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**Supramolecular stereoelectronic effect in hemiketals**

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## Cartesian coordinates of all located stationary points:

16

MePropOL\_-gg\_PBE0-D3\_CCT

C	0.397718000	1.505148000	-0.237747000
H	1.342273000	1.933405000	0.096176000
H	-0.405623000	1.996722000	0.310074000
C	0.392338000	0.011538000	0.025863000
H	0.276368000	1.697418000	-1.303864000
O	-0.738189000	-0.634975000	-0.519376000
C	-1.988631000	-0.129543000	-0.114455000
H	-2.224974000	0.820608000	-0.605508000
H	-2.034677000	0.007580000	0.969544000
H	-2.734568000	-0.865921000	-0.411496000
C	1.578397000	-0.684353000	-0.612103000
H	1.573704000	-0.536440000	-1.691959000
H	2.507826000	-0.294426000	-0.198349000
H	1.521038000	-1.757631000	-0.418198000
O	0.415579000	-0.133102000	1.427909000
H	0.480579000	-1.073438000	1.615972000

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MePropOL\_tg\_tors180\_PBE0-D3\_CCT

C	0.437893000	1.449516000	-0.435378000
H	1.385954000	1.900077000	-0.134236000
H	-0.367924000	2.026114000	0.017799000
C	0.382585000	-0.005449000	0.013768000
H	0.359692000	1.516732000	-1.521414000
O	-0.751167000	-0.669156000	-0.455923000
C	-1.994798000	-0.123343000	-0.079510000
H	-2.212001000	0.809563000	-0.611393000
H	-2.045571000	0.054223000	0.996927000
H	-2.748435000	-0.859665000	-0.355297000
C	1.560438000	-0.802629000	-0.511717000
H	1.574361000	-0.791525000	-1.601923000
H	2.500432000	-0.384277000	-0.146563000
H	1.470160000	-1.832184000	-0.167788000
O	0.333862000	-0.071676000	1.433311000
H	1.105066000	0.379032000	1.781806000

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MePropOL\_+gg\_PBE0-D3\_CCT

C	0.504234000	1.406351000	-0.544236000
H	1.442193000	1.862458000	-0.227437000
H	-0.315504000	2.041297000	-0.198588000
C	0.395415000	-0.000714000	0.025449000
H	0.473869000	1.377219000	-1.633493000
O	-0.747085000	-0.670158000	-0.472485000
C	-1.990706000	-0.150470000	-0.087655000
H	-2.179879000	0.846929000	-0.503106000
H	-2.096849000	-0.111851000	1.002136000
H	-2.747430000	-0.829399000	-0.478710000
C	1.561808000	-0.871506000	-0.382486000
H	1.572273000	-1.000171000	-1.464207000

H	2.499448000	-0.420748000	-0.059323000
H	1.453961000	-1.848009000	0.088320000
O	0.390708000	0.039360000	1.433410000
H	-0.075580000	0.826690000	1.720580000

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MePropOL-MeCN\_ang\_-gg\_PBE0-D3\_CCT

C	-2.954544000	-0.528175000	-0.373139000
H	-3.117466000	-1.500592000	-0.837478000
H	-3.232199000	0.238162000	-1.096659000
C	-1.494590000	-0.387708000	0.019204000
H	-3.592584000	-0.440627000	0.506753000
O	-1.261205000	0.791459000	0.775664000
C	-1.584776000	1.997525000	0.131575000
H	-2.667258000	2.167663000	0.091305000
H	-1.182705000	2.029750000	-0.884985000
H	-1.134043000	2.798645000	0.717715000
C	-1.044303000	-1.513627000	0.932113000
H	-1.637662000	-1.526687000	1.846805000
H	-1.149077000	-2.469926000	0.419901000
H	0.002711000	-1.365757000	1.200611000
O	-0.764750000	-0.372860000	-1.172716000
H	0.177830000	-0.363249000	-0.950829000
C	3.202391000	-0.058345000	-0.177853000
N	2.119465000	-0.231601000	-0.514924000
C	4.567409000	0.163816000	0.249585000
H	5.036532000	0.919047000	-0.381459000
H	5.136808000	-0.763004000	0.176306000
H	4.580967000	0.508064000	1.283991000

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MePropOL-MeCN\_tg\_PBE0-D3\_CCT

C	-1.017480000	-0.054327000	1.473325000
H	0.038638000	0.106627000	1.695996000
H	-1.239796000	-1.107436000	1.646235000
C	-1.305338000	0.324113000	0.024267000
H	-1.615494000	0.554384000	2.153429000
O	-2.671606000	0.235568000	-0.279757000
C	-3.250201000	-1.039981000	-0.149475000
H	-3.401843000	-1.319154000	0.900008000
H	-2.645785000	-1.805707000	-0.640827000
H	-4.225031000	-0.988974000	-0.633990000
C	-0.929597000	1.767052000	-0.259883000
H	-1.488988000	2.447395000	0.383671000
H	0.138367000	1.914462000	-0.092141000
H	-1.160606000	1.989766000	-1.301083000
O	-0.624631000	-0.545257000	-0.851734000
H	0.307239000	-0.563921000	-0.598149000
C	3.391891000	-0.248192000	-0.060106000
N	2.254629000	-0.385906000	-0.127096000
C	4.826585000	-0.074936000	0.022005000
H	5.293921000	-0.406063000	-0.905709000
H	5.226104000	-0.661340000	0.849707000
H	5.065605000	0.976440000	0.183657000

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MePropOL-MeCN\_+gg\_PBE0-D3\_CCT

C	1.179613000	-0.700660000	1.371159000
H	1.089847000	-1.786347000	1.417873000
H	0.196912000	-0.274362000	1.578835000
C	1.680849000	-0.285564000	-0.006582000
H	1.874955000	-0.367447000	2.142231000
O	1.926997000	1.114754000	-0.049913000
C	0.796356000	1.938344000	0.023495000
H	0.286366000	1.871586000	0.992956000
H	0.074929000	1.711237000	-0.768028000
H	1.145900000	2.962413000	-0.107643000
C	3.017609000	-0.913975000	-0.333112000
H	3.777004000	-0.576924000	0.372091000
H	2.939925000	-2.000198000	-0.294157000
H	3.310353000	-0.613904000	-1.338912000
O	0.784278000	-0.679890000	-1.003247000
H	-0.123026000	-0.587695000	-0.684493000
N	-2.061009000	-0.345232000	-0.209710000
C	-3.194193000	-0.215069000	-0.084504000
C	-4.623933000	-0.051631000	0.071194000
H	-5.150209000	-0.701027000	-0.628805000
H	-4.920119000	-0.311736000	1.087672000
H	-4.903774000	0.983438000	-0.126267000

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MePropOL-amide\_-gg\_PBE0-D3\_CCT

C	-3.062840000	1.015253000	-0.721644000
H	-2.748356000	1.692589000	-1.515652000
H	-3.282266000	1.614266000	0.162189000
C	-1.954727000	0.018855000	-0.429117000
H	-3.967662000	0.493778000	-1.035238000
O	-2.377986000	-0.984339000	0.480736000
C	-2.787370000	-0.526222000	1.743561000
H	-3.775544000	-0.051293000	1.712235000
H	-2.067808000	0.180369000	2.166877000
H	-2.848136000	-1.400959000	2.391103000
C	-1.539302000	-0.751442000	-1.668677000
H	-2.380653000	-1.321809000	-2.062941000
H	-1.182819000	-0.061204000	-2.433574000
H	-0.737302000	-1.443972000	-1.410264000
O	-0.886041000	0.753846000	0.093798000
H	-0.104741000	0.173614000	0.147410000
O	1.462426000	-0.740449000	0.124744000
C	2.639438000	-0.412601000	0.055119000
C	3.724316000	-1.443479000	-0.100538000
H	3.533292000	-2.012272000	-1.010782000
H	3.664067000	-2.139024000	0.736719000
H	4.728010000	-1.020795000	-0.145721000
N	3.037394000	0.870676000	0.109148000
H	4.019621000	1.069428000	0.076782000
C	2.101899000	1.959910000	0.273733000
H	1.617248000	1.923006000	1.251480000

H	1.317325000	1.913471000	-0.480974000
H	2.638284000	2.901963000	0.177469000

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MePropOL-amide\_tg\_PBE0-D3\_CCT

C	1.753129000	-1.629702000	0.256560000
H	0.746295000	-2.048533000	0.290609000
H	2.149019000	-1.629124000	1.272023000
C	1.700231000	-0.211709000	-0.298971000
H	2.380917000	-2.263340000	-0.371829000
O	2.977574000	0.351135000	-0.443259000
C	3.728332000	0.482745000	0.739199000
H	4.109255000	-0.481467000	1.095697000
H	3.144052000	0.952934000	1.533499000
H	4.579398000	1.118679000	0.496493000
C	1.100561000	-0.184494000	-1.693934000
H	1.690060000	-0.793415000	-2.380407000
H	0.079020000	-0.566403000	-1.667353000
H	1.091386000	0.844676000	-2.052964000
O	0.967373000	0.621686000	0.570309000
H	0.132869000	0.174121000	0.792558000
O	-1.506798000	-0.600540000	0.829705000
C	-2.546611000	-0.340891000	0.236598000
H	-3.854674000	-1.878033000	0.886173000
C	-3.556159000	-1.418086000	-0.056005000
H	-3.074469000	-2.189878000	-0.657006000
H	-4.442955000	-1.059504000	-0.578483000
N	-2.856881000	0.893840000	-0.194976000
H	-3.754501000	1.028689000	-0.622265000
C	-2.023505000	2.050922000	0.044862000
H	-0.973729000	1.795077000	-0.090320000
H	-2.153419000	2.435870000	1.059675000
H	-2.291413000	2.831798000	-0.665161000

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MePropOL-amide\_+gg\_PBE0-D3\_CCT

C	1.985660000	-1.031714000	-1.187772000
H	2.164141000	-0.609298000	-2.177035000
H	1.006957000	-1.513370000	-1.207044000
C	2.036240000	0.074799000	-0.143265000
H	2.749053000	-1.782040000	-0.979760000
O	1.975852000	-0.468488000	1.172269000
C	0.762663000	-1.056851000	1.542932000
H	0.498169000	-1.917482000	0.915503000
H	-0.064370000	-0.338600000	1.515588000
H	0.883922000	-1.406058000	2.568527000
C	3.350129000	0.824527000	-0.175920000
H	4.176373000	0.153230000	0.057211000
H	3.504013000	1.263077000	-1.161397000
H	3.320963000	1.620613000	0.567741000
O	1.015347000	1.005185000	-0.356239000
H	0.232870000	0.563392000	-0.728979000
O	-1.338008000	-0.248559000	-1.148520000
C	-3.038158000	-1.560132000	-0.118604000

H	-2.370088000	-2.298600000	0.327550000
H	-3.356714000	-1.949175000	-1.085084000
H	-3.908185000	-1.432879000	0.525529000
N	-2.631751000	0.773373000	0.385921000
H	-3.379194000	0.665139000	1.045824000
C	-1.973969000	2.056759000	0.271998000
H	-1.850283000	2.312532000	-0.780511000
H	-0.983455000	2.046697000	0.730010000
H	-2.591648000	2.813179000	0.752527000
C	-2.261864000	-0.292235000	-0.343990000

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MePropOL-CN\_-gg\_PBE0-D3\_CCT

C	-2.194859000	-0.712457000	-0.600339000
H	-2.148715000	-1.623542000	-1.199139000
H	-2.517216000	0.102300000	-1.251252000
C	-0.816460000	-0.403038000	-0.025416000
H	-2.924763000	-0.840554000	0.201343000
O	-0.929235000	0.760160000	0.823524000
C	-0.883642000	1.986263000	0.153010000
H	-1.713007000	2.113345000	-0.559107000
H	0.054845000	2.119334000	-0.390793000
H	-0.969685000	2.761692000	0.917721000
C	-0.345480000	-1.499124000	0.919397000
H	-1.015823000	-1.581762000	1.777791000
H	-0.315982000	-2.452941000	0.389727000
H	0.660110000	-1.259199000	1.264387000
O	0.037831000	-0.211190000	-1.076711000
H	1.010639000	-0.153456000	-0.755802000
N	3.778129000	0.046699000	0.078240000
C	2.667762000	-0.022288000	-0.266161000

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MePropOL-CN\_tg\_PBE0-D3\_CCT

C	-0.225514000	-0.049703000	1.467449000
H	0.853171000	0.019913000	1.616395000
H	-0.520771000	-1.079714000	1.673520000
C	-0.546247000	0.311481000	0.018541000
H	-0.740223000	0.620365000	2.160950000
O	-1.957211000	0.293035000	-0.203581000
C	-2.547478000	-0.973974000	-0.140660000
H	-2.636120000	-1.345788000	0.890271000
H	-1.985292000	-1.705226000	-0.727231000
H	-3.554934000	-0.877225000	-0.552502000
C	-0.128108000	1.740584000	-0.288486000
H	-0.628795000	2.450559000	0.374421000
H	0.953200000	1.824690000	-0.172196000
H	-0.392943000	1.964505000	-1.322442000
O	0.044680000	-0.581237000	-0.856341000
H	1.047723000	-0.586996000	-0.676934000
N	3.864219000	-0.333602000	0.067721000
C	2.756631000	-0.469097000	-0.266665000

18

MePropOL-CN\_+gg\_PBE0-D3\_CCT

C	0.436084000	-0.655881000	1.364218000
H	0.372338000	-1.741818000	1.451353000
H	-0.569262000	-0.261667000	1.511909000
C	0.962101000	-0.287423000	-0.021843000
H	1.103207000	-0.271168000	2.139468000
O	1.226639000	1.125343000	-0.082592000
C	0.088555000	1.940251000	0.013440000
H	-0.284912000	2.015732000	1.043357000
H	-0.730845000	1.577120000	-0.613176000
H	0.381339000	2.938990000	-0.319668000
C	2.323676000	-0.909484000	-0.279562000
H	3.055025000	-0.562412000	0.452799000
H	2.244970000	-1.996125000	-0.231769000
H	2.653556000	-0.621231000	-1.278393000
O	0.111493000	-0.696879000	-1.019536000
H	-0.862930000	-0.618311000	-0.742946000
N	-3.651594000	-0.264974000	0.093325000
C	-2.561480000	-0.426131000	-0.284452000

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MePropOL-NCO\_-gg\_PBE0-D3\_CCT

C	-1.378300000	-0.362153000	-0.014594000
O	-1.325016000	0.809899000	0.825009000
C	-1.019833000	2.001590000	0.156606000
H	-1.726395000	2.226434000	-0.655381000
H	-0.009709000	1.986428000	-0.260935000
H	-1.088997000	2.797605000	0.902143000
O	-0.543494000	-0.280461000	-1.098160000
H	0.422493000	-0.281026000	-0.791604000
C	3.113223000	-0.092980000	-0.083312000
N	1.951799000	-0.210336000	-0.282845000
O	4.296474000	0.023251000	0.124306000
C	-2.801657000	-0.499481000	-0.541915000
H	-3.046605000	0.363345000	-1.164459000
H	-2.886799000	-1.397279000	-1.156686000
H	-3.511899000	-0.555324000	0.284882000
C	-1.002044000	-1.504902000	0.916825000
H	-1.128242000	-2.458854000	0.400928000
H	0.045770000	-1.389085000	1.195702000
H	-1.624259000	-1.493848000	1.814427000

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MePropOL-NCO\_tg\_PBE0-D3\_CCT

C	-0.782981000	-0.010517000	1.483567000
H	0.293322000	0.085608000	1.634445000
H	-1.058513000	-1.042638000	1.706987000
C	-1.092861000	0.316308000	0.024623000
H	-1.318914000	0.660978000	2.159321000
O	-2.494131000	0.237322000	-0.228805000
C	-3.037276000	-1.049972000	-0.152116000
H	-3.138314000	-1.402569000	0.884351000
H	-2.433308000	-1.771660000	-0.708148000
H	-4.036654000	-1.000874000	-0.591020000
C	-0.717540000	1.752635000	-0.300004000

H	-1.241401000	2.456629000	0.351143000
H	0.360946000	1.863560000	-0.180485000
H	-0.985009000	1.954567000	-1.337920000
O	-0.446687000	-0.568617000	-0.822857000
H	0.538890000	-0.508052000	-0.624305000
C	3.284875000	-0.226240000	-0.066087000
N	2.105036000	-0.248411000	-0.174517000
O	4.485618000	-0.199949000	0.050081000

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MePropOL-NCO\_+gg\_PBE0-D3\_CCT

C	1.457667000	-0.303608000	-0.012501000
O	1.769959000	1.094927000	-0.111393000
C	0.666465000	1.954883000	0.011828000
H	0.377015000	2.106331000	1.060856000
H	-0.209931000	1.583793000	-0.526682000
H	0.965045000	2.920733000	-0.403440000
O	0.591225000	-0.710312000	-1.000716000
H	-0.363843000	-0.566828000	-0.725703000
N	-1.927255000	-0.258017000	-0.269984000
C	-3.094667000	-0.188425000	-0.078732000
O	-4.282545000	-0.114135000	0.119574000
C	0.913181000	-0.620766000	1.378437000
H	0.846273000	-1.703040000	1.503061000
H	1.569851000	-0.210881000	2.149713000
H	-0.094718000	-0.219495000	1.490042000
C	2.794549000	-0.981060000	-0.256024000
H	3.138017000	-0.722392000	-1.258385000
H	3.536246000	-0.649194000	0.472609000
H	2.674545000	-2.062888000	-0.189953000

23

MePropOL-MeCOO\_-gg\_PBE0-D3\_CCT

C	3.112204000	-0.202062000	0.527075000
H	3.341232000	-1.019151000	1.213667000
H	3.222094000	0.738104000	1.070572000
C	1.680320000	-0.335908000	0.017651000
H	3.817853000	-0.217285000	-0.305823000
O	1.430276000	0.721977000	-0.921043000
C	1.009723000	1.936800000	-0.348288000
H	1.725359000	2.316884000	0.395193000
H	0.023239000	1.851227000	0.114828000
H	0.959520000	2.655438000	-1.170358000
C	1.491786000	-1.608688000	-0.797776000
H	2.090722000	-1.576284000	-1.710783000
H	1.785554000	-2.476211000	-0.203085000
H	0.436288000	-1.699440000	-1.055679000
O	0.851500000	-0.293350000	1.108754000
H	-0.106634000	-0.482797000	0.823349000
O	-1.532763000	-0.901242000	0.358424000
O	-2.262573000	1.226655000	0.347056000
H	-4.096761000	-1.325491000	0.253996000
C	-3.738726000	-0.500212000	-0.365951000
H	-3.597314000	-0.895371000	-1.375762000

H	-4.479229000	0.299638000	-0.392124000
C	-2.390881000	0.009807000	0.166703000

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MePropOL-MeCOO\_tg\_PBE0-D3\_CCT

C	-1.162896000	0.473074000	1.435909000
H	-0.116149000	0.763087000	1.534278000
H	-1.286797000	-0.494978000	1.924201000
C	-1.493519000	0.361920000	-0.051775000
H	-1.804097000	1.210318000	1.926222000
O	-2.870896000	0.039295000	-0.239556000
C	-3.234983000	-1.249554000	0.167122000
H	-3.290270000	-1.344532000	1.261271000
H	-2.536419000	-1.999489000	-0.212334000
H	-4.230716000	-1.442448000	-0.239395000
C	-1.311455000	1.702966000	-0.745464000
H	-1.938639000	2.473946000	-0.290808000
H	-0.261142000	1.988201000	-0.678214000
H	-1.586009000	1.589215000	-1.794953000
O	-0.729047000	-0.619189000	-0.654861000
H	0.243986000	-0.391150000	-0.491601000
O	1.620094000	0.314520000	-0.143608000
C	2.723594000	-0.308072000	-0.072583000
O	2.930406000	-1.508056000	-0.265903000
H	3.757960000	0.989635000	1.313853000
C	3.915669000	0.584200000	0.310533000
H	3.975483000	1.436020000	-0.371498000
H	4.849892000	0.022413000	0.287951000

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MePropOL-MeCOO\_+gg\_PBE0-D3\_CCT

C	0.780441000	-0.603141000	1.232349000
H	0.077616000	-1.424564000	1.090222000
H	0.176923000	0.275740000	1.459378000
C	1.584538000	-0.380526000	-0.042264000
H	1.450916000	-0.808578000	2.070538000
O	2.476206000	0.746834000	0.134443000
C	1.826909000	1.982085000	0.228292000
H	1.424544000	2.169743000	1.234192000
H	1.004006000	2.059678000	-0.488638000
H	2.565734000	2.757474000	0.007888000
C	2.532739000	-1.535859000	-0.311524000
H	3.266749000	-1.635085000	0.490652000
H	1.959979000	-2.459493000	-0.400529000
H	3.052607000	-1.347879000	-1.252046000
O	0.782655000	-0.205806000	-1.141432000
H	-0.156137000	0.071928000	-0.877397000
O	-1.564492000	0.654211000	-0.541497000
H	-4.181049000	0.916234000	-0.849862000
C	-3.825083000	0.531077000	0.109185000
H	-3.730545000	1.387873000	0.781432000
H	-4.547998000	-0.177848000	0.513576000
C	-2.449261000	-0.126699000	-0.080937000
O	-2.327499000	-1.318595000	0.224735000