

Investigation of the thermal deconstruction of β - β' and 4-O-5 linkages in lignin model oligomers by density functional theory (DFT)

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Supporting Information

S.1.Optimized geometries of the initial stereoisomers of MC1

RRRSSRRR			H 5.70262269	1.43698305	-0.93965458
O 1.81714707	4.75311763	-0.83164502	H 6.54186447	0.26538051	0.09460078
C 2.86768026	4.16621231	-0.19099402	O 5.96391264	-0.38001978	-1.78668221
C 5.13923862	3.23738791	1.09943302	H 5.59540852	-1.25815709	-1.63809541
C 3.96153308	5.02610689	0.01132056	O 4.55735491	-1.33404827	0.51272878
C 2.91855949	2.85208212	0.24506845	C 3.48449406	-2.16729491	0.38645025
C 4.06888201	2.38097281	0.88932897	C 1.29479930	-3.90339947	0.15959529
C 5.08959316	4.55990981	0.65900090	C 3.08588004	-2.65096183	-0.86945143
H 6.02742481	2.87639841	1.60675288	C 2.81060435	-2.62220479	1.51777429
H 2.07646289	2.18227214	0.10996788	C 1.72631029	-3.48286759	1.41180416
H 5.91576147	5.24183334	0.81710906	C 1.99147705	-3.50770413	-0.98074654
C 0.63722544	3.98078479	-0.96768191	H 1.21917004	-3.78531942	2.32183330
H-0.08829029	4.60638873	-1.48416352	H 1.67411165	-3.88081057	-1.94497233
H 0.25364721	3.69799059	0.01636398	O 3.82523826	-2.21554997	-1.91389587
H 0.82160484	3.07640180	-1.55421387	O 3.16772907	-2.14410187	2.75730034
O 3.90027738	6.30961942	-0.41958165	C 3.37017004	-2.49351197	-3.23186913
H 3.03773421	6.44318545	-0.83112714	H 4.06042101	-1.97335857	-3.89201140
C 4.14693337	0.92823331	1.28373870	H 2.35749767	-2.10815750	-3.37363428
H 4.98542268	0.79290542	1.98065069	H 3.40226547	-3.56739541	-3.43345011
C 4.42001620	0.04009411	0.06004220	C 4.39949749	-2.67610592	3.25856467
H 3.57654267	0.10209820	-0.63756878	H 4.56169051	-2.21137987	4.22908269
C 5.72711598	0.39066358	-0.63404214	H 4.31082900	-3.75880643	3.37654641

H 5.22078775 -2.43524154 2.58187862
C 0.04893148 -4.76577052 0.04068534
C-1.17871821 -4.04640922 0.60365263
C-1.70054484 -3.23912436 -0.59787008
C-1.11295668 -3.98647937 -1.81096645
O-0.29363704 -5.04545089 -1.30339752
H 0.22233563 -5.72978705 0.52932576
H-0.94963918 -3.40867175 1.45812101
H-1.35054642 -2.20824190 -0.57894522
H-0.51257103 -3.30815150 -2.42443400
H-1.87821009 -4.44738017 -2.43896502
C-3.24538100 -3.28807396 -0.43203379
O-3.50436982 -4.12850352 0.68501508
C-2.37216267 -4.95216975 0.89825439
H-3.70740560 -3.72486254 -1.32657650
H-2.37707693 -5.80711784 0.20811329
H-2.41234674 -5.31874915 1.92417853
C-3.81295239 -1.90950071 -0.19692880
C-4.54846550 0.73991471 0.18426744
C-4.07991282 -1.10515663 -1.30121889
C-3.94845932 -1.41976932 1.09680187
C-4.32916323 -0.09076322 1.28422710
C-4.45072621 0.22373045 -1.10863943
H-3.97229825 -1.51379302 -2.29797790
H-3.76881595 -2.08467486 1.92980266
O-4.71463624 1.10406439 -2.10914541
O-4.48732098 0.50520499 2.49376968
C-4.32587071 -0.29682126 3.64826536
H-4.52447298 0.35637726 4.49462685
H-3.30563043 -0.68668142 3.71829339
H-5.03430207 -1.12973548 3.64830699
C-4.56867903 0.64269092 -3.44046166

H-4.78843448 1.49550194 -4.07941202
H-5.27698419 -0.16335199 -3.65096538
H-3.54598235 0.29969657 -3.62180851
O-4.87582478 2.05727694 0.35797114
O 2.93044791 0.55886419 1.90456866
H 3.05094250 -0.30197112 2.32948677
C-3.80973220 2.91068151 0.81474949
H-3.27226744 2.40491151 1.62050779
C-4.51563458 4.11995954 1.39959190
H-3.77585034 4.84361387 1.74820848
H-5.12447022 4.59036046 0.62006577
O-5.29482955 3.74918030 2.51564959
H-5.77938107 2.95414060 2.26639622
C-2.87331588 3.27262682 -0.34714223
H-2.24408767 4.10065188 0.00383891
O-3.62049821 3.78956968 -1.42299373
H-4.27085091 3.11012584 -1.65680943
C-1.94976483 2.13373121 -0.78548754
C-0.22684968 0.08637128 -1.62060595
C-1.29700627 1.32809834 0.15969933
C-1.70978111 1.91184775 -2.13417224
C-0.85310930 0.89059749 -2.55309495
C-0.45121863 0.30968128 -0.25016362
H-1.45510250 1.48800421 1.21846401
H-2.19544717 2.54439516 -2.86646000
H-0.65814096 0.71493844 -3.60472356
O 0.20649840 -0.56044083 0.56477797
O 0.59786986 -0.92166336 -2.00886267
H 0.94219893 -1.35855026 -1.21403367
C 0.04649179 -0.38709149 1.96271707
H 0.64926765 -1.16008192 2.43492899
H 0.41676449 0.59305075 2.27183190

H-1.00721528 -0.51132135 2.23732622

RRRSSRSS

O-0.10291281 -2.86870208 0.12065349

C-1.29568747 -2.40743016 -0.36426268

C-3.56794313 -1.38537694 -1.57601710

C-1.17217295 -1.52460969 -1.44404166

C-2.54958524 -2.74168144 0.12487766

C-3.70214410 -2.22237786 -0.47267884

C-2.30991984 -1.02369305 -2.04907380

H-4.43835782 -0.97110202 -2.06938690

H-2.65936859 -3.40208563 0.97505549

H-2.19873986 -0.34874834 -2.88979883

C-0.13467659 -3.71758015 1.25322982

H-0.67389608 -4.64203264 1.03009812

H 0.90260698 -3.94265622 1.49246611

H-0.60242949 -3.21500861 2.10484728

O 0.05580544 -1.16819636 -1.91432718

H 0.73542085 -1.48065908 -1.30174109

C-5.06417601 -2.60717885 0.10972085

H-5.46133517 -3.44610237 -0.47340703

C-6.10328871 -1.48118592 0.04478244

H-6.14043675 -1.02466484 -0.94618361

C-7.50046937 -1.95252235 0.40360421

H-7.80340922 -2.75111537 -0.27678701

H-7.49413126 -2.34699250 1.42529100

O-8.43318142 -0.90387663 0.25752888

H-8.04455571 -0.12628219 0.67359677

O-5.80894763 -0.46465645 1.02169998

C-4.79316777 0.40468098 0.72453356

C-2.70124215 2.14945295 0.14845231

C-4.94409615 1.37844682 -0.26325631

C-3.59523774 0.32301523 1.43575794

C-2.54573237 1.19314833 1.15101416

C-3.89454590 2.24821964 -0.55918243

H-1.62528877 1.15032817 1.71876756

H-3.99081119 3.01863883 -1.31183561

O-6.14740728 1.37582105 -0.89394560

O-3.54008871 -0.65824764 2.37781455

C-6.36444383 2.35021167 -1.89661148

H-7.37548898 2.18308344 -2.26051930

H-5.65277859 2.23252395 -2.71950748

H-6.28224429 3.36052183 -1.48636205

C-2.31159414 -0.82965754 3.06120281

H-2.45276034 -1.68116991 3.72461988

H-1.50131076 -1.03764809 2.35549250

H-2.05749863 0.05765201 3.64654931

C-1.59803076 3.16957031 -0.09299297

C-0.19287713 2.56866338 -0.21288964

C-0.03624317 2.30063578 -1.72813703

C-1.18372781 3.12113139 -2.35012604

O-1.77124284 3.88590200 -1.30260650

H-1.64460438 3.90939598 0.71177345

H-0.06770663 1.66826427 0.38016186

H-0.12375645 1.24179111 -1.96810442

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H-0.84486921 3.82527583 -3.11158192

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O 1.51838315 3.94387851 -1.15018547

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H 1.43836940 3.24833750 -3.04841329

H 0.53791621 4.51088280 0.53679789

H 1.66432493 3.14781051 0.76457796

C 2.46041786 1.80397911 -1.83126147
C 4.40054008 -0.14037123 -1.38747490
C 2.41101033 0.60530511 -2.54013424
C 3.50515813 2.05985131 -0.95008862
C 4.47237533 1.08281341 -0.72554456
C 3.38857223 -0.36319743 -2.32542048
H 1.60078912 0.41709645 -3.23199102
H 3.54711837 3.01998378 -0.45717876
O 3.43312167 -1.57285566 -2.94258419
O 5.51431497 1.22120876 0.14148543
C 5.58014806 2.42398697 0.88382444
H 6.43419590 2.31902539 1.55112795
H 5.73610336 3.28226838 0.22468212
H 4.66534688 2.57173114 1.46779859
C 2.57535997 -1.77838169 -4.05610688
H 2.83591884 -2.75785627 -4.45056320
H 1.52580614 -1.76861611 -3.75408149
H 2.75079289 -1.01430636 -4.81897250
O 5.34241242 -1.10215589 -1.13630078
O-4.95198192 -3.08141758 1.43387217
H-4.72161510 -2.31397221 1.97968062
C 4.89460223 -2.24267469 -0.38142004
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C 5.88701180 -3.33832329 -0.72326466

SSRSSRRR

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C-2.31623324 -3.96672278 0.34474984
C-4.42257771 -3.30851227 -1.33137756
C-2.90251294 -4.95559631 -0.46440718
C-2.77894233 -2.66188803 0.30072222
C-3.84872168 -2.32255615 -0.53974890
C-3.95107336 -4.62090007 -1.30100220

H 5.64731901 -4.24088391 -0.15682263
H 6.89359742 -3.00773201 -0.44444599
O 5.80926609 -3.67021419 -2.09179690
H 5.74229812 -2.84048203 -2.57837808
C 4.86472248 -1.90967186 1.11748922
H 4.78688043 -2.86057988 1.65733254
O 6.09610291 -1.34693635 1.50781913
H 6.24725742 -0.58816798 0.92374921
C 3.67735041 -1.03628914 1.53107071
C 1.53788198 0.57768518 2.34632611
C 3.87986192 -0.01508512 2.46342821
C 2.39425863 -1.24782480 1.03665307
C 1.32833380 -0.44089085 1.43363445
C 2.82282082 0.78812419 2.86241848
H 4.87605375 0.13624289 2.85778648
H 2.19706921 -2.05213309 0.33767204
H 0.32958479 -0.60098921 1.04001228
O 2.90297373 1.82164355 3.75553036
O 0.50016539 1.35990382 2.75948932
H 0.84319803 1.99025644 3.40594989
C 4.09752047 1.94246884 4.50854079
H 4.94352914 2.19777378 3.86492607
H 4.31291007 1.01196729 5.04052766
H 3.92815024 2.74671349 5.22051747

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H-2.29737692 -1.90910302 0.91157653
H-4.39383485 -5.39668463 -1.91336210
C-0.76927057 -3.53866353 2.09913127
H-1.55815242 -3.24023025 2.79658900
H-0.32432306 -2.65660648 1.63533329
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O-2.43255190 -6.22516152 -0.42699171
H-1.71594365 -6.25819355 0.21914405
C-4.36945221 -0.90486727 -0.61434672
H-5.38860981 -0.93209520 -1.02083290
C-4.42814133 -0.22564709 0.75834204
H-3.45384483 -0.27546786 1.24871042
C-5.49563152 -0.84144750 1.64574304
H-5.38004354 -1.92705576 1.65915276
H-6.47513252 -0.60275135 1.20910445
O-5.41395782 -0.39213320 2.97820618
H-5.16586945 0.53953377 2.95293848
O-4.78073350 1.16616079 0.59711668
C-3.74268346 2.05880745 0.57920163
C-1.57502718 3.81329407 0.50055875
C-2.96067049 2.27429411 1.72042433
C-3.47034336 2.79544199 -0.57146359
C-2.39439483 3.68131695 -0.60982087
C-1.86649762 3.12891613 1.67831666
H-2.18110300 4.26627454 -1.49195047
H-1.23905603 3.26639671 2.55089972
O-3.35015999 1.57662149 2.81951726
O-4.28252543 2.54291948 -1.64129568
C-2.48890158 1.55644248 3.94205271
H-1.49748835 1.18911542 3.66054828
H-2.40279631 2.55030354 4.39002266
H-2.94530877 0.87165069 4.65368278
C-4.07441891 3.30526562 -2.81891943
H-3.08309898 3.11380185 -3.24002426
H-4.18970692 4.37225493 -2.61397701
H-4.83926931 2.98316985 -3.52165924
C-0.32247777 4.66679669 0.43207144
C 0.94662050 3.80349821 0.43346851

C 1.14031523 3.47365689 -1.05674731
C 0.46985831 4.66987570 -1.75853321
O-0.23801384 5.41524462 -0.76694621
H-0.32542466 5.38510279 1.25761112
H 0.83490865 2.90496824 1.03823665
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H 1.20773296 5.34168957 -2.20329047
C 2.66448136 3.47759702 -1.21867125
O 3.10611101 4.49547138 -0.33789567
C 2.22827048 4.58156125 0.78441230
H 2.95693177 3.78906150 -2.22637404
H 2.02870532 5.64117410 0.95990931
H 2.71581157 4.16094642 1.66989845
C 3.30161936 2.12997273 -0.93018197
C 4.47397660 -0.34685944 -0.46366294
C 4.18351566 1.98024408 0.13199129
C 3.02094336 1.06113980 -1.78117326
C 3.62360471 -0.17345077 -1.55905086
C 4.77086309 0.73478902 0.36277837
H 4.42868620 2.84105301 0.73763881
H 2.34450872 1.20398111 -2.61465327
O 5.63955122 0.46271371 1.37153223
O 3.44371718 -1.27358019 -2.33488955
C 2.55395614 -1.16045888 -3.43070655
H 2.52579893 -2.14434745 -3.89562834
H 2.92204068 -0.42759612 -4.15451722
H 1.55007044 -0.88119368 -3.09537488
C 5.98029988 1.51813353 2.25004118
H 6.47085777 2.33399930 1.71194787
H 6.66845864 1.09085591 2.97566031
H 5.09392707 1.90097265 2.76508610

O 5.03541921 -1.57293628 -0.22988866
O-3.54408588 -0.16618006 -1.51195307
H-3.98153131 0.68178700 -1.68578029
C 4.52624309 -2.29775864 0.90776286
H 4.36502720 -1.59923189 1.73184092
C 5.64988917 -3.24000302 1.29492220
H 5.32604180 -3.87804404 2.12012561
H 5.89477049 -3.87593460 0.43745012
O 6.77502028 -2.51532417 1.74297377
H 6.88757390 -1.77065065 1.14072990
C 3.23047441 -3.02575339 0.52709783
H 3.01366421 -3.74681239 1.32404855
O 3.44498283 -3.79414666 -0.63582057
H 3.76615847 -3.17890749 -1.31196162
C 2.03338363 -2.08478626 0.37793763

SSRSSRSS

O-3.85358031 3.85960224 0.68167508
C-3.39017848 2.82309933 -0.08366332
C-2.21000506 0.76417547 -1.51032869
C-2.02527369 2.55914953 0.07967198
C-4.15349261 2.05868930 -0.94907504
C-3.57262247 1.00456763 -1.65933056
C-1.43583855 1.53463602 -0.64260822
H-1.72551850 -0.03708834 -2.05627039
H-5.21113538 2.24700629 -1.07591566
H-0.37490667 1.34014981 -0.51597546
C-5.16468957 4.32820561 0.41848558
H-5.30984114 5.19901398 1.05339284
H-5.26896439 4.61102972 -0.63238554
H-5.90963164 3.56729348 0.66632069
O-1.29230227 3.32307929 0.94055364
H-1.88387770 3.98565440 1.32015219

C-0.13838705 -0.34487124 -0.01591123
C 1.13987449 -2.29357422 -0.67781803
C 1.80609925 -1.02098139 1.24624048
C 0.72656452 -0.15963674 1.05179793
C 0.07866612 -1.42575871 -0.88743165
H 1.30959480 -3.12504977 -1.34974192
H 2.46941437 -0.83498010 2.08259911
H 0.53699786 0.66694214 1.72736698
O-0.80927254 -1.49819505 -1.91409285
O-1.17853711 0.49494121 -0.19972551
H-1.81257065 0.13692625 -0.85522336
C-0.90497041 -2.71795987 -2.62699173
H-0.98131951 -3.56394316 -1.93945575
H-1.81451790 -2.64727583 -3.22005948
H-0.04030309 -2.85792585 -3.28384777

C-4.46672438 0.16946740 -2.57916930
H-4.30609408 0.50364194 -3.61032319
C-4.16401862 -1.33301412 -2.52917501
H-3.09070867 -1.52723259 -2.58859898
C-4.85250576 -2.11688214 -3.63052563
H-4.56624455 -1.71151474 -4.60359345
H-5.93727962 -2.01589735 -3.51556445
O-4.45176138 -3.46929106 -3.60475089
H-4.41187441 -3.73438060 -2.67823696
O-4.67839766 -1.89223606 -1.30509860
C-3.87175400 -1.76471161 -0.20556442
C-2.20960332 -1.46057016 2.00085200
C-4.22906322 -0.89594142 0.82237488
C-2.70627593 -2.52837635 -0.09803773
C-1.86398616 -2.36686639 0.99730092
C-3.39540937 -0.74022670 1.93217227

<u>H-0.94742039</u>	<u>-2.93753165</u>	<u>1.07901038</u>	<u>C 2.70632230</u>	<u>2.52843457</u>	<u>-0.09811889</u>
<u>H-3.65417052</u>	<u>-0.08045051</u>	<u>2.74809144</u>	<u>C 4.22903871</u>	<u>0.89594544</u>	<u>0.82231185</u>
<u>O-5.40510622</u>	<u>-0.23386110</u>	<u>0.64431025</u>	<u>H 3.65412803</u>	<u>0.08051668</u>	<u>2.74804356</u>
<u>O-2.48562639</u>	<u>-3.38180400</u>	<u>-1.13062307</u>	<u>H 0.94750078</u>	<u>2.93770671</u>	<u>1.07894340</u>
<u>C-5.78238150</u>	<u>0.69372912</u>	<u>1.64322843</u>	<u>O 5.40504568</u>	<u>0.23380245</u>	<u>0.64425559</u>
<u>H-5.02553712</u>	<u>1.47751893</u>	<u>1.75624257</u>	<u>O 2.48571302</u>	<u>3.38187116</u>	<u>-1.13070518</u>
<u>H-6.72128969</u>	<u>1.13087025</u>	<u>1.30703421</u>	<u>C 1.33618866</u>	<u>4.21006804</u>	<u>-1.06633726</u>
<u>H-5.93816959</u>	<u>0.19347340</u>	<u>2.60302654</u>	<u>H 0.41926294</u>	<u>3.61562456</u>	<u>-1.05390697</u>
<u>C-1.33604377</u>	<u>-4.20992000</u>	<u>-1.06626766</u>	<u>H 1.36487882</u>	<u>4.84609543</u>	<u>-0.17711544</u>
<u>H-1.36492064</u>	<u>-4.82481114</u>	<u>-1.96286498</u>	<u>H 1.36508542</u>	<u>4.82493672</u>	<u>-1.96294907</u>
<u>H-1.36466687</u>	<u>-4.84593013</u>	<u>-0.17703191</u>	<u>C 5.78230414</u>	<u>-0.69373751</u>	<u>1.64322799</u>
<u>H-0.41915895</u>	<u>-3.61541113</u>	<u>-1.05387742</u>	<u>H 5.02543128</u>	<u>-1.47749068</u>	<u>1.75630533</u>
<u>C-1.26382317</u>	<u>-1.28769529</u>	<u>3.17932222</u>	<u>H 5.93812699</u>	<u>-0.19342387</u>	<u>2.60298980</u>
<u>C 0.10321162</u>	<u>-0.76126098</u>	<u>2.73433990</u>	<u>H 6.72118904</u>	<u>-1.13093628</u>	<u>1.30704416</u>
<u>C-0.10320678</u>	<u>0.76143481</u>	<u>2.73430863</u>	<u>O 4.67839316</u>	<u>1.89216211</u>	<u>-1.30519887</u>
<u>C-1.23163060</u>	<u>0.96319193</u>	<u>3.75985490</u>	<u>O-5.83516857</u>	<u>0.38361984</u>	<u>-2.31284428</u>
<u>O-1.72366251</u>	<u>-0.33047782</u>	<u>4.11728321</u>	<u>H-6.01803138</u>	<u>-0.05477080</u>	<u>-1.46798751</u>
<u>H-1.18114078</u>	<u>-2.23962920</u>	<u>3.71244577</u>	<u>C 4.16400043</u>	<u>1.33286301</u>	<u>-2.52923651</u>
<u>H 0.39385148</u>	<u>-1.13889840</u>	<u>1.75851617</u>	<u>H 3.09069003</u>	<u>1.52707688</u>	<u>-2.58866346</u>
<u>H-0.39383953</u>	<u>1.13903371</u>	<u>1.75846706</u>	<u>C 4.85247238</u>	<u>2.11666986</u>	<u>-3.63064286</u>
<u>H-2.04055145</u>	<u>1.56455745</u>	<u>3.33015362</u>	<u>H 4.56620147</u>	<u>1.71124422</u>	<u>-4.60368322</u>
<u>H-0.87856406</u>	<u>1.44086370</u>	<u>4.67666583</u>	<u>H 5.93724813</u>	<u>2.01569798</u>	<u>-3.51568661</u>
<u>C 1.26383193</u>	<u>1.28788264</u>	<u>3.17927068</u>	<u>O 4.45172070</u>	<u>3.46907842</u>	<u>-3.60494427</u>
<u>O 1.72365603</u>	<u>0.33070916</u>	<u>4.11728283</u>	<u>H 4.41183690</u>	<u>3.73422069</u>	<u>-2.67844524</u>
<u>C 1.23163966</u>	<u>-0.96297771</u>	<u>3.75989200</u>	<u>C 4.46671560</u>	<u>-0.16961943</u>	<u>-2.57915278</u>
<u>H 1.18116355</u>	<u>2.23984661</u>	<u>3.71234225</u>	<u>H 4.30610736</u>	<u>-0.50384196</u>	<u>-3.61029458</u>
<u>H 0.87858750</u>	<u>-1.44062745</u>	<u>4.67671932</u>	<u>O 5.83516101</u>	<u>-0.38374680</u>	<u>-2.31280230</u>
<u>H 2.04056231</u>	<u>-1.56434583</u>	<u>3.33019877</u>	<u>H 6.01800677</u>	<u>0.05466958</u>	<u>-1.46795532</u>
<u>C 2.20961445</u>	<u>1.46069128</u>	<u>2.00079338</u>	<u>C 3.57260930</u>	<u>-1.00468201</u>	<u>-1.65928362</u>
<u>C 3.87175859</u>	<u>1.76470522</u>	<u>-0.20564681</u>	<u>C 2.02527194</u>	<u>-2.55916346</u>	<u>0.07982104</u>
<u>C 3.39538606</u>	<u>0.74029048</u>	<u>1.93211572</u>	<u>C 4.15347921</u>	<u>-2.05877076</u>	<u>-0.94898127</u>
<u>C 1.86403438</u>	<u>2.36699006</u>	<u>0.99723290</u>	<u>C 2.20999117</u>	<u>-0.76428094</u>	<u>-1.51028566</u>

C 1.43583245 -1.53469063 -0.64251568
C 3.39017097 -2.82313079 -0.08351768
H 5.21111993 -2.24710031 -1.07581886
H 1.72550104 0.03695008 -2.05627169
H 0.37490032 -1.34019906 -0.51588680
O 3.85357954 -3.85959362 0.68187169

O 1.29230837 -3.32303088 0.94076347
H 1.88388172 -3.98559188 1.32038965
C 5.16467314 -4.32823559 0.41867097
H 5.90963683 -3.56732820 0.66645791
H 5.30982204 -5.19901979 1.05361198
H 5.26891881 -4.61110470 -0.63219072

S.2.Optimized geometries of the initial stereoisomers of MC2

RSSRRSSR

C 1.88429498 4.02396804 -1.21780430
C 2.29284171 2.13306786 0.78668251
C 0.84277555 3.70341490 -0.34742435
C 3.09492240 3.34860292 -1.13857644
C 3.29194733 2.38251461 -0.16221359
C 1.06674181 2.77771029 0.66313307
H 3.89623043 3.53582834 -1.84309569
H 0.28361238 2.54177330 1.37311489
O 4.48644479 1.68258021 -0.16205294
C 4.41533988 0.30726543 -0.30634060
C 4.43990135 -2.44951590 -0.33730811
C 5.59423216 -0.36079738 0.01843531
C 3.27133813 -0.37793636 -0.67860661
C 3.26555323 -1.76774357 -0.64618559
C 5.60673445 -1.75797071 -0.02788811
H 4.47388999 -3.53362110 -0.30528913
H 2.38059426 0.16621997 -0.95868254
C 1.94805197 -2.51281362 -0.79394358
O 0.90969861 -1.67036993 -1.26300094
C 0.29002840 -1.01116113 -0.14513584
C 0.79716530 -1.70085361 1.13226049
C 1.45985497 -2.97410579 0.58872087

H 2.04881096 -3.33923487 -1.50402154
H 0.51136193 0.05868266 -0.16360571
H -0.78749510 -1.13812875 -0.25215532
C 0.28722950 -3.98107137 0.57940483
O -0.83411374 -3.34436289 1.19085416
C -0.36469087 -2.24255023 1.95956299
H 0.54462777 -4.88693936 1.13750784
H -0.00995044 -4.26437688 -0.43317919
H 0.00725556 -2.60811818 2.92878407
H 1.48139959 -1.06740698 1.69487566
H 2.28325479 -3.32265501 1.21149305
H 1.73843216 4.77530320 -1.98727015
C -0.52099803 4.32968083 -0.53367662
O -1.31191068 4.08477017 0.62367071
C -2.64596040 3.78170976 0.24319767
C -2.50290741 3.04729079 -1.07860706
C -1.33813558 3.78545790 -1.75769005
H -0.39300919 5.41232108 -0.65430440
H -3.09857261 3.18710708 1.03937277
H -3.22656509 4.70394803 0.11288469
H -3.41459190 3.06634888 -1.67719978
H -1.68092252 4.61388649 -2.37892385

C	-0.71156288	2.67277963	-2.58483029	O	6.69953600	0.32316026	0.41898818
O	-0.78326759	1.52533720	-1.75743032	O	2.42077561	1.21923572	1.79000584
C	-1.95346931	1.60671027	-0.94049045	O	-3.06718131	-2.84938915	-2.79120527
H	0.33323181	2.82456904	-2.85324826	O	-5.54200956	-2.66766511	-1.86595686
H	-1.29794455	2.52577650	-3.50162993	O	-5.14424118	-0.87355208	2.04764214
H	-1.61641651	1.44183303	0.09127718	O	-4.45922642	1.60904603	2.60787849
C	-2.94889308	0.52107644	-1.28553097	C	-5.56200580	-2.19756285	1.75779480
C	-4.70256876	-1.60963946	-1.69691972	H	-5.24677564	-2.87943170	2.55272215
C	-4.25783293	0.58599931	-0.82385508	H	-5.16325824	-2.53224440	0.79722568
C	-2.51877682	-0.61115388	-1.98295139	H	-6.64823508	-2.16810964	1.70748176
C	-3.38417168	-1.67651443	-2.17057458	C	-1.70802732	-3.03391377	-3.15663370
C	-5.13758383	-0.47316780	-1.03971254	H	-1.04805551	-2.89351087	-2.29553213
H	-4.59910625	1.45314497	-0.26664297	H	-1.63219021	-4.05204607	-3.53207608
H	-1.49840425	-0.64724729	-2.34218002	H	-1.42069766	-2.33050133	-3.94311451
H	-6.15810253	-0.44075592	-0.67726352	C	7.83246745	-2.28314001	-0.56484115
C	-1.47007095	-1.23642609	2.17883736	H	7.55990799	-2.60178027	-1.57557624
C	-3.47543065	0.67414595	2.49685651	H	8.62898833	-2.91947102	-0.18404165
C	-2.80803747	-1.59888684	1.99835466	H	8.16496635	-1.24416883	-0.57825925
C	-1.14958338	0.06971793	2.53310347	C	3.60914772	1.26583265	2.58064896
C	-2.15213589	1.02713456	2.68981992	H	3.31787508	0.98012576	3.59064243
C	-3.80507682	-0.65088846	2.17139943	H	4.02288983	2.27653740	2.59309672
H	-3.04146592	-2.61352338	1.70517730	H	4.35439561	0.56127131	2.20633907
H	-0.11158487	0.36108810	2.66216826	H	6.48770535	1.26439332	0.39692251
H	-1.91542121	2.05432844	2.94565553	H	-5.30403945	1.15876208	2.48261988
O	6.72720832	-2.45686878	0.31765854	H	-5.05621909	-3.35295111	-2.34131621

S.3.Optimized geometries of the radical species produced from the RRRSSRRR stereoisomer of MC1

β - β' Cleavage

O	1.49946136	4.90709098	-0.86300285	C	4.84237974	3.54129002	1.14238293
C	2.56091653	4.36733216	-0.19926890	C	3.61581228	5.27175007	0.01498296

C 2.65574601	3.05990445	0.24955906	C 2.27196504	-3.53527819	-1.03063601
C 3.81139772	2.64086235	0.91967062	H 1.10593286	-3.70748722	2.16001051
C 4.74907648	4.85664444	0.68792042	H 2.13338982	-3.99277809	-2.00165801
H 5.73352315	3.22100237	1.67144723	O 4.01678161	-2.06124694	-1.84081401
H 1.84306309	2.35589828	0.10725287	O 2.86053994	-1.90572460	2.73244232
H 5.54421867	5.57241281	0.85525471	C 3.65206236	-2.32682621	-3.18921647
C 0.35300084	4.08759269	-1.01181581	H 4.31463199	-1.71324577	-3.79548899
H -0.38363960	4.67734983	-1.55394145	H 2.61253697	-2.03596428	-3.36193363
H -0.04160104	3.80484810	-0.03206466	H 3.79999631	-3.38212262	-3.43206556
H 0.58506770	3.18270054	-1.57988538	C 4.04081331	-2.37111838	3.39734141
O 3.51122678	6.54825783	-0.42874829	H 4.07059899	-1.86494861	4.36023818
H 2.65166319	6.64283651	-0.85703832	H 3.97673270	-3.45156757	3.54738277
C 3.93314760	1.19768790	1.33989740	H 4.92777680	-2.12239439	2.81207745
H 4.75645070	1.10638078	2.06242479	C 0.49471628	-5.10941825	-0.20072559
C 4.28114914	0.29819364	0.14177467	C -0.49423768	-5.32908234	0.91001038
H 3.47082597	0.32404352	-0.59640636	C -1.33113793	-3.01885310	-0.85456009
C 5.61220228	0.68722184	-0.48553847	C -0.67564386	-3.81142568	-1.92492056
H 5.56955991	1.73289565	-0.79083594	O -0.10916045	-5.06365531	-1.48368796
H 6.38829363	0.58798809	0.28796605	H 1.111105643	-6.01914980	-0.25459827
O 5.94201031	-0.06783023	-1.62448734	H -0.08780577	-5.57190284	1.88429843
H 5.61895739	-0.96588131	-1.49102665	H -0.75099280	-2.31217023	-0.27177521
O 4.43440414	-1.06431620	0.62992498	H 0.09696318	-3.20662830	-2.40581226
C 3.43949560	-1.97253033	0.41609438	H -1.40309459	-4.11041211	-2.68455491
C 1.48836271	-3.96937401	0.04259970	C -2.69052792	-3.35618595	-0.32476270
C 3.22720200	-2.54054400	-0.85357865	O -2.61857752	-4.09660099	0.88519716
C 2.67794716	-2.44702094	1.47976284	C -1.97637868	-5.37070727	0.73292438
C 1.69523696	-3.41699664	1.29978168	H -3.23404703	-3.95600049	-1.07088989

H -2.23229028	-5.78763988	-0.24839362	C -4.85695391	3.90050299	1.23523069
H -2.41932097	-6.00279796	1.50267643	H -4.19295420	4.71657764	1.52761585
C -3.44069596	-2.06423744	-0.08676604	H -5.51355369	4.25399728	0.43317708
C -4.53701383	0.46494023	0.22248018	O -5.58993863	3.52795035	2.38161495
C -3.83787126	-1.34366770	-1.21152309	H -6.00096256	2.67864733	2.18520703
C -3.62575939	-1.55911151	1.19258045	C -3.15271837	3.11196071	-0.47590804
C -4.18425149	-0.28691381	1.34314513	H -2.60703677	4.01826018	-0.18248488
C -4.39374889	-0.07996918	-1.05546107	O -3.95959307	3.49076264	-1.56649467
H -3.67150356	-1.76210254	-2.19607297	H -4.53245427	2.73312551	-1.75878284
H -3.32419046	-2.15645818	2.04123313	C -2.11713884	2.05418070	-0.86869385
O -4.78756881	0.72053059	-2.08103401	C -0.16251152	0.18555765	-1.62217768
O -4.38220635	0.33090089	2.53635530	C -1.41658006	1.32811053	0.10550693
C -4.10969705	-0.40820801	3.71211563	C -1.81942322	1.83386051	-2.20667855
H -4.37734804	0.24231385	4.54133676	C -0.84615760	0.90329644	-2.58477510
H -3.04898514	-0.66846718	3.77980825	C -0.46170058	0.39547092	-0.26427342
H -4.71061908	-1.32106801	3.74784963	H -1.62260351	1.47878632	1.15696098
C -4.58553175	0.23979326	-3.39848427	H -2.34850371	2.39942297	-2.96361153
H -4.92792880	1.03113853	-4.06211324	H -0.60366289	0.73655336	-3.62790381
H -5.17413946	-0.66481726	-3.57451827	O 0.24670491	-0.39616166	0.58527363
H -3.52561652	0.03918540	-3.57912431	O 0.79165124	-0.72172256	-1.96629641
O -5.01252024	1.74177406	0.35376023	H 1.14451091	-1.11078356	-1.15127796
O 2.71509569	0.80067123	1.93288874	C -0.03514978	-0.27997933	1.97111057
H 2.82059100	-0.08807784	2.30129928	H 0.59201418	-1.01343481	2.47258737
C -4.03414132	2.73219289	0.72369131	H 0.22309667	0.71911001	2.32919122
H -3.43796952	2.34590683	1.55399206	H -1.09106979	-0.50391031	2.15504063
<u>β-β' bottomC_α-C_β</u>					
O 2.66040799	4.60349874	-0.85924713	C 3.58221672	3.79730272	-0.26082776

C 5.63909030	2.38788154	0.95097994	C 2.56086678	-3.02678571	1.56918443
C 4.82984403	4.41287097	-0.05631466	C 1.43540969	-3.82074862	1.66400978
C 3.37328471	2.48594483	0.13502435	C 1.33698728	-3.93360266	-0.76690946
C 4.41392297	1.77294153	0.74193811	H 1.04668122	-4.06333679	2.64650929
C 5.85066225	3.70774629	0.55132355	H 0.90017901	-4.35053992	-1.66325929
H 6.44433446	1.83831364	1.42609635	O 3.11277668	-2.82352152	-1.98752744
H 2.41233487	2.00348199	-0.00375755	O 3.12395669	-2.52100657	2.71825719
H 6.80056658	4.20305887	0.70921706	C 2.50921035	-3.17641176	-3.22431569
C 1.37724000	4.04224306	-1.07299510	H 3.15171707	-2.75132816	-3.99194424
H 0.76060488	4.81882820	-1.52167632	H 1.50924773	-2.74253618	-3.29749159
H 0.94034274	3.72386287	-0.12380517	H 2.46722606	-4.26321266	-3.33670380
H 1.43527180	3.18084551	-1.74347441	C 4.36352169	-3.13690163	3.08446643
O 5.02139006	5.69626457	-0.44779971	H 4.69810519	-2.63734604	3.99155402
H 4.19873834	6.01230055	-0.84093671	H 4.20062461	-4.19871942	3.28512376
C 4.21031446	0.32168181	1.08933900	H 5.10033160	-3.01112516	2.28963034
H 5.05120056	-0.01163814	1.71223758	C -0.38574302	-5.04953726	0.62445709
C 4.20634386	-0.56174705	-0.16618056	C -3.51494994	-4.06848853	0.74164943
H 3.28456821	-0.39555362	-0.73696914	C -2.58706266	-3.38274856	-0.20750689
C 5.43164399	-0.35662645	-1.04320408	C -1.84922959	-4.36410679	-1.12881628
H 5.47258373	0.68311842	-1.36898738	O -1.17461735	-5.40717589	-0.41278063
H 6.32641593	-0.55880680	-0.43566836	H -0.66914171	-5.46762380	1.58455472
O 5.41416489	-1.16253980	-2.19621167	H -3.21736506	-4.65753450	1.59629789
H 4.98362900	-1.99478906	-1.96947985	H -1.85257194	-2.73905483	0.29062560
O 4.25256760	-1.94920626	0.26305238	H -1.14849600	-3.80550360	-1.75749141
C 3.09676567	-2.66440399	0.33041088	H -2.56625518	-4.88439157	-1.76518903
C 0.78323004	-4.26913446	0.49621767	C -3.57713003	-2.56080300	-1.05865664
C 2.48418988	-3.16007943	-0.84027208	O -4.78510730	-3.32299889	-1.04046474

C -4.91512628	-3.93052493	0.23964324	H -2.64672059	2.79813857	1.87867680
H -3.26433181	-2.52025305	-2.10559279	C -3.54831114	4.72491582	1.73449975
H -5.43423807	-4.88474030	0.10808382	H -2.70351277	5.26655757	2.16466916
H -5.53274647	-3.30058130	0.89953961	H -4.01146088	5.35336713	0.96662103
C -3.79284094	-1.14211687	-0.57498914	O -4.44424531	4.44661960	2.78813113
C -4.14218531	1.50891606	0.21040049	H -5.09087369	3.82063824	2.44464357
C -3.97753170	-0.15234588	-1.53329205	C -2.02004017	3.69516847	-0.01422241
C -3.82476578	-0.82146937	0.78271322	H -1.24836148	4.33847660	0.42694546
C -4.01138072	0.50369121	1.17264703	O -2.59673051	4.44812077	-1.05534339
C -4.15335044	1.17251058	-1.14245948	H -3.36197956	3.94379676	-1.37091601
H -3.95009325	-0.42085367	-2.58075191	C -1.35299968	2.41853901	-0.52940682
H -3.67720143	-1.59465901	1.52619423	C -0.26319414	0.01639280	-1.47423421
O -4.28733153	2.21529001	-2.00420806	C -0.90932031	1.43938625	0.37086355
O -4.02350786	0.93141353	2.46241477	C -1.18337060	2.20338073	-1.88932620
C -4.08568625	-0.04982250	3.47927443	C -0.63556378	1.00699585	-2.36236313
H -4.19113933	0.49518363	4.41438093	C -0.38736355	0.24361732	-0.09290891
H -3.17263535	-0.65230243	3.51129146	H -1.00751336	1.59515031	1.43734602
H -4.94822538	-0.70682232	3.33368416	H -1.49486412	2.96916754	-2.58897969
C -4.26618723	1.92411703	-3.39113115	H -0.50959267	0.82642898	-3.42374679
H -4.37237614	2.88011494	-3.89944083	O 0.00529797	-0.80462262	0.68233547
H -5.09962140	1.27071228	-3.66242894	O 0.20663377	-1.18128466	-1.91365515
H -3.31859692	1.45766614	-3.67566261	H 0.45282387	-1.71293032	-1.14022265
O -4.24627852	2.82590728	0.56556712	C -0.03070023	-0.61191004	2.08653049
O 2.99109935	0.17436131	1.79698181	H 0.34751058	-1.53157759	2.52709689
H 3.01155733	-0.67998480	2.25054274	H 0.61250844	0.22404886	2.37162632
C -3.05449686	3.44022743	1.09457769	H -1.06028857	-0.43540457	2.41646495

β - β' bottomC_g-O

O 2.97673532	4.57079532	-1.88441300	C 3.60508875	-2.23665792	0.84339622
C 3.66943681	4.01242684	-0.85024796	C 1.51208427	-3.86619839	-0.11327815
C 5.20161680	3.13229981	1.28448864	C 3.77605940	-3.00417471	-0.32695526
C 4.69292105	4.82787819	-0.34041995	C 2.42178442	-2.37687017	1.56708634
C 3.42832393	2.76225030	-0.30454082	C 1.37980940	-3.14984519	1.09380935
C 4.20413763	2.31539878	0.77019528	C 2.75660296	-3.81557897	-0.79056007
C 5.45250299	4.38503122	0.72711046	H 0.46434710	-3.16831079	1.66880075
H 5.79453490	2.79609971	2.12864483	H 2.87219412	-4.37790202	-1.70816325
H 2.63087758	2.13548582	-0.68507812	O 4.98072360	-2.84848685	-0.92757166
H 6.22415423	5.03563854	1.11923260	O 2.25057164	-1.66908404	2.73807783
C 1.81195007	3.89052027	-2.31770436	C 5.17795272	-3.44148491	-2.19973006
H 1.36588540	4.51133080	-3.09164352	H 6.16566146	-3.12252432	-2.52429891
H 1.10899719	3.76391052	-1.48991765	H 4.42423715	-3.09042032	-2.90972702
H 2.06488982	2.90942475	-2.73130214	H 5.14437999	-4.53217644	-2.13079322
O 4.92005926	6.04914732	-0.88154807	C 3.07313798	-2.12506376	3.81797287
H 4.27626757	6.18549021	-1.58727712	H 2.83270482	-1.49664879	4.67376219
C 3.96771763	0.93533457	1.33355186	H 2.83524740	-3.16702225	4.04549286
H 4.29852265	0.91353470	2.37937427	H 4.12915541	-2.02625026	3.56296852
C 4.75802684	-0.14419440	0.58047708	C 0.40661461	-4.54394174	-0.69819902
H 4.35977682	-0.24649668	-0.43642041	C -0.98657592	-4.17502498	-0.33416006
C 6.25630217	0.10882056	0.53577334	C -1.42408672	-2.78604441	-0.91538100
H 6.45118561	1.06376237	0.04787174	C -0.60862023	-2.26775110	-2.09419953
H 6.62782143	0.16748885	1.56978862	O -0.52748651	-3.12143319	-3.15788682
O 6.93936755	-0.88421743	-0.18923045	H 0.57366864	-5.12167435	-1.60105498
H 6.49165216	-1.72450936	-0.03468660	H -1.08835116	-4.10757844	0.75264530
O 4.59714913	-1.40694394	1.27922381	H -1.38767081	-2.02496356	-0.13005033

H 0.43601836	-2.04949913	-1.79830266	O 2.57614620	0.64819246	1.26810148
H -0.98009652	-1.28077805	-2.42161315	H 2.33652800	0.01682782	1.96309943
C -2.89693766	-3.04763616	-1.34451900	C -4.77519219	2.40795973	1.18550490
O -3.26956919	-4.27175310	-0.74131182	H -4.36226006	1.75206719	1.95608569
C -2.11239071	-5.09021989	-0.81817148	C -5.76636569	3.35087243	1.84214072
H -2.92402635	-3.17317205	-2.43684068	H -5.24102331	4.01102543	2.53532607
H -1.93550931	-5.40531138	-1.85544911	H -6.24252811	3.96316567	1.06868697
H -2.27311824	-5.96595669	-0.19074296	O -6.71756100	2.62901478	2.59381536
C -3.78025367	-1.90370112	-0.94484773	H -7.01217308	1.89674812	2.04058421
C -5.01394152	0.43980917	-0.12244948	C -3.66700517	3.15030820	0.42242440
C -3.92535691	-0.85278580	-1.84350143	H -3.28597159	3.92313860	1.10071590
C -4.29188850	-1.82338774	0.34685215	O -4.21688061	3.84241591	-0.67270340
C -4.92194499	-0.64795030	0.75170573	H -4.67870334	3.18419568	-1.21315840
C -4.54540932	0.32376097	-1.42942623	C -2.47354554	2.27844454	0.02258811
H -3.53629905	-0.95342963	-2.84814413	C -0.14621020	0.84407167	-0.64407374
H -4.18454778	-2.67376927	1.00682781	C -1.90295250	1.38012031	0.93429447
O -4.71301739	1.41932652	-2.21569980	C -1.88894785	2.41811147	-1.22769770
O -5.45247076	-0.43757041	1.98323162	C -0.74040720	1.69596809	-1.55969332
C -5.42520697	-1.51411384	2.90047105	C -0.76207008	0.65975172	0.60774836
H -5.92310958	-1.15436372	3.79775122	H -2.34982191	1.24645143	1.91062668
H -4.39676827	-1.80070144	3.14184622	H -2.31960107	3.11301098	-1.93752874
H -5.95956529	-2.38109374	2.50237171	H -0.26907849	1.80808067	-2.53034938
C -4.17790076	1.37109366	-3.52701676	O -0.15328517	-0.24645745	1.42492897
H -4.37049952	2.34824415	-3.96518543	O 0.99918132	0.18229392	-0.96352881
H -4.67571120	0.59972283	-4.12069045	H 1.54993034	0.10621743	-0.15919315
H -3.10024808	1.18468846	-3.49912114	C -0.81302382	-0.57352287	2.63182558
O -5.57642937	1.61780982	0.28667938	H -0.19962685	-1.33427737	3.10886969

H -0.88544903 0.29649906 3.29150389

H -1.81777014 -0.96232210 2.42667573

β - β' bottom C_{β} - C_{γ}

O 2.08987724 4.49212483 -0.97073575

H 5.70647341 -1.75253336 -1.58098619

C 3.18893782 3.91052192 -0.41014502

O 4.68255582 -1.59337876 0.61006187

C 5.56515001 2.99957754 0.68992617

C 3.51558017 -2.29820220 0.52276937

C 4.32571807 4.73799841 -0.40958860

C 1.08735606 -3.67900114 0.36438164

C 3.24988493 2.63429085 0.12636931

C 3.04231767 -2.76740875 -0.71489518

C 4.45220548 2.17195097 0.67715979

C 2.80052841 -2.62094981 1.67228051

C 5.50690119 4.28089438 0.14264825

C 1.59290370 -3.30757584 1.60094716

H 6.49323694 2.64820649 1.12818115

C 1.82957652 -3.44501471 -0.79298221

H 2.37829758 1.98852600 0.14371933

H 1.04332538 -3.49229659 2.51797255

H 6.36656233 4.93930225 0.14698301

H 1.44374147 -3.78776368 -1.74382013

C 0.85988670 3.79767960 -0.86178252

O 3.83268141 -2.48968446 -1.77677980

H 0.10457241 4.42950538 -1.32480718

O 3.24487445 -2.16985894 2.89400621

H 0.61098669 3.62821404 0.18982500

C 3.30354964 -2.68345209 -3.08174222

H 0.89823344 2.83692213 -1.38316097

H 4.05124916 -2.28082852 -3.76128891

O 4.25396525 5.98392178 -0.93839954

H 2.36271186 -2.13843306 -3.19591629

H 3.35195096 6.11918091 -1.25356876

H 3.15260411 -3.74704563 -3.28401301

C 4.52574529 0.76113139 1.20809541

C 4.39490934 -2.86502248 3.38904705

H 5.40466330 0.67230042 1.86182836

H 4.63892679 -2.41114725 4.34752708

C 4.69524912 -0.24784316 0.05961576

H 4.15361626 -3.92134272 3.52962841

H 3.86283952 -0.14544842 -0.64543519

H 5.23102759 -2.75709567 2.69613249

C 6.03139829 -0.08982579 -0.64827244

C -0.34514110 -4.17646886 0.25679261

H 6.13490012 0.93846974 -0.99618926

C -1.26097510 -2.99335871 0.19253420

H 6.82550665 -0.28693766 0.08686346

C -2.05115483 -3.01065831 -1.06660972

O 6.16927325 -0.92825236 -1.76948747

C -1.37867530 -4.15740128 -1.84552059

O -0.58580115	-4.90972379	-0.93213958	H -4.99524446	2.02804875	-3.93750665
H -0.57123487	-4.83129655	1.10910775	H -5.57403802	0.37189960	-3.62657678
H -1.34227722	-2.25329466	0.97389515	H -3.81757671	0.72130031	-3.63961101
H -1.92508037	-2.07777662	-1.62794113	O -4.88204775	2.20801306	0.52802860
H -0.73427168	-3.73463143	-2.62487485	O 3.34559040	0.49769796	1.93843363
H -2.08956431	-4.84003430	-2.31532889	H 3.43975115	-0.35303645	2.38958841
C -3.58098667	-3.12187781	-0.78802196	C -3.76825248	2.96405663	1.04070335
O -3.87349991	-4.01791414	0.27090769	H -3.25070338	2.36307630	1.79234699
C -3.64259757	-5.32844220	0.02065699	C -4.40576669	4.15784592	1.72652858
H -4.08835612	-3.46768009	-1.69983345	H -3.62611078	4.80537726	2.13303891
H -3.80060786	-5.68600229	-0.99214196	H -4.98331687	4.72692001	0.98971200
H -3.84588453	-5.96872201	0.86624314	O -5.20864667	3.74263141	2.80927266
C -4.08678814	-1.75211578	-0.40489162	H -5.74579482	3.00761784	2.49315713
C -4.63862561	0.89420459	0.23419478	C -2.81872988	3.36892668	-0.09945732
C -4.34471565	-0.83790213	-1.42205234	H -2.16023779	4.14985352	0.30199016
C -4.15252762	-1.37283482	0.93119996	O -3.54199262	3.97305894	-1.14336715
C -4.44068069	-0.04479994	1.24838964	H -4.24060448	3.35099909	-1.39592800
C -4.62495673	0.48682209	-1.10029548	C -1.93679165	2.21995622	-0.58539678
H -4.29172492	-1.15791387	-2.45481360	C -0.29590810	0.12113746	-1.45486021
H -3.97516517	-2.11317317	1.69806106	C -1.18990540	1.47477074	0.33871320
O -4.86747437	1.46496107	-2.01216810	C -1.82015438	1.92595915	-1.93521823
O -4.52344751	0.44633688	2.51030075	C -1.01523170	0.86895866	-2.36838996
C -4.34937136	-0.46090819	3.58218790	C -0.36466305	0.44555710	-0.08687644
H -4.47227924	0.12430962	4.49035624	H -1.23447802	1.71929016	1.39298471
H -3.34920206	-0.90490432	3.56373880	H -2.35951788	2.52773683	-2.65537079
H -5.10052941	-1.25484720	3.54923739	H -0.92195083	0.62656085	-3.42093961
C -4.80679150	1.11164387	-3.38220254	O 0.43236399	-0.31497787	0.71006992

O 0.48855532	-0.90730609	-1.86807774	H 1.06382580	-0.77315405	2.56781662
H 0.87759056	-1.33127826	-1.08676568	H 0.77067208	0.95695353	2.31163140
C 0.40031903	-0.04957439	2.10209235	H -0.61848891	-0.17262417	2.48764630

β - β' bottom C_{γ} -O

O 1.89267601	4.58667327	-1.13584084	H 6.54500328	0.25872612	0.70980680
C 2.78954945	4.09432867	-0.23600256	O 6.26005187	-0.19663676	-1.29080274
C 4.73433924	3.36938837	1.60415693	H 5.85489350	-1.07101129	-1.28135428
C 3.68160075	5.06132646	0.26247169	O 4.50329996	-1.27793831	0.73811969
C 2.87434988	2.77920295	0.18903121	C 3.45951005	-2.08769941	0.40072443
C 3.86148085	2.41105922	1.11340375	C 1.33877082	-3.81252871	-0.24688030
C 4.64652050	4.69624182	1.18089743	C 3.21553093	-2.44545747	-0.93783941
H 5.49585610	3.08703790	2.32274990	C 2.65472151	-2.63925517	1.38985476
H 2.17722007	2.03080053	-0.17246542	C 1.60694030	-3.50370679	1.07820571
H 5.32019116	5.45689833	1.55521114	C 2.15335004	-3.28313832	-1.25444637
C 1.02054313	3.65692401	-1.75714153	H 1.00919315	-3.88081169	1.89873037
H 0.39140064	4.23004839	-2.43435465	H 1.92703503	-3.52461134	-2.28494801
H 0.39580020	3.15369391	-1.01575171	O 4.07025447	-1.91173991	-1.83972789
H 1.58886399	2.91093765	-2.32073056	O 2.84300692	-2.26059644	2.69934748
O 3.58831834	6.34562972	-0.15966998	C 3.78411131	-2.07407218	-3.22350702
H 2.86890956	6.39507827	-0.80089826	H 4.54796504	-1.50250530	-3.74567954
C 3.98563018	0.96354094	1.51469257	H 2.79364543	-1.67640166	-3.45693750
H 4.74054006	0.87717710	2.30828770	H 3.84852317	-3.12716948	-3.50945925
C 4.45414085	0.11337514	0.32560917	C 3.98366822	-2.86079162	3.32257381
H 3.74482099	0.21192479	-0.50272924	H 4.01662421	-2.47527677	4.33967447
C 5.85975230	0.47759685	-0.12188765	H 3.86428509	-3.94688276	3.34193415
H 5.90502214	1.54779839	-0.32903804	H 4.89495245	-2.59024856	2.78650779

C 0.20242669	-4.72499355	-0.69179804	H -4.30829352	1.10830760	4.62509554
C -0.96923161	-4.86640648	0.28689540	H -3.06830968	0.00000288	3.98326411
C -1.65849863	-3.49656269	0.04052097	H -4.76318155	-0.54606755	4.13544016
C -1.45210680	-3.29791391	-1.47558149	C -4.39373454	-0.06315580	-3.21933355
O -0.41524685	-4.20035013	-1.86339632	H -4.59070549	0.67352615	-3.99537247
H 0.61188089	-5.69999321	-0.96885815	H -5.03898728	-0.93292721	-3.37115926
H -0.66191142	-4.95141575	1.32964603	H -3.34125781	-0.35979698	-3.25431920
H -1.12144203	-2.72111207	0.59294685	O -4.90737449	1.95020009	0.27228728
H -1.17118414	-2.26853273	-1.71375570	O 2.73003318	0.51420734	1.98552488
H -2.34160652	-3.56888972	-2.05060494	H 2.83971343	-0.36740019	2.36962656
C -3.15349196	-3.43098330	0.48485972	C -3.88399306	2.93402559	0.52561118
O -3.15332732	-3.96434400	1.74237954	H -3.25317380	2.59160799	1.34930355
C -1.82379938	-6.02974260	-0.08703345	C -4.64336511	4.16103071	0.99568757
H -3.71513584	-4.08608083	-0.19999379	H -3.94327210	4.98093216	1.16898076
H -1.83134602	-6.38914958	-1.10802864	H -5.35036633	4.46303372	0.21561571
H -2.52133383	-6.44364208	0.62667731	O -5.29633469	3.90405491	2.21955521
C -3.67003928	-2.00201881	0.42989198	H -5.70988512	3.03673750	2.14135215
C -4.51200334	0.64377342	0.32944040	C -3.07057878	3.19103343	-0.74721181
C -3.98181724	-1.42553309	-0.79882546	H -2.50050334	4.11326318	-0.57854243
C -3.80265936	-1.28156217	1.61187657	O -3.94214965	3.47543813	-1.81898006
C -4.23842027	0.04223747	1.55858602	H -4.52156628	2.70429607	-1.90745416
C -4.39766154	-0.09553030	-0.84822856	C -2.06879019	2.09313736	-1.11471538
H -3.89976316	-2.00658137	-1.70733276	C -0.13411256	0.21453343	-1.88396704
H -3.57886328	-1.76722103	2.55121297	C -1.42546736	1.30448585	-0.15060080
O -4.69053853	0.57656142	-1.98930349	C -1.72981072	1.92441273	-2.45236039
O -4.40523216	0.84625163	2.63775008	C -0.76301174	0.99482962	-2.83701136
C -4.11628098	0.30742007	3.91527761	C -0.48338534	0.35824870	-0.53097731

H -1.66343267	1.41004440	0.89885619	H 1.08850314	-1.17798268	-1.45329159
H -2.22414431	2.53272824	-3.19957379	C -0.08465643	-0.37631778	1.69365707
H -0.48531408	0.86742997	-3.87697898	H 0.51847154	-1.14088453	2.17943038
O 0.16674094	-0.50079120	0.30118599	H 0.23047405	0.60598820	2.05142733
O 0.80972287	-0.69211722	-2.24511053	H -1.14614055	-0.55013951	1.89982918

β - β' bottomC $_{\alpha}$ -C $_{\beta}$ α -side

C -4.49685634	-0.10323774	1.03071694	C 1.01611826	1.85345871	-0.47688519
C -3.31366151	0.62284631	0.49177564	C 1.10469577	-0.13654012	-1.84163151
C -3.13139514	-0.06004669	-0.87495443	H -0.76949654	-0.75271786	-2.71140691
C -4.57874700	-0.41154167	-1.23547082	H -0.92706496	2.80505396	-0.35166655
O -5.27749694	-0.56105597	0.01149590	O 1.90251820	-1.11543981	-2.34153185
H -5.03438327	0.12396862	1.94208371	O 1.73547103	2.71226205	0.29155647
H -2.43056254	0.52929651	1.11979610	C 1.07511573	3.85944754	0.78934751
H -2.51043311	-0.95254328	-0.80631291	H 1.82698378	4.42225437	1.33751674
H -4.67410563	-1.34511025	-1.78863326	H 0.25917420	3.58424544	1.46547569
H -5.05741515	0.39746449	-1.79675424	H 0.67896386	4.46940541	-0.02732258
C -2.48802428	1.04400192	-1.71676060	C 1.29655796	-2.09750403	-3.16294882
O -3.07794869	2.24957566	-1.25740634	H 2.08737618	-2.79567232	-3.42916495
C -3.55074399	2.09889573	0.08243109	H 0.88768881	-1.64457082	-4.07037357
H -2.72612644	0.95283138	-2.78100020	H 0.50678648	-2.62459681	-2.62007409
H -4.61363269	2.35511075	0.09881854	O 3.07315437	0.63588874	-0.73745011
H -3.01442743	2.79006752	0.73984721	C 3.41835191	0.21282259	0.59599410
C -0.98183997	1.02075713	-1.52469251	H 2.82102068	0.78437343	1.31058293
C 1.73869344	0.78229792	-1.00164583	C 4.87263024	0.61527506	0.75376465
C -0.25863325	-0.02427098	-2.09416565	H 5.23222504	0.31014041	1.73861668
C -0.35147206	1.97430079	-0.73515408	H 5.46942592	0.10456408	-0.00962430

O 5.01451171	2.01698397	0.67393143	C -0.46075613	-1.31458533	1.85956157
H 4.49642192	2.30616841	-0.08555204	H 1.27493125	-0.17674989	2.36322603
C 3.19789629	-1.30013367	0.76010643	H 1.85227937	-3.31419686	-0.48640054
H 3.70922372	-1.59756999	1.68316721	H -0.57780967	-3.88245158	-0.33068938
O 3.84474323	-1.99449540	-0.27929460	O -1.35943246	-0.71038938	2.69540685
H 3.49579797	-1.63772321	-1.10959708	O -2.31908241	-2.65362527	1.13037599
C 1.72424076	-1.68523910	0.88803587	H -2.78092440	-2.00895027	1.68601886
C -0.99896056	-2.34685786	1.07420889	C -0.95296740	0.48539751	3.32980436
C 0.88077518	-0.98402969	1.75884617	H -1.82925927	0.86896645	3.84869174
C 1.19876466	-2.74380386	0.16123532	H -0.15569985	0.29758758	4.05427198
C -0.15645475	-3.06541733	0.24382628	H -0.60842959	1.21595896	2.58771693

β - β' bottom C_g-C_{ph} phenyl-side

O -4.32165487	1.16064687	-1.65963931	O -5.93799512	0.21850723	0.20079909
C -3.74380788	0.32665196	-0.74468529	H -6.06156722	0.81009017	-0.55110937
C -2.83923744	-1.41211676	1.21583405	C -0.48722472	-1.28724976	0.29428379
C -4.63515242	-0.15655656	0.22777215	H -0.35471884	-2.20133598	0.88967027
C -2.41257322	-0.05226082	-0.72528833	C 0.33865460	-0.17541018	0.96040274
C -1.95295973	-0.92673977	0.26588420	H 0.24294466	0.74895494	0.38061248
C -4.17920792	-1.02522299	1.20167299	C -0.04961483	0.05815412	2.41178144
H -2.49019220	-2.09969706	1.97889806	H -1.10963949	0.30665257	2.46814237
H -1.71819472	0.28836921	-1.48267816	H 0.11465667	-0.87928416	2.96334872
H -4.88451509	-1.39754689	1.93414777	O 0.66272777	1.11826219	3.00369819
C -3.49548031	1.66868423	-2.68919711	H 1.55293386	1.11413372	2.63454286
H -4.13330591	2.29110802	-3.31234133	O 1.73287090	-0.57602092	0.98239100
H -3.07538819	0.85517471	-3.28709024	C 2.56018604	-0.11142471	-0.00177498
H -2.68455766	2.27349032	-2.27321841	C 4.29165222	0.76647484	-1.90613749

C 2.96515384	1.23552350	-0.01641005	H 2.15868906	3.80129812	1.80466281
C 3.07856564	-0.99581302	-0.94616392	H 2.36594101	3.84058153	0.03329141
C 3.96840686	-0.56173434	-1.93403465	H 3.78278174	3.58424174	1.09673247
C 3.84261861	1.69870636	-1.00064949	C 3.24582608	-3.09267064	0.10734238
H 4.34225525	-1.26376176	-2.66870516	H 2.83930397	-4.09592652	-0.00373614
H 4.16181496	2.73187910	-1.03784770	H 4.33196352	-3.11888241	-0.01062877
O 2.45073144	1.99720800	0.97750013	H 2.98123779	-2.68320760	1.08368626
O 2.66606000	-2.30523824	-0.93766968	O -0.05637437	-1.49404461	-1.03422470
C 2.71483196	3.38904104	0.96594852	H 0.80280641	-1.93711501	-1.02270363

β -O-4 bottomC _{α} -C _{β} α -side

O 1.90198698	1.20309115	0.00000027	C 1.55157344	2.57276574	-0.00000093
C 0.88335472	0.29187159	0.00000110	H 2.48734180	3.12685367	-0.00000449
C -0.96110262	-1.79049985	0.00000142	H 0.97354800	2.82568092	0.89332547
C 1.32554171	-1.04529116	0.00000028	H 0.97354281	2.82567786	-0.89332468
C -0.46107417	0.59495851	0.00000173	O 2.65306222	-1.32593686	-0.00000108
C -1.42091992	-0.45319713	0.00000013	H 3.13229317	-0.48871758	-0.00000852
C 0.39241962	-2.07444482	0.00000038	C -2.79530303	-0.17230189	-0.00000330
H -1.68110577	-2.60072230	0.00000172	H -3.54970455	-0.94804944	-0.00000329
H -0.80885632	1.61849128	0.00000150	O -3.20561013	1.12580232	0.00000806
H 0.75397751	-3.09540035	-0.00000033	H -4.16348763	1.16936704	-0.00005023

β -O-4 bottomC _{α} -C _{β} β -side

C -3.70358450	-2.89712055	0.78342462	O -4.52365423	-4.02030722	-1.17905751
H -2.71961815	-2.49508112	0.55769515	H -4.90309282	-3.13960023	-1.28784554
C -4.20194007	-4.16787068	0.20205799	O -4.70300293	-1.96367088	0.95531617
H -3.43353604	-4.93827719	0.27094688	C -4.31906442	-0.65808439	0.75757413
H -5.08493069	-4.49997888	0.76141275	C -3.32966446	1.88771830	0.22503587

C -4.31238440	-0.16583284	-0.55608584	O 0.84427302	4.30646501	0.23446140
C -3.89568802	0.15132253	1.80867732	C -0.52199366	4.55969051	0.51388501
C -3.40800174	1.42936594	1.53001944	H 1.10141325	3.80546449	-1.74886287
C -3.81817882	1.10808058	-0.82519983	H -0.94901814	5.25148172	-0.22497840
H -3.06196257	2.02881385	2.36500889	H -0.58325166	5.01026624	1.50469218
H -3.78990109	1.50121510	-1.83151943	C 2.05312275	2.35409829	-0.49820942
O -4.75486256	-1.03318123	-1.49755503	C 3.92517578	0.36476570	0.00828536
O -3.83204700	-0.24971340	3.10167193	C 2.58054309	1.61983840	-1.55701416
C -4.60646628	-0.66123224	-2.86257580	C 2.47652201	2.13289304	0.80710184
H -4.96166476	-1.51211611	-3.43953048	C 3.42334659	1.13814846	1.05587722
H -3.55567476	-0.47250436	-3.09403804	C 3.52337397	0.62636827	-1.30303107
H -5.21532176	0.21722467	-3.09074982	H 2.23800411	1.81556659	-2.56528012
C -4.79564409	-1.17760958	3.60211765	H 2.07483522	2.74925485	1.59914394
H -4.83566965	-1.00454430	4.67603177	O 4.09868283	-0.15299383	-2.25465892
H -5.77514209	-0.99260202	3.15783899	O 3.90738115	0.82170445	2.28515818
H -4.49309649	-2.20519701	3.39959344	C 3.48996969	1.61482650	3.37975376
C -2.65070828	3.21833018	-0.06127317	H 4.01549769	1.22448358	4.24807578
C -1.19309914	3.19275748	0.40621555	H 2.41011424	1.53267454	3.53853113
C -0.44824748	2.58838286	-0.79599479	H 3.75551020	2.66441758	3.22639775
C -1.38242471	2.90124461	-1.98160965	C 3.67296157	0.02679632	-3.59376025
O -2.56828039	3.49958591	-1.44615622	H 4.21962318	-0.70670431	-4.18281456
H -3.22021624	4.03355321	0.39533021	H 3.91689899	1.03290338	-3.94600132
H -1.04413308	2.61132077	1.31652827	H 2.59814812	-0.15372994	-3.68621815
H -0.30776877	1.51351445	-0.69257924	O 4.83129345	-0.63234680	0.24651773
H -1.63586299	1.98492487	-2.52310728	C 4.31790942	-1.82168893	0.87813934
H -0.95104132	3.61809656	-2.68364705	H 3.65196660	-1.52955490	1.69352687
C 0.92392745	3.31575493	-0.78302199	C 5.54146298	-2.48616429	1.48091482

H 5.25178850	-3.42493525	1.95758381	C 0.61035591	-1.74492113	-2.32345218
H 6.25856287	-2.70593121	0.68288872	C 0.12596703	-1.10908933	-0.05568809
O 6.10996937	-1.66826726	2.48078896	H 1.62048927	-1.55739038	1.39922461
H 6.14112854	-0.77331812	2.12412456	H 2.51065639	-2.70652112	-2.62714084
C 3.60032226	-2.71098645	-0.14818931	H 0.29947468	-1.79995782	-3.36025322
H 3.45263068	-3.68895438	0.32468261	O -0.80713711	-0.52770840	0.75858357
O 4.44591695	-2.94178054	-1.25093731	O -1.43299232	-0.63422842	-1.80847142
H 4.67826374	-2.07021556	-1.60461242	H -1.89048410	-0.27170012	-1.03444851
C 2.23218373	-2.17720463	-0.57753121	C -0.45202009	-0.34105556	2.11722667
C -0.24386379	-1.15872765	-1.40875753	H -1.29951242	0.14689577	2.59227084
C 1.34826848	-1.61645722	0.35382255	H -0.27151821	-1.30254240	2.60679737
C 1.84086736	-2.25399100	-1.90705675	H 0.44325321	0.28674661	2.18993968

β -O-4 bottomC _{α} -C_{Ph} α -side

C -2.87734173	-3.39758106	1.27265367	C -3.71673753	0.28230614	1.66200986
H -2.36856147	-4.33217245	1.07160006	C -3.21337330	1.56957249	1.53799078
C -3.63739775	-2.75514579	0.15998592	C -3.62832871	1.48786964	-0.83155129
H -2.97347490	-2.25727325	-0.56488431	H -2.85115952	2.06989642	2.42960078
C -4.49469660	-3.79057050	-0.55119994	H -3.59327328	1.97642124	-1.79555001
H -3.87484800	-4.65575824	-0.79799081	O -4.65165488	-0.52394448	-1.72531198
H -5.27209144	-4.11548440	0.15200680	O -3.68090392	-0.33436078	2.89121666
O -5.05297384	-3.31703149	-1.75086311	C -4.42847296	-0.06262625	-3.05267062
H -5.31061062	-2.39853724	-1.60745299	H -4.79754873	-0.85367632	-3.70162996
O -4.54536949	-1.73669101	0.68410221	H -3.36043242	0.08878833	-3.22501970
C -4.14131659	-0.43962418	0.54806106	H -4.98463602	0.85945609	-3.23930329
C -3.11492504	2.15284090	0.28034699	C -4.97087438	-0.57820900	3.46997297
C -4.15473453	0.20310286	-0.69937667	H -4.78812134	-1.06573056	4.42526047

H -5.48445323	0.37268172	3.62826655	O 4.12016088	0.63675210	2.25894287
H -5.56019241	-1.22766374	2.82147352	C 3.75734874	1.38540343	3.40315778
C -2.37254485	3.46916003	0.11134321	H 4.28014673	0.92512582	4.23822685
C -0.91792985	3.32842369	0.57019488	H 2.67786041	1.34082676	3.57835207
C -0.20499422	2.78651977	-0.68021052	H 4.06635657	2.42946017	3.30209911
C -1.11976069	3.24714102	-1.83218390	C 3.71265921	0.14571700	-3.64270251
O -2.27313641	3.86134145	-1.24508583	H 4.21043838	-0.58196093	-4.28030336
H -2.90007833	4.27075155	0.63736235	H 3.99434021	1.15584920	-3.95304018
H -0.79847348	2.66684091	1.42884855	H 2.62881461	0.01811176	-3.71522194
H -0.12190893	1.70127037	-0.66659619	O 4.92770768	-0.75425657	0.12961890
H -1.42146406	2.39349625	-2.44699924	O -2.26535079	-2.65243573	2.22040793
H -0.65066124	3.99565057	-2.47425516	H -2.80055092	-1.87313796	2.45028679
C 1.20452196	3.43352487	-0.61110196	C 4.37580315	-1.94830808	0.71976662
O 1.17384682	4.34909313	0.47734058	H 3.73883801	-1.66499802	1.56073953
C -0.17712251	4.64608125	0.78536249	C 5.58088896	-2.68974540	1.26753332
H 1.41406866	3.98369736	-1.53716768	H 5.25977459	-3.63558101	1.70874284
H -0.57050923	5.41731312	0.10917312	H 6.27270349	-2.90404241	0.44605517
H -0.21319182	5.01586591	1.81034364	O 6.20312150	-1.94164559	2.28989926
C 2.28032617	2.39358522	-0.39823828	H 6.26144265	-1.03287677	1.97385082
C 4.06421561	0.29376202	-0.03673279	C 3.60272412	-2.75970208	-0.33021575
C 2.74487528	1.68619971	-1.50448627	H 3.41821927	-3.74981884	0.10256142
C 2.72172335	2.08708834	0.88314881	O 4.42104459	-2.97898612	-1.45641014
C 3.62421032	1.03650278	1.05914568	H 4.68415424	-2.10327171	-1.77649875
C 3.64480945	0.63854418	-1.32344644	C 2.25535036	-2.14579248	-0.71581682
H 2.39005533	1.94819008	-2.49342081	C -0.16763084	-0.96406272	-1.47292435
H 2.36931940	2.68169643	1.71417126	C 1.42086710	-1.56341345	0.24731205
O 4.16152603	-0.11806856	-2.32549223	C 1.83887592	-2.16376338	-2.03980448

C 0.63179160	-1.57523126	-2.41926574	O -1.33241003	-0.35742283	-1.83382716
C 0.22602795	-0.97026335	-0.12566139	H -1.74310449	0.01006650	-1.03671183
H 1.71156870	-1.55161678	1.28904140	C -0.27718241	-0.25894726	2.08124130
H 2.47108129	-2.63003059	-2.78460899	H -1.09215075	0.25560626	2.58675106
H 0.30066167	-1.58291226	-3.45130350	H -0.16580722	-1.25722956	2.51002927
O -0.64747654	-0.34207623	0.71548863	H 0.65247845	0.31241728	2.18307650

β -O-4 bottomC _{α} -C_{Ph} phenyl-side

O -1.70204643	0.39151922	0.00005131	H -0.81442357	-2.22683702	-0.00025417
C -0.42685787	-0.09391925	-0.00007434	H 2.64251093	1.35038315	0.00000482
C 2.28585693	-0.79248833	0.00008171	C -2.75833160	-0.54885512	0.00006585
C 0.56516567	0.90282983	-0.00003496	H -3.68028655	0.02748828	0.00001058
C -0.07043026	-1.44051089	-0.00012617	H -2.71814988	-1.17721824	0.89443145
C 1.27967787	-1.71938930	0.00002234	H -2.71812830	-1.17732283	-0.89423269
C 1.90522306	0.55645076	-0.00000111	O 0.20602457	2.21240869	-0.00002101
H 3.33205158	-1.07151376	0.00023157	H -0.75722212	2.25889099	-0.00003385

β -O-4 bottomC _{β} -O β -side

O 2.96719965	0.78764196	-0.63221133	C 2.86672899	2.18219636	-0.84722794
C 1.87015938	0.14746969	-0.13046507	H 3.83122961	2.50060929	-1.23547292
C -0.18835284	-1.39215193	0.90730844	H 2.65525995	2.70506994	0.08960741
C 2.05738075	-1.23101615	0.06614620	H 2.08391084	2.40687462	-1.57722866
C 0.66060921	0.74458681	0.18193212	O 3.24586121	-1.80592491	-0.24141450
C -0.37760960	-0.03192920	0.70682277	H 3.83167205	-1.11713342	-0.57768506
C 1.02731280	-1.99371779	0.58488626	C -1.73123187	0.60019049	0.97491194
H -0.98824580	-1.99451551	1.32561082	H -2.21093759	0.03582602	1.78734191
H 0.50364659	1.80698178	0.05124943	C -2.57779515	0.51406040	-0.25513077
H 1.19514063	-3.05203407	0.74109957	H -2.37971675	1.23618257	-1.04377761

C -3.25168807	-0.75785010	-0.63505078	H -4.93313488	0.08626155	-1.11877703
H -2.55915811	-1.41888476	-1.17081931	O -1.52513768	1.94936805	1.36638598
H -3.57135230	-1.29808829	0.26788143	H -2.37868985	2.39127625	1.36154482
O -4.33951145	-0.55351729	-1.52093186			

β-O-4 bottomC_β-O_α-side

O -4.89219304	-2.98884645	0.59513124	C -1.99871820	2.55303756	-1.74510782
C -4.60377471	-1.78754210	0.51479953	O -3.28454239	2.84202191	-1.18330545
C -3.82563406	0.94444430	0.26054710	H -4.03135064	3.03061005	0.68958052
C -4.52975418	-1.10781183	-0.78628570	H -1.67302544	1.84369571	1.49119663
C -4.30102637	-0.95596588	1.67870903	H -0.72372822	1.19445280	-0.62317667
C -3.92573548	0.36697885	1.52465087	H -2.07243591	1.69978942	-2.42572247
C -4.14954551	0.21639131	-0.89580107	H -1.69191557	3.43381525	-2.31354040
H -3.69869944	0.93851108	2.41856728	C 0.18081164	3.16858376	-0.40203815
H -4.10259337	0.71652253	-1.85311758	O -0.09347884	3.98533735	0.73013813
O -4.83779882	-1.90103009	-1.80897263	C -1.48496977	3.95110158	0.99189576
O -4.29930196	-1.42584154	2.93139580	H 0.30146894	3.80683327	-1.28627332
C -4.73165655	-1.36830700	-3.12091999	H -2.02108285	4.65757281	0.34332250
H -5.01079564	-2.17798750	-3.78979905	H -1.63802159	4.23416478	2.03359816
H -3.70402212	-1.05483204	-3.32327119	C 1.44562273	2.37254631	-0.18396790
H -5.41768551	-0.52705521	-3.25240598	C 3.59745847	0.65060482	0.16189484
C -4.91486700	-2.66853589	3.29082489	C 2.12181196	1.88471938	-1.29858114
H -4.93503838	-2.65635111	4.37863507	C 1.85472754	2.04298771	1.10275641
H -5.92660495	-2.72863839	2.89176066	C 2.94186296	1.18433967	1.27207894
H -4.33526917	-3.51228143	2.92335160	C 3.20443666	1.02584292	-1.12427899
C -3.33766032	2.37638982	0.15010731	H 1.78629926	2.16165537	-2.28998681
C -1.90273271	2.51868227	0.66610390	H 1.33085060	2.47307533	1.94490607
C -1.04574723	2.23264633	-0.57751915	O 3.92947101	0.48383493	-2.13638071

O 3.42658060	0.77935257	2.47460306	O 4.65159325	-2.33112299	-1.49498385
C 2.84945185	1.33992021	3.63814539	H 4.75918372	-1.39441792	-1.71802330
H 3.40046550	0.91967745	4.47616961	C 2.32682216	-2.00038017	-0.84259070
H 1.79196577	1.07072822	3.72423770	C -0.25437115	-1.27719355	-1.66428377
H 2.94798171	2.42895920	3.63819968	C 1.33926132	-1.69987200	0.10512020
C 3.52539336	0.77967368	-3.46155804	C 1.99252177	-1.96412350	-2.18930774
H 4.19789537	0.22342091	-4.11124525	C 0.70918261	-1.60177504	-2.60016111
H 3.62194862	1.84962990	-3.66587724	C 0.06483964	-1.33603102	-0.29859720
H 2.49502710	0.45581682	-3.63326130	H 1.56932867	-1.73108577	1.16178733
O 4.63897839	-0.22272297	0.31738652	H 2.74580097	-2.21425802	-2.92547611
C 4.29075941	-1.55111045	0.75532046	H 0.44097887	-1.57288410	-3.64990965
H 3.56468527	-1.47571051	1.56820581	O -0.96843154	-1.00253303	0.53355403
C 5.58164245	-2.11095381	1.32322402	O -1.50122874	-0.90150258	-2.05641906
H 5.42003860	-3.13765604	1.65802480	H -2.04838397	-0.76895522	-1.26749845
H 6.34535270	-2.11520675	0.53831394	C -0.69143943	-0.96102939	1.92120663
O 5.99533290	-1.36555763	2.44792231	H -1.61883327	-0.66986435	2.40930867
H 5.91292964	-0.43501494	2.21066992	H -0.38400909	-1.94514539	2.28637173
C 3.74651062	-2.38152214	-0.41640035	H 0.09497347	-0.22612808	2.12863723
H 3.73356654	-3.42699415	-0.08673403			

β-O-4 bottomO-C_{PhO}-side

O -3.01604171	0.99100755	0.69698603	C -1.47248726	-1.94864176	-0.70004284
C -2.02326485	0.24718839	0.12997232	H 0.50031398	-2.15862229	-1.52264153
C -0.20504045	-1.48333703	-1.05024078	H -0.47830042	1.73909737	-0.05481643
C -2.38223751	-1.09124371	-0.11032968	H -1.77280968	-2.97166986	-0.88870717
C -0.76228381	0.70585660	-0.20923221	C -2.74167096	2.35382448	0.96205846
C 0.15657944	-0.16772403	-0.80230501	H -3.64722718	2.76679483	1.39966555

H -2.50142437	2.88771825	0.03858328	C 2.59559867	-1.06380270	0.84797501
H -1.91363123	2.45173883	1.66984209	H 1.63461555	-1.41251972	1.22519032
O -3.61795601	-1.53181931	0.22442938	H 2.95535086	-1.78733196	0.10294293
H -4.10597104	-0.79321932	0.60814563	O 3.47461961	-0.97024484	1.93981011
C 1.54828661	0.32238601	-1.10049415	H 4.26329098	-0.50791108	1.63656831
H 2.01419682	-0.34754912	-1.83609220	O 3.64411892	0.88181636	-0.08155696
C 2.43064135	0.30200076	0.17144083	O 1.49425458	1.64042201	-1.59581391
H 1.96125369	0.99758733	0.89934982	H 2.39365167	1.98739047	-1.58167950

β-O-4 bottomO-C_{Ph} phenyl-side

C -4.64750006	-1.81728856	0.89405609	C -3.56444766	2.17584297	-0.07048513
C -3.98975243	0.75459731	0.26836025	C -2.12947594	2.45405032	0.38246870
C -4.66256088	-1.46007638	-0.44225041	C -1.28100894	1.99695693	-0.81610526
C -4.33505621	-0.96385776	1.92399894	C -2.26875630	2.06993590	-1.99688597
C -4.01006864	0.35915385	1.59746185	O -3.54716019	2.42977051	-1.46306506
C -4.32748797	-0.13669164	-0.75592153	H -4.27764809	2.88037310	0.36889861
H -3.76692195	1.04540982	2.40226888	H -1.86080023	1.93186439	1.30122921
H -4.33583574	0.21880742	-1.77712314	H -0.91120144	0.98105405	-0.69198003
O -4.98513409	-2.41044802	-1.34477452	H -2.33221938	1.10196184	-2.50281050
O -4.29733304	-1.32741976	3.22591808	H -2.00005990	2.83487483	-2.72882669
C -4.89813836	-2.06029985	-2.71687151	C -0.09668206	3.00202610	-0.83469276
H -5.15693382	-2.96132684	-3.26754778	O -0.37425865	3.97182672	0.16760464
H -3.88108038	-1.75040144	-2.97260072	C -1.75977099	3.93331487	0.46236083
H -5.60813068	-1.26570512	-2.96332437	H -0.03707051	3.49956549	-1.81099941
C -4.62491492	-2.68370697	3.48906470	H -2.33134981	4.50621104	-0.28068531
H -4.54757625	-2.81348089	4.56583005	H -1.90559906	4.37739596	1.44733896
H -5.64340791	-2.90464671	3.15787664	C 1.21233938	2.30626294	-0.54736809
H -3.92691888	-3.35397006	2.97884905	C 3.45235645	0.75028273	-0.02304273

C 1.86748936	1.66816802	-1.59700547	O 6.00814339	-0.76990348	2.46317501
C 1.68590075	2.21090844	0.75581410	H 5.86270680	0.10608251	2.08805259
C 2.81688412	1.43489159	1.01334697	C 3.71814230	-2.32869383	-0.10974069
C 2.99402353	0.89266391	-1.33413131	H 3.76496838	-3.30552070	0.38587475
H 1.48105642	1.76369761	-2.60385158	O 4.58277927	-2.42048519	-1.21836833
H 1.17381570	2.75234451	1.53884927	H 4.63749649	-1.53013252	-1.59643543
O 3.70371452	0.21899058	-2.27602930	C 2.26824094	-2.08118234	-0.53284441
O 3.36651259	1.25381366	2.24263381	C -0.37502477	-1.62248624	-1.35232305
C 2.80619212	1.97278784	3.32445251	C 1.29969410	-1.67062711	0.39355419
H 3.40765705	1.71927712	4.19424212	C 1.88599374	-2.28436606	-1.85157658
H 1.76697271	1.67717576	3.49967396	C 0.57209390	-2.05363674	-2.26177843
H 2.85125707	3.05026353	3.14363942	C -0.00514068	-1.43855362	-0.01021640
C 3.23528810	0.27576187	-3.61172429	H 1.56651391	-1.51290944	1.43021439
H 3.90725305	-0.35313518	-4.19206804	H 2.62530280	-2.61896380	-2.56813169
H 3.27406569	1.30025294	-3.99227747	H 0.26747995	-2.21074543	-3.29003945
H 2.21518938	-0.11235934	-3.68100701	O -1.02609396	-1.02116703	0.79640598
O 4.53689013	-0.04565056	0.22712140	O -1.65172233	-1.37589485	-1.74727104
C 4.26326220	-1.29658939	0.88821598	H -2.17884011	-1.12731954	-0.97199452
H 3.56147482	-1.11801287	1.70639283	C -0.71131488	-0.72570745	2.14317972
C 5.59577402	-1.70390854	1.48865624	H -1.64128036	-0.40775239	2.60965279
H 5.49331393	-2.66908250	1.98903595	H -0.33163642	-1.61267344	2.65913489
H 6.33427469	-1.80260948	0.68599549	H 0.03357098	0.07707662	2.19168562

β - β' top C_{α} - C_{β}

O 1.56313573	4.47419125	-1.46374462	C 3.34027649	5.20005645	-0.16133655
C 2.51478705	4.12974485	-0.55162887	C 2.70925205	2.86632103	-0.01949106
C 4.54572950	3.71443725	1.29172053	C 3.73951613	2.65486004	0.90668622

C 4.34831981	4.98915528	0.75910633	H 2.29019172	-3.66955172	-1.99230398
H 5.34031059	3.55335929	2.01199480	O 4.30204706	-1.87028180	-1.69501646
H 2.06481798	2.03883341	-0.29605260	O 3.11521901	-1.93579036	2.87104374
H 4.96837820	5.82782026	1.05018881	C 3.96760741	-2.08402879	-3.05992322
C 0.73348326	3.43590459	-1.95874806	H 4.67742147	-1.48898733	-3.63005210
H 0.03383642	3.90287874	-2.64816128	H 2.94809880	-1.74263866	-3.26002762
H 0.18156743	2.95853871	-1.14609498	H 4.07275993	-3.13921568	-3.32515405
H 1.32806188	2.68335143	-2.48557439	C 4.31320869	-2.39595491	3.50628669
O 3.13977740	6.43258619	-0.68793409	H 4.33211668	-1.93854668	4.49351333
H 2.40285607	6.37328601	-1.30814185	H 4.28370978	-3.48404096	3.60275676
C 3.98174075	1.25965593	1.42280097	H 5.18935914	-2.09097045	2.93195050
H 4.73963308	1.29878488	2.21730249	C 0.48294763	-4.66528935	-0.22136691
C 4.52010216	0.35993966	0.30121545	C -0.84829639	-3.93566541	0.08853029
H 3.80380234	0.33505777	-0.52662363	C -1.11239547	-3.30781672	-1.24427734
C 5.88916333	0.80216952	-0.18726067	C -0.37645632	-4.06263629	-2.29546729
H 5.84564268	1.85197328	-0.48051589	O 0.39595860	-5.03761065	-1.58772812
H 6.59380660	0.70763707	0.65165824	H 0.58935840	-5.59094078	0.35200332
O 6.33745372	0.07041669	-1.30315425	H -0.72195559	-3.18143517	0.87159525
H 6.01692048	-0.83396545	-1.21178869	H -1.74703382	-2.45364631	-1.42956012
O 4.68675240	-0.98729857	0.81590401	H 0.26901079	-3.40196244	-2.89081435
C 3.70059744	-1.89340630	0.55372599	H -1.03014022	-4.60454656	-2.98984884
C 1.66747600	-3.75535072	0.05309474	C -3.75737934	-3.56282573	0.05937657
C 3.47799570	-2.37138103	-0.74586963	O -3.09395999	-4.23996681	1.02419667
C 2.93524597	-2.41525533	1.59456705	C -1.93134606	-4.92273578	0.55637169
C 1.92770804	-3.33928576	1.35253694	H -3.87840072	-4.06448206	-0.89692669
C 2.46201759	-3.29244346	-0.99376581	H -2.20044070	-5.61463745	-0.25183731
H 1.33361177	-3.68749358	2.19136733	H -1.57503942	-5.49875599	1.41140360

C -4.08935240	-2.21006773	0.23140363	H -3.79656493	4.81071007	1.42158467
C -4.65852629	0.51747690	0.48539394	H -5.25300975	4.39432299	0.49328532
C -4.56738108	-1.47630248	-0.88155677	O -5.19961038	3.82405945	2.49328524
C -3.89318412	-1.55946040	1.47273019	H -5.72565232	3.02311566	2.39447735
C -4.19966871	-0.21379079	1.59227796	C -3.13051995	2.97614474	-0.54922512
C -4.82634540	-0.12469382	-0.75038634	H -2.49254216	3.85817790	-0.40721021
H -4.69027656	-1.98093757	-1.83060649	O -4.03144206	3.32207536	-1.57563785
H -3.52864186	-2.13761793	2.30974229	H -4.68047723	2.60394757	-1.62503976
O -5.22577662	0.68258385	-1.77028193	C -2.20843096	1.82440696	-0.95547967
O -4.06129751	0.50942410	2.73318413	C -0.28053118	-0.04827201	-1.76446829
C -3.73786876	-0.18984828	3.92023979	C -1.47754325	1.10103590	-0.00242211
H -3.74533154	0.55252838	4.71473386	C -1.98692760	1.56827472	-2.30284666
H -2.74484159	-0.64486232	3.85556160	C -1.02477642	0.63844069	-2.70658675
H -4.47995940	-0.96535369	4.12927327	C -0.53662568	0.16108617	-0.39818259
C -5.19171137	0.14330258	-3.08000394	H -1.63430343	1.27125309	1.05402754
H -5.44052247	0.96439161	-3.74929169	H -2.54609624	2.12687635	-3.04329270
H -5.93085954	-0.65435569	-3.19336574	H -0.82549993	0.45630982	-3.75643026
H -4.19120729	-0.23379048	-3.31281974	O 0.20828371	-0.61332688	0.43620764
O -4.97242601	1.84186059	0.58994879	O 0.69521375	-0.91459943	-2.14622075
O 2.76517978	0.74910909	1.93364673	H 1.03977292	-1.35358307	-1.35232231
H 2.94649130	-0.08194427	2.39481726	C 0.00106099	-0.43953664	1.82923213
C -3.88455474	2.76879743	0.76891608	H 0.66455510	-1.14358804	2.32643659
H -3.22924114	2.40028249	1.56045121	H 0.26773114	0.57495524	2.13317928
C -4.55338692	4.04097763	1.25814760	H -1.04201931	-0.66284150	2.08055916

β - β' topC_g-O

O 1.71932121	4.82809496	-0.80010033	C 2.79903627	4.23613729	-0.21549378
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C 5.13177348	3.29902587	0.95390260	C 2.77866580	-2.57138337	1.50593966
C 3.90786586	5.08970261	-0.07778332	C 1.72043865	-3.47081530	1.44176556
C 2.86537036	2.92359446	0.22366171	C 1.90433735	-3.49582482	-0.95793204
C 4.04634192	2.44841945	0.80692388	H 1.25485418	-3.78773344	2.36958840
C 5.06678109	4.61948383	0.50952152	H 1.57840634	-3.89176595	-1.90985188
H 6.04381353	2.93494399	1.41457232	O 3.66392339	-2.15426357	-1.95995019
H 2.01265140	2.25888743	0.13764027	O 3.16724492	-2.07787375	2.72976120
H 5.90452281	5.29682052	0.61891298	C 3.19560753	-2.48025602	-3.26206223
C 0.52567924	4.06713115	-0.86324652	H 3.85856930	-1.95638130	-3.94674460
H -0.22068163	4.69671102	-1.34372712	H 2.17002805	-2.12823900	-3.39876272
H 0.19491863	3.79702519	0.14332911	H 3.25766163	-3.55761353	-3.43644163
H 0.66727918	3.15622087	-1.45170683	C 4.40921284	-2.60866216	3.20668297
O 3.83080769	6.37141859	-0.51144607	H 4.59709856	-2.13357594	4.16748876
H 2.94674895	6.50860086	-0.87320710	H 4.32062234	-3.68975536	3.33878290
C 4.13808832	0.99803954	1.20752018	H 5.21392875	-2.37795356	2.50674878
H 5.01049793	0.86447318	1.86194615	C 0.06849350	-4.84961161	0.13515344
C 4.34523214	0.09818354	-0.02028769	C -1.24580184	-4.11827803	0.47203200
H 3.47495180	0.16768467	-0.68331308	C -1.52023694	-3.44355473	-0.89223004
C 5.63005010	0.42702911	-0.76538110	C -1.05195310	-4.53036240	-1.87242298
H 5.60739259	1.47252747	-1.07406997	O -0.12376921	-5.35766612	-1.17433270
H 6.46878827	0.29442012	-0.06584721	H 0.23739836	-5.70566329	0.79587836
O 5.81739097	-0.35015273	-1.92253299	H -1.08873542	-3.38754162	1.26872280
H 5.44282820	-1.22270886	-1.75828875	H -0.82446437	-2.59521497	-0.94870956
O 4.48011312	-1.27318992	0.44195022	H -0.57657580	-4.09571154	-2.75703851
C 3.40551783	-2.10804230	0.35193842	H -1.88944371	-5.15551276	-2.19948996
C 1.26886303	-3.92077042	0.20871199	C -2.87018228	-2.92407071	-1.26799384
C 2.97148128	-2.60338033	-0.88885659	O -3.38496809	-4.50140897	1.57937903

C -2.35245073	-5.08525100	0.89485538	H -3.18012484	2.34914406	1.85539670
H -3.21679320	-3.19435636	-2.26154230	C -4.54922463	3.98161408	1.74999095
H -2.74354427	-5.67448628	0.04981419	H -3.83221621	4.72881397	2.09591777
H -1.95531708	-5.83908687	1.60313305	H -5.20884433	4.44685546	1.01010089
C -3.48365316	-1.76966784	-0.68497858	O -5.26724129	3.54007591	2.88094164
C -4.44477439	0.67557382	0.28934024	H -5.78319675	2.77624267	2.60177027
C -4.17538488	-0.88493860	-1.53733385	C -2.97415076	3.28333442	-0.11382517
C -3.35061733	-1.44628588	0.67754008	H -2.35661075	4.12163564	0.23411149
C -3.86165917	-0.25042281	1.16165099	O -3.81371888	3.81555069	-1.11090335
C -4.61123539	0.33869233	-1.06008647	H -4.46637913	3.13145985	-1.32552688
H -4.26524987	-1.13578319	-2.58521478	C -2.03698750	2.20503310	-0.66201538
H -2.89144360	-2.15393562	1.35071318	C -0.31702388	0.22430797	-1.65451926
O -5.15480692	1.31588300	-1.83741351	C -1.29762281	1.40132404	0.21577633
O -3.77122780	0.13640999	2.46260129	C -1.88370002	2.01851671	-2.02918961
C -3.58868534	-0.88725016	3.42825675	C -1.02217537	1.03416648	-2.52498990
H -3.74901485	-0.41708537	4.39579589	C -0.46765637	0.40505399	-0.26900364
H -2.57679368	-1.30172507	3.39184454	H -1.39736775	1.52939687	1.28550179
H -4.31019328	-1.69424835	3.27612772	H -2.43582457	2.65028378	-2.71407293
C -5.22967835	1.07396167	-3.23165165	H -0.89162572	0.88750046	-3.59071520
H -5.64365933	1.97886509	-3.67114015	O 0.23208734	-0.47982676	0.49462651
H -5.89035229	0.22950465	-3.44530889	O 0.51286926	-0.75220346	-2.11513065
H -4.23452260	0.88250319	-3.64437904	H 0.92612089	-1.17847092	-1.34830074
O -4.84516088	1.91234272	0.70764860	C 0.11510470	-0.33258089	1.90155637
O 2.95421146	0.63823746	1.89144666	H 0.70968950	-1.12803085	2.34400559
H 3.08330127	-0.22965165	2.29961004	H 0.51487260	0.63268161	2.21974042
C -3.80431136	2.82990403	1.09913939	H -0.93323442	-0.43331577	2.20038241

β - β' top C_{β} - C_{γ}

O 1.62233517	4.89610993	-0.80642524	C 3.47108399	-2.03080908	0.39956857
C 2.69044545	4.32753982	-0.17889207	C 1.43860755	-3.96760176	0.27040268
C 4.99623926	3.43886100	1.07849211	C 3.08589401	-2.58479344	-0.83230861
C 3.77085283	5.20746422	0.01086080	C 2.85362873	-2.50188572	1.55562021
C 2.77086871	3.01403795	0.25482542	C 1.84841653	-3.45837458	1.49734498
C 3.93905565	2.56337714	0.88173309	C 2.07074515	-3.53938591	-0.89615355
C 4.91589610	4.76140843	0.64227480	H 1.39798990	-3.78358300	2.42901566
H 5.89828725	3.09306433	1.57156141	H 1.79073514	-3.96411757	-1.84946648
H 1.93948978	2.32870708	0.12972781	O 3.76651627	-2.12577414	-1.90561919
H 5.73155016	5.45814735	0.79002138	O 3.20089578	-1.97064867	2.77552146
C 0.46281013	4.09474050	-0.94841332	C 3.31976924	-2.48800104	-3.20618656
H -0.27638580	4.70270052	-1.46658531	H 3.95276481	-1.93185349	-3.89373641
H 0.08310040	3.80043383	0.03375329	H 2.27610410	-2.19602628	-3.34470683
H 0.67311629	3.19657471	-1.53573987	H 3.44459558	-3.56122944	-3.37243879
O 3.67997899	6.49001954	-0.41751324	C 4.46879073	-2.41895333	3.26995249
H 2.81041343	6.60741392	-0.81911853	H 4.61791763	-1.92105429	4.22595828
C 4.05234189	1.11121065	1.26860385	H 4.44417837	-3.50162790	3.41550471
H 4.92561123	0.98615066	1.92371282	H 5.26439028	-2.14859624	2.57395978
C 4.28485515	0.22872235	0.03202067	C 0.29247132	-4.96687761	0.25146666
H 3.40281726	0.25619533	-0.61900285	C -1.01533817	-4.28631571	0.70595630
C 5.54043886	0.62642090	-0.73013302	C -1.46564745	-3.10949237	-0.09305741
H 5.45479258	1.66730080	-1.04314545	C -0.42007025	-5.12968523	-2.05116485
H 6.39404870	0.54624532	-0.04052254	O 0.20322183	-5.67745867	-0.97766411
O 5.75658162	-0.14479724	-1.88580279	H 0.52278749	-5.75405279	0.97485720
H 5.44139074	-1.03859653	-1.71084971	H -0.82766626	-3.97372141	1.74374013
O 4.49732965	-1.13740464	0.48288575	H -0.85893741	-2.26883724	-0.39081909

H -0.56219234	-4.05746170	-2.09998937	O 2.87295813	0.72605836	1.94663325
H -0.31464268	-5.73097410	-2.94263091	H 3.01833276	-0.14146486	2.34941436
C -2.92554716	-3.25796264	-0.39413509	C -3.93695691	2.81791884	0.77295128
O -3.35957777	-4.26132396	0.51955035	H -3.38638399	2.32548407	1.57864972
C -2.27830844	-5.17032183	0.67425963	C -4.68223282	4.00188230	1.36050363
H -3.08480177	-3.61845268	-1.42552463	H -3.96708465	4.74860605	1.71194887
H -2.23865791	-5.86206353	-0.17541312	H -5.30548993	4.45386755	0.58136541
H -2.44209655	-5.73264006	1.59297469	O -5.44969253	3.60189927	2.47454949
C -3.65595328	-1.95385318	-0.20012997	H -5.89803240	2.78512868	2.22708948
C -4.59159506	0.62934963	0.14604595	C -3.00540127	3.21336098	-0.38266009
C -3.95432223	-1.18142262	-1.31483641	H -2.41494436	4.06731928	-0.02640039
C -3.87616501	-1.47897167	1.08987406	O -3.76248812	3.69885288	-1.46566826
C -4.35796870	-0.18442371	1.25969925	H -4.38336311	2.99431375	-1.70470116
C -4.43068208	0.11821080	-1.13937310	C -2.02399343	2.11852947	-0.81122594
H -3.78034718	-1.58282340	-2.30439204	C -0.16971267	0.18089441	-1.63240173
H -3.65672856	-2.12458147	1.92985144	C -1.32492833	1.35951676	0.13976532
O -4.72754700	0.97362557	-2.15251598	C -1.76532774	1.90472121	-2.15817969
O -4.59713408	0.40608306	2.45818332	C -0.84614837	0.93628612	-2.57062226
C -4.38008204	-0.36615046	3.62365155	C -0.40787529	0.40147479	-0.26417798
H -4.64677550	0.27504163	4.46036712	H -1.49425471	1.51431975	1.19783714
H -3.32975969	-0.66212785	3.70913001	H -2.28547101	2.50343275	-2.89514890
H -5.01153402	-1.25890991	3.62451974	H -0.64117666	0.76604549	-3.62119683
C -4.54650425	0.50490435	-3.47726126	O 0.32143858	-0.40558618	0.55406780
H -4.81997710	1.33274774	-4.12815461	O 0.71803045	-0.77798341	-2.01031809
H -5.19932959	-0.34904722	-3.67780784	H 1.09287322	-1.17368963	-1.20850231
H -3.50316105	0.22761494	-3.65219354	C 0.05462724	-0.33485872	1.94426827
O -4.97483764	1.93255450	0.31012215	H 0.69510089	-1.07759571	2.41496595

H 0.30919381 0.65359326 2.33344859 H -0.99892752 -0.57328223 2.13194707

β - β' topC_y-O

O 1.80691532 4.85730698 -0.77021010 H 5.39274014 -1.24165947 -1.74724064

C 2.85779065 4.23704549 -0.16270064 O 4.46638049 -1.31009363 0.45725397

C 5.13439256 3.23649928 1.06359219 C 3.41316553 -2.17262222 0.38495606

C 3.97444353 5.06924958 0.03101584 C 1.32162751 -4.03264186 0.27358137

C 2.88827697 2.91490105 0.25043542 C 3.00670388 -2.71923616 -0.84561213

C 4.04041469 2.40825987 0.86336271 C 2.78267410 -2.61052542 1.54664355

C 5.10532030 4.56714392 0.64588395 C 1.74270496 -3.53162272 1.49719657

H 6.02457651 2.84730665 1.54578957 C 1.96072978 -3.63753364 -0.89989940

H 2.02907879 2.26586976 0.12209886 H 1.27250226 -3.83030963 2.42878494

H 5.95011275 5.22759373 0.79657577 H 1.63879697 -4.05911253 -1.84255693

C 0.62772155 4.09096076 -0.94185752 O 3.69358727 -2.28241880 -1.92319791

H -0.09578166 4.73429015 -1.43918115 O 3.14869650 -2.07900470 2.76147044

H 0.23767147 3.77087725 0.02808661 C 3.21153636 -2.62126452 -3.21777098

H 0.81915570 3.20932329 -1.55925855 H 3.84574567 -2.07734178 -3.91392335

O 3.93269065 6.36109800 -0.37701075 H 2.17324624 -2.30029237 -3.33107789

H 3.06625896 6.51965839 -0.77109251 H 3.30258619 -3.69622633 -3.39370988

C 4.09094291 0.94991426 1.23972434 C 4.40477772 -2.55855090 3.25652851

H 4.95416643 0.78422709 1.89902951 H 4.57130455 -2.05596812 4.20723621

C 4.29111199 0.06068372 0.00269646 H 4.34958314 -3.63863218 3.41266184

H 3.40637666 0.11199866 -0.64343702 H 5.20553577 -2.31801011 2.55558027

C 5.55385160 0.41915446 -0.76679907 C 0.13353123 -4.97668463 0.22318121

H 5.49750607 1.46180106 -1.08074092 C -1.19316913 -4.21723288 0.46189048

H 6.40871368 0.31459522 -0.08193983 C -1.60917982 -3.19338969 -0.62376712

O 5.74040002 -0.35991063 -1.92232911 C -1.13649559 -3.46319984 -2.00785176

O 0.07512871	-5.78412768	-0.87726413	H -4.65438786	1.58883587	-4.10651389
H 0.21324297	-5.69142048	1.06783872	H -5.15042012	-0.07972456	-3.72685356
H -1.06734392	-3.67120051	1.40186882	H -3.42225015	0.38603754	-3.63885464
H -1.28471294	-2.19455863	-0.32559513	O -4.86720847	2.05526128	0.33936473
H -1.09135763	-2.65100897	-2.72146432	O 2.89181030	0.61170482	1.90966994
H -1.05069205	-4.48073826	-2.37569124	H 3.00419447	-0.25727884	2.31995265
C -3.19005901	-3.25492627	-0.52226671	C -3.81550341	2.90282322	0.83814320
O -3.49341883	-4.14737765	0.53581355	H -3.29729558	2.38409419	1.64831577
C -2.43738385	-5.08798790	0.59462616	C -4.53977064	4.09982674	1.42576679
H -3.58386594	-3.66327660	-1.46148258	H -3.81141240	4.81805718	1.80800613
H -2.50332426	-5.80650717	-0.23244124	H -5.12801896	4.58365829	0.63867950
H -2.50890003	-5.62122094	1.54321138	O -5.34848034	3.70694551	2.51292113
C -3.77327556	-1.89301190	-0.27248640	H -5.82470743	2.91625873	2.23535000
C -4.52974129	0.74332521	0.14559540	C -2.84957271	3.28765179	-0.29174576
C -4.01471214	-1.06747538	-1.36643577	H -2.23311556	4.11112665	0.09113990
C -3.94413254	-1.43250181	1.02898045	O -3.56832062	3.82207388	-1.37830189
C -4.33643645	-0.11027457	1.23398951	H -4.20890523	3.14491224	-1.64361718
C -4.39526735	0.25624167	-1.15461800	C -1.90900886	2.16039527	-0.72417721
H -3.88131758	-1.45729993	-2.36736309	C -0.13907981	0.14630315	-1.54535261
H -3.78091532	-2.11423234	1.85200786	C -1.27174093	1.34697575	0.22533256
O -4.63532805	1.15637349	-2.14340866	C -1.63417816	1.95993120	-2.06934999
O -4.53184410	0.45936791	2.45062034	C -0.75453297	0.95536019	-2.48137583
C -4.39422451	-0.36522078	3.59204844	C -0.40371842	0.34475182	-0.17798869
H -4.62011473	0.26850542	4.44633035	H -1.45797641	1.48945813	1.28205310
H -3.37301658	-0.74879721	3.68065583	H -2.10768903	2.59846080	-2.80443631
H -5.09569832	-1.20326306	3.55622496	H -0.52955873	0.79923561	-3.53020465
C -4.45058388	0.72318239	-3.47964753	O 0.24117465	-0.53192419	0.63989767

O 0.71897705	-0.83340546	-1.92851048	H 0.65008756	-1.15389983	2.51025890
H 0.98443408	-1.33365365	-1.14124040	H 0.39773415	0.59913832	2.36622170
C 0.04799556	-0.38156765	2.03575761	H -1.00953544	-0.52329993	2.28637404

β - β' topC $_{\alpha}$ -C $_{\beta}$ α -side

O -4.47503800	3.38868037	0.38716562	H -3.11778227	-3.20737785	0.31595246
C -4.54691256	2.09088474	-0.03433910	O -2.31722078	-2.81766288	2.18667993
C -4.98145288	-0.50737995	-0.89696218	H -1.36913463	-2.94372562	2.06599498
C -5.85803945	1.59573617	-0.13118476	O -0.75515780	-2.30952763	-0.14712960
C -3.46803734	1.28644054	-0.35816102	C 0.49890393	-1.77367143	-0.07375789
C -3.68483085	-0.02681115	-0.79022482	C 3.10592142	-0.75008201	0.05139896
C -6.06900284	0.29992554	-0.56404127	C 1.10179349	-1.50820744	1.16489993
H -5.15491635	-1.52088192	-1.24270570	C 1.24006472	-1.56239092	-1.23248918
H -2.45309805	1.66041055	-0.31520991	C 2.53157105	-1.05087166	-1.17760511
H -7.08736784	-0.05920058	-0.64495001	C 2.39206999	-0.99328199	1.22530391
C -3.18973500	3.97053064	0.48357442	H 3.05577302	-0.89606495	-2.11337158
H -3.34289623	4.99431532	0.81669834	H 2.86991896	-0.79236919	2.17461798
H -2.68915218	3.96939262	-0.48870541	O 0.33699979	-1.79786853	2.24632619
H -2.57480672	3.43465155	1.21244329	O 0.66126444	-1.80457827	-2.45590129
O -6.90947284	2.39091985	0.18638326	C 0.83215095	-1.46472561	3.53148831
H -6.56247650	3.25043328	0.45353479	H 0.04068614	-1.72874502	4.22915463
C -2.49126209	-0.90025449	-1.09176607	H 1.04283294	-0.39389567	3.59944895
H -2.81616993	-1.74989143	-1.70825205	H 1.73669267	-2.03391850	3.76156101
C -1.88520889	-1.46905000	0.20081294	C 0.53933287	-3.19308778	-2.77769064
H -1.53534205	-0.64642186	0.83390085	H 0.06985205	-3.24102232	-3.75831199
C -2.84897828	-2.36150799	0.96569314	H 1.53125723	-3.65017115	-2.82058898
H -3.75733232	-1.80315094	1.19381795	H -0.07929584	-3.70365857	-2.03765894

C 4.53366563	-0.22739492	0.13740930	H 4.92482302	2.13466744	2.25293690
C 4.82091524	0.95634093	-0.79644784	C 5.74328896	3.04865833	-0.12219991
C 4.52112779	2.20218764	0.07968787	O 6.58803275	2.50822769	-1.04202683
C 4.34664457	1.60665367	1.49541941	C 6.31615820	1.11048273	-1.10879882
O 4.84498502	0.27400206	1.42563061	H 5.77287716	4.12817696	-0.07265156
H 5.22171978	-1.05925491	-0.04296739	H 6.91799508	0.59901895	-0.34986112
H 4.22371972	0.94378125	-1.70605172	H 6.59972582	0.76348802	-2.10127185
H 3.60629063	2.71490052	-0.23001433	O -1.53599660	-0.12297921	-1.78303887
H 3.28771781	1.59666657	1.77863682	H -0.87017039	-0.70860163	-2.16895610

β - β' topC $_{\alpha}$ -C $_{Ph}$ phenyl-side

C 0.74042642	1.59654433	2.31488508	H 0.98562501	-2.33233872	3.51197034
C -1.10640396	0.06233575	1.07980685	H 1.95591564	-2.28039962	2.00449352
C 0.91149546	0.24043834	2.41559594	O -2.01986302	-0.72329966	0.43092574
C -0.27846753	2.26366122	1.68366266	C -1.93726444	-0.73981675	-1.00933343
C -1.23241675	1.45455087	1.04920272	H -1.78192522	0.28055631	-1.36741763
C -0.06236159	-0.54647955	1.78413312	C -3.31344792	-1.19245609	-1.46019022
H 1.75064810	-0.19379619	2.94144674	H -3.33493147	-1.27147935	-2.54905240
H -0.34627454	3.34341436	1.68463667	H -3.52303209	-2.17911750	-1.03402393
O -0.07065009	-1.90119209	1.78091625	O -4.29416860	-0.24679110	-1.09044688
O -2.30375325	1.91920047	0.35784215	H -4.11447510	-0.00362135	-0.17520268
C -2.52124908	3.31688094	0.34239457	C -0.81684245	-1.67953748	-1.47604193
H -3.43173670	3.47098804	-0.23169419	H -0.95261820	-1.82819505	-2.55366853
H -1.69125378	3.84031151	-0.14256301	O -0.99209189	-2.94977193	-0.88984945
H -2.65424747	3.70303526	1.35696068	H -0.97315988	-2.81162681	0.06866410
C 0.99502851	-2.56214221	2.44297486	C 0.59153596	-1.13253479	-1.23449547
H 0.82342828	-3.62651283	2.29757770	C 3.16286605	-0.16361011	-0.67366462

C 0.89055334	0.22648095	-1.40866199	O 2.55516941	2.01062635	-1.21844514
C 1.60298859	-1.99038037	-0.82612453	O 4.39567115	0.31609592	-0.37485829
C 2.88368486	-1.51071817	-0.54742310	H 4.38380128	1.27087539	-0.51263422
C 2.15622983	0.70707565	-1.11966765	C 1.58476599	2.96172654	-1.60551738
H 0.12692683	0.91714432	-1.74123578	H 2.08230870	3.92880407	-1.59146498
H 1.38358704	-3.04380392	-0.70700695	H 1.21627658	2.75456282	-2.61471763
H 3.67691812	-2.17477168	-0.22428158	H 0.74898153	2.96491281	-0.89867423

β -O-4 topC _{α} -C _{β} α -side

C 2.57185567	0.97479184	0.02164059	H 0.13182390	1.98286180	0.01054519
H 2.57367582	2.05346475	0.08309824	H 2.28889527	-1.76741473	0.08087933
O 3.81663122	0.44981939	-0.03520210	H 0.15274840	-2.97669464	0.02389836
H 3.77206960	-0.48811304	-0.24321069	O -2.29754147	0.73303969	-0.01143351
C 1.38719464	0.21881566	0.02443258	O -2.20935140	-1.90422017	-0.01987387
C -1.03938340	-1.21890474	-0.00343642	H -2.93019777	-1.26319379	-0.02581267
C 0.13525051	0.90024926	0.01454481	C -2.40373900	2.14261765	-0.00470817
C 1.36862051	-1.19578581	0.03403726	H -3.46730103	2.36870422	-0.01254233
C 0.16957879	-1.89374010	0.01459435	H -1.94543812	2.56200199	0.89557330
C -1.04333880	0.19319436	0.00092235	H -1.93041636	2.57184340	-0.89251702

β -O-4 topC _{α} -C _{β} β -side

O 4.23009943	1.58104703	-2.01006967	H 4.95334075	-2.21417020	1.50596609
C 4.36158618	0.58621459	-1.06541920	H 2.28854154	0.44769354	-0.55999561
C 4.78459344	-1.42773189	0.77729023	H 6.87775772	-1.25151119	0.25857751
C 5.65731453	0.10559508	-0.84802663	C 4.04691233	2.88845752	-1.44909848
C 3.28103234	0.04767659	-0.38322590	H 4.00104568	3.57899379	-2.28975987
C 3.48698559	-0.97827558	0.54028985	H 4.89477782	3.14013182	-0.80381281
C 5.86827914	-0.89999366	0.08570744	H 3.11522358	2.93506135	-0.88712338

O 6.70111470	0.62806488	-1.53660630	H 0.23632511	-2.70839814	4.82144415
H 6.33206834	1.23117175	-2.19488104	H -1.24387236	-3.56341609	4.31220066
C 2.31255955	-1.63754008	1.22348323	H 0.30161644	-3.86143975	3.45611754
H 2.66494942	-2.12388125	2.14337023	C -4.51554779	-1.34801627	0.30152080
C 1.69360191	-2.73325591	0.33868621	C -4.12126013	0.11472395	0.08297940
H 1.22345379	-2.26753997	-0.53521765	C -3.70798784	0.10018818	-1.39312648
C 2.68842613	-3.79820931	-0.09670891	C -4.74152373	-0.86481342	-1.98166994
H 3.50457208	-3.33181755	-0.64827243	O -5.12704687	-1.74671916	-0.91811066
H 3.10724743	-4.26762811	0.80588044	H -5.24664316	-1.48527968	1.10300242
O 2.10858333	-4.76279215	-0.94162245	H -3.30644050	0.42660231	0.73430332
H 1.19785552	-4.89779273	-0.65510491	H -2.69328918	-0.26858919	-1.53054533
O 0.67717563	-3.43605915	1.10175904	H -4.33705929	-1.46020123	-2.80390130
C -0.62060936	-3.03741368	0.94544704	H -5.63027030	-0.33286198	-2.33565001
C -3.23721439	-2.11811857	0.59410043	C -3.84853394	1.57801765	-1.76057323
C -1.33534671	-3.35571833	-0.21791260	O -4.99477920	2.01821192	-1.04501989
C -1.27419365	-2.34688746	1.96329128	C -5.25270674	1.14828030	0.06596754
C -2.57429035	-1.89014780	1.79406921	H -4.03918657	1.74437228	-2.82465022
C -2.63438866	-2.88702344	-0.39832136	H -6.22829049	0.67468113	-0.08252828
H -3.01785546	-1.29534077	2.58542326	H -5.28528101	1.74270863	0.98213670
H -3.18406359	-3.09178350	-1.30732076	C -2.57348054	2.28513337	-1.32211745
O -0.65273461	-4.10028642	-1.12231955	C -0.16256465	3.18295642	-0.28733484
O -0.58739464	-2.01220428	3.10554132	C -1.38043451	1.94939320	-1.96096495
C -1.24202361	-4.32672372	-2.38980035	C -2.57705707	3.10676364	-0.20300655
H -0.50295026	-4.88007765	-2.96459814	C -1.36038268	3.55474078	0.31855780
H -1.46233581	-3.37830297	-2.88903225	C -0.16728707	2.38900037	-1.43623993
H -2.15843069	-4.91552290	-2.29625588	H -1.40042010	1.30544690	-2.83137421
C -0.30673111	-3.11649339	3.97130082	H -3.52099978	3.36346544	0.25692378

O 1.05196261	2.07363007	-1.92998401	O 1.02155187	3.59150360	0.26939730
O -1.23517651	4.32312346	1.43058122	O 1.34698359	-0.65007847	1.53109310
C -2.41384575	4.62735176	2.15530374	H 0.75308488	-0.99991422	2.20974222
H -2.09319092	5.20455245	3.01950346	C 1.57230531	2.72015475	1.18997203
H -2.91078769	3.71260149	2.49100005	H 1.09605841	1.75136825	1.29348757
H -3.10249913	5.22276291	1.55011358	C 2.23963439	3.42598582	2.30780042
C 1.11513892	1.17228226	-3.02223800	H 2.78811825	2.71188361	2.92220429
H 2.17538876	1.03062947	-3.22045896	H 2.94634812	4.16428301	1.90793871
H 0.61977065	1.59033152	-3.90335257	O 1.29172676	4.07510733	3.15790521
H 0.65526760	0.21372151	-2.75951841	H 0.60876885	4.44329416	2.58376462

β -O-4 topC_α-C_{Ph} α-side

O -1.85880970	0.60694989	-1.77639271	H -3.35322443	2.15979318	-2.46558753
C -1.25581692	1.74565385	-1.29500307	C 1.65887819	2.83448406	0.86416647
C -0.14908726	4.11432232	-0.37542237	H 1.78028840	3.78142432	1.40921095
C -1.81852405	2.97015327	-1.68282066	C 2.88453178	2.62966684	-0.05685693
C -0.15771950	1.71310529	-0.45263254	H 2.60490717	1.95798100	-0.87179143
C 0.41323736	2.90280144	0.00943045	C 3.39322738	3.93994820	-0.62367507
C -1.25926500	4.15195667	-1.21494022	H 2.55737388	4.49704643	-1.05222298
H 0.27326505	5.04474569	-0.00992308	H 3.81310030	4.52742054	0.20490353
H 0.24708168	0.75527254	-0.13722122	O 4.34425070	3.75352029	-1.64479743
H -1.71128305	5.09035962	-1.51192296	H 4.87476907	2.98324829	-1.41043618
C -1.03558083	-0.15414922	-2.64855146	O 4.00036050	2.03732173	0.65851104
H -1.64752751	-0.97438218	-3.02030738	C 4.05012564	0.67079161	0.57317480
H -0.17588624	-0.56782960	-2.11237915	C 3.71036025	-2.08796694	0.34249354
H -0.68626553	0.46343501	-3.48213503	C 4.25838160	0.03593568	-0.65845607
O -2.89757491	3.01558264	-2.49686107	C 3.85669394	-0.11372232	1.70706560

C 3.68093249	-1.48699270	1.59650187	H -0.66937036	-3.91141396	-1.58943289
C 4.06649334	-1.33694823	-0.77620030	H 1.46191200	-5.57718847	-0.07253945
H 3.44380865	-2.04530725	2.49531883	H 1.03123166	-5.33876735	1.64072880
H 4.15673601	-1.83384338	-1.73206012	C -1.49015015	-2.55000736	-0.17307171
O 4.58452692	0.86060347	-1.68490194	C -3.56258706	-0.88990390	0.68732112
O 3.70838631	0.49283035	2.92996076	C -2.69342353	-2.53249205	-0.86737671
C 4.54290978	0.34110153	-3.00284307	C -1.30117057	-1.71248463	0.92453963
H 4.73567739	1.18576998	-3.66021670	C -2.33883278	-0.89280742	1.36773857
H 3.55549488	-0.07709190	-3.22096176	C -3.71714429	-1.68394258	-0.44784545
H 5.30896091	-0.42516775	-3.14683119	H -2.82418585	-3.18248497	-1.72270059
C 4.90921600	1.08835643	3.43107777	H -0.35944998	-1.72387656	1.45717686
H 4.65543566	1.52408348	4.39532788	O -4.91671646	-1.55223003	-1.08770803
H 5.67579616	0.32087802	3.56239888	O -2.27222086	-0.08920548	2.45045354
H 5.26522201	1.86407202	2.75055154	C -1.02916317	0.00390631	3.13078905
C 3.17853474	-3.50352237	0.15722679	H -1.18732345	0.71846631	3.93513097
C 1.71010614	-3.52383685	0.59007652	H -0.24416929	0.37514657	2.46751250
C 1.01259323	-2.90959156	-0.63312077	H -0.74928714	-0.96465335	3.55655142
C 1.90812891	-3.40553115	-1.78716675	C -5.12458380	-2.32242755	-2.25737622
O 3.13577954	-3.86756806	-1.21348144	H -6.11940110	-2.06521617	-2.61357797
H 3.79662644	-4.24265585	0.67313473	H -5.08271477	-3.39108514	-2.03158360
H 1.53297530	-2.95983377	1.50470569	H -4.38485168	-2.07583331	-3.02507711
H 0.99660647	-1.82049954	-0.59001397	O -4.65378786	-0.20136113	1.13486577
H 2.11382186	-2.60797929	-2.50755162	O 1.49881113	1.76744025	1.77147012
H 1.45981072	-4.24740288	-2.32085465	H 2.30219945	1.65009906	2.29698456
C -0.40381506	-3.51153861	-0.60305862	C -4.60734811	1.23855770	1.22015677
O -0.33775634	-4.60527264	0.32320154	H -3.84204932	1.54282638	1.93773211
C 1.01669924	-4.88202063	0.65119957	C -5.98928420	1.59601815	1.76658194

H -6.04869625	2.67566853	1.91150941	C -4.32241716	1.84083925	-0.10934324
H -6.74596406	1.29865605	1.02939423	H -4.09367386	2.89571622	-0.18256868
O -6.22409787	0.99114805	3.01743977	O -4.93171034	1.33649600	-1.21734426
H -6.01634532	0.05619180	2.91684405	H -5.10777708	0.38789373	-1.09322024

β -O-4 topC_g-C_{ph} phenyl-side

C -1.27967380	-1.71939174	0.00002217	H -2.64251411	1.35037734	0.00000792
C -0.56516764	0.90282986	-0.00003431	O 1.70204737	0.39152170	0.00004673
C 0.07043354	-1.44050898	-0.00012724	O -0.20603160	2.21240946	-0.00002143
C -2.28585483	-0.79249302	0.00008199	H 0.75721473	2.25889581	-0.00003109
C -1.90522419	0.55644688	0.00000071	C 2.75833254	-0.54885319	0.00006905
C 0.42685838	-0.09391666	-0.00007517	H 3.68028774	0.02748993	0.00002488
H 0.81442954	-2.22683276	-0.00025732	H 2.71814233	-1.17721963	0.89443211
H -3.33204892	-1.07152080	0.00023003	H 2.71813849	-1.17731813	-0.89423201

β -O-4 topC_g-O β -side

C -2.30980850	0.81872639	0.20553722	C -0.24780296	-0.57151195	-0.24413912
H -1.87259652	1.14328439	1.14491596	C 2.50887102	-0.89658882	0.10219522
C -3.71341711	1.21040910	-0.12213855	C 0.59022723	0.55028272	-0.18565383
H -3.93458790	2.21624246	0.23570496	C 0.30761319	-1.83955547	-0.13815369
H -3.85915746	1.19502950	-1.21038437	C 1.68171761	-2.00150001	0.03934484
O -4.66210110	0.35278729	0.51053646	C 1.95530214	0.38887037	-0.01692759
H -4.42688969	-0.54943535	0.26510004	H 0.16270010	1.54137381	-0.27747237
C -1.73570501	-0.38492055	-0.47336052	H -0.32965051	-2.71205243	-0.20786187
H -1.92713081	-0.30909190	-1.55050403	H 2.12656584	-2.98499085	0.12688091
O -2.48670089	-1.55286126	-0.09125734	O 2.87399024	1.39607811	0.05660235
H -2.27443942	-1.74252966	0.83056666	O 3.84393394	-1.04858101	0.27600352

H 4.24656291 -0.17206281 0.28829450
C 2.40284837 2.72395448 -0.06374520
H 3.27721928 3.36564610 0.01298212

H 1.91803178 2.87806728 -1.03200800
H 1.70131899 2.96213687 0.74095304

β-O-4 topC_β-O_β-side

O 4.95699159 2.62062819 -0.88140535
C 4.76653199 1.43412155 -0.24360859
C 4.66193843 -0.95301884 1.16217823
C 5.94712528 0.86411194 0.25901116
C 3.54531201 0.79919844 -0.06092043
C 3.49244010 -0.40926226 0.64267782
C 5.88913269 -0.32564389 0.96263805
H 4.62117210 -1.87342236 1.73538551
H 2.62973046 1.25575580 -0.41732712
H 6.80797522 -0.73652822 1.36228252
C 3.80991593 3.26731588 -1.41870702
H 4.16493619 4.20840952 -1.83237897
H 3.05528968 3.45252374 -0.65169651
H 3.37026093 2.65858707 -2.21391590
O 7.13389617 1.49253235 0.07395819
H 6.96059306 2.30840085 -0.41181987
C 2.17567683 -1.12980435 0.85428649
H 2.19152557 -1.59700602 1.84583817
C 1.88656974 -2.25615164 -0.15036960
H 1.32320854 -1.83242803 -0.98945494
C 3.07612286 -3.01474830 -0.70768637
H 3.77008250 -2.32349781 -1.18645123

H 3.60508592 -3.52090217 0.11097440
O 2.64634009 -3.93802542 -1.68370853
H 1.81643193 -4.31913475 -1.37164787
O 1.07673181 -3.27533309 0.47962327
C -0.25668243 -2.99055440 0.58635624
C -2.93563325 -2.23811096 0.70566066
C -1.09047644 -3.17818085 -0.52231043
C -0.79742215 -2.51899663 1.78006271
C -2.13545071 -2.14562297 1.83730841
C -2.43077737 -2.80096753 -0.46533757
H -2.50795334 -1.71460081 2.76068760
H -3.08344702 -2.90785699 -1.32135729
O -0.47260274 -3.68999432 -1.61923191
O -0.00809727 -2.32539048 2.87784417
C -1.23372092 -3.81494714 -2.80425440
H -0.55584721 -4.21401037 -3.55516413
H -1.61038760 -2.84014204 -3.13153689
H -2.07340039 -4.50115155 -2.66234867
C 0.51951500 -3.52277483 3.44678708
H 1.10356429 -3.21705485 4.31311304
H -0.29603619 -4.17699187 3.76813377
H 1.15668080 -4.04625078 2.73187527

C	-4.26840416	-1.50611232	0.69463156	C	-2.65922585	3.30701857	0.19535500
C	-3.95040066	-0.01185974	0.56845855	C	-1.44593524	3.86277582	0.57013532
C	-3.76935065	0.12311755	-0.94668378	C	-0.30645585	2.45454521	-1.12209046
C	-4.86447996	-0.81317814	-1.46467415	H	-1.60129772	1.23105044	-2.29894582
O	-5.05592519	-1.80722557	-0.45120382	H	-3.58786016	3.58142486	0.67659603
H	-4.85926984	-1.75166683	1.58095103	O	0.86542064	2.07705768	-1.64373383
H	-3.04884466	0.26333984	1.11475181	O	-1.28841656	4.78198245	1.52156829
H	-2.78474609	-0.21003316	-1.26368574	C	-2.44432346	5.25141964	2.19255754
H	-4.58395517	-1.30843368	-2.39767457	H	-2.09435095	5.99727922	2.90115487
H	-5.80782577	-0.27951104	-1.61877141	H	-2.93990249	4.43663433	2.72794269
C	-3.99349818	1.62007704	-1.14321726	H	-3.14425534	5.70774222	1.48746478
O	-5.03966061	1.94613827	-0.24100889	C	0.87259164	0.92721197	-2.47587786
C	-5.08889377	0.98242170	0.82519803	H	1.91978693	0.69558422	-2.66272357
H	-4.33489158	1.87927265	-2.15082980	H	0.36557718	1.12640356	-3.42403700
H	-6.06743881	0.49389236	0.79932455	H	0.39920862	0.09052358	-1.95396140
H	-4.97619992	1.50314543	1.77845448	O	0.90977089	3.87255818	0.32383405
C	-2.69860699	2.35151152	-0.82220873	O	1.05741960	-0.25576308	0.74947205
C	-0.18533962	3.44150432	-0.04745222	H	1.10273903	0.38725339	1.46430190
C	-1.53127585	1.96026347	-1.50316488				

β -O-4 topO-C_{PhO}-side

O	-2.17096352	1.34155916	0.10560108	O	-4.55449142	0.59546263	-1.14840456
C	-2.26913064	0.08355285	-0.38135194	H	-4.45354587	1.50213669	-0.84438090
H	-2.00972191	0.04302666	-1.44952034	C	-1.48043165	-0.94007948	0.46018219
C	-3.81261521	-0.23998279	-0.31417729	H	-1.83140664	-1.94523623	0.21183827
H	-3.92918882	-1.25963446	-0.68262440	O	-1.78806205	-0.75356273	1.82755653
H	-4.11845080	-0.18830003	0.73350804	H	-1.61044246	0.17036432	2.03872467

C 0.00522494	-0.87132074	0.17278585	H 2.66335861	-2.87458548	-0.55917185
C 2.75919962	-0.76901547	-0.29883923	O 2.81094569	1.53501862	-0.01212625
C 0.67864066	0.35820376	0.21159262	O 4.09203945	-0.71127710	-0.53030622
C 0.72061730	-2.02688959	-0.10396190	H 4.36985891	0.20967151	-0.45626182
C 2.09455584	-1.97931861	-0.34116478	C 2.16517627	2.76614417	0.25184067
C 2.04219013	0.40790328	-0.01855680	H 2.93773470	3.52998665	0.20989468
H 0.12758255	1.26919456	0.41633019	H 1.40062793	2.97362205	-0.50213735
H 0.20883981	-2.98225710	-0.13042708	H 1.70844526	2.75922185	1.24556694

β-O-4 topO-C_{Ph} phenyl-side

O -3.43228931	3.67398102	0.54626726	H -2.14813169	-1.71701775	-1.11765168
C -3.54241327	2.45443712	-0.04657483	C -2.35792124	-1.75375981	1.01772265
C -3.99187002	0.08712217	-1.42514385	H -1.84442364	-1.26378070	1.85250307
C -4.61443104	2.36034339	-0.95303385	C -3.84390762	-1.86585089	1.31772163
C -2.71053557	1.36821468	0.16667413	H -4.26831056	-0.87443789	1.47221749
C -2.93826967	0.17322013	-0.52738635	H -4.34997440	-2.32587494	0.45691372
C -4.83350162	1.17994412	-1.63807349	O -4.06395474	-2.60761999	2.49619130
H -4.15728456	-0.83187363	-1.97676436	H -3.50677936	-3.39138995	2.44740920
H -1.85234043	1.44466108	0.82270477	O -1.92295501	-3.14105068	0.96830418
H -5.65639662	1.13343609	-2.34048359	C -0.61542821	-3.30319504	0.60382182
C -2.35560365	3.87064038	1.44786465	C 2.00302820	-3.10276545	-0.32010377
H -2.43513704	4.89804132	1.79470218	C 0.41782108	-2.95938219	1.49249829
H -1.39965987	3.72498178	0.94002275	C -0.30043364	-3.69510730	-0.69911232
H -2.43799850	3.18702289	2.29804414	C 1.01090098	-3.58786592	-1.16058877
O -5.41637325	3.43221626	-1.16198682	C 1.72569582	-2.85285343	1.02451629
H -5.08803148	4.15720769	-0.61578206	H 1.20765620	-3.81034719	-2.20354378
C -2.02549306	-1.00516840	-0.29226789	H 2.52842060	-2.53047272	1.67341083

O 0.02084489	-2.65178748	2.74748228	H 4.93198802	1.30485070	-0.41798787
O -1.27215981	-4.04861196	-1.58631979	H 5.04287881	-1.07310466	-2.35799343
C 1.00003483	-2.15812285	3.64258724	H 3.69696295	-0.78066310	-3.48647127
H 0.47885400	-1.96326065	4.57654947	C 2.94943578	2.09945013	-0.52631845
H 1.43912632	-1.22899490	3.26538486	C 1.04670789	3.87799867	0.22932380
H 1.78812211	-2.89753062	3.81001776	C 3.22637365	2.99523465	0.50492862
C -2.07951579	-5.16268156	-1.20365428	C 1.72585265	2.10380321	-1.19179771
H -2.73134087	-5.36581592	-2.05085478	C 0.73432180	3.01455879	-0.79990439
H -1.44653186	-6.03325279	-1.01151398	C 2.24708576	3.91957569	0.89774421
H -2.67463444	-4.93040232	-0.32035916	H 4.19378342	2.96607215	0.99089805
C 3.30775036	-2.61831753	-0.92098306	H 1.55472165	1.40425787	-1.99916017
C 3.08888626	-1.17732829	-1.40451266	O 2.39608506	4.83990521	1.88245039
C 3.50305903	-0.33522878	-0.19066836	O -0.50026349	3.10763518	-1.33862386
C 4.61665265	-1.19800707	0.41631502	C -0.83487056	2.19831617	-2.37959511
O 4.35267547	-2.54935048	0.03866076	H -1.88489774	2.37914731	-2.60393782
H 3.62595253	-3.28492088	-1.72835387	H -0.70979580	1.16724736	-2.04257982
H 2.05510258	-0.99919837	-1.70362495	H -0.22398888	2.39364693	-3.26619690
H 2.68555344	-0.18713081	0.51478049	C 3.64480716	4.88741821	2.54195276
H 4.64610901	-1.14095831	1.50732653	H 3.56795831	5.68978982	3.27190148
H 5.60023335	-0.90774056	0.03077882	H 4.45397608	5.10966352	1.83982829
C 3.95362414	1.00571516	-0.81322335	H 3.85614670	3.94555522	3.05785008
O 4.07494081	0.76616678	-2.21493231	O -0.69558450	-0.48293632	-0.28130156
C 4.04252834	-0.63117093	-2.46361203	H -0.06784560	-1.21091683	-0.23221886

S.4.Optimized geometries of the radical species produced from the RSSRRSSR stereoisomer of MC2

4-O-5C₂-OC₂-side

C 3.86666386	-0.75107923	1.67601687	H -0.50517190	0.17488673	1.71442804
C 4.18579296	1.05296733	-0.44619127	H -0.70940127	-0.90545945	-1.81716437
C 3.09236477	-0.87272463	0.51862022	C -2.33737894	-0.52592750	-0.47445304
C 4.79913870	0.28068786	1.78435167	C -5.04610745	0.04497078	-0.07285711
C 4.91950326	1.13936881	0.72020437	C -3.30447231	-1.50873185	-0.65093909
C 3.24629806	0.02017856	-0.53483267	C -2.73334088	0.76150443	-0.10228842
H 5.41088272	0.39067033	2.67247505	C -4.07564974	1.04215657	0.10156436
H 2.63957901	-0.07093142	-1.42754355	C -4.65457223	-1.22580211	-0.45430193
H 3.74612199	-1.46042823	2.48823409	H -3.01539502	-2.50924483	-0.95526541
C 2.03246559	-1.93928085	0.45793203	H -1.97460173	1.52438792	0.01186325
O 1.79112090	-2.32244220	-0.88455357	H -5.41741674	-1.98228281	-0.59119595
C 0.53579378	-2.97094732	-0.88517560	O 4.31460796	1.89719094	-1.49407329
C -0.35419636	-2.09168109	-0.00812055	O -4.58617609	2.25417186	0.47307745
C 0.64031090	-1.53020598	1.04264064	O -6.35811301	0.32583616	0.12866098
H 2.38409840	-2.81891270	1.01637124	C -3.67411184	3.32200547	0.64159611
H 0.19783100	-3.05758774	-1.91826493	H -3.13884282	3.52699449	-0.28968899
H 0.62916010	-3.97791147	-0.45407932	H -4.26833133	4.18864054	0.92148815
H -1.17465018	-2.65004776	0.44032663	H -2.95490560	3.09776358	1.43455171
H 0.50439331	-1.96246103	2.03413743	C 5.28142605	2.92060580	-1.33900767
C 0.33234460	-0.03649103	1.03543466	H 5.25994092	3.50313475	-2.25705145
O -0.03498434	0.24609399	-0.30465707	H 6.27806098	2.49368619	-1.19177615
C -0.86703134	-0.81952345	-0.73777387	H 5.03569082	3.56033306	-0.48591448
H 1.17761210	0.60023047	1.29526395	H -6.42774713	1.25542995	0.37665078

4-O-5C₄-OO-side

O -4.11085138	2.93153970	1.08236810	C -3.57530372	-0.90686346	-0.08493656
C -3.88093344	1.75254558	0.76037563	C -4.92002355	1.06113558	-0.00332812

C -2.67442558	1.02471164	1.06383961	C 5.24999437	1.28219533	-0.78899129
C -2.52396193	-0.25922357	0.63296061	C 3.86350394	-0.50632618	0.07514663
C -4.76047455	-0.27132493	-0.39984632	C 3.21533742	0.68048823	-1.91872742
H -3.46648894	-1.93854005	-0.40288444	C 4.35559276	1.47538357	-1.82698261
H -1.91130293	1.52247509	1.64787851	C 5.00025669	0.28276357	0.16346018
C -1.26404214	-1.05520527	0.93203458	H 3.65653286	-1.28369400	0.79811792
O -0.28933233	-0.29201969	1.60451690	H 2.52288302	0.83375852	-2.73998604
C 0.48610638	0.41524440	0.63421025	H 4.56837794	2.24741834	-2.55589832
C 0.39859582	-0.37757082	-0.68502685	O -5.70114793	-0.92676847	-1.13391159
C -0.55680028	-1.54324903	-0.34058139	O -6.00339111	1.76456446	-0.30036240
H -1.53017929	-1.88901811	1.59013511	O 5.95904378	0.18729552	1.13124301
H 0.09204106	1.42708111	0.50277302	O 6.36437884	2.04904217	-0.69569242
H 1.50266156	0.48152782	1.02120252	C 5.77289272	-0.78739643	2.13999536
C 0.41244344	-2.72587656	-0.09916725	H 5.74230114	-1.79172481	1.70859118
O 1.72947799	-2.20331478	-0.15661929	H 4.85004097	-0.59943009	2.69596590
C 1.69651046	-1.11603219	-1.06178115	H 6.62697205	-0.70109699	2.80742152
H 0.28597420	-3.48897950	-0.87619486	C -6.97268365	-1.07522401	-0.50228710
H 0.28363662	-3.18926930	0.87990093	H -6.85853191	-1.59408156	0.45395453
H 1.58802533	-1.49856260	-2.08912778	H -7.57433537	-1.68066482	-1.17654217
H 0.03693802	0.24397239	-1.50376328	H -7.45147618	-0.10794070	-0.34737471
H -1.25660716	-1.76499727	-1.14544697	H -5.85325252	2.64865561	0.08781126
C 2.96153807	-0.30444140	-0.97265545	H 6.85562731	1.76599558	0.08485963

4-O-5O-C₅O-side

C 3.48079149	-0.83813154	1.72776798	C 4.42016580	0.14158608	1.81129720
C 4.02980858	0.70303476	-0.56251834	C 4.76006348	0.97916083	0.67798319
C 2.78360834	-1.06729975	0.50808656	C 3.06242442	-0.30620841	-0.60721375

H 4.96882989	0.34082445	2.72393621	C -5.28016565	0.20617350	-0.07517743
H 2.52737907	-0.47413413	-1.53277524	C -3.61540908	-1.44035825	-0.62123068
O 5.62307269	1.87275001	0.76580125	C -2.93565031	0.81085906	-0.11866240
H 3.25269491	-1.45623239	2.59062389	C -4.26299060	1.15930837	0.07944009
C 1.69325129	-2.09676900	0.49063132	C -4.95020299	-1.08937033	-0.43085847
O 1.42371046	-2.51637612	-0.83185597	H -3.37472318	-2.45963503	-0.90497663
C 0.13637673	-3.10130239	-0.80352392	H -2.14215640	1.53978702	-0.02015711
C -0.70033834	-2.14902139	0.04805409	H -5.74842991	-1.81103386	-0.55290574
C 0.32546636	-1.60807249	1.07923176	O 4.21510628	1.36562394	-1.69972104
H 2.02048934	-2.96648075	1.08015277	O -4.71475550	2.40083947	0.42663364
H -0.21209349	-3.20408708	-1.83140923	O -6.57664237	0.55307002	0.12009926
H 0.18331455	-4.09681182	-0.34039412	C -3.75323538	3.42740041	0.57734882
H -1.54681907	-2.64835402	0.51725982	H -3.20896809	3.59063680	-0.35695049
H 0.17728838	-2.00908207	2.08182928	H -4.30603873	4.32574011	0.84147250
C 0.08803129	-0.10157461	1.03149695	H -3.04578687	3.18346423	1.37503691
O -0.26336613	0.16009093	-0.31582697	C 5.14738513	2.44225835	-1.83818895
C -1.14892142	-0.87395559	-0.71915306	H 5.04139441	2.75818112	-2.87356597
H 0.95967387	0.50486784	1.27679007	H 6.16267463	2.10443949	-1.63869221
H -0.73881819	0.16538850	1.70374669	H 4.90313653	3.25647006	-1.15827997
H -0.99566685	-0.99900261	-1.79522945	H -6.60247035	1.48942951	0.35068453
C -2.60244385	-0.50144448	-0.46435060			

4-O-5O-C₅C₅-side

C -3.97611135	1.57965739	1.38125838	C -2.68339180	-0.26614933	0.67513939
C -3.71877035	-0.58349695	-0.20544384	C -4.87331401	0.18610504	-0.29471181
C -5.01102590	1.32641371	0.51620680	H -3.65965695	-1.44996579	-0.85487243
C -2.82440878	0.84794943	1.50893613	H -2.04994450	1.09497919	2.22534140

C -1.44321582	-1.14545472	0.77652976	C 4.16580793	1.78830996	-1.54160283
O -0.42706873	-0.54168315	1.55166104	C 4.79777982	0.26551324	0.21346195
C 0.28972342	0.35730894	0.70586962	H 3.43972986	-1.37571277	0.56865231
C 0.19386686	-0.20117575	-0.72801544	H 2.33026256	1.32712658	-2.55291647
C -0.77036074	-1.40212429	-0.57828585	H 4.38611154	2.67244707	-2.12682530
H -1.71027328	-2.07892617	1.28085402	O -5.82540896	-0.14300681	-1.21420039
H -0.15613530	1.35585647	0.75615304	O -6.12411359	2.10087368	0.39053201
H 1.31243457	0.40718624	1.07858067	O 5.75423001	-0.00395907	1.15080872
C 0.18757570	-2.61718500	-0.57273121	O 6.17683467	2.14348492	-0.32631853
O 1.51054544	-2.10603848	-0.54099822	C 5.56254190	-1.14281939	1.96845380
C 1.48414626	-0.87347413	-1.23461201	H 5.52461276	-2.05308513	1.36371503
H 0.04911516	-3.21824206	-1.47934582	H 4.64136409	-1.05217388	2.55097070
H 0.06022856	-3.25654964	0.30173900	H 6.41780209	-1.18322323	2.63879629
H 1.36963485	-1.06390247	-2.31373624	C -7.07760251	-0.54293734	-0.66196373
H -0.16704034	0.55224519	-1.42765886	H -6.94295765	-1.42195778	-0.02441463
H -1.48886533	-1.46910436	-1.39319783	H -7.71414316	-0.79831700	-1.50670940
C 2.75669237	-0.10172192	-1.00793801	H -7.53109704	0.26750751	-0.08981495
C 5.05665173	1.41234233	-0.55181167	H -6.04827889	2.85002068	0.98933404
C 3.65514134	-0.48765951	-0.01000507	H 6.66615863	1.72306463	0.39092381
C 3.02007172	1.02949131	-1.76997527			

β-β' Cleavage

C 1.57703434	3.40225063	-2.22315188	C 1.04827563	2.91405060	0.06882008
C 2.31870124	2.38089451	0.26081354	H 3.53666477	2.76045411	-2.87397467
C 0.66163159	3.40798794	-1.17121125	H 0.35250489	2.91116846	0.89749683
C 2.83324373	2.83516518	-2.05344728	O 4.41231971	1.64529488	-0.72102100
C 3.19532193	2.29953173	-0.82726243	C 4.36062933	0.28829653	-0.45413487

C 4.45495111	-2.37441817	0.26351210	C -3.35479110	2.18010629	-0.82625672
C 5.58378334	-0.26945177	-0.08519803	C -1.34017583	3.37454786	-2.66076508
C 3.20218928	-0.46816563	-0.49269058	H -0.70934706	5.02479144	-1.49612429
C 3.23907907	-1.79932011	-0.09324821	H -3.32460866	3.73878451	0.62673943
C 5.62779375	-1.62456784	0.25369142	H -3.28273053	4.30686861	-1.04233003
H 4.52084572	-3.41043422	0.57917773	H -4.37367835	2.08625671	-1.18007601
H 2.27021292	-0.01728765	-0.80376355	H -1.56376956	4.03870116	-3.48649212
C 1.93284503	-2.54995099	0.09510842	C -1.45866351	1.89810124	-2.86248240
O 0.86764052	-1.94972555	-0.62838205	O -1.26627891	1.19679493	-1.65322862
C 0.16033123	-1.01899203	0.21309378	C -2.44229536	0.99498341	-0.85298144
C 0.80097352	-1.09295022	1.60646395	H -0.67680055	1.54272314	-3.54769984
C 1.49193015	-2.45961734	1.56233861	H -2.42382737	1.63948653	-3.32320558
H 2.03146500	-3.58329990	-0.25180373	H -2.02339921	0.85238134	0.15284401
H 0.20651766	-0.01870523	-0.22545372	C -3.14027452	-0.29334605	-1.27201203
H -0.88627193	-1.33462140	0.24654789	C -4.31603518	-2.74683340	-1.93970897
C 0.34142875	-3.40738917	1.95736434	C -4.46299415	-0.56000693	-0.94035139
O -0.68509479	-2.61253144	2.55788127	C -2.39728127	-1.27300556	-1.94460450
C -0.22975936	-1.27513057	2.71587123	C -2.97535276	-2.48897702	-2.26738357
H 0.66849444	-4.17024742	2.66821696	C -5.05116119	-1.77999736	-1.28070112
H -0.08833355	-3.90002030	1.08002698	H -5.04875018	0.16771484	-0.39111855
H 0.26952943	-1.17358984	3.69029818	H -1.36254421	-1.07040252	-2.18822932
H 1.48492952	-0.26423473	1.79019227	H -6.08460516	-1.99482616	-1.03511647
H 2.33643489	-2.53327063	2.24754727	C -1.37757831	-0.29527061	2.64704435
H 1.29498514	3.79838748	-3.19255116	C -3.44868581	1.56533525	2.47235277
C -0.75371847	3.93158031	-1.39506432	C -2.69111935	-0.73556734	2.47536800
O -1.50013043	3.63285698	-0.21543501	C -1.11114773	1.06845302	2.72714817
C -2.90263673	3.52870833	-0.36336312	C -2.14397165	1.99941924	2.63590491

C -3.72073284	0.19221883	2.39413528	C -0.97207816	-3.35142751	-3.21050591
H -2.87941997	-1.79824533	2.40531405	H -0.39271623	-3.12832039	-2.31060740
H -0.08852049	1.41231351	2.84970744	H -0.64558120	-4.29172538	-3.64902014
H -1.94832124	3.06437282	2.68149111	H -0.83913021	-2.54418555	-3.93691024
O 6.79641137	-2.20498389	0.65475740	C 7.79574419	-2.29048153	-0.35740539
O 6.70801512	0.49337868	-0.01877521	H 7.42546559	-2.87959671	-1.20198858
O 2.60751752	1.87355375	1.49326237	H 8.64566583	-2.79694952	0.09591534
O -2.34831941	-3.52000099	-2.90271684	H 8.09608080	-1.29839804	-0.69771951
O -4.87909590	-3.93797657	-2.26587747	C 3.88323399	2.17818080	2.05637429
O -5.04516520	-0.10581740	2.24254871	H 3.73474929	2.24363197	3.13336175
O -4.46597259	2.46532651	2.37899273	H 4.25102102	3.13517711	1.67950702
C -5.40738486	-1.47676156	2.27504671	H 4.60605813	1.38943788	1.83866351
H -5.12042082	-1.92507955	3.23037191	H 6.47147183	1.39041801	-0.28472530
H -4.93820677	-2.02055071	1.45158448	H -5.29001942	1.96886904	2.30157029
H -6.48923536	-1.50651678	2.16383302	H -4.20533304	-4.46988776	-2.70667625

β - β' bottom C_{α} - C_{β}

C 1.81866875	3.74025549	-1.79966606	C 4.44181518	-2.43107088	-0.03610882
C 2.49954609	2.33256041	0.52407544	C 5.65813635	-0.34995856	-0.14931648
C 0.86393119	3.58934238	-0.76564869	C 3.27164349	-0.40216199	-0.57600084
C 3.04888192	3.12161435	-1.70103062	C 3.25194090	-1.76930800	-0.32567136
C 3.38543668	2.38836553	-0.56500478	C 5.64485262	-1.73509360	0.03588110
C 1.24574004	2.90208793	0.40880308	H 4.46316894	-3.49760837	0.16247679
H 3.76255140	3.15574683	-2.51554814	H 2.36052784	0.11922841	-0.83509913
H 0.54979255	2.80543842	1.23156789	C 1.91808459	-2.48685768	-0.22145992
O 4.57135541	1.67197925	-0.56055885	O 0.87168672	-1.76759273	-0.85766778
C 4.46109710	0.29660156	-0.45274175	C 0.21072760	-0.91246222	0.09327772

C 0.83017981	-1.19759937	1.46873507	H -0.55465855	2.38926366	-3.34580795
C 1.48102670	-2.56752082	1.24826179	H -1.69643889	1.09117298	-3.76549531
H 1.97818302	-3.47260766	-0.69413877	H -2.02084689	1.20698573	0.06651066
H 0.31517108	0.13056514	-0.21385057	C -3.16658791	-0.01850615	-1.28046211
H -0.85183585	-1.16870537	0.08450605	C -4.57266075	-2.40052672	-1.70260618
C 0.30531586	-3.52573667	1.51723140	C -4.49858616	-0.13117184	-0.90358278
O -0.69248051	-2.79502275	2.23311688	C -2.53209467	-1.11307833	-1.88012174
C -0.22279062	-1.48668006	2.53579859	C -3.22415962	-2.29664399	-2.07783501
H 0.61059089	-4.39205172	2.10913875	C -5.20320822	-1.31470545	-1.12314973
H -0.14244140	-3.87633541	0.58160803	H -5.00231246	0.69025075	-0.40690755
H 0.25557758	-1.49422528	3.52549612	H -1.48955582	-1.02555366	-2.15992041
H 1.53916530	-0.42498668	1.76650125	H -6.24414136	-1.41140750	-0.83785135
H 2.32231264	-2.75356946	1.91581885	C -1.36492965	-0.49558479	2.54299184
H 1.55887012	4.29184227	-2.69618104	C -3.42899637	1.37766471	2.46085010
C -0.45793336	4.04257225	-0.92309881	C -2.68236890	-0.92279941	2.36991735
O -1.36029507	3.72730420	0.02318445	C -1.09320326	0.86103369	2.69223398
C -2.73169625	3.69920326	-0.36234249	C -2.12294639	1.79928269	2.64585164
C -3.07633257	2.54849558	-1.32813189	C -3.71028871	0.00936780	2.34471949
C -2.62056636	2.75093166	-2.74090595	H -2.87550991	-1.97985838	2.24936695
H -0.80396903	4.57472105	-1.80330206	H -0.06882962	1.19295885	2.83027737
H -3.28140512	3.56950030	0.57078215	H -1.92280921	2.86080864	2.73485082
H -3.00597751	4.66152686	-0.81116516	O 6.78670526	-2.40535546	0.36919287
H -4.16285457	2.43381016	-1.28193811	O 6.81232437	0.35363163	0.00353937
H -3.15334027	3.31586681	-3.49181696	O 2.78058077	1.65278911	1.67334456
C -1.45600610	1.85996600	-3.01418426	O -2.70543840	-3.43371165	-2.62405899
O -1.15759391	1.26056977	-1.76033345	O -5.24747087	-3.56235395	-1.89970790
C -2.34826140	1.22782378	-0.97744422	O -5.03751189	-0.28067788	2.21100977

O -4.44180222	2.28769640	2.37998591	H 7.39822704	-2.88554255	-1.55278427
C -5.40494228	-1.65043586	2.24164558	H 8.61251356	-3.00715972	-0.25247789
H -5.08747526	-2.10896727	3.18239703	H 8.13209280	-1.40412165	-0.86675974
H -4.96751142	-2.18838914	1.39731154	C 4.05774536	1.86816082	2.27266387
H -6.48985751	-1.67487339	2.16568411	H 3.90890007	1.79179242	3.34895266
C -1.32502874	-3.41976007	-2.95659580	H 4.43530846	2.86301667	2.02604385
H -0.71214694	-3.16258303	-2.08793255	H 4.77343898	1.10826043	1.95262282
H -1.08964775	-4.42290024	-3.30484981	H 6.61254757	1.28393772	-0.15840110
H -1.12979335	-2.69927427	-3.75614027	H -5.27210662	1.79668844	2.34151875
C 7.78774785	-2.41523271	-0.64470722	H -4.63753044	-4.19131787	-2.30416217

β - β' bottom C_g -O

C 2.38353686	4.24100047	-1.18566788	H 4.51025497	-3.56387388	-0.42592532
C 2.33177766	2.09826847	0.58655310	H 2.59558204	0.22427160	-1.10388551
C 1.15207814	3.85179534	-0.62201585	C 2.07300776	-2.44166360	-1.11322097
C 3.53279553	3.49790895	-0.96764844	O 1.06941349	-1.53032972	-1.52222696
C 3.50620675	2.39862692	-0.11935128	C 0.44196907	-0.97264266	-0.35570575
C 1.16466291	2.78023053	0.28424066	C 0.83945226	-1.85188638	0.84231957
H 4.46052277	3.73236591	-1.47545522	C 1.50090608	-3.06490094	0.16950988
H 0.26797839	2.49003745	0.81287311	H 2.20220505	-3.17073463	-1.91838926
O 4.65177939	1.63517003	0.00183577	H 0.73505883	0.06964069	-0.22226856
C 4.55522011	0.27311095	-0.23271812	H -0.63429611	-1.00732121	-0.51814094
C 4.50824390	-2.47898225	-0.40612123	C 0.30521513	-4.02500207	-0.03226785
C 5.67311450	-0.44930260	0.17980356	O -0.84813542	-3.39681862	0.52838699
C 3.43972773	-0.35653937	-0.76114285	C -0.39025247	-2.46457890	1.50502915
C 3.39025492	-1.74512849	-0.79707583	H 0.48368482	-4.98018876	0.47264508
C 5.65433024	-1.84193013	0.05696498	H 0.09510237	-4.21729447	-1.08684560

H -0.08420574	-3.01725985	2.40719822	H -1.72424085	-0.48752849	-2.19477726
H 1.50382889	-1.33118737	1.53063060	H -6.33717580	0.10775371	-0.50984831
H 2.27791274	-3.51776799	0.78426619	C -1.47362573	-1.47706097	1.86518258
H 2.41601300	5.08834268	-1.86102936	C -3.45227259	0.36147655	2.56139117
C -0.05097253	4.55866654	-1.02347411	C -2.82320285	-1.82239620	1.72616400
O -1.44248837	3.56854221	1.67006237	C -1.13090106	-0.22768057	2.36944525
C -2.48669745	3.75571830	0.80995174	C -2.12080719	0.69113718	2.72324254
C -2.32318663	3.20357085	-0.60485839	C -3.80526597	-0.91271130	2.08591758
C -1.31881175	3.93256188	-1.54591278	H -3.07810251	-2.79485443	1.32595372
H 0.11771617	5.57644117	-1.36197369	H -0.08837691	0.05915167	2.46643926
H -3.34250546	3.25950270	1.31431153	H -1.86445386	1.67104146	3.10949716
H -2.75615605	4.82471442	0.79465348	O 6.71339764	-2.59318994	0.47891535
H -3.30160054	3.30882332	-1.08506431	O 6.74632109	0.17530135	0.73388151
H -1.86251848	4.71911179	-2.07337142	O 2.24914862	1.09622033	1.51065546
C -1.00136080	2.76610891	-2.50353114	O -3.48464301	-2.50023230	-2.72575894
O -0.86063436	1.64862526	-1.64998179	O -5.95440993	-2.09076472	-1.84805367
C -1.90953164	1.71278139	-0.68753966	O -5.14989005	-1.12440176	2.02738124
H -0.07003536	2.88956976	-3.05597163	O -4.42535685	1.26973174	2.84924607
H -1.83191466	2.61172623	-3.20701866	C -5.59217943	-2.39486901	1.58131902
H -1.47968624	1.37646625	0.26104187	H -5.24711474	-3.17912995	2.26142930
C -3.03701771	0.76253940	-1.05387107	H -5.23947482	-2.59580620	0.56776529
C -5.00728620	-1.14601736	-1.59677576	H -6.67909722	-2.35599822	1.58191336
C -4.33589652	0.93268462	-0.58861800	C -2.12892281	-2.89832343	-2.88734689
C -2.72831133	-0.37199007	-1.80982137	H -1.60987421	-2.86718820	-1.92422100
C -3.69511209	-1.33148372	-2.05394236	H -2.15628587	-3.91625593	-3.27049011
C -5.32242418	-0.01236349	-0.86990098	H -1.61348817	-2.25220516	-3.60215581
H -4.59788363	1.79346791	0.01736361	C 7.91082204	-2.40676955	-0.27060448

H 7.74008014	-2.66110453	-1.32111854	H 3.64053097	2.05259156	2.72586857
H 8.64537017	-3.08780843	0.15487047	H 4.07678112	0.39063742	2.22517287
H 8.26940080	-1.37964169	-0.18911153	H 6.56061110	1.12213498	0.74935091
C 3.25754615	1.05075285	2.51890586	H -5.27674398	0.83653208	2.70757742
H 2.77896020	0.65404073	3.41398797	H -5.53935383	-2.78634919	-2.37334073

β - β' bottom C_{β} - C_{γ}

C 2.07909871	4.05478378	-0.91357236	C 1.02290501	-1.77371118	0.65500405
C 2.52161815	2.03235808	0.95452828	C 1.69142900	-2.99393170	0.01093940
C 1.05648177	3.67838128	-0.04294179	H 2.41839983	-3.12841305	-2.06727054
C 3.29929166	3.39509248	-0.88062390	H 0.75290303	0.10522063	-0.46836206
C 3.51796974	2.37287692	0.03285690	H -0.50129930	-1.10343049	-0.75727669
C 1.29150380	2.68303150	0.89483225	C 0.49715457	-3.95284513	-0.18897232
H 4.09273512	3.63686082	-1.57742648	O -0.61986463	-3.40562813	0.52002277
H 0.51715897	2.40333251	1.59746404	C -0.14807103	-2.39138124	1.40759587
O 4.72840798	1.69996505	-0.00577371	H 0.71853061	-4.95254075	0.19529569
C 4.68341716	0.34862455	-0.30140170	H 0.21075794	-4.03080129	-1.24156164
C 4.73284861	-2.38634814	-0.65017390	H 0.22127311	-2.86867036	2.32772146
C 5.84473419	-0.35081504	0.01950860	H 1.69915515	-1.20287978	1.29063864
C 3.57245475	-0.29060014	-0.82196122	H 2.46364028	-3.43481306	0.64087826
C 3.57560686	-1.67412085	-0.95373317	H 1.91425394	4.84395290	-1.63928020
C 5.87114665	-1.73351797	-0.18656354	C -0.31248335	4.32448242	-0.16368259
H 4.77491790	-3.46661707	-0.74307519	O -1.17291403	3.86682465	0.87168094
H 2.69879515	0.28313384	-1.09467168	C -2.47820398	3.66840838	0.33645661
C 2.27238825	-2.38850158	-1.27520312	C -2.25228903	3.18558087	-1.10608408
O 1.27011884	-1.48725096	-1.71111034	C -1.00420581	3.93311157	-1.43700828
C 0.56532135	-0.96719929	-0.57590793	H -0.19518685	5.41751077	-0.08786949

H -2.99089332	2.94933535	0.97710267	H -1.70468253	1.84083833	2.62478279
H -3.03358923	4.61421864	0.33783952	O 6.97255294	-2.46694822	0.14811418
H -3.07747721	3.46009670	-1.76992481	O 6.91713025	0.28400652	0.56473567
H -0.53424455	3.94974285	-2.40913249	O 2.65617057	1.03208974	1.87098989
C -1.72330853	1.53099127	-3.48301245	O -4.34622117	-2.67820514	-1.63670404
O -1.21726988	1.27301893	-2.25473635	O -6.67974276	-1.60485289	-0.98737403
C -2.03561687	1.65667941	-1.14547224	O -4.92643866	-1.17829297	2.04746259
H -1.08271674	1.20234754	-4.28804908	O -4.25483281	1.32144631	2.57135808
H -2.80085410	1.56869446	-3.60024831	C -5.33022621	-2.51184638	1.79736054
H -1.42392779	1.38676450	-0.27754559	H -4.93731954	-3.18092340	2.56909704
C -3.31744217	0.83852066	-1.11615061	H -4.98873747	-2.84540654	0.81335994
C -5.58488499	-0.80201529	-1.03041816	H -6.41714898	-2.50824169	1.82007436
C -4.55644997	1.35783541	-0.76209814	C -3.09158043	-3.29635875	-1.89589362
C -3.22044115	-0.52123005	-1.43576784	H -2.40191681	-3.14207478	-1.05961411
C -4.33419665	-1.33705599	-1.37864626	H -3.29965267	-4.35736966	-2.01511668
C -5.68794760	0.54047356	-0.72255639	H -2.65436262	-2.90379507	-2.81845888
H -4.67063054	2.40403313	-0.50750388	C 8.13105815	-2.19218288	-0.63518201
H -2.26351887	-0.92186937	-1.74000751	H 7.92552116	-2.38935833	-1.69168230
H -6.65961625	0.93734880	-0.45444667	H 8.90534850	-2.87012823	-0.28138485
C -1.25223173	-1.42001365	1.74496848	H 8.45720670	-1.15930577	-0.50508211
C -3.26728479	0.42108390	2.32712296	C 3.83301936	1.02822516	2.68107029
C -2.59033266	-1.82576629	1.72749656	H 3.53512588	0.63823661	3.65333966
C -0.93556893	-0.11103106	2.08937782	H 4.22063191	2.04257884	2.79812972
C -1.94126797	0.81109536	2.37836070	H 4.60030016	0.38152142	2.25158119
C -3.59027390	-0.91231429	2.02445138	H 6.70299317	1.22284144	0.62908267
H -2.82752926	-2.84861264	1.46430146	H -5.09908149	0.87990377	2.41199351
H 0.10217698	0.20521947	2.12325565	H -6.41505249	-2.48096323	-1.29369059

β - β' bottomC_y-O

C 1.97161290	4.11681751	-0.71043724	C 0.56137881	-4.07986305	-0.36524474
C 2.34277248	1.91521683	0.95428407	O -0.57385799	-3.58605991	0.35535881
C 0.90523854	3.65081938	0.06231336	C -0.13732731	-2.58587386	1.27570468
C 3.18797283	3.45010490	-0.70226595	H 0.80169370	-5.08863447	-0.01842930
C 3.37375500	2.33851443	0.10911615	H 0.28470249	-4.12302795	-1.42252133
C 1.11071060	2.56259504	0.90020207	H 0.22910419	-3.07851815	2.18877286
H 4.01070263	3.76778190	-1.33131436	H 1.68193714	-1.35163202	1.21352599
H 0.31847336	2.22273954	1.55485309	H 2.50658010	-3.54699030	0.50655817
O 4.59828097	1.69361931	0.06899909	H 1.84241907	4.98868858	-1.34200250
C 4.60676085	0.35195326	-0.26992109	C -0.42635676	4.37122645	0.03481410
C 4.75924635	-2.36919447	-0.69100990	O -1.28268812	3.84878897	1.04528558
C 5.78314611	-0.31688524	0.06207124	C -2.59618650	3.67348106	0.52702848
C 3.53334686	-0.30919257	-0.83894083	C -2.37925229	3.28182309	-0.93507836
C 3.58624864	-1.68820005	-1.00580912	C -1.24552124	4.28545216	-1.29410427
C 5.86279443	-1.69141534	-0.18169233	H -0.23057668	5.42882839	0.24911539
H 4.84041820	-3.44459258	-0.81054951	H -3.08786453	2.90879039	1.13183945
H 2.64828459	0.24330477	-1.11834759	H -3.16551043	4.60884656	0.60050929
C 2.31485008	-2.43730469	-1.37461637	H -3.25214010	3.49183498	-1.55621129
O 1.29035352	-1.55463269	-1.79706981	H -1.77440899	5.24263756	-1.37179677
C 0.55833711	-1.09301915	-0.65476009	C -0.50157431	4.09310008	-2.56462298
C 1.02726692	-1.92139205	0.55630916	O -1.13999149	1.43030271	-1.98597888
C 1.73214369	-3.10284428	-0.11836770	C -2.04850409	1.77592096	-1.03437745
H 2.49834411	-3.14428774	-2.18845061	H 0.31649193	3.39508801	-2.63970820
H 0.71013938	-0.01886476	-0.51053641	H -0.93788172	4.46662389	-3.48171608
H -0.50078264	-1.26189262	-0.84987660	H -1.48373483	1.51275935	-0.10321078

C -3.29064217	0.87896474	-1.06811378	O -6.53727814	-1.71443473	-1.21153346
C -5.47818343	-0.86441337	-1.16013111	O -4.94551226	-1.48659824	1.89748908
C -4.55394033	1.30382558	-0.67181999	O -4.32619499	0.99678424	2.56329349
C -3.12747450	-0.43481685	-1.51570272	C -5.31781521	-2.80199268	1.52874168
C -4.20181754	-1.30581988	-1.53971563	H -4.93371990	-3.52552479	2.25432992
C -5.64538302	0.43647573	-0.72560015	H -4.94177145	-3.04623099	0.53117219
H -4.72127983	2.31151835	-0.31448028	H -6.40464913	-2.81844243	1.51947264
H -2.15385316	-0.74998444	-1.86094382	C -2.86246242	-3.15798794	-2.19357598
H -6.63642305	0.76131775	-0.43214616	H -2.20890696	-3.05892731	-1.32083849
C -1.26517085	-1.64485331	1.62481123	H -3.02232801	-4.21052309	-2.41730541
C -3.32152759	0.13089170	2.27165969	H -2.41165841	-2.66497953	-3.05939605
C -2.59512590	-2.07219363	1.57244102	C 8.14777581	-2.05981899	-0.58349666
C -0.97681209	-0.34396463	2.02263219	H 7.97566774	-2.23320365	-1.65007508
C -2.00353354	0.54463754	2.34458030	H 8.93590298	-2.72111088	-0.22875050
C -3.61574380	-1.19194126	1.90012115	H 8.43467545	-1.02070050	-0.41601869
H -2.80926346	-3.08684554	1.26232969	C 3.58082301	0.83167318	2.68313171
H 0.05431787	-0.00964626	2.08039844	H 3.24395610	0.35046120	3.60034425
H -1.79023656	1.56559346	2.64534483	H 3.91072329	1.84895299	2.90505077
O 6.98015965	-2.39614071	0.16142046	H 4.40331523	0.25633432	2.25397128
O 6.81793693	0.33688375	0.65490818	H 6.56952515	1.26538081	0.74180179
O 2.45631504	0.85176662	1.80174867	H -5.16107069	0.55355838	2.36383800
O -4.14915236	-2.61622455	-1.92132106	H -6.23123674	-2.54195778	-1.60275067

β - β' bottom C_{α} - C_{Ph} α -side

C 4.12564963	0.63888314	0.39146677	C 2.17425410	-0.71344405	0.35961189
O 4.29540997	-0.31311617	-0.56788339	C 2.77924618	0.53688667	1.05138354
C 3.39214147	-1.37897310	-0.27955504	H 4.65297831	1.56351250	0.19862037

H 3.17875672	-1.89724557	-1.21428807	C -1.25199305	0.54480546	-0.30974301
H 3.87175131	-2.07200574	0.41958234	C -2.57623090	0.22097912	-0.05557759
H 1.67333749	-1.38057726	1.05914942	C -1.99439995	-2.10699629	0.11908994
H 2.84658115	0.43714775	2.13795425	H 0.07640182	-2.57280282	-0.16287602
C 1.80513556	1.64957285	0.65094955	H -0.94850401	1.56618319	-0.49732252
O 1.38017786	1.29342732	-0.65180293	H -2.30470799	-3.13163367	0.28249295
C 1.16542006	-0.11081956	-0.65844267	O -3.61291275	1.10878911	0.00735348
H 2.26440130	2.63689820	0.59724149	O -4.25128591	-1.42242292	0.40951221
H 0.95158225	1.68097122	1.34268026	C -3.32038995	2.47226533	-0.22884147
H 1.39504081	-0.44486624	-1.67467800	H -2.90472325	2.61314829	-1.23045397
C -0.28137240	-0.45964821	-0.33971314	H -4.26467053	3.00504403	-0.14554152
C -2.95440957	-1.11170216	0.16173353	H -2.61635441	2.85360734	0.51631114
C -0.66314611	-1.77950368	-0.12808670	H -4.76241483	-0.60463295	0.38803922

β - β' bottom C_{α} - C_{β} phenyl-side

C -1.03475902	4.19841914	1.93644246	C -2.19935816	-0.12943935	0.83697542
C -1.08239691	2.53041541	-0.33989182	C -2.17608325	-1.51770132	0.77527005
C 0.04993547	4.01787959	1.11436511	C -4.37957004	-1.50713897	-0.22691901
C -2.18570188	3.47970357	1.60866241	H -3.28877392	-3.28218587	0.19524943
C -2.20528336	2.65168268	0.49486178	H -1.37108372	0.41171092	1.27187251
C 0.08514623	3.22312710	-0.00257160	C -0.90257001	-2.25497930	1.14683376
H -3.07771653	3.53080655	2.22213319	O -0.04447161	-1.46307720	1.95057650
H 0.96218271	3.11072483	-0.62959266	C 0.90254594	-0.76404338	1.13185227
O -3.36114905	1.93649609	0.23559731	C 0.68627969	-1.23424288	-0.31709473
C -3.28173359	0.55676117	0.31628294	C -0.08377066	-2.54564587	-0.11745771
C -3.27259419	-2.19896455	0.25565876	H -1.14052586	-3.16196174	1.71037790
C -4.38186274	-0.10959059	-0.22035534	H 0.76100780	0.31541087	1.23828868

H 1.90406125	-1.01769844	1.48773874	O -5.41809678	-2.20353389	-0.77332953
C 1.05876183	-3.56939772	0.06002449	O -5.42285440	0.57896082	-0.76120109
O 2.27745168	-2.92458659	-0.31753732	O -1.04377942	1.71864314	-1.42880174
C 1.97256529	-1.71105028	-0.98863578	O 6.46515589	-0.28025944	0.60148395
H 0.90504542	-4.45205709	-0.56691707	O 6.16660604	2.06141523	-0.58273677
H 1.16178276	-3.88602821	1.10102505	C 6.66003636	-1.51662603	1.26072381
H 1.76282620	-1.92009563	-2.04821920	H 6.64443992	-2.34468040	0.54664289
H 0.14188732	-0.49774627	-0.90918191	H 5.89153479	-1.67606329	2.02237603
H -0.72160966	-2.79446796	-0.96546995	H 7.63773324	-1.45870364	1.73325797
H -1.00808726	4.84396869	2.80501123	C -6.65320172	-2.07786611	-0.07303348
C 3.11747067	-0.73355988	-0.89512968	H -6.53794607	-2.42777723	0.95726092
C 5.16736524	1.14917160	-0.68733462	H -7.36548636	-2.71260143	-0.59646065
C 4.27186658	-1.04275127	-0.17411611	H -7.00473713	-1.04514495	-0.07933504
C 2.99975788	0.50949292	-1.50749176	C -2.12464798	1.79767974	-2.36163467
C 4.02179143	1.44967631	-1.40414649	H -1.69285105	1.61310454	-3.34404016
C 5.28947056	-0.10480318	-0.07261437	H -2.57688242	2.79145924	-2.34139376
H 4.34731158	-2.01477724	0.29403697	H -2.87874726	1.03830563	-2.14826067
H 2.10219945	0.75247035	-2.06790118	H -5.24354730	1.52081299	-0.65265308
H 3.94874804	2.42215999	-1.87579715	H 6.86957732	1.67133802	-0.04961614

β - β' top C_{α} - C_{β}

C 1.76417953	3.87166984	-1.47403161	H 3.72144679	3.27739672	-2.17414473
C 2.30079171	2.22922527	0.71416867	H 0.34492747	2.75777315	1.39182690
C 0.79694409	3.69666421	-0.48383577	O 4.43963062	1.67468160	-0.29644182
C 2.97189115	3.19207558	-1.39678703	C 4.38079126	0.29199048	-0.31379294
C 3.23771627	2.36085633	-0.31764735	C 4.44885151	-2.46089525	-0.15135175
C 1.07703530	2.88364509	0.60542734	C 5.58642685	-0.33645671	-0.00621236

C 3.22924929	-0.43170895	-0.56298301	H -0.31627211	5.50450153	-0.58969318
C 3.25086970	-1.81687502	-0.44451611	H -3.36115194	3.88572362	0.75846565
C 5.61787464	-1.73254085	0.05130932	H -2.82774740	5.56716871	0.55183804
H 4.50281077	-3.53996684	-0.05167512	H -3.65715977	4.49610676	-1.85200667
H 2.31230462	0.07981767	-0.81963525	H -1.13823953	4.81330574	-2.64198104
C 1.93677695	-2.57563673	-0.49618634	C -1.22411252	2.71665837	-2.45080102
O 0.91263837	-1.79201839	-1.09139483	O -1.35051720	1.62180819	-1.55190951
C 0.17477314	-1.08860511	-0.07413271	C -2.61613223	1.31042822	-1.16102694
C 0.76676603	-1.50798218	1.28019201	H -0.21794452	2.62747454	-2.86377964
C 1.42900059	-2.84141851	0.92750218	H -1.94979704	2.60067652	-3.26412519
H 2.04263071	-3.49226775	-1.08537907	H -3.19008432	2.06977985	-0.64285255
H 0.22554137	-0.01114945	-0.25692978	C -3.15091269	0.03078284	-1.38702748
H -0.87172762	-1.39159247	-0.14821524	C -4.29579767	-2.50574802	-1.75065410
C 0.23396689	-3.80504925	1.01704896	C -4.45542391	-0.25676207	-0.92341079
O -0.72685559	-3.20897033	1.89102217	C -2.43294881	-0.98610915	-2.07403621
C -0.30834538	-1.90333466	2.28736198	C -3.00032068	-2.23178974	-2.23709864
H 0.51398917	-4.78239233	1.41546686	C -5.01734505	-1.50553099	-1.11167830
H -0.22944808	-3.94220024	0.03308798	H -5.01221953	0.51623718	-0.40583412
H 0.13281560	-1.96781669	3.29129704	H -1.43416568	-0.77187482	-2.43219842
H 1.46553462	-0.76816173	1.66940452	H -6.01912868	-1.73008022	-0.76492016
H 2.23352796	-3.11628864	1.61004605	C -1.47086283	-0.93563891	2.30290985
H 1.56951429	4.52604935	-2.31762790	C -3.55859135	0.90226268	2.16723792
C -0.51838041	4.42173024	-0.58486362	C -2.78773371	-1.39071585	2.23622573
O -1.33939880	4.12093429	0.53019644	C -1.21217461	0.43074970	2.32799895
C -2.66413367	4.53172381	0.21198173	C -2.25319364	1.35171820	2.25055238
C -2.74803753	4.41306347	-1.27496663	C -3.82750234	-0.47253679	2.18486621
C -1.39362743	4.11678363	-1.83178002	H -2.97094465	-2.45575955	2.19688015

H -0.18679646	0.78331783	2.37764541	H -0.40831344	-2.80603231	-2.64293946
H -2.05679327	2.41752098	2.22065896	H -0.83969330	-4.05967272	-3.84725839
O 6.76631410	-2.39040754	0.38501921	H -1.16060293	-2.34181875	-4.19610194
O 6.70310710	0.38868994	0.27177325	C 7.81801589	-2.27388129	-0.56944328
O 2.49057115	1.43218545	1.80239973	H 7.49386820	-2.67139414	-1.53607119
O -2.41705358	-3.29907313	-2.85573085	H 8.64320499	-2.87174168	-0.18738815
O -4.83569461	-3.74023646	-1.91427571	H 8.13474064	-1.23577471	-0.68018470
O -5.15666293	-0.78566198	2.12326544	C 3.72473327	1.55580350	2.51093165
O -4.58257289	1.79565345	2.03374164	H 3.49471760	1.37517313	3.55994050
C -5.49781458	-2.15902932	2.18927762	H 4.13461989	2.56147669	2.39474378
H -5.15453692	-2.59477205	3.13199751	H 4.44838825	0.81471179	2.16613866
H -5.06440477	-2.70780959	1.34885211	H 6.47737343	1.32303165	0.18711340
H -6.58349532	-2.20561695	2.13621378	H -5.40924820	1.29856297	2.06861989
C -1.12549655	-3.10435197	-3.41214963	H -4.18668550	-4.28370817	-2.37808981

β - β' topC_α-O

C 2.04093685	4.05699787	-0.71198741	C 5.79863640	-0.40511594	0.03226127
C 2.44791943	1.90192707	1.00414214	C 3.53052087	-0.33868809	-0.82443248
C 0.98914114	3.59621683	0.08194687	C 3.54652367	-1.71932942	-0.98910589
C 3.26369579	3.39934530	-0.70443741	C 5.83804640	-1.78149678	-0.20944130
C 3.46124166	2.30541648	0.12441114	H 4.75770653	-3.50738930	-0.81602488
C 1.21374529	2.53913538	0.95442374	H 2.65505753	0.23693581	-1.09216899
H 4.07261079	3.70036217	-1.35875911	C 2.25420284	-2.44187391	-1.33682986
H 0.42069733	2.19941114	1.60656035	O 1.24621984	-1.54222770	-1.76127180
O 4.67100197	1.63702019	0.05738140	C 0.52409622	-1.05954423	-0.62078124
C 4.63393286	0.29357039	-0.27815148	C 0.98547540	-1.88357645	0.59722294
C 4.70752284	-2.43010600	-0.69602096	C 1.66828420	-3.08257220	-0.06919410

H 2.41595557	-3.16218589	-2.14376858	H -1.37803461	1.25660823	-1.12644934
H 0.68809565	0.01434125	-0.49059336	C -3.49564715	0.89198839	-1.09056947
H -0.53789233	-1.22327071	-0.80998769	C -5.70838882	-0.84930355	-1.22052358
C 0.48171601	-4.04496904	-0.29803215	C -4.80719374	1.34972078	-0.83157960
O -0.64105196	-3.52812235	0.42528011	C -3.33027416	-0.47926435	-1.41826492
C -0.18416349	-2.52460472	1.33311599	C -4.40896573	-1.32961242	-1.47633730
H 0.71054007	-5.05365879	0.05702306	C -5.89245471	0.48703511	-0.89813401
H 0.19728720	-4.09474673	-1.35299252	H -4.97602233	2.38371922	-0.55583023
H 0.18339013	-3.01374383	2.24752136	H -2.33483876	-0.84309488	-1.62930671
H 1.65362828	-1.31754786	1.24465690	H -6.89959718	0.83253379	-0.69736978
H 2.43959917	-3.53163958	0.55611250	C -1.29539775	-1.56170784	1.67536448
H 1.89737324	4.90967715	-1.36728289	C -3.30857233	0.28672612	2.23974364
C -0.37773333	4.23165518	-0.01893332	C -2.63521667	-1.95791772	1.62429585
O -1.21032822	3.74036895	1.01710576	C -0.97870144	-0.25856790	2.04234090
C -2.54572515	3.69998007	0.54531491	C -1.98218664	0.66647964	2.32321238
C -2.42999997	3.21254166	-0.90981311	C -3.63435076	-1.03787023	1.90790813
C -1.15620006	3.97143990	-1.35948342	H -2.87566714	-2.97449927	1.34023697
H -0.26029068	5.31699451	0.10346988	H 0.05995588	0.04976803	2.09771503
H -3.11978242	3.03118565	1.18743246	H -1.74323516	1.69321925	2.57821636
H -2.98613314	4.70715319	0.57601442	O 6.94360610	-2.51446043	0.11310294
H -3.28919972	3.57524740	-1.48421589	O 6.86211312	0.22304165	0.60241523
H -1.48260275	4.94445709	-1.73929852	O 2.57883427	0.85276146	1.86455943
C -0.35115558	3.33008768	-2.49617259	O -4.35359338	-2.66451163	-1.76503577
O 0.39567126	2.22548153	-2.16863215	O -6.76781675	-1.69614793	-1.27428271
C -2.34968605	1.72612367	-1.04242524	O -4.97433149	-1.28561324	1.87401332
H 0.27082695	4.07215863	-3.01545802	O -4.29551384	1.19333125	2.46907061
H -1.06199263	2.95726025	-3.25801752	C -5.39011892	-2.60731358	1.58593539

H -5.04355068	-3.29536909	2.36330735	H 8.88203438	-2.89026883	-0.31582911
H -5.01321026	-2.93371162	0.61266838	H 8.42011291	-1.17829792	-0.49913432
H -6.47709582	-2.58429133	1.56305720	C 3.73333605	0.82930449	2.70574841
C -3.06662822	-3.22238329	-1.99923659	H 3.41908969	0.37897348	3.64629090
H -2.41848290	-3.09381405	-1.12660082	H 4.09350705	1.84389720	2.88987974
H -3.22882580	-4.28193776	-2.18477081	H 4.52688107	0.22480167	2.26269942
H -2.60498399	-2.76313140	-2.87833784	H 6.63939401	1.15784024	0.69106064
C 8.10363253	-2.21039450	-0.65674783	H -5.13658645	0.77029961	2.25265475
H 7.90538480	-2.38275028	-1.71898461	H -6.44266522	-2.55574892	-1.56956450

β - β' top C_{β} - C_{γ}

C 1.48046723	3.69629148	-1.83017534	H 2.31174122	-0.11843765	-1.01055709
C 2.19447708	2.19231938	0.40371397	C 2.21485521	-2.78865515	-0.45824208
C 0.58719462	3.56980419	-0.76981333	O 1.06888573	-2.19363605	-1.04450900
C 2.70675542	3.04560056	-1.79835587	C 0.37978588	-1.40230480	-0.06417504
C 3.06295748	2.29002779	-0.69398315	C 1.08261353	-1.63297359	1.28525953
C 0.95228726	2.81636249	0.34296160	C 1.84286488	-2.93669884	1.02389681
H 3.40634033	3.11120328	-2.62255396	H 2.38333993	-3.74816440	-0.95542626
H 0.28407355	2.72092049	1.19194980	H 0.38470754	-0.35313332	-0.36968106
O 4.30734067	1.68536842	-0.69762698	H -0.65728353	-1.74936128	-0.02744883
C 4.37121017	0.30588220	-0.63254019	C 0.76617004	-3.99824092	1.33816269
C 4.71228378	-2.41110707	-0.31955924	O -0.30474634	-3.33868490	2.02256098
C 5.64741156	-0.18813564	-0.36318627	C 0.11338515	-2.03156798	2.39158586
C 3.28138655	-0.53334134	-0.77301218	H 1.16198958	-4.79722320	1.97063944
C 3.44263747	-1.90142419	-0.57234361	H 0.35452857	-4.43813747	0.42575112
C 5.81679951	-1.56839280	-0.23224157	H 0.65715204	-2.07626904	3.34657797
H 4.87362788	-3.47210024	-0.15947112	H 1.72394716	-0.79696969	1.56078999

H 2.72326612	-3.05009229	1.65626452	C -1.05616868	-1.08871940	2.53061189
H 1.21982263	4.30326246	-2.69029513	C -3.15743019	0.73828739	2.67121949
C -0.75977085	4.24157813	-0.85103418	C -2.35863949	-1.51093757	2.26523252
O -1.04022972	4.81474973	0.42172151	C -0.81481608	0.23945357	2.87427412
C -2.12345414	5.62222109	0.46568521	C -1.86448126	1.15222604	2.94566708
C -2.37915106	2.39157430	-0.18362340	C -3.40534626	-0.60124820	2.34195563
C -1.92133490	3.29681597	-1.28102203	H -2.52786267	-2.54491680	1.99677432
H -0.69365136	5.05335368	-1.58857272	H 0.20061843	0.57481700	3.06169274
H -2.30993032	6.04457269	1.44170668	H -1.69361961	2.19439749	3.19044197
H -2.39113681	6.16291768	-0.43752087	O 7.03982825	-2.09663530	0.06424958
H -2.92464309	2.70384125	0.69460343	O 6.70226624	0.65344028	-0.19469742
H -2.73852084	3.93442374	-1.63513976	O 2.49004804	1.46911221	1.52168731
C -1.51569984	2.26743346	-2.35187151	O -3.78823908	-3.05591109	-2.80850175
O -1.11208561	1.11790679	-1.62160718	O -6.29236920	-2.34877952	-2.32341364
C -2.05064795	0.97892202	-0.54684245	O -4.71707548	-0.88646311	2.11358534
H -0.68140687	2.57127915	-2.98369948	O -4.18393183	1.63076443	2.69734379
H -2.38046897	2.02723708	-2.98233952	C -5.01206326	-2.15545401	1.55400019
H -1.53271172	0.46027092	0.26659799	H -4.80902334	-2.95080875	2.27680062
C -3.23047745	0.12541952	-1.00227087	H -4.42553541	-2.31452597	0.64484566
C -5.29472641	-1.53078110	-1.89959236	H -6.07059487	-2.14278639	1.30451026
C -4.55448881	0.46175468	-0.76697401	C -2.45717322	-3.49441977	-3.02285009
C -2.93234507	-1.05417463	-1.69918762	H -1.92877377	-3.61138324	-2.07198217
C -3.95286059	-1.87795727	-2.13797924	H -2.53166632	-4.45551138	-3.52585714
C -5.58731555	-0.36444558	-1.21967212	H -1.91130862	-2.78839905	-3.65405179
H -4.79461748	1.37383712	-0.23239140	C 8.01900095	-1.94127827	-0.95950420
H -1.89599640	-1.28818436	-1.90900255	H 7.67961397	-2.42509985	-1.88041163
H -6.62713292	-0.11462788	-1.04571027	H 8.91846760	-2.43566840	-0.59779873

H 8.22739730	-0.88694431	-1.14692051	H 4.50232591	1.00019131	1.80556597
C 3.75002873	1.71249384	2.15016812	H 6.38372641	1.55527777	-0.32287945
H 3.59049710	1.57963253	3.21945839	H -4.99286086	1.14785058	2.48443363
H 4.08500486	2.73377195	1.95635645	H -5.88806439	-3.09742843	-2.77844640

β - β' topC_γ-O

C 2.05812827	4.03715103	-1.26709678	C 1.40209968	-3.18062395	0.29011370
C 2.19336311	2.15827912	0.78685911	H 2.05341331	-3.30247376	-1.81387394
C 0.98118357	3.88783611	-0.39888494	H 0.54537267	-0.06947056	-0.12450560
C 3.19314760	3.24979582	-1.12468660	H -0.79735042	-1.20403670	-0.37073873
C 3.26343645	2.31217220	-0.10950149	C 0.21350906	-4.15524846	0.12993295
C 1.06257831	2.95359949	0.62986013	O -0.91024809	-3.57499117	0.79011432
H 4.03867099	3.34357576	-1.79515526	C -0.43879991	-2.58656251	1.69851385
H 0.25030091	2.83007420	1.33991942	H 0.44142323	-5.12813102	0.57695964
O 4.42634887	1.57163621	0.00609866	H -0.06346506	-4.30295902	-0.91660655
C 4.35749854	0.20800402	-0.20394987	H -0.08617578	-3.07866250	2.61798679
C 4.38487068	-2.53994917	-0.39052434	H 1.42838340	-1.41699575	1.61287292
C 5.51169236	-0.48114230	0.16468156	H 2.20228540	-3.61521918	0.88818330
C 3.23942904	-0.44746220	-0.68621054	H 2.01889187	4.77758604	-2.05903926
C 3.23384637	-1.83718777	-0.73600584	C -0.23478097	4.77758442	-0.57815700
C 5.52807902	-1.87268810	0.03843664	O -0.61546491	5.45114538	0.54887097
H 4.41765406	-3.62404865	-0.42089748	C -2.55603443	3.44734839	1.02013040
H 2.37241584	0.11819440	-0.99676051	C -2.35868946	3.16491819	-0.42681969
C 1.92964647	-2.56630927	-1.01429889	C -1.48754337	4.12812511	-1.26210860
O 0.90117064	-1.67470149	-1.40984336	H 0.04445469	5.57061673	-1.29795984
C 0.28095835	-1.12499261	-0.23538481	H -1.96780968	4.18936238	1.54510994
C 0.74638531	-1.96717810	0.96476365	H -3.35425173	2.95179748	1.55866973

H -3.34327384	3.19118241	-0.91220409	O 6.62162688	-2.59611859	0.41605253
H -2.10045061	4.96217214	-1.60786886	O 6.58792818	0.17632777	0.67284722
C -1.07520528	3.20209425	-2.40719426	O 2.17516363	1.22034155	1.77608153
O -0.80344065	1.95849484	-1.78674566	O -3.01014084	-2.39819178	-3.12640338
C -1.76181308	1.75629929	-0.74939607	O -5.42732156	-2.36233231	-2.05511252
H -0.17484060	3.51394956	-2.93868419	O -5.21083475	-1.23993107	2.01988820
H -1.90036970	3.10331486	-3.12490207	O -4.51585635	1.15194655	2.87881096
H -1.21211970	1.37587075	0.11824858	C -5.63176199	-2.49878673	1.51979600
C -2.79458529	0.72092515	-1.15156762	H -5.31177221	-3.30248497	2.18894265
C -4.57492669	-1.34041285	-1.77093132	H -5.24031034	-2.66968092	0.51382485
C -4.07353273	0.70545969	-0.61024232	H -6.71839805	-2.46207023	1.48463497
C -2.40833104	-0.30010053	-2.02890853	C -1.67716594	-2.52250431	-3.59849902
C -3.28349321	-1.33155792	-2.32134166	H -0.96539425	-2.51897619	-2.76778147
C -4.96786381	-0.31638996	-0.93121321	H -1.63376522	-3.46941779	-4.13214167
H -4.38963523	1.47626570	0.08460321	H -1.43368177	-1.70543023	-4.28356410
H -1.41136405	-0.27694211	-2.45055171	C 7.78715427	-2.37166761	-0.37305287
H -5.96771250	-0.33801599	-0.51482091	H 7.58547402	-2.61936904	-1.41961027
C -1.53490737	-1.60471886	2.03278805	H 8.55247814	-3.03878322	0.01867819
C -3.53443075	0.24090822	2.63260648	H 8.12297222	-1.33690222	-0.29249665
C -2.87607841	-1.95069506	1.84546488	C 3.30584431	1.14598136	2.64658910
C -1.20699913	-0.34530684	2.52289454	H 2.92165048	0.85105170	3.62229888
C -2.20750752	0.57699757	2.82601278	H 3.79449451	2.11928367	2.72714115
C -3.86944115	-1.03391108	2.15266996	H 4.01894600	0.39682117	2.29667938
H -3.11493162	-2.92488386	1.44078637	H 6.38132484	1.11887294	0.68299083
H -0.16803016	-0.05869618	2.65194156	H -5.36376885	0.71879770	2.71897043
H -1.96775100	1.56497961	3.20002666	H -4.96918771	-2.96762589	-2.65140719

β - β' topC $_{\alpha}$ -C $_{\beta}$ α -side

C 0.35787124	3.85217885	-0.84375415	O -0.74965929	-3.92256626	0.04837940
C 1.15759770	1.92796553	1.01084248	C -0.62545284	-2.81439323	0.92951407
C -0.59879476	3.18077430	-0.08186747	H 0.91871779	-5.10694696	-0.25346476
C 1.70067233	3.52166635	-0.72275648	H 0.31328677	-4.22430085	-1.67624165
C 2.10043827	2.54894735	0.18276523	H -0.25670297	-3.16333572	1.90528205
C -0.19194865	2.23175281	0.84708658	H 0.88797335	-1.22702467	0.96883160
H 2.45751812	3.98530294	-1.34383587	H 2.19883150	-3.24714903	0.46052516
H -0.92456116	1.71057997	1.45064967	H 0.05218637	4.61001290	-1.55742283
O 3.43430560	2.17818696	0.21295995	C -2.06151243	3.45387680	-0.30704948
C 3.70989438	0.87180099	-0.15866928	O -2.83717179	2.84316527	0.70146560
C 4.38526376	-1.75397249	-0.66674125	C -4.16973710	2.83727380	0.22424041
C 4.97753778	0.42102741	0.20143825	C -4.05834664	2.43643489	-1.26152314
C 2.79988060	0.04391518	-0.79091497	C -2.63678101	2.93110593	-1.65833532
C 3.11849362	-1.29038595	-1.01012435	H -2.22853077	4.54198037	-0.27557608
C 5.32053190	-0.90464359	-0.08193495	H -4.74545273	2.13168314	0.82219070
H 4.67221002	-2.78859876	-0.82323716	H -4.60212794	3.84407923	0.31718219
H 1.83328704	0.42605773	-1.08474622	H -4.85962475	2.89149457	-1.84836191
C 2.02416249	-2.23649989	-1.47578101	H -2.65268225	3.73524937	-2.39355362
O 0.92350324	-1.53529150	-2.02982248	C -1.97638249	1.67810040	-2.24661232
C -0.05304921	-1.26287425	-1.01227393	O -2.67045044	0.56389183	-1.68653334
C 0.43917160	-1.94051567	0.27763062	C -3.95784853	0.95695110	-1.48460877
C 1.43309328	-2.97181759	-0.26477685	H -0.91812093	1.57257024	-2.01177186
H 2.40434028	-2.91811750	-2.24230823	H -2.10584293	1.65764239	-3.33328083
H -0.17165051	-0.18473489	-0.87844601	H -4.59559979	0.21335846	-1.02843087
H -1.01231363	-1.66286996	-1.34692344	C -1.94446621	-2.10723658	1.12216746
C 0.50401951	-4.15742010	-0.60178079	C -4.32659653	-0.70173466	1.45498074

C -3.10107274	-2.54927766	0.48065769	H -5.23858623	-4.16905906	-0.34431765
C -1.98624800	-0.96331884	1.91275617	H -4.79942617	-3.06017428	-1.67553938
C -3.17443228	-0.25575727	2.07693520	H -6.51273093	-3.29647324	-1.23527457
C -4.28421210	-1.84476263	0.64744808	C 7.64616303	-0.83114014	-0.40250189
H -3.04556041	-3.42912939	-0.14570574	H 7.54716995	-1.00076750	-1.47897168
H -1.08065369	-0.60905680	2.39611412	H 8.53158812	-1.34419884	-0.03218235
H -3.21829755	0.64933765	2.67127987	H 7.72712631	0.23772344	-0.19925665
O 6.53720792	-1.40179016	0.28688804	C 2.58341614	1.21303421	2.79056574
O 5.85218337	1.23426886	0.85358402	H 2.33837076	0.73458746	3.73763643
O 1.47774157	0.96745474	1.92049267	H 2.71767495	2.28564829	2.94713358
O -5.48044159	-2.14862703	0.05536188	H 3.50017153	0.77573028	2.39126973
O -5.49557796	-0.01293906	1.59244065	H 5.43338752	2.09775576	0.95455688
C -5.49697171	-3.23562231	-0.85161116	H -6.18462633	-0.50748440	1.13199928

β - β' topC $_{\alpha}$ -C $_{\text{Ph}}$ phenyl-side

C 1.27961793	-1.71940422	-0.00000033	H 2.64267065	1.35032334	0.00000090
C 0.56530546	0.90279898	-0.00000011	O -1.70210452	0.39168562	0.00000278
C 2.28593573	-0.79262286	-0.00000016	O 0.20632753	2.21224797	-0.00000236
C -0.07054644	-1.44047699	0.00000043	C -2.75863461	-0.54877107	-0.00000171
C -0.42696626	-0.09382889	0.00000036	H -2.71860300	-1.17706309	0.89439902
C 1.90536454	0.55640384	0.00000041	H -3.68046137	0.02782237	-0.00000335
H 3.33207727	-1.07189165	-0.00000029	H -2.71859774	-1.17705998	-0.89440437
H -0.81434601	-2.22700255	0.00000094	H -0.75698202	2.25881013	0.00001043

β'' - β''' Cleavage

C 2.41339141	3.92634224	-1.39909383	C 1.44702699	3.70290038	-0.42168495
C 2.83043419	1.96245716	0.51747542	C 3.56999550	3.15056312	-1.44803699

C 3.77719062	2.16612482	-0.49517077	H 1.50766058	-0.74708703	0.72792913
C 1.66826435	2.71646285	0.53711734	H 2.32744596	-4.58260052	-1.15527515
H 4.31845451	3.29596054	-2.21732904	H 2.25904778	4.70014066	-2.14411899
H 0.92985856	2.52452940	1.30566707	C 0.14384814	4.46350964	-0.44038642
O 4.93273550	1.40467126	-0.54145640	O -0.37755894	4.53173649	0.87950504
C 4.72127844	0.03041163	-0.52910010	C -1.78583702	4.63512394	0.78280676
C 4.18984561	-2.64539945	-0.20532251	C -2.15744935	3.66467700	-0.32978554
C 5.45837612	-0.68680555	0.40726155	C -0.98567795	3.82721482	-1.32522981
C 3.78251978	-0.57398496	-1.34156655	H 0.33259223	5.48264339	-0.80279476
C 3.46609502	-1.91640076	-1.14641904	H -2.20822229	4.38268434	1.75635944
C 5.19933683	-2.05064809	0.54712738	H -2.07968004	5.66068613	0.52066845
H 3.98088647	-3.68763845	-0.00198324	H -3.12926992	3.88127108	-0.77311299
H 3.25068624	0.01965191	-2.07362307	H -1.22847593	4.47961605	-2.16425349
C 2.32090738	-2.52235376	-1.96162761	C -0.73203802	2.39388391	-1.76246470
O 1.37595679	-1.55600169	-2.37979158	O -0.92102317	1.63845285	-0.57825904
C 0.78688146	-0.68238737	-1.38914103	C -2.05320352	2.17116254	0.09907491
C 0.82015886	-1.17675910	0.01106220	H 0.27675379	2.20473084	-2.12930377
C 1.69023029	-3.71799707	-1.30088748	H -1.45697350	2.09755949	-2.53338628
H 2.75321820	-2.86955954	-2.91228200	H -1.83033508	2.09992505	1.16803454
H 1.27418503	0.29416699	-1.43755524	C -3.30208881	1.36189626	-0.19443537
H -0.24631234	-0.56122558	-1.72087153	C -5.58433258	-0.17505354	-0.67821463
C 0.21984353	-3.98044250	-1.23833836	C -4.50654824	1.66854026	0.42953397
O -0.60733558	-2.93672834	-0.74113354	C -3.24007884	0.27312136	-1.06238355
C -0.13122117	-2.25989868	0.41672728	C -4.37246491	-0.48843690	-1.30581237
H 0.06103217	-4.88170081	-0.63164545	C -5.64427831	0.90190959	0.19132267
H -0.17911305	-4.18276445	-2.24140881	H -4.56092552	2.49445554	1.13204245
H 0.38531670	-2.98520907	1.06693904	H -2.28960952	0.00653445	-1.50185751

H -6.58652581	1.12253953	0.67825408	H -4.66469931	-4.26728300	1.07191723
C -1.33958260	-1.70956922	1.17259657	H -4.91082853	-3.09940328	-0.26044456
C -3.54279432	-0.72263476	2.58622965	H -6.27755943	-3.55285119	0.79263748
C -2.59189293	-2.31722158	1.03122930	C -3.21215731	-1.97521501	-2.75792607
C -1.20305509	-0.62582358	2.03234967	H -2.43778435	-2.20868905	-2.02118958
C -2.29806838	-0.14324684	2.74695351	H -3.45274989	-2.86186237	-3.34095533
C -3.68525145	-1.82058032	1.72397882	H -2.85992871	-1.18492020	-3.42774313
H -2.69650584	-3.15508140	0.35503375	C 7.24602904	-2.93566147	1.28709084
H -0.24223232	-0.13668958	2.14222718	H 7.43619169	-3.41573136	0.32225258
H -2.20506953	0.70262670	3.41837458	H 7.60974908	-3.57417877	2.08992721
O 5.84415226	-2.79275246	1.49539127	H 7.75050181	-1.96913217	1.32750222
O 6.34903043	-0.06493113	1.22422166	C 3.71472253	1.46369556	2.62468423
O 3.04306477	0.99135935	1.45983665	H 3.95769212	0.58664565	3.22130530
O -4.42251300	-1.58530388	-2.12208874	H 3.06869944	2.14178364	3.18987038
O -6.69028943	-0.93369073	-0.90864742	H 4.63643310	1.98657708	2.35232766
O -4.96076580	-2.30100650	1.65064541	H 6.36842567	0.86638732	0.97123504
O -4.61997255	-0.23497179	3.25090134	H -5.39796778	-0.71037138	2.93288242
C -5.20611232	-3.36945985	0.75745685	H -6.46137074	-1.58790447	-1.57955753

β'' - β''' bottom C_α - C_β

C -1.78552329	3.98876125	1.35862778	H -0.00444118	2.57758673	-1.15417155
C -2.07408493	2.21371759	-0.77762188	O -4.31018741	1.72526901	0.00218043
C -0.68685608	3.66989356	0.56142126	C -4.24546257	0.37740131	0.31179219
C -3.00200922	3.35779292	1.14038334	C -4.42909389	-2.32772904	0.85543734
C -3.13293564	2.44289929	0.10535157	C -5.49248117	-0.25564838	0.23765667
C -0.84761030	2.81548441	-0.51968473	C -3.09128515	-0.30668338	0.63647604
H -3.85445063	3.52496375	1.78774482	C -3.16149015	-1.69800604	0.88693295

C -5.57273566	-1.62257214	0.53607179	H 3.40869786	4.52904606	0.61113704
H -4.52360841	-3.38989392	1.05020330	H 3.43431667	2.60472136	2.07753652
H -2.14359018	0.20952606	0.71827996	H 1.63241896	3.96170041	2.92232637
C -2.01815705	-2.48390878	1.14454876	C 0.61189518	2.06996922	2.57831233
O -0.73146625	-2.09563492	1.02030462	O 0.78410763	1.11760991	1.54269047
C -0.20772133	-1.46188164	-0.16872125	C 2.07826044	1.28995981	0.96397816
C -0.94149374	-1.79274813	-1.47240421	H -0.45869412	2.20309117	2.73248748
C -1.26169266	-3.24265854	-1.66171321	H 1.06753020	1.71045063	3.51074100
H -2.12819430	-3.49455886	1.52296787	H 1.92812087	1.26412119	-0.12188977
H -0.17382875	-0.37888175	-0.01497080	C 3.01879574	0.16727444	1.35759366
H 0.82050978	-1.82548161	-0.21899698	C 4.75975555	-1.91222052	2.02965216
C -0.56332356	-3.74815033	-2.87618122	C 4.38751302	0.29207247	1.14713471
O 0.44012088	-2.78395757	-3.13832915	C 2.51160202	-1.01682904	1.90238254
C -0.05305856	-1.51183462	-2.73301588	C 3.37823183	-2.04969056	2.23263446
H -1.24768794	-3.82862547	-3.73870077	C 5.25793409	-0.74115708	1.48758521
H -0.07874758	-4.71950459	-2.74392489	H 4.78859547	1.20039051	0.70825423
H -0.71656742	-1.11757902	-3.51504957	H 1.44370648	-1.10814911	2.06080208
H -1.84284446	-1.17457435	-1.52614139	H 6.32651081	-0.65624168	1.32959781
H -2.08382446	-3.75320759	-1.18158653	C 1.12725950	-0.57736341	-2.58990988
H -1.67693360	4.68353980	2.18500602	C 3.34596066	1.10835513	-2.40283829
C 0.69057165	4.14817903	0.94408612	C 2.38055297	-1.10202934	-2.25213424
O 1.55287213	4.04660043	-0.17978936	C 1.00137236	0.78326155	-2.83432585
C 2.84514746	3.65614357	0.25515816	C 2.10824246	1.63027507	-2.73300275
C 2.58309734	2.69242074	1.40198462	C 3.48192607	-0.26835253	-2.16507490
C 1.35438600	3.30852964	2.09436008	H 2.47595082	-2.16867585	-2.10257635
H 0.63434269	5.19627656	1.26374538	H 0.03364326	1.19182544	-3.10245867
H 3.36875903	3.21659517	-0.59456083	H 2.02085305	2.69661541	-2.90867298

O -6.76746532	-2.27893652	0.45227201	H 1.53812813	-4.49658614	3.33680809
O -6.60519243	0.43299527	-0.12708831	H 1.20342557	-2.77482686	3.66117735
O -2.13137957	1.33668808	-1.81769658	C -7.72250844	-1.89095068	1.43554850
O 3.01215343	-3.25255487	2.76282306	H -7.32712271	-2.07952867	2.43846615
O 5.59957383	-2.93340801	2.34332954	H -8.60182100	-2.50988315	1.26768085
O 4.75418484	-0.66385984	-1.87966317	H -7.98796624	-0.83768977	1.33113867
O 4.43561438	1.91813419	-2.29878229	C -3.31855067	1.28078219	-2.60630544
C 4.94047311	-2.02411276	-1.52617270	H -3.00018703	1.00259518	-3.61069980
H 4.73141319	-2.67388983	-2.38079701	H -3.81087858	2.25493655	-2.63483874
H 4.29695265	-2.29068248	-0.68331974	H -4.00932979	0.52679190	-2.22227422
H 5.98190456	-2.12471820	-1.22928128	H -6.34974275	1.35251894	-0.26982339
C 1.62401463	-3.48583463	2.94446325	H 5.19765065	1.35544781	-2.11030629
H 1.08343238	-3.39807367	1.99904524	H 5.06660042	-3.64991898	2.70908183

β'' - β''' bottomC $_{\alpha}$ -O

C 2.34380609	3.34817742	-1.14924783	C 3.83529064	-0.92252178	0.68815200
C 2.68463987	2.01314670	1.27461753	C 3.67285060	-2.23911251	0.20327955
C 1.29090870	3.29672846	-0.23325757	C 5.48644061	-1.81114540	-1.38088090
C 3.52767786	2.67741206	-0.88648813	H 4.46172522	-3.65806965	-1.24827972
C 3.69457736	1.98900623	0.30893655	H 3.22223552	-0.54783977	1.49141454
C 1.47395083	2.63835644	0.97525592	C 2.65604636	-3.08862353	0.70331783
H 4.33446214	2.65745431	-1.61061361	O -0.23812970	-2.22227018	-0.29431659
H 0.67991945	2.61489981	1.71117473	C 0.37007850	-1.16493614	0.32803910
O 4.86617110	1.25881405	0.50257932	C 0.88387314	-1.45550548	1.73426829
C 4.74977276	-0.07224813	0.10837111	C 1.73990849	-2.74489022	1.83679702
C 4.53268993	-2.65419664	-0.84533779	H 2.56057989	-4.07255155	0.25658880
C 5.60632756	-0.49035240	-0.91040157	H 1.23306343	-0.93242445	-0.33183134

H -0.25276134	-0.26264438	0.29198842	C -5.33598684	-0.91064292	-2.17313942
C 0.66422744	-3.82775650	2.08496637	C -4.53323063	1.24197907	-1.46651895
O -0.52891838	-3.16361568	2.49193251	C -2.98586456	-0.59100410	-1.68024058
C -0.24151568	-1.79794285	2.72768053	C -4.02711581	-1.41082410	-2.07899382
H 0.97244317	-4.53322850	2.86205146	C -5.58354394	0.41257163	-1.86500350
H 0.44340068	-4.37330944	1.16527653	H -4.75101363	2.27302697	-1.21192765
H 0.15802649	-1.67756381	3.74633258	H -1.97753498	-0.97555865	-1.58108191
H 1.40127700	-0.56303232	2.09113385	H -6.59954997	0.78137654	-1.93749664
H 2.34299063	-2.63626473	2.75049764	C -1.46654045	-0.93701436	2.58073459
H 2.22826105	3.89084212	-2.08189824	C -3.61042819	0.77936392	2.10502403
C -0.01229659	3.98813297	-0.55487322	C -2.60428241	-1.41646310	1.92931860
O -0.88431620	3.89896092	0.56153264	C -1.42197985	0.38222404	3.01668806
C -2.21763978	3.95782269	0.08367509	C -2.49186873	1.24235071	2.77689189
C -2.18639982	3.11132165	-1.17963428	C -3.67764591	-0.56496414	1.70608683
C -0.80865076	3.44084255	-1.79071392	H -2.62508319	-2.45070267	1.61134830
H 0.20530955	5.04862469	-0.74446990	H -0.54127553	0.75173226	3.53258587
H -2.87641231	3.56359666	0.85946191	H -2.46341646	2.27883191	3.09226431
H -2.49931765	4.99519051	-0.14135906	O 6.32637434	-2.27264645	-2.35335665
H -3.00180711	3.33241967	-1.86714745	O 6.52521862	0.34831021	-1.44717740
H -0.87233658	4.20645236	-2.56481371	O 2.78407441	1.40908044	2.49454163
C -0.39253626	2.09322650	-2.36276770	O -3.91815808	-2.73887312	-2.38063013
O -0.83404066	1.15177334	-1.40567949	O -6.35137802	-1.73648347	-2.53920022
C -2.08360841	1.59836756	-0.86973043	O -4.84403114	-0.90529086	1.09382536
H 0.67967597	1.95461291	-2.49559134	O -4.63545708	1.62582090	1.81889590
H -0.89717178	1.93342029	-3.32556041	C -5.07689368	-2.27801433	0.83634281
H -2.00048579	1.45409280	0.21277610	H -5.09531924	-2.84368280	1.77283205
C -3.23522201	0.75411193	-1.37955748	H -4.31332295	-2.69111693	0.17286975

H -6.04512610	-2.33175486	0.34215874	H 6.29672967	-0.61521691	-3.61502996
C -2.64592446	-3.34043899	-2.19188275	C 4.02322739	1.51646044	3.19672710
H -2.31300825	-3.23542995	-1.15575628	H 3.77519811	1.43845367	4.25389004
H -2.76805986	-4.39069188	-2.44629714	H 4.49378276	2.48123169	2.99671712
H -1.89845481	-2.88324963	-2.84540385	H 4.70724381	0.71477810	2.91323073
C 6.11643242	-1.69145861	-3.63701936	H 6.49437007	1.17141935	-0.94295627
H 5.09640535	-1.89306935	-3.97863805	H -5.27376174	1.13709051	1.28121228
H 6.82749482	-2.16870351	-4.30844976	H -5.96996060	-2.60136274	-2.73366806

β'' - β''' bottom C_{β} - C_{γ}

C 2.17881617	3.94896519	-1.21858862	C 2.02510145	-2.49551372	-1.07618329
C 2.44280564	2.01062310	0.76510800	O 1.07739009	-1.52838038	-1.49977716
C 1.08884956	3.64317567	-0.40399631	C 0.46560277	-0.95550283	-0.34017673
C 3.37139611	3.24830973	-1.08685913	C 0.59796921	-1.98377848	0.80292198
C 3.50046701	2.26322955	-0.11776956	C 1.41018323	-3.06699832	0.16855426
C 1.24177513	2.69011283	0.59457905	H 2.14417576	-3.22711645	-1.88013387
H 4.21179356	3.43210307	-1.74521285	H 0.93527590	-0.00457658	-0.08257651
H 0.42169855	2.46358905	1.26422662	H -0.57524870	-0.76556273	-0.57760895
O 4.68020940	1.54011072	-0.06301112	C -1.93480012	-4.28167634	0.35612244
C 4.57229543	0.16806902	-0.22750170	O -1.46510022	-3.02701948	0.19830207
C 4.44142811	-2.58642436	-0.25912875	C -0.77954503	-2.42587869	1.30216066
C 5.65430637	-0.56271813	0.25511910	H -2.01624677	-4.68546884	1.35835808
C 3.45943416	-0.45311164	-0.76602182	H -2.56609087	-4.61443066	-0.45516181
C 3.36507987	-1.83854073	-0.73224231	H -0.66221137	-3.18275161	2.08705903
C 5.59245656	-1.95968052	0.20661475	H 1.14491055	-1.54861698	1.64936901
H 4.40517610	-3.66970854	-0.21578092	H 1.79089349	-3.93546800	0.68839902
H 2.65047950	0.13752015	-1.17171604	H 2.08955206	4.71587119	-1.98133525

C -0.24382188	4.32645388	-0.61824117	C -3.01858688	-1.43398883	1.84023514
O -1.06204048	4.11955717	0.52748204	C -1.08249740	-0.04333845	2.18248415
C -2.40444003	3.88128152	0.13210824	C -1.91067212	1.01719599	2.56106016
C -2.28473571	3.14980361	-1.19552387	C -3.83649054	-0.39137026	2.23233057
C -1.07045777	3.82505983	-1.85354220	H -3.45118001	-2.37311820	1.51775176
H -0.06410142	5.40199551	-0.73610751	H -0.01107418	0.12362889	2.16311062
H -2.88514444	3.30108158	0.92344215	H -1.49898425	1.98400620	2.83048467
H -2.94220655	4.82966744	0.00667449	O 6.61184895	-2.71782643	0.70711133
H -3.18630793	3.21928241	-1.80616449	O 6.72706603	0.05863951	0.81664943
H -1.35917542	4.67465955	-2.47372261	O 2.48809627	1.05952431	1.74194991
C -0.49344602	2.69176457	-2.69012941	O -3.18454603	-2.85598894	-2.44236538
O -0.69695435	1.51480921	-1.92639942	O -5.59142630	-2.50236505	-1.39477441
C -1.81341477	1.68769156	-1.05200319	O -5.19731523	-0.43025481	2.29970080
H 0.57341633	2.77487549	-2.89815388	O -4.09770511	1.89630540	2.88021085
H -1.03680892	2.62789716	-3.64148697	C -5.82428065	-1.68968705	2.11186565
H -1.42930611	1.53952092	-0.03382146	H -5.45800564	-2.40873273	2.85052253
C -2.87835841	0.63896371	-1.28633587	H -5.65165276	-2.07197833	1.10286463
C -4.71641185	-1.45716676	-1.38939777	H -6.88869025	-1.52127894	2.26012707
C -4.15788536	0.79685010	-0.76709762	C -1.88213538	-3.09295948	-2.96406392
C -2.53423766	-0.56364448	-1.91239898	H -1.11971700	-2.90671143	-2.20326834
C -3.43306581	-1.61600701	-1.93272229	H -1.86698094	-4.13876007	-3.26412032
C -5.08367299	-0.24321387	-0.83853259	H -1.69925679	-2.45882295	-3.83604099
H -4.44158684	1.72230132	-0.27586612	C 7.83762757	-2.61322966	-0.01149638
H -1.54948541	-0.66579110	-2.34869830	H 7.69232989	-2.92511268	-1.05026431
H -6.08443127	-0.13244589	-0.43827912	H 8.53630108	-3.28905939	0.47794523
C -1.62713645	-1.26466070	1.80293423	H 8.22627709	-1.59424446	0.02088979
C -3.28185944	0.85493818	2.56910439	C 3.59679145	1.09592571	2.64172345

H 3.22927037	0.72112758	3.59592581	H 6.57640249	1.01047809	0.76513146
H 3.95420293	2.12079215	2.76609328	H -5.00663267	1.57132660	2.86545227
H 4.40838562	0.45570394	2.29231408	H -5.15879997	-3.24050203	-1.84168895

β'' - β''' bottomC_y-O

C 2.12396095	3.95261533	-1.43707793	H 3.01613753	-3.05796543	-2.50580884
C 2.25728052	2.12282560	0.66134566	H 0.70623283	-0.18642592	-1.07736729
C 0.98190503	3.67088818	-0.69166996	H -0.33729061	-1.35750018	-1.89700056
C 3.32098247	3.29773244	-1.16259391	C 0.95040581	-4.35315542	-1.59006349
C 3.38481089	2.37501388	-0.13106053	O -1.42953286	-3.16625321	-0.51565613
C 1.06404135	2.76689992	0.36361285	C -0.56332734	-2.62548994	0.40217967
H 4.21295004	3.47538285	-1.75094073	H 0.61026483	-5.27215899	-1.13340664
H 0.19404901	2.54629338	0.96871508	H 0.58109223	-4.10524661	-2.57683379
O 4.57241090	1.70425375	0.09977787	H -0.35899144	-3.51026107	1.04811489
C 4.55797737	0.33318467	-0.09585730	H 1.36765783	-1.71074444	0.57808610
C 4.67130138	-2.41310829	-0.30226936	H 2.24772985	-3.78741808	0.00689165
C 5.58371143	-0.34975344	0.55262491	H 2.07945595	4.67164724	-2.24798017
C 3.61065891	-0.32925097	-0.85838580	C -0.34748453	4.27908215	-1.06542535
C 3.65022305	-1.71636818	-0.94484384	O -1.12386076	4.47983637	0.10888634
C 5.64146816	-1.74148697	0.43355281	C -2.49187929	4.34885352	-0.23460993
H 4.73694174	-3.49483312	-0.35316866	C -2.51442675	3.17978858	-1.20910708
H 2.84280831	0.22839575	-1.37755324	C -1.22633460	3.40258419	-2.02724827
C 2.56709894	-2.45640495	-1.71180104	H -0.17018857	5.24905431	-1.54691392
O 1.65689926	-1.55993397	-2.32570884	H -3.05055783	4.17526286	0.68615919
C 0.62441165	-1.22858251	-1.39176382	H -2.86221458	5.26580918	-0.71190196
C 0.77633285	-2.19184367	-0.20489997	H -3.41425457	3.14485365	-1.82372951
C 1.66939559	-3.32088848	-0.79455514	H -1.40942337	3.93578254	-2.96063717

C -0.74622701	1.98138107	-2.27280310	O 6.49383094	0.31286542	1.31696333
O -1.07390331	1.27612820	-1.08778525	O 2.25347550	1.20932851	1.67263498
C -2.25030712	1.82194228	-0.50288855	O -4.41263178	-2.31283496	-2.21442830
H 0.33009186	1.88834818	-2.43308337	O -6.50116746	-1.91235389	-0.65534401
H -1.27195426	1.55092708	-3.13624091	O -4.52310502	-1.11490225	2.96434123
H -2.02196763	2.00813398	0.55182432	O -3.31425619	1.11106521	3.67406206
C -3.39412042	0.83617454	-0.56883540	C -5.20322021	-2.31708317	2.64767280
C -5.49256536	-0.99771335	-0.63659564	H -4.65692772	-3.17961365	3.04090149
C -4.51637806	1.02050635	0.22901286	H -5.33736836	-2.41891794	1.56847022
C -3.31790856	-0.27714909	-1.40868750	H -6.17691230	-2.24962629	3.12775112
C -4.36163456	-1.18899717	-1.44385790	C -3.33815237	-2.54281231	-3.11052744
C -5.56745913	0.10631574	0.19387716	H -2.40392446	-2.69366483	-2.56475134
H -4.56423392	1.86464250	0.91018323	H -3.59016435	-3.44901931	-3.65654601
H -2.42166174	-0.43407166	-1.99365595	H -3.23776526	-1.70765336	-3.81016293
H -6.44310407	0.22571208	0.82071969	C 7.92907331	-2.24005814	0.61802027
C -1.26006400	-1.58468082	1.28026646	H 8.00140581	-2.51104294	-0.43971157
C -2.62828179	0.22362262	2.90908367	H 8.57122927	-2.89246895	1.20652409
C -2.57597962	-1.85885077	1.68330782	H 8.23073630	-1.20102516	0.75835962
C -0.64419382	-0.41661221	1.70257429	C 3.25887554	1.32946438	2.68000400
C -1.32916414	0.48342723	2.52453603	H 2.80058417	0.99780937	3.61071170
C -3.25143070	-0.96792392	2.49447737	H 3.57763923	2.36962719	2.78032124
H -3.05786411	-2.76158106	1.32902066	H 4.11677068	0.69399043	2.45533923
H 0.36701158	-0.16532764	1.41036091	H 6.29729589	1.25599598	1.25743690
H -0.85715032	1.39876888	2.86391147	H -4.18624057	0.73446801	3.84633426
O 6.60163880	-2.45693427	1.08892390	H -6.27656452	-2.58099151	-1.31440244

β'' - β''' bottomC $_{\alpha}$ -C $_{Ph}$ α -side

C 3.80871998	0.43032623	1.03681546	C -0.28044579	-0.54401845	-0.70484086
O 3.05083199	-0.16693324	1.99340602	C -2.93291687	-0.91540221	0.08059538
C 1.83196397	-0.58993488	1.37931430	C -1.06394001	0.56074783	-0.36339455
C 2.18764287	-0.91501735	-0.07868174	C -0.83090595	-1.81902094	-0.65635518
C 3.44388546	-0.04167689	-0.33896507	C -2.15386136	-2.00628587	-0.26287870
H 4.80416074	0.70058838	1.36142982	C -2.38175507	0.37328383	0.02621712
H 1.44920437	-1.43900946	1.94238747	H -0.62345128	1.54725537	-0.41348703
H 1.11274248	0.23311192	1.42695885	H -0.22910736	-2.67958459	-0.92997193
C 2.91435597	1.04979684	-1.30167820	H -2.59823784	-2.99291069	-0.22052001
O 1.50035727	1.00020574	-1.20417325	O -3.25192420	1.36398036	0.38205637
C 1.16539324	-0.37099176	-1.09398163	O -4.22267600	-1.08999196	0.46193331
H 3.21809999	0.83124833	-2.33361491	C -2.77046340	2.69429817	0.35970185
H 3.23789938	2.05392402	-1.02990263	H -2.45307984	2.97567535	-0.64818662
H 1.34050492	-0.86261163	-2.06352176	H -1.93445750	2.81643707	1.05411496
H 2.37747634	-1.97930557	-0.21617658	H -3.60069908	3.32343226	0.67162136
H 4.25636288	-0.60151863	-0.81181742	H -4.59616891	-0.22144674	0.65369767

β'' - β''' bottomC_α-C_{Ph} phenyl-side

C -0.18211460	-3.37581197	-1.59152628	C -2.91786593	-0.18583421	-0.22939773
C -1.12110707	-2.40079392	0.85212541	C -2.90522031	2.59171353	-0.03006497
C 0.66124138	-3.35225907	-0.47950176	C -4.10494686	0.49427865	0.05943123
C -1.45251460	-2.82674134	-1.50606262	C -1.71177520	0.48739564	-0.42101725
C -1.89310699	-2.28639555	-0.30696530	C -1.78299537	1.85457665	-0.30406606
C 0.15679637	-2.94341785	0.74699516	C -4.10103332	1.88829272	0.15355827
H -2.09979412	-2.75102077	-2.37175601	H -2.91263344	3.67103340	0.06188007
H 0.75996246	-2.99623599	1.64431464	H -0.78795426	-0.03945345	-0.64214661
O -3.07179626	-1.55952666	-0.29131197	H 0.17360171	-3.76705192	-2.53863865

C 2.13806893	-3.63756612	-0.64644401	H 4.42737738	0.30092059	1.57904266
O 2.78104726	-3.88580421	0.59151827	H 1.27690441	1.73618243	-0.94299609
C 3.38618761	-2.69787442	1.10573245	H 5.21254935	2.63242972	1.92851661
C 3.34463999	-1.64351529	-0.00530114	O -5.23555566	2.57087189	0.47579458
C 2.92255698	-2.43677023	-1.25453099	O -5.25914811	-0.19481792	0.27344422
H 2.26914882	-4.52939306	-1.26479990	O -1.48793426	-1.91383818	2.06247653
H 2.85495383	-2.36721826	2.00455320	O 2.03255972	4.36051702	-0.65282850
H 4.41120035	-2.94829354	1.38657544	O 4.13854470	4.75227328	0.88761633
H 4.32235957	-1.18381308	-0.14942236	C 0.85274693	4.20453205	-1.42022981
H 3.78604942	-2.81792490	-1.80156803	H 0.06036527	3.74278355	-0.82392864
C 2.15648826	-1.38637479	-2.04545952	H 0.55381023	5.20487611	-1.72461240
O 1.45530987	-0.63411534	-1.06840039	H 1.04313946	3.59218958	-2.30630972
C 2.26005675	-0.53742915	0.10896605	C -6.26300743	2.52299538	-0.51169308
H 1.42496890	-1.77691327	-2.75141236	H -5.89700013	2.94011028	-1.45474075
H 2.86524281	-0.74514242	-2.58528563	H -7.07698131	3.13744641	-0.13225005
H 1.58763566	-0.74677873	0.94872346	H -6.61147012	1.50088954	-0.66527209
C 2.80919334	0.86668891	0.27900553	C -2.84816991	-2.02729061	2.47311742
C 3.70471227	3.48166928	0.69598603	H -2.82735037	-2.10676718	3.55871571
C 3.90844259	1.11856551	1.09020435	H -3.30697254	-2.92318904	2.04831431
C 2.14014266	1.93891365	-0.32219246	H -3.42049741	-1.14279735	2.18776381
C 2.58804174	3.23402787	-0.11817353	H -5.07162132	-1.13253566	0.14371838
C 4.35614246	2.42253475	1.29979541	H 3.54918311	5.34252747	0.40280366

β'' - β''' top C_α - C_β

C 3.45536738	3.67180505	-1.24051686	C 4.33742748	2.60422445	-1.33025564
C 3.70775907	1.88724202	0.89164582	C 4.42241881	1.68288897	-0.29491541
C 2.62070418	3.79069086	-0.12877306	C 2.78349342	2.92797001	0.94562238

H 4.93171274	2.43210963	-2.21958567	H 3.35607076	4.36092192	-2.07252343
H 2.15240563	3.01747188	1.82029180	C 1.41461502	4.68712736	-0.20617260
O 5.18777082	0.54603075	-0.48705498	O 0.87282871	4.90720116	1.08203029
C 4.52071041	-0.66818620	-0.51507743	C -0.50097833	5.20123500	0.91041156
C 3.44780588	-3.20959316	-0.45513507	C -0.99056441	4.22813932	-0.16078085
C 5.36975559	-1.76564525	-0.65027127	C 0.26291725	4.04729808	-1.06089236
C 3.15039870	-0.82567894	-0.36727805	H 1.68971826	5.65171134	-0.65523637
C 2.61344163	-2.10620019	-0.29679123	H -0.99256714	5.08445287	1.87684073
C 4.81591998	-3.04883409	-0.64594778	H -0.62547781	6.23892764	0.57107419
H 3.06226452	-4.22325767	-0.41170509	H -1.84894798	4.61901924	-0.70543441
H 2.49948076	0.03245615	-0.28086058	H 0.17582893	4.54877153	-2.02472559
C 1.14851370	-2.29460917	0.06887362	C 0.34362909	2.52924203	-1.20555516
O 0.44212163	-1.06230963	0.09067112	O -0.08763965	2.05331493	0.05793250
C 0.53042468	-0.47706040	1.39848436	C -1.26321038	2.78877525	0.36570751
C 0.95466367	-1.58893634	2.28893798	H 1.33755775	2.12916416	-1.39797593
C 1.02519043	-2.86078220	1.50798937	H -0.33626210	2.19030221	-1.99715077
H 0.64687728	-2.93648857	-0.66236442	H -1.35709215	2.78065747	1.45622262
H 1.23836146	0.36012354	1.40688855	C -2.48116486	2.12571842	-0.26717601
H -0.46109153	-0.06675257	1.63260130	C -4.66153842	0.88793829	-1.49776668
C -0.17295295	-3.80886142	1.69064993	C -3.71564334	2.76071790	-0.32210121
O -1.40823333	-3.28921932	1.22134704	C -2.34532467	0.84238244	-0.80655230
C -1.99970713	-2.34868015	1.99958372	C -3.41937794	0.23861444	-1.44063833
H -0.27023288	-4.08488735	2.74711152	C -4.80767670	2.13843645	-0.92618825
H -0.00618688	-4.71714827	1.10796439	H -3.84438938	3.74821147	0.10888311
H -1.45077228	-1.98938213	2.86084223	H -1.38964534	0.33624432	-0.73409028
H 1.25079128	-1.46863249	3.32037044	H -5.78171733	2.61073917	-0.96019412
H 1.91318487	-3.44472881	1.77133506	C -3.27099880	-1.85651016	1.65854198

C -5.74226510	-0.73769670	0.91712301	H -4.62569248	-3.31161928	-1.96776674
C -4.02325464	-2.41694066	0.59666674	H -6.35370306	-3.68103600	-2.22128930
C -3.80991078	-0.75017378	2.35631600	C -2.14145130	-1.67887297	-1.98759072
C -5.02256752	-0.20573337	1.98365760	H -1.82735173	-1.83699554	-0.95205090
C -5.23303108	-1.85999643	0.23611679	H -2.30825943	-2.63572495	-2.48038140
H -3.61798907	-3.26896549	0.06854062	H -1.36137330	-1.12386504	-2.51771370
H -3.24690272	-0.31071454	3.17235396	C 6.27399770	-4.29751144	-2.00062286
H -5.43162351	0.66053161	2.48922628	H 5.53910978	-4.35975514	-2.80905286
O 5.61131861	-4.15336712	-0.74721974	H 6.83329984	-5.22930901	-1.94351625
O 6.71496888	-1.60094447	-0.75468122	H 6.95789727	-3.46702612	-2.18118048
O 3.75823619	1.04745013	1.95766807	C 5.02577541	0.53426663	2.36195550
O -3.37790543	-0.98230297	-2.04983809	H 4.97177135	0.41315260	3.44272940
O -5.72504986	0.28532018	-2.09870357	H 5.82468663	1.23544906	2.11124790
O -6.00743715	-2.29593970	-0.80582023	H 5.22105269	-0.43492268	1.89847805
O -6.91730885	-0.16614340	0.55405334	H 6.89924263	-0.65413127	-0.72883003
C -5.58996509	-3.46965324	-1.47565666	H -7.08950889	-0.38123352	-0.37218010
H -5.51520938	-4.30928027	-0.77880832	H -5.46875863	-0.61862578	-2.32523022

β'' - β''' topC_g-O

C 1.74596086	3.53007547	-2.24515798	O 4.54858644	1.67547379	-0.80049719
C 2.33141568	2.11979673	0.08337283	C 4.59630145	0.32389776	-0.50086194
C 0.76365751	3.36148892	-1.27333223	C 4.81545225	-2.30803483	0.27996463
C 3.00462215	2.95918014	-2.07901071	C 5.72307857	-0.07446671	0.21225585
C 3.29466678	2.24313177	-0.92795385	C 3.60430685	-0.57244288	-0.85759553
C 1.07042504	2.66398201	-0.10902187	C 3.69561166	-1.89247728	-0.43725505
H 3.77208942	3.04708862	-2.83822309	C 5.83368016	-1.41528518	0.59449255
H 0.31894846	2.53418977	0.65887583	H 4.92116678	-3.33420003	0.61643977

H 2.75159990	-0.23341754	-1.43242727	H -1.84380476	3.30813007	-3.25599725
C 2.53627016	-2.83958024	-0.67806922	C -1.06056930	1.44731070	-2.44134547
O 1.74458120	-2.42283185	-1.77639766	O -1.25699921	0.86733096	-1.16277820
C 0.57146968	-1.74382769	-1.33182136	C -2.50380805	1.33368770	-0.65767159
C 0.63492497	-1.67624746	0.20830672	H -0.00062316	1.37062313	-2.68816655
C 1.58262466	-2.85570183	0.53206547	H -1.64755276	0.91413337	-3.20209687
H 2.91600758	-3.84170642	-0.89909472	H -2.35872365	1.47907422	0.41732572
H 0.53381479	-0.74422945	-1.76852414	C -3.61207942	0.31776105	-0.86620499
H -0.30080310	-2.31363222	-1.66447502	C -5.65277303	-1.57391666	-1.12682248
C 0.85829781	-4.22518014	0.69440684	C -4.92358453	0.64077983	-0.53657293
O 0.11731408	-4.46806606	-0.42761376	C -3.31751530	-0.96594488	-1.33111240
C -0.70981917	-1.72447164	0.84529503	C -4.33061698	-1.90598128	-1.46049223
H 0.20678296	-4.13165921	1.57521946	C -5.94324419	-0.30011716	-0.66930405
H 1.62356674	-4.99551128	0.85717200	H -5.16082822	1.63071333	-0.15950377
H -1.33899481	-2.56692076	0.57151709	H -2.28918597	-1.21108678	-1.56239647
H 1.16065373	-0.75957281	0.48787201	H -6.96979884	-0.06278959	-0.41659993
H 2.11883404	-2.69158956	1.46900851	C -1.27496570	-0.74033386	1.68589262
H 1.52624473	4.08816836	-3.14943362	C -2.54558579	1.25665645	3.21972221
C -0.64212677	3.85736876	-1.49750776	C -2.64591341	-0.86050602	2.05441055
O -1.26741292	4.06459151	-0.24057143	C -0.56606682	0.39316533	2.15073312
C -2.66069002	3.88937099	-0.40964056	C -1.19847380	1.37165440	2.90264415
C -2.78192924	2.69765211	-1.35124735	C -3.26493198	0.11918871	2.79515281
C -1.56998423	2.87425494	-2.29403836	H -3.20629400	-1.71503353	1.69459846
H -0.60412088	4.81059089	-2.04159488	H 0.48364054	0.51329261	1.91597960
H -3.09727443	3.72331816	0.57686026	H -0.66141504	2.24666241	3.25050437
H -3.10964129	4.78696649	-0.85659800	O 6.89884617	-1.84342136	1.33293109
H -3.73170296	2.68112486	-1.88547166	O 6.68681300	0.82016674	0.56269945

O 2.56993885	1.40961894	1.22862228	H -2.43664117	-3.00885991	-3.01893363
O -4.17740323	-3.18760089	-1.90207713	C 8.14660898	-1.81688712	0.64476743
O -6.63923758	-2.49920361	-1.24813285	H 8.10124526	-2.45878814	-0.24025189
O -4.57491436	0.12336816	3.17922906	H 8.88673935	-2.20663351	1.34091864
O -3.16941962	2.22280318	3.93663613	H 8.41305787	-0.79950890	0.35446089
C -5.34073615	-1.03207411	2.88265904	C 3.53023374	1.97988414	2.11505478
H -4.90282340	-1.91309567	3.36100500	H 3.55446438	1.33680966	2.99239383
H -5.40592338	-1.18807322	1.80290570	H 3.22401327	2.98976243	2.40176897
H -6.33395840	-0.84967488	3.28655529	H 4.52387878	2.00825939	1.66326571
C -2.86585979	-3.62357574	-2.22234573	H 6.45143078	1.67285995	0.17691528
H -2.21469276	-3.59678224	-1.34471227	H -4.08293034	1.94292367	4.07487092
H -2.96314095	-4.65008372	-2.56720120	H -6.24285921	-3.30908958	-1.59199515

β'' - β''' top C_{β} - C_{γ}

C 1.90732480	4.11296678	-1.18212726	C 3.57897674	-1.60190087	-0.93959833
C 2.19962962	2.19862088	0.82773254	C 5.86460866	-1.48835744	-0.13471951
C 0.82372795	3.78550609	-0.37043739	H 4.94980587	-3.27482267	-0.81944075
C 3.12159720	3.45713300	-1.02168609	H 2.50082483	0.26662409	-0.95493828
C 3.26133529	2.49328919	-0.03579134	C 2.43403066	-2.47970857	-1.40910678
C 0.98165630	2.83959005	0.63757931	O 1.43805289	-1.78838919	-2.14964256
H 3.97009428	3.66480160	-1.66216985	C 0.52824420	-0.97553104	-1.55273407
H 0.14977237	2.57417086	1.27592490	C 1.43164973	-2.60314927	0.97447395
O 4.47229524	1.83463473	0.07621659	C 1.89822118	-3.34192218	-0.23639546
C 4.49875105	0.48319443	-0.20811304	H 2.83395001	-3.18051184	-2.14741249
C 4.79750912	-2.21357756	-0.65262696	H -0.12994386	-0.49570683	-2.26025922
C 5.71491209	-0.12225262	0.10742083	H 0.28603733	-1.06016923	-0.50475735
C 3.43374787	-0.23376098	-0.73104499	C 0.66940352	-4.20446123	-0.59183635

O -0.43592979	-3.64695500	0.10047307	C -3.33500107	-0.31416019	-1.09138007
C 0.03611735	-3.02781221	1.30244102	C -4.33474702	-1.23091271	-1.37559981
H 0.82514492	-5.24185948	-0.27284548	C -6.01212566	0.35405511	-0.68671786
H 0.43440565	-4.18733865	-1.65804382	H -5.27432213	2.25789112	-0.02630665
H 0.05791837	-3.79676408	2.09755765	H -2.28977212	-0.57624281	-1.19376794
H 2.08711174	-2.07081598	1.64801484	H -7.05789616	0.59065500	-0.53236141
H 2.74493160	-3.98974986	0.02414977	C -0.94292681	-1.94771697	1.70828292
H 1.79847848	4.86366870	-1.95740294	C -2.82683283	-0.02106650	2.41870923
C -0.53156872	4.37840780	-0.65326178	C -2.30986784	-2.26021920	1.67177933
O -1.27813622	4.47644917	0.54965249	C -0.53315959	-0.68523932	2.10783258
C -2.64903115	4.43901806	0.19762589	C -1.47976988	0.27217492	2.48000967
C -2.72576733	3.34577183	-0.86096638	C -3.24549085	-1.29843745	2.00580565
C -1.40947539	3.53863227	-1.64758596	H -2.61800772	-3.24604121	1.34578732
H -0.40078117	5.38410387	-1.07482357	H 0.51478480	-0.40958650	2.10793283
H -3.22175508	4.22405318	1.10081320	H -1.17756691	1.26487338	2.79365114
H -2.96753711	5.40769131	-0.21166055	O 7.02335978	-2.13632741	0.18002744
H -3.61418390	3.41710819	-1.48843448	O 6.72976907	0.59485605	0.65732152
H -1.54704678	4.07743799	-2.58537672	O 2.27801416	1.25105571	1.80382728
C -0.94933620	2.10522011	-1.86904196	O -4.13209086	-2.50109182	-1.83546747
O -1.29329860	1.44222126	-0.66565618	O -6.65226487	-1.81809639	-1.42492795
C -2.56524763	1.92752907	-0.24800904	O -4.59763599	-1.44384824	1.95067312
H 0.12454577	1.98773612	-2.02095711	O -3.75170064	0.92844454	2.71755951
H -1.48582196	1.66420582	-2.72211310	C -5.11051622	-2.69746554	1.53787396
H -2.52106809	2.00814068	0.84081753	H -4.86274430	-3.47146464	2.27099291
C -3.66867006	0.95412672	-0.61347014	H -4.71711141	-2.97893088	0.55725002
C -5.68126848	-0.90000149	-1.17019185	H -6.18946020	-2.57643282	1.47076664
C -5.00610061	1.27886180	-0.41133559	C -2.78899472	-2.88077752	-2.11425405

H -2.16895173	-2.83782664	-1.21515043	C 3.40112593	1.29012585	2.68338656
H -2.83797275	-3.90434788	-2.47996400	H 3.04525847	0.93193063	3.64867309
H -2.36346382	-2.23280917	-2.88668867	H 3.77348926	2.31157922	2.78871683
C 8.15724359	-1.73766988	-0.58637988	H 4.20121633	0.63731947	2.32771166
H 7.97086704	-1.91142986	-1.65056193	H 6.43657656	1.51144445	0.73168199
H 8.98363985	-2.36275862	-0.25386737	H -4.62080149	0.57039338	2.49208570
H 8.39677016	-0.68719191	-0.41621839	H -6.22637719	-2.59539398	-1.80670964

β'' - β''' topC_v-O

C 1.65518653	4.04866192	-1.25927167	O 1.97323330	-2.40590138	-2.43934620
C 2.25724433	1.99985450	0.52234751	C 0.44236750	-0.90151400	-0.50778362
C 0.70192529	3.64710215	-0.32492155	C 1.10871758	-1.77800135	0.49895125
C 2.88338203	3.40389305	-1.33728394	C 1.78041615	-3.02225859	-0.09865941
C 3.18615523	2.37616015	-0.45535035	H 3.12593731	-3.74297313	-1.59700365
C 1.01511389	2.62095428	0.55935099	H -0.07384413	-0.00261759	-0.20355652
H 3.62664275	3.68637692	-2.07276198	H 0.51401212	-1.09593218	-1.57267260
H 0.29463270	2.29804584	1.30179988	C 0.58292120	-3.95077617	-0.32423151
O 4.44433788	1.80796326	-0.53583874	O -0.38212727	-3.59319339	0.66792651
C 4.56125842	0.43009253	-0.54562301	C 0.09536996	-2.48297328	1.43034408
C 4.97579525	-2.28708702	-0.37613412	H 0.84144480	-5.00635436	-0.20952917
C 5.74286302	-0.04066919	0.02771735	H 0.14976509	-3.79379640	-1.31708101
C 3.60850341	-0.42845001	-1.06312381	H 0.63741418	-2.86685683	2.30672063
C 3.80488732	-1.80185675	-0.94975451	H 1.81699415	-1.19020431	1.09173704
C 5.95387568	-1.41901493	0.09887203	H 2.43218094	-3.45245836	0.66804840
H 5.15550917	-3.35246041	-0.27417198	H 1.43377351	4.86101902	-1.94432655
H 2.70183493	-0.03023720	-1.50292977	C -0.65552734	4.30967336	-0.29613216
C 2.69048545	-2.75937069	-1.32929814	O -1.28909491	4.02738066	0.94469291

C -2.69054051	3.94658590	0.73876505	C -1.78526436	0.52107444	2.76910554
C -2.82159747	3.26283053	-0.61366577	C -3.39256167	-1.11032343	2.02002349
C -1.65139493	3.85810842	-1.42016753	H -2.57469872	-2.96156146	1.27592603
H -0.51106541	5.39446219	-0.38182209	H 0.27641006	-0.04876692	2.58241929
H -3.11936928	3.37416938	1.56400998	H -1.58082470	1.50788343	3.17056608
H -3.13568717	4.94999766	0.72011560	O 7.07190375	-1.92838700	0.69230279
H -3.78323576	3.43618413	-1.09621907	O 6.66205708	0.81976239	0.54044382
H -1.95484517	4.71443056	-2.02349523	O 2.52354837	1.00370814	1.42376233
C -1.22555512	2.67583285	-2.27675335	O -3.94051259	-2.72775709	-1.93214000
O -1.34691289	1.55827478	-1.41821475	O -6.48366196	-2.10320525	-1.54502126
C -2.46484020	1.76152398	-0.54555915	O -4.72186474	-1.35303792	1.84995209
H -0.19522459	2.71384409	-2.63124241	O -4.10629389	1.04984300	2.76290588
H -1.89928415	2.57899916	-3.13862443	C -5.11167118	-2.66477067	1.48387607
H -2.09578577	1.52551830	0.45824263	H -4.83292432	-3.37631937	2.26720318
C -3.58374973	0.79427415	-0.87028561	H -4.65595529	-2.96475164	0.53686038
C -5.54199961	-1.14484770	-1.33561154	H -6.19245217	-2.63743169	1.36428357
C -4.92491040	1.07549668	-0.64453684	C -2.57777904	-3.12421673	-2.01998693
C -3.21801948	-0.47897640	-1.32076722	H -2.06829096	-2.97875587	-1.06175085
C -4.18438799	-1.44144681	-1.54001246	H -2.58777636	-4.18083759	-2.27902997
C -5.90512289	0.11002525	-0.88678470	H -2.06001164	-2.55936858	-2.80098267
H -5.22874186	2.04531035	-0.26730618	C 8.28975597	-1.65455251	0.00377485
H -2.16847025	-0.69779373	-1.46582789	H 8.25090367	-2.07002385	-1.00772777
H -6.95528626	0.31713659	-0.72045951	H 9.07691967	-2.14746340	0.57087916
C -1.03955054	-1.60130724	1.88529488	H 8.48287111	-0.58185128	-0.04053166
C -3.10151075	0.16247303	2.52911625	C 3.49657395	1.33604312	2.41158241
C -2.36618548	-1.98771649	1.69782233	H 3.59650385	0.46031965	3.05040645
C -0.75522470	-0.35902817	2.44523668	H 3.15679163	2.19170495	3.00174459

H 4.46507723	1.56117364	1.95918856	H -4.92976209	0.63775876	2.46987300
H 6.35410767	1.71745186	0.36377550	H -6.03551603	-2.88558472	-1.88904149

β'' - β''' topC $_{\alpha}$ -C $_{\beta}$ α -side

C 0.99254658	3.87764960	-1.40471831	H 0.75581478	-0.49412336	1.34832174
C 1.90119501	2.47718307	0.83318923	H -0.95508592	-0.95769868	1.22102399
C 0.15368648	3.69516318	-0.30661001	C 0.18059809	-4.51413513	0.15761131
C 2.25741417	3.30415321	-1.41327199	O -0.65844780	-4.71348346	1.29307192
C 2.69427257	2.57850936	-0.31605259	C -0.74189807	-3.52815872	1.95989237
C 0.62176155	3.02387297	0.81642198	H 0.65781624	-5.46547863	-0.07338390
H 2.90548334	3.36802769	-2.27902716	H -0.44182380	-4.20223499	-0.68903057
H -0.01949158	2.87809744	1.67587677	H -1.26940784	-3.58565687	2.90198438
O 3.89404275	1.89291575	-0.40565286	H 1.05979460	-2.48200153	2.54544100
C 3.79944133	0.51298959	-0.45322946	H 2.11869067	-3.79963524	0.86251415
C 3.84776965	-2.24389730	-0.43939162	H 0.63997481	4.42121453	-2.27458920
C 5.02749247	-0.14071388	-0.35803828	C -1.29646444	4.07442648	-0.41326975
C 2.60937107	-0.18885330	-0.54889603	O -1.85450223	4.27963096	0.87125504
C 2.62686032	-1.57906685	-0.51348662	C -3.25206503	4.11229178	0.73170111
C 5.04493235	-1.53683648	-0.37253336	C -3.41168075	2.88376647	-0.16153346
H 3.91127472	-3.32617811	-0.42488255	C -2.17698001	2.97162940	-1.09763390
H 1.66366941	0.33044090	-0.62359822	H -1.39162835	5.00062849	-0.99768013
C 1.30932464	-2.34104869	-0.57740809	H -3.68025722	3.99794930	1.72803819
O 0.18725203	-1.49181189	-0.38623756	H -3.69333880	4.99774231	0.25299118
C 0.06484809	-1.27966188	1.02324462	H -4.35659345	2.88756902	-0.70326544
C 0.42541280	-2.63379967	1.66767651	H -2.43110777	3.26593955	-2.11598769
C 1.16374017	-3.39585292	0.53239189	C -1.61472038	1.55315602	-1.04182909
H 1.19711049	-2.78313492	-1.57236402	O -1.87114787	1.13350202	0.28884173

C -3.19796578	1.53896724	0.58964462	O -4.37672794	-3.04551122	-0.93903409
H -0.54383746	1.47070266	-1.22280542	O -6.95215459	-2.48964106	-0.77815096
H -2.14572647	0.90986074	-1.75530973	C -3.01083752	-3.42589592	-0.90556617
H -3.23205800	1.69231061	1.67261114	H -2.60860621	-3.33374402	0.10735149
C -4.20515548	0.46532710	0.20304389	H -2.97858983	-4.46736168	-1.21945120
C -6.05870797	-1.52205293	-0.45227157	H -2.41704746	-2.81104194	-1.58920921
C -5.57022667	0.71623554	0.27553224	C 7.12255866	-2.06368590	-1.33714271
C -3.76109666	-0.80020186	-0.19248206	H 6.65329951	-2.39728251	-2.26774040
C -4.68216496	-1.78277371	-0.52395627	H 7.98045256	-2.69514768	-1.11467337
C -6.49622912	-0.27385867	-0.04722448	H 7.44317773	-1.02542953	-1.43240871
H -5.92838913	1.68968254	0.59478491	C 3.59838164	1.90465243	2.41985666
H -2.69683773	-0.99771696	-0.24295593	H 3.53792317	1.78786742	3.50078581
H -7.56245772	-0.09260930	0.00976157	H 3.99619386	2.89325980	2.18019809
O 6.21747178	-2.22388975	-0.24788170	H 4.25033783	1.13119880	2.00897774
O 6.18337376	0.56130932	-0.22221423	H 5.96276358	1.50070260	-0.24040268
O 2.26593955	1.76443032	1.93056953	H -6.45477671	-3.28320402	-1.01039496

β'' - β''' topC_α-C_{Ph} phenyl-side

C 1.27974544	-1.71944302	0.00028561	H 2.64260346	1.35037661	-0.00051952
C 0.56524598	0.90280970	-0.00012778	O -1.70210334	0.39153052	0.00047518
C -0.07046909	-1.44052601	0.00011263	O 0.20615846	2.21238988	0.00028944
C 2.28585477	-0.79257049	-0.00016297	C -2.75849885	-0.54875395	-0.00037006
C 1.90525833	0.55648930	-0.00018395	H -2.71922322	-1.17717379	0.89405468
C -0.42685588	-0.09393581	-0.00000721	H -2.71770760	-1.17724661	-0.89460310
H -0.81439462	-2.22690055	0.00060901	H -3.68042572	0.02770010	-0.00134732
H 3.33209001	-1.07150412	-0.00047738	H -0.75706750	2.25896677	-0.00111091