0.29342900	-1.16885100	-1.68887500
H	-8.90539600	0.51096800	-0.17991400	C	0.21698700	-2.17702900	-0.57236600
H	-8.87994900	1.15867500	-1.82590200	C	0.35791900	-1.78497400	0.70775500
H	-0.19521900	-1.26203600	4.50075700	C	0.84092200	-0.45187100	1.08191200
H	-1.14280600	0.20639400	4.21467500	C	-0.21096100	-2.42838200	1.94543000
H	-1.65492300	-1.31471200	3.50191100	C	-0.84195800	-1.20857000	2.66834800
H	6.64705900	-1.43435300	-1.29959300	C	0.10141200	-0.01115500	2.34528600
H	8.09329500	-0.53831300	0.52097400	C	3.12174200	3.53151800	1.84792200
H	7.21251100	-1.50511600	1.71023400	C	-0.29546200	-3.51742300	-1.02864100
H	8.19574400	-2.29743700	0.47011900	O	-0.72629500	-0.72089600	-2.16384600
H	6.57773200	1.21236300	0.65037600	O	3.52265600	-0.18356600	-2.63818800
H	6.90968000	0.62945400	-1.68363600	O	-2.18078300	-0.97197900	2.24893300
H	4.24727900	1.80394700	1.16220200	H	2.54149800	-1.70710000	-0.18320000
H	4.80094300	1.71990100	-2.17828900	H	4.23520800	-0.76779900	1.24597200
H	4.30758700	4.16925300	0.34732900	C	8.74528500	-0.75137200	0.04128300
H	5.89831900	3.63623200	0.91006000	H	5.03276400	0.93421600	-1.13283200
H	5.56727400	3.74163100	-0.82433500	C	1.07500200	0.26232000	3.50167900
H	4.44025200	-0.53341900	-0.66414600	C	-6.73212600	1.39723100	-0.26483300
H	4.87739200	-0.54233700	1.02829300	C	-7.91579300	1.47228100	0.70699700

C	-5.38433800	-0.63448700	0.68654300	H	-7.10885200	1.70582800	-1.24657600
O	-6.24074700	-0.78535100	1.82289900	H	-8.69892200	0.76497300	0.41977600
C	-4.75926300	-2.01363300	0.32356000	H	-7.60627700	1.22886300	1.72326900
C	-3.74588400	-1.86734200	-0.79048100	H	-8.34952500	2.47668800	0.70197100
O	-3.74638400	-2.47963000	-1.83445100	H	-4.56216500	0.03731200	0.94119500
O	-2.80260600	-0.95463700	-0.49020300	H	-5.68708000	-1.01399100	2.57788100
C	-5.79105900	-3.09478200	0.01590800	H	-4.17564900	-2.30473700	1.20565600
C	-6.18842300	-0.03285100	-0.46182300	H	-2.13221900	-0.88719600	-1.21542400
H	0.37634800	2.79603000	-2.33242800	H	-5.31524000	-4.07461900	-0.04925200
H	2.55607800	2.34727500	-1.49989100	H	-6.53675700	-3.12025000	0.81060800
H	-2.05394800	2.75493500	-2.16336700	H	-6.29616200	-2.90721700	-0.93252700
H	-0.70906100	2.03421500	0.47617200	H	-7.02822800	-0.69443700	-0.69398500
H	-5.52061700	3.76144200	-2.22336600	H	-5.53993300	-0.03409600	-1.34437200
H	-3.95698200	3.18218100	-2.81457100	B3LYP Energy = -2081.90785492 a.u.			
H	-5.33685200	2.08963300	-2.72389200	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf L			
H	-3.08717400	2.07485700	0.68415000	C	0.74513000	2.61551500	-0.89933800
H	-5.27480600	2.16196900	1.14964000	C	1.94028900	2.30844600	-0.36265100
H	-6.12655800	3.39066200	0.23104600	C	-1.72438200	2.55562300	-0.94809000
H	7.19457600	1.88365300	-1.01785700	C	-0.54758500	2.33440000	-0.31890000
H	7.20216000	-0.56120900	-1.44440600	C	-4.22619800	2.60430000	-0.85615100
H	6.98312700	-2.81233900	-0.38523000	C	-4.44405300	3.08822000	-2.26317300
H	6.54723300	-2.04940400	1.13767100	C	-3.01077300	2.34772700	-0.32538000
H	5.03048700	-1.81180200	-1.50353800	C	-5.46885400	2.47231600	-0.01067200
H	4.50978000	-2.75283700	-0.11249900	O	7.15885700	1.79635100	-0.29748700
H	6.69380700	0.47547600	1.36345700	C	7.14907300	-0.51488600	-0.88376500
H	1.25520200	2.01576800	1.22628700	C	6.49246700	-1.86108900	-0.57273400
H	5.37516700	2.50448100	1.10720700	C	4.98577500	-1.78864100	-0.78963200
H	-0.94979700	-3.20626300	1.76040700	C	4.30785200	-0.70667300	0.07438800
H	0.58935300	-2.84844500	2.56366400	C	5.03474900	0.65787600	0.03815100
H	-0.90360900	-1.37380600	3.74389400	C	6.57655700	0.53557800	0.06016500
H	-0.52653400	0.86879000	2.18631400	C	2.80375500	-0.66536300	-0.29873000
H	4.06655900	4.01056700	2.10802600	C	1.87975300	0.06574100	0.66863000
H	2.51297800	4.24912000	1.28607300	C	2.12530200	1.54302800	0.94128200
H	2.57714400	3.31718600	2.77440300	C	3.43319800	1.92403800	1.61603700
H	-1.24288400	-3.41722900	-1.56559600	C	4.64365200	1.55383900	1.19607200
H	0.41990900	-3.98672800	-1.71136000	C	2.53346000	-0.25730600	-1.72076900
H	-0.43731700	-4.18413900	-0.17976100	O	1.20894400	-0.40609200	-2.17202100
H	-2.20991400	-0.87885000	1.28272200	C	0.15519300	-1.14572200	-1.73389800
H	9.27757700	0.15904600	-0.23650300	C	0.19724200	-2.19990700	-0.68019600
H	8.84694700	-0.88547300	1.12358300	C	0.37415100	-1.90129300	0.62078100
H	9.22897000	-1.60048300	-0.44890300	C	0.80511500	-0.59201500	1.14786300
H	0.52798300	0.56969500	4.39634000	C	-0.09860900	-2.73711100	1.77663400
H	1.64860000	-0.63710000	3.74159500	C	-0.57434400	-1.69495600	2.82688000
H	1.78780100	1.04725700	3.24833800				

C	-0.13036500	-0.28289100	2.31313100	H	4.24156800	3.17104900	3.18586900
C	3.27532400	2.84611900	2.79696800	H	2.70036400	3.73512200	2.51382000
C	-0.31592800	-3.53627100	-1.16292100	H	2.72358600	2.35980600	3.60721000
O	-0.87852000	-0.94671800	-2.34401400	H	-1.38657800	-3.50411100	-1.38109000
O	3.29147500	0.19368600	-2.52674100	H	0.19412400	-3.83483400	-2.08228200
O	-1.96886700	-1.74901500	3.08450400	H	-0.13864900	-4.30661400	-0.41480300
H	2.48831800	-1.71111900	-0.27278900	H	-2.41293700	-1.49613800	2.25579200
H	4.33330700	-1.05723000	1.11232100	H	9.12855500	0.37880300	-1.01180200
C	8.67411600	-0.58597400	-0.78443500	H	8.98027300	-0.87570600	0.22654000
H	4.79756800	1.14594000	-0.91160700	H	9.07083900	-1.32961900	-1.48099200
C	0.36771400	0.57444900	3.47725200	H	-0.31074300	0.44125600	4.32379300
C	-6.58600000	1.57200300	-0.58213700	H	1.36923500	0.26872000	3.79065000
C	-7.85740200	1.71147200	0.26252500	H	0.38712900	1.64064800	3.25373700
C	-5.76272500	-0.66208800	0.48364300	H	-6.82605300	1.94487300	-1.58389200
O	-6.97557900	-1.02601200	1.14598200	H	-8.65985900	1.08251400	-0.13095800
C	-4.93014500	-1.94797500	0.19069800	H	-7.68352100	1.40955700	1.29656300
C	-3.55251800	-1.52848300	-0.26908900	H	-8.20284000	2.74943300	0.25757100
O	-2.72290900	-1.05132700	0.48975700	H	-5.15583000	-0.03426600	1.14422100
O	-3.32733800	-1.68242000	-1.56707000	H	-6.74906600	-1.36058100	2.02077300
C	-5.64562200	-2.93009700	-0.73503700	H	-4.76668000	-2.42204800	1.16443000
C	-6.12895800	0.11387700	-0.77974400	H	-2.40924100	-1.37834400	-1.79328300
H	0.73718800	3.11527500	-1.86518700	H	-5.09396900	-3.86947000	-0.80524600
H	2.84237500	2.57256500	-0.90178300	H	-6.63781000	-3.14043900	-0.33401200
H	-1.69612800	2.93470800	-1.96544400	H	-5.75476600	-2.52755600	-1.74186400
H	-0.57867300	1.93623900	0.68944900	H	-6.91870600	-0.43822200	-1.29787100
H	-5.11603600	3.95283100	-2.26960400	H	-5.26202800	0.11507200	-1.44666400
H	-3.52133900	3.36967900	-2.76762800	B3LYP Energy = -2081.90496323 a.u.			
H	-4.92786700	2.31349500	-2.86767100				
H	-2.97821200	1.98520200	0.69945100	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf M			
H	-5.19720500	2.13364500	0.99330200	C	-0.56315500	-2.10061000	-1.68141400
H	-5.89600500	3.47729000	0.11101800	C	-1.81291600	-2.05066800	-1.18941100
H	6.81119700	2.46928800	0.29726000	C	1.88525900	-2.16645600	-1.56841600
H	6.87478900	-0.22430900	-1.90657600	C	0.68489200	-2.01721100	-0.95922900
H	6.92333100	-2.63912500	-1.20967100	C	4.37600900	-2.19364200	-1.45460600
H	6.71575000	-2.14275400	0.46440700	C	4.60236400	-2.54827300	-2.89920400
H	4.80172800	-1.58599100	-1.84716600	C	3.15516700	-2.05779700	-0.89387800
H	4.51941300	-2.75266700	-0.56279700	C	5.61913800	-1.96304100	-0.63478100
H	6.88728500	0.26774200	1.08271600	O	-6.76931100	-1.07848800	-1.86108100
H	1.32903500	1.86350900	1.60392300	C	-6.50425700	1.33252400	-1.48121900
H	5.47773400	1.93118300	1.78669800	C	-5.93624300	2.33120900	-0.46995500
H	-0.90921000	-3.41827900	1.52075500	C	-4.43821600	2.12322500	-0.28754500
H	0.72690300	-3.33219200	2.18069500	C	-4.08139000	0.69655800	0.17589600
H	-0.09678100	-1.89675300	3.78664800	C	-4.75062600	-0.39839500	-0.68170100
H	-1.03578900	0.17032400	1.89784400	C	-6.23735400	-0.08563500	-0.97501400

C	-2.54177100	0.63815100	0.31203200	H	-6.27757800	-1.01800100	-2.68889000
C	-1.87456000	-0.60554400	0.86520000	H	-5.96108900	1.45879100	-2.42908900
C	-2.21742000	-1.97172900	0.28110700	H	-6.13273000	3.35383400	-0.80505800
C	-3.65761200	-2.44348000	0.42528800	H	-6.45663300	2.20752700	0.48842800
C	-4.71014800	-1.76385400	-0.02848600	H	-3.94372900	2.33111700	-1.24041600
C	-1.75576100	1.00120700	-0.93274100	H	-4.03903400	2.83782500	0.43923200
O	-0.47333000	1.41892200	-0.59494400	H	-6.80324200	-0.22105000	-0.04555400
C	-0.32464900	2.41012700	0.41039400	H	-1.59845000	-2.69207900	0.81066300
C	-0.06440300	1.97192900	1.77914400	H	-5.67817900	-2.24831600	0.05278100
C	-0.21834000	0.71287900	2.28830900	H	1.37281200	0.94061100	3.78037500
C	-0.87715600	-0.49671300	1.78290800	H	-0.18765200	0.44334700	4.43444900
C	0.48928300	0.33760900	3.57962700	H	1.00519900	-1.66514200	4.30808400
C	0.84723800	-1.13761400	3.36636800	H	-0.05523800	-2.52928600	2.00195700
C	-0.37630400	-1.68703300	2.61660800	H	-4.85827300	-4.14606900	0.99312300
C	-3.81337500	-3.83212200	0.98854200	H	-3.24034100	-4.55011300	0.39013500
C	0.55058000	3.06402200	2.62844000	H	-3.42922300	-3.90355900	2.01077000
O	-0.30486100	3.55383700	0.03061200	H	1.64245000	3.05388800	2.53559200
O	-2.06069400	0.89004400	-2.08137100	H	0.20251000	4.03775200	2.28964200
O	2.05322700	-1.29229600	2.62214100	H	0.29674300	2.94942300	3.68074800
H	-2.31477000	1.43021900	1.03115400	H	2.13593600	-0.57747500	1.97158500
H	-4.46452200	0.57541000	1.19583100	H	-8.38991800	0.83636000	-2.44521400
C	-7.99434700	1.56422400	-1.73579900	H	-8.56162400	1.47023800	-0.80359400
H	-4.23694700	-0.42430700	-1.65128200	H	-8.16697900	2.56749700	-2.13425800
C	-1.45920200	-2.15671700	3.60218700	H	-1.10673500	-3.01601500	4.17794700
C	6.54403200	-0.85665000	-1.19744700	H	-1.72163300	-1.36006500	4.30298400
C	7.82099600	-0.75174800	-0.35788800	H	-2.37188700	-2.44114500	3.08090700
C	5.48433300	1.23693500	-0.07707400	H	6.84378400	-1.16743500	-2.20390700
O	6.64010400	2.00441700	0.26899400	H	8.49088500	0.01377300	-0.75538800
C	4.25392700	2.18229400	-0.20865400	H	7.59718500	-0.48466600	0.67757000
C	2.99550500	1.34467200	-0.19354300	H	8.35229000	-1.70777900	-0.35431100
O	2.63106700	0.73393900	0.79309300	H	5.25927600	0.52923500	0.72755300
O	2.31921800	1.32193400	-1.34373500	H	6.53140200	2.31750200	1.17380900
C	4.36586900	3.17014000	-1.36744400	H	4.21017500	2.73797900	0.73421100
C	5.80738800	0.48587100	-1.36835700	H	1.50201000	0.80433200	-1.22013200
H	-0.46788600	-2.19514600	-2.76123200	H	3.54455600	3.88848300	-1.34480000
H	-2.63536500	-2.08426900	-1.89364700	H	5.30649800	3.71531500	-1.27931700
H	1.88745100	-2.36090400	-2.63717700	H	4.34564400	2.66610400	-2.33386200
H	0.66475700	-1.80929900	0.10335600	H	6.41194400	1.15234000	-1.99002400
H	5.39435000	-3.29930500	-2.98231500	H	4.87978200	0.30378000	-1.91769800
H	3.71163000	-2.94060000	-3.38712800	B3LYP Energy = -2081.90900706 a.u.			
H	4.93890400	-1.67603600	-3.47023600				
H	3.10621300	-1.81794000	0.16379800	(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf N			
H	5.34150700	-1.72530600	0.39659800	C	-0.01971300	-1.97619200	-1.33498000
H	6.20375700	-2.89171400	-0.59789200	C	-1.21236100	-1.59117500	-0.84497000

C	2.41358400	-2.31399900	-1.30274300	O	4.01547800	2.31834300	-0.36797100
C	1.27678800	-1.89694800	-0.69946000	C	6.52580000	2.64935100	0.63091000
C	4.87603100	-2.72749300	-1.21688900	C	6.68207400	-0.21841800	-0.48796700
C	5.01699400	-3.22629000	-2.62908200	H	-0.01971500	-2.42550300	-2.32623200
C	3.71219700	-2.31231900	-0.67183500	H	-2.09387900	-1.75716100	-1.44854600
C	6.14790800	-2.73476000	-0.40715800	H	2.33536400	-2.69673000	-2.31639200
O	-5.70789400	-3.84886300	0.29036700	H	1.34686300	-1.50758200	0.31163800
C	-7.07166100	-1.89964000	0.11221400	H	5.40716900	-4.25025300	-2.63019700
C	-7.17892800	-0.42975700	0.52417600	H	4.08326800	-3.21681500	-3.18809200
C	-5.96160500	0.35588100	0.05254400	H	5.74090000	-2.61884300	-3.18201600
C	-4.63445500	-0.20752700	0.59936100	H	3.73152200	-1.95079400	0.35295400
C	-4.51177700	-1.73638700	0.43444900	H	5.91568800	-2.64718800	0.65744200
C	-5.82109000	-2.49494800	0.74797300	H	6.63390600	-3.70922200	-0.53923200
C	-3.50139800	0.63434000	-0.03250200	H	-4.92693000	-4.24044200	0.69590800
C	-2.04435200	0.43928200	0.34205300	H	-6.94159700	-1.94520700	-0.97722500
C	-1.44368200	-0.95408000	0.51271800	H	-8.08903800	0.00701900	0.10318800
C	-2.15025000	-1.95772700	1.41625500	H	-7.27326200	-0.36383000	1.61558200
C	-3.43570100	-2.29891300	1.33556000	H	-5.94645400	0.33596400	-1.04195300
C	-3.50554200	0.63367500	-1.55668500	H	-6.04592900	1.40667700	0.34653300
O	-3.11030700	1.83390900	-2.08397000	H	-5.96901400	-2.48973100	1.83976300
C	-3.47073000	3.03560900	-1.43796900	H	-0.46819700	-0.80682600	0.95581700
C	-2.48295300	3.61005900	-0.52625700	H	-3.76798500	-3.06078400	2.03953800
C	-1.49247600	2.93988100	0.13583600	H	-0.15382800	4.67318100	0.19577700
C	-1.21035700	1.51699600	0.39416600	H	-0.53405600	3.98475900	1.77631800
C	-0.34361500	3.74200500	0.72532600	H	1.65496100	3.04232800	1.28645700
C	0.83835500	2.78396500	0.61612200	H	0.81517500	0.65619700	0.41647600
C	0.23034300	1.41717000	0.93057700	H	-1.73608000	-3.43184900	2.94268200
C	-1.22247900	-2.65160600	2.37903100	H	-0.38587700	-3.10964200	1.83977800
C	-2.60591300	5.11417900	-0.39268400	H	-0.78720700	-1.94273800	3.09143200
O	-4.49973800	3.55650100	-1.78491200	H	-1.94528200	5.62645500	-1.10080300
O	-3.70190900	-0.29615800	-2.28732500	H	-3.62629100	5.41908500	-0.61631800
O	1.41812000	2.82423300	-0.70499500	H	-2.35252900	5.45387800	0.61074800
H	-3.73818500	1.65828000	0.27042400	H	0.81381900	2.41355200	-1.33588600
H	-4.60132600	0.00664900	1.67329300	H	-8.23858400	-3.73413500	0.18898700
C	-8.32508900	-2.69025400	0.49188600	H	-8.48290900	-2.66306600	1.57544100
H	-4.28516900	-1.95287600	-0.61335100	H	-9.20988400	-2.26213000	0.01305600
C	0.27921700	1.16091200	2.44708100	H	1.31931100	1.07047600	2.76508500
C	7.17582300	-1.64655900	-0.79909300	H	-0.18661000	1.98083600	2.99886100
C	8.54774500	-1.97169900	-0.19576800	H	-0.24615200	0.24726800	2.72268400
C	6.35048000	0.10118800	0.96755200	H	7.29233600	-1.68261500	-1.88810200
O	7.56486700	0.06463900	1.72447300	H	9.27564100	-1.19255000	-0.43721100
C	5.67556500	1.48900000	1.14625000	H	8.49439100	-2.04463300	0.89047900
C	4.25412500	1.44617800	0.61109200	H	8.91957000	-2.92040600	-0.59414500
O	3.40945100	0.68878600	1.05130300	H	5.65164400	-0.64334000	1.35955800

H	7.33392700	0.13840400	2.65700300	O	1.70931400	2.29484600	-0.34808400
H	5.54194400	1.60520800	2.22876100	H	-3.55663900	1.73370500	0.42458800
H	3.04875200	2.32785000	-0.59263000	H	-4.69276000	0.06191100	1.61136400
H	6.60251900	2.64400600	-0.45644800	C	-8.73526100	-1.83834100	0.03913400
H	6.09625900	3.60673900	0.92996600	H	-4.61893000	-1.63022600	-0.90193600
H	7.52936200	2.57258300	1.05184700	C	0.31150000	0.47586400	2.61424600
H	7.43973000	0.49032700	-0.83468000	C	6.84699200	-2.07154800	0.11493500
H	5.78198600	-0.02981900	-1.08231100	C	8.09722300	-2.36250000	0.94961000
B3LYP Energy = -2081.90371954 a.u.				C	6.85463200	0.46986100	-0.18655700
(2R, 3R, 5S, 13R, 16S, 17R, 18S, 21S, 22S, 26S, 27S)-a4-2,Conf O				O	6.60006700	0.43590900	-1.59462600
C	-0.16166900	-2.16449400	-1.32874900	C	6.43888900	1.81432700	0.45459400
C	-1.34748700	-1.67731700	-0.92015800	C	4.93280000	1.95418200	0.56597900
C	2.22960000	-2.70670500	-1.05756000	O	4.34413900	2.21171300	1.59497800
C	1.03562700	-2.34394600	-0.53691500	O	4.30899300	1.77470100	-0.60896900
C	4.67446400	-3.11160900	-0.72389100	C	7.03312100	3.01744600	-0.29337800
C	5.03277100	-3.18289400	-2.18326500	C	6.20916600	-0.73047300	0.50934200
C	3.42452300	-2.88522500	-0.26672800	H	-0.08193500	-2.46689400	-2.37091500
C	5.83019800	-3.23008400	0.23515200	H	-2.16437600	-1.63008200	-1.62762600
O	-6.22328700	-3.39346300	-0.13417500	H	2.29411900	-2.85731700	-2.13146600
C	-7.35862500	-1.21855200	-0.20693900	H	0.97771600	-2.18459400	0.53585100
C	-7.26153200	0.19814000	0.36219500	H	5.76583500	-3.97544400	-2.36134000
C	-5.91414900	0.81984100	0.01668400	H	4.17314500	-3.36163200	-2.82783100
C	-4.71396200	-0.01029700	0.51826900	H	5.49852700	-2.24324100	-2.50114500
C	-4.82199300	-1.50772700	0.16655500	H	3.28987800	-2.80505000	0.81028100
C	-6.23905800	-2.06311300	0.40310100	H	5.46072600	-3.27642600	1.26506900
C	-3.44628800	0.72218400	0.02336100	H	6.36076900	-4.17080900	0.04015600
C	-2.05032600	0.29089900	0.42448800	H	-6.95605500	-3.88137900	0.25361100
C	-1.65372800	-1.18105900	0.48217000	H	-7.18320400	-1.17044900	-1.28960500
C	-2.55901700	-2.19370400	1.17225400	H	-8.07000300	0.81835300	-0.03552700
C	-3.86896000	-2.34625500	0.98328200	H	-7.39681000	0.16354900	1.45076700
C	-3.37226800	0.87231600	-1.49176300	H	-5.85665500	0.92203600	-1.07230700
O	-2.81630500	2.06073300	-1.88018800	H	-5.84126700	1.83008100	0.43079000
C	-3.04204600	3.22806700	-1.11895600	H	-6.41019300	-2.11236000	1.48981600
C	-2.03371000	3.56136800	-0.11480900	H	-0.72229700	-1.21486500	1.03094200
C	-1.15987700	2.69895000	0.48670700	H	-4.33486800	-3.18910600	1.48455000
C	-1.07774000	1.23242800	0.59640300	H	0.38993100	4.22274500	0.75557100
C	0.06875300	3.27196000	1.17523900	H	-0.11148700	3.41933900	2.24539900
C	1.11796500	2.18434200	0.96379200	H	1.96298900	2.25764300	1.64320100
C	0.32617800	0.88486700	1.12931300	H	0.80164200	0.10478300	0.53365900
C	-1.79172500	-3.16691300	2.03241900	H	-2.44419000	-3.93684800	2.44665400
C	-1.97448400	5.04386300	0.19028700	H	-1.00549200	-3.66055200	1.45033100
O	-3.96923400	3.92321700	-1.44700000	H	-1.29453800	-2.65409500	2.86325000
O	-3.63618400	0.04595100	-2.31966900	H	-1.26405500	5.55369500	-0.46991800
				H	-2.95317700	5.48970700	0.02251700

H	-1.67573600	5.23309500	1.22011900
H	1.06285300	2.06722500	-1.02751900
H	-8.82240100	-2.82469600	-0.42270400
H	-8.92877900	-1.94371000	1.11213900
H	-9.52235300	-1.20783800	-0.38209400
H	1.32252000	0.22397900	2.94240800
H	-0.05667200	1.29263200	3.23903600
H	-0.33120300	-0.38436500	2.79720700
H	7.14625500	-1.99711500	-0.93453100
H	8.81818400	-1.54282000	0.88749800
H	7.83496900	-2.49655400	2.00430700
H	8.59682900	-3.27275500	0.60703100
H	7.94321000	0.40797800	-0.09953000
H	5.66045600	0.63535400	-1.70756300
H	6.80806700	1.81297300	1.48221900
H	3.32875800	1.91979800	-0.50516100
H	6.75524800	3.95548600	0.19214400
H	8.12324100	2.94510300	-0.29875300
H	6.68636900	3.04004600	-1.32619200
H	5.14652200	-0.73342200	0.24692900
H	6.26432800	-0.60432600	1.59708100

B3LYP Energy = -2081.90978620 a.u.