

Hydrogen Abstraction from n-Butanol by the Methyl Radical: High Level Ab Initio Abstraction Pathways and the Importance of Low Energy Rotational Conformers[†]

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Supplementary Information

S1. Coordinates (xyz) for the n-butanol conformers computed at the ROCBS-QB3 level

TGt

C	1.448269000	0.519321000	0.222466000
C	0.006316000	0.707080000	-0.225741000
H	2.068883000	1.333937000	-0.177345000
H	1.504454000	0.562194000	1.320885000
C	-0.962227000	-0.319899000	0.370974000
H	-0.310973000	1.721822000	0.044931000
H	-0.021570000	0.648884000	-1.320179000
H	-0.592918000	-1.322828000	0.140854000
H	-0.951070000	-0.229109000	1.464527000
C	-2.395802000	-0.158568000	-0.140864000
H	-3.063925000	-0.900712000	0.304620000
H	-2.795546000	0.832729000	0.096817000
H	-2.442485000	-0.280954000	-1.227497000
O	1.903979000	-0.745306000	-0.260078000
H	2.793981000	-0.891112000	0.072002000

TGg

C	1.458349000	0.518812000	0.219498000
C	0.011616000	0.705669000	-0.237459000
H	2.090053000	1.315022000	-0.198961000
H	1.521820000	0.590691000	1.308736000
C	-0.964386000	-0.298542000	0.384142000
H	-0.300378000	1.730497000	0.002396000
H	-0.027812000	0.626188000	-1.333494000
H	-0.589696000	-1.309665000	0.200669000
H	-0.964276000	-0.166840000	1.473036000
C	-2.392924000	-0.162746000	-0.148555000
H	-3.062529000	-0.890209000	0.318170000
H	-2.798841000	0.834972000	0.047173000
H	-2.429206000	-0.326327000	-1.230410000
O	1.986149000	-0.767264000	-0.103749000
H	1.995742000	-0.845370000	-1.063086000

TTt

C	1.319353000	0.479579000	0.000001000
C	0.035431000	-0.335058000	0.000002000
H	1.347379000	1.128875000	-0.888107000
H	1.347383000	1.128873000	0.888109000
C	-1.229761000	0.528792000	-0.000001000
H	0.043581000	-0.989921000	-0.878434000
H	0.043578000	-0.989916000	0.878442000
H	-1.221253000	1.187962000	0.876608000
H	-1.221254000	1.187957000	-0.876614000
C	-2.518660000	-0.298095000	0.000000000
H	-3.404189000	0.343178000	-0.000005000
H	-2.573981000	-0.942453000	-0.882700000
H	-2.573986000	-0.942446000	0.882704000
O	2.417934000	-0.430670000	-0.000003000
H	3.231090000	0.081950000	0.000010000

TTg

C	-1.325721000	0.491736000	0.021250000
C	-0.039375000	-0.330849000	-0.022765000
H	-1.353377000	1.098323000	0.939069000
H	-1.358972000	1.183207000	-0.824869000
C	1.232078000	0.523912000	0.024040000
H	-0.036540000	-1.032582000	0.823155000
H	-0.051222000	-0.941064000	-0.932746000
H	1.226739000	1.222626000	-0.821053000
H	1.222309000	1.142317000	0.929775000
C	2.518404000	-0.306179000	-0.010971000
H	3.405551000	0.332025000	0.019421000
H	2.571307000	-0.989687000	0.842116000
H	2.573744000	-0.909939000	-0.921850000
O	-2.499610000	-0.307738000	-0.096504000
H	-2.514969000	-0.915047000	0.649695000

TGg'

C	1.457866000	0.515508000	0.241193000
C	0.008751000	0.716665000	-0.203291000
H	2.078434000	1.330741000	-0.137544000
H	1.520671000	0.539239000	1.339682000
C	-0.955803000	-0.358689000	0.309700000
H	-0.325544000	1.702186000	0.146044000
H	-0.019177000	0.740742000	-1.298721000
H	-0.629623000	-1.340787000	-0.053124000
H	-0.904569000	-0.398090000	1.405469000
C	-2.405457000	-0.126964000	-0.125331000
H	-3.066149000	-0.912893000	0.250278000
H	-2.781205000	0.830629000	0.248077000
H	-2.490976000	-0.112933000	-1.216050000
O	2.044741000	-0.678938000	-0.272843000
H	1.628070000	-1.426453000	0.165004000

GGt

C	1.177372000	0.119209000	0.606164000
C	0.072772000	1.009260000	0.051233000
H	1.941346000	0.747122000	1.086405000
H	0.775044000	-0.557537000	1.373299000
C	-1.079380000	0.251835000	-0.626344000
H	-0.315940000	1.625075000	0.872060000
H	0.526864000	1.695681000	-0.671449000
H	-1.735499000	0.983766000	-1.109845000
H	-0.664223000	-0.370054000	-1.424153000
C	-1.911754000	-0.616131000	0.323382000
H	-2.747191000	-1.083199000	-0.205320000
H	-1.318200000	-1.421646000	0.764574000
H	-2.329482000	-0.022338000	1.143409000
O	1.738848000	-0.620476000	-0.478966000
H	2.402432000	-1.218110000	-0.123867000

GGg

C	1.177839000	0.087626000	0.624805000
C	0.081232000	0.999195000	0.070103000
H	1.942586000	0.695205000	1.128929000
H	0.771680000	-0.600094000	1.369792000
C	-1.067534000	0.261070000	-0.633151000
H	-0.312992000	1.608295000	0.894135000
H	0.540776000	1.704994000	-0.635160000
H	-1.701673000	0.999296000	-1.135825000
H	-0.644806000	-0.373542000	-1.417906000
C	-1.931477000	-0.591752000	0.301721000
H	-2.760249000	-1.051286000	-0.243496000
H	-1.357093000	-1.401125000	0.759868000
H	-2.359936000	0.012804000	1.108043000
O	1.768233000	-0.745074000	-0.372526000
H	2.175478000	-0.170787000	-1.029045000

GTt

C	-1.036615000	-0.359730000	0.310597000
C	-0.094918000	0.698998000	-0.245217000
H	-0.709830000	-1.364085000	0.008141000
H	-1.025582000	-0.320849000	1.410840000
C	1.347873000	0.596640000	0.269668000
H	-0.109166000	0.634583000	-1.339162000
H	-0.510377000	1.677972000	0.015048000
H	1.898290000	1.478367000	-0.074635000
H	1.347808000	0.652195000	1.365348000
C	2.099292000	-0.663019000	-0.178371000
H	3.139416000	-0.639648000	0.158051000
H	1.648546000	-1.575351000	0.221500000
H	2.105368000	-0.748322000	-1.269693000
O	-2.342438000	-0.083542000	-0.195599000
H	-2.938758000	-0.763857000	0.129287000

GTg'

C	-1.039680000	-0.363053000	0.333822000
C	-0.101053000	0.683883000	-0.266129000
H	-0.706918000	-1.372772000	0.085403000
H	-1.038864000	-0.278567000	1.431547000
C	1.343991000	0.613521000	0.251152000
H	-0.117253000	0.578955000	-1.356909000
H	-0.510250000	1.678441000	-0.043139000
H	1.887251000	1.490485000	-0.115996000
H	1.342393000	0.696897000	1.345064000
C	2.103690000	-0.651989000	-0.164315000
H	3.142506000	-0.613591000	0.174390000
H	1.657424000	-1.556692000	0.256813000
H	2.113448000	-0.763791000	-1.253083000
O	-2.364331000	-0.270326000	-0.184078000
H	-2.696776000	0.609072000	0.021352000

GTg

C	-1.043665000	-0.357571000	0.339219000
C	-0.100238000	0.687285000	-0.257177000
H	-0.712874000	-1.374273000	0.087154000
H	-1.046723000	-0.277063000	1.429805000
C	1.347326000	0.607472000	0.251977000
H	-0.105634000	0.589242000	-1.352062000
H	-0.517645000	1.674028000	-0.031631000
H	1.891241000	1.485463000	-0.111734000
H	1.347689000	0.685915000	1.346031000
C	2.105150000	-0.656967000	-0.171079000
H	3.144154000	-0.622459000	0.167462000
H	1.657247000	-1.563508000	0.244178000
H	2.115872000	-0.761955000	-1.260841000
O	-2.398530000	-0.158469000	-0.059866000
H	-2.436523000	-0.248954000	-1.017069000

GGg'

C	1.194904000	0.144429000	0.594927000
C	0.087527000	1.020078000	0.003596000
H	1.979804000	0.781159000	1.009142000
H	0.807810000	-0.468228000	1.420918000
C	-1.080773000	0.248226000	-0.629842000
H	-0.295569000	1.674569000	0.797425000
H	0.538624000	1.669262000	-0.754161000
H	-1.743012000	0.966082000	-1.124526000
H	-0.696118000	-0.392060000	-1.433254000
C	-1.901216000	-0.591895000	0.355824000
H	-2.742756000	-1.075974000	-0.146823000
H	-1.305223000	-1.381080000	0.823673000
H	-2.308049000	0.030086000	1.159312000
O	1.842458000	-0.672159000	-0.379962000
H	1.222169000	-1.351572000	-0.659031000

GG'g'

C	1.363857000	0.380128000	-0.228018000
C	0.107162000	1.011938000	0.374298000
H	1.374051000	0.530069000	-1.311247000
H	2.253655000	0.882676000	0.178195000
C	-1.229383000	0.586129000	-0.255042000
H	0.087208000	0.812295000	1.455531000
H	0.215807000	2.099363000	0.274911000
H	-2.005601000	1.278682000	0.089882000
H	-1.166284000	0.722579000	-1.341780000
C	-1.671167000	-0.849041000	0.055762000
H	-2.645260000	-1.062299000	-0.393674000
H	-0.949319000	-1.575062000	-0.318566000
H	-1.768409000	-0.999974000	1.136603000
O	1.465160000	-1.032244000	-0.044304000
H	1.460065000	-1.205304000	0.902577000

G'Gt

C	1.353872000	0.394291000	0.221352000
C	0.091598000	1.009733000	-0.369356000
H	2.231307000	0.921055000	-0.180745000
H	1.353447000	0.532432000	1.313520000
C	-1.235162000	0.568601000	0.271076000
H	0.188279000	2.097117000	-0.265256000
H	0.077564000	0.800202000	-1.445464000
H	-1.157944000	0.686056000	1.359671000
H	-2.016566000	1.266958000	-0.050062000
C	-1.679042000	-0.860481000	-0.062141000
H	-2.640181000	-1.088015000	0.408581000
H	-1.799645000	-0.986901000	-1.142764000
H	-0.942705000	-1.591754000	0.270815000
O	1.413623000	-0.993520000	-0.114146000
H	2.209861000	-1.361860000	0.279291000

GG'g

C	-1.312517000	0.366950000	0.319366000
C	-0.102981000	1.031587000	-0.345894000
H	-1.186241000	0.357414000	1.412907000
H	-2.209480000	0.952294000	0.104646000
C	1.280447000	0.591730000	0.161104000
H	-0.180879000	0.857891000	-1.425498000
H	-0.189604000	2.114979000	-0.197119000
H	2.037228000	1.185705000	-0.362806000
H	1.373341000	0.856827000	1.221592000
C	1.620368000	-0.894366000	-0.016227000
H	2.670392000	-1.083798000	0.222546000
H	1.033255000	-1.535403000	0.650465000
H	1.447266000	-1.225194000	-1.044368000
O	-1.601653000	-0.940783000	-0.173903000
H	-0.893960000	-1.529851000	0.098764000

S2. Transition States and products structures for the reaction of the TGt conformer

rad_α

C	1.446987000	0.530539000	0.196141000
C	0.036379000	0.684844000	-0.248115000
H	1.774436000	0.913288000	1.161537000
C	-0.951599000	-0.322241000	0.389164000
H	-0.291678000	1.706322000	-0.024178000
H	-0.004913000	0.571037000	-1.339373000
H	-0.587285000	-1.334903000	0.191424000
H	-0.938993000	-0.193628000	1.477615000
C	-2.380682000	-0.166002000	-0.135728000
H	-3.057582000	-0.888419000	0.328790000
H	-2.772373000	0.835476000	0.069874000
H	-2.422224000	-0.320610000	-1.218448000
O	2.057763000	-0.620633000	-0.250101000
H	2.932002000	-0.686333000	0.144794000

TS_{α,(H3)}

C	-0.806036000	0.420871000	0.399262000
C	0.376491000	-0.421388000	-0.015805000
H	-1.862392000	-0.273663000	0.183453000
H	-0.833485000	0.624350000	1.479249000
C	1.737544000	0.233278000	0.270907000
H	0.311490000	-1.386676000	0.500403000
H	0.290614000	-0.630370000	-1.088896000
H	1.761549000	1.213766000	-0.212897000
H	1.827167000	0.416501000	1.348621000
C	2.919022000	-0.615568000	-0.205724000
H	3.872951000	-0.127586000	0.012419000
H	2.928266000	-1.595596000	0.282183000
H	2.872463000	-0.784982000	-1.285941000
O	-0.859549000	1.594331000	-0.371710000
H	-1.548321000	2.164675000	-0.017895000
C	-3.049329000	-1.070764000	-0.084701000
H	-3.874412000	-0.468685000	0.288857000
H	-3.041783000	-1.189623000	-1.165105000
H	-2.893871000	-1.995333000	0.465598000

TS_{$\alpha_1(H4)$}			
C	-0.941734000	-0.693748000	0.489836000
C	0.509951000	-0.376124000	0.767909000
H	-1.471308000	-1.063631000	1.378258000
H	-1.548713000	0.408884000	0.216310000
C	1.255170000	0.251510000	-0.417574000
H	0.552651000	0.293525000	1.635260000
H	1.019594000	-1.303993000	1.064398000
H	1.156036000	-0.407966000	-1.283857000
H	0.767715000	1.194464000	-0.689255000
C	2.735114000	0.504273000	-0.119341000
H	3.242631000	0.952374000	-0.977872000
H	2.860830000	1.182396000	0.731066000
H	3.254616000	-0.428224000	0.122937000
O	-1.051420000	-1.569104000	-0.603309000
H	-1.976910000	-1.805179000	-0.715808000
C	-2.265797000	1.636375000	-0.089268000
H	-3.296544000	1.428184000	0.188865000
H	-2.113734000	1.769715000	-1.157339000
H	-1.791736000	2.398575000	0.524132000

rad_{β}			
C	1.473861000	0.561194000	0.076225000
C	0.006362000	0.739440000	-0.083593000
H	2.007617000	1.276111000	-0.566719000
H	1.770987000	0.788082000	1.119899000
C	-0.970893000	-0.269422000	0.417308000
H	-0.350892000	1.724524000	-0.369420000
H	-0.557928000	-1.270693000	0.262639000
H	-1.081092000	-0.165691000	1.512843000
C	-2.356544000	-0.155491000	-0.230173000
H	-3.046337000	-0.896953000	0.181507000
H	-2.792360000	0.834316000	-0.061915000
H	-2.296253000	-0.313326000	-1.310256000
O	1.837677000	-0.786752000	-0.241897000
H	2.728124000	-0.936675000	0.087994000

TS _{β , (H6)}

C	1.426006000	0.653279000	0.115627000
C	0.104378000	0.090904000	-0.347341000
H	1.642167000	1.587259000	-0.421862000
H	1.374012000	0.886153000	1.189978000
C	-0.403761000	-1.118681000	0.413540000
H	-0.758737000	1.068279000	-0.168821000
H	0.089033000	-0.052871000	-1.431645000
H	0.378309000	-1.888070000	0.395363000
H	-0.537143000	-0.851535000	1.470032000
C	-1.708164000	-1.694264000	-0.144819000
H	-2.029212000	-2.571074000	0.423811000
H	-2.517398000	-0.959081000	-0.108586000
H	-1.586032000	-2.001818000	-1.187890000
O	2.446618000	-0.320739000	-0.139436000
H	3.278775000	0.025201000	0.197529000
C	-1.653833000	2.123061000	0.045688000
H	-2.004311000	1.989619000	1.066443000
H	-1.062449000	3.024080000	-0.099960000
H	-2.427715000	1.983974000	-0.705070000

TS _{β , (H7)}

C	1.376867000	-0.721879000	0.592519000
C	-0.034809000	-0.194130000	0.660835000
H	2.017348000	-0.159516000	1.287411000
H	1.393977000	-1.779417000	0.908918000
C	-1.042662000	-0.862619000	-0.255946000
H	-0.378506000	-0.129378000	1.698025000
H	0.061976000	1.070064000	0.307768000
H	-0.689148000	-0.786567000	-1.288065000
H	-1.068471000	-1.939551000	-0.027431000
C	-2.457916000	-0.290367000	-0.134534000
H	-3.153431000	-0.814572000	-0.795414000
H	-2.837304000	-0.383462000	0.888169000
H	-2.481514000	0.769700000	-0.400848000
O	1.849549000	-0.597702000	-0.750348000
H	2.724682000	-0.992386000	-0.796653000
C	0.269663000	2.396938000	-0.080577000
H	0.982967000	2.301691000	-0.894236000
H	-0.704944000	2.771423000	-0.383790000
H	0.669111000	2.885930000	0.805153000

rad_γ

C	-1.402684000	0.501923000	-0.298653000
C	0.005340000	0.703394000	0.250275000
H	-2.036706000	1.350998000	-0.006486000
H	-1.365856000	0.463999000	-1.396630000
C	0.969652000	-0.355849000	-0.166970000
H	0.366915000	1.693921000	-0.058600000
H	-0.071925000	0.746112000	1.351518000
H	0.574636000	-1.353523000	-0.322339000
C	2.439781000	-0.167848000	-0.014933000
H	3.006176000	-0.924499000	-0.564066000
H	2.762168000	0.820100000	-0.366675000
H	2.758712000	-0.235413000	1.039639000
O	-1.913444000	-0.718995000	0.236094000
H	-2.759094000	-0.899452000	-0.183425000

TS_{γ,(H8)}

C	-1.717135000	-0.729751000	0.140317000
C	-0.326245000	-1.052656000	-0.387259000
H	-2.456733000	-1.342298000	-0.394851000
H	-1.773812000	-0.992337000	1.207549000
C	0.825430000	-0.440558000	0.391362000
H	-0.222271000	-2.148976000	-0.381838000
H	-0.272410000	-0.749778000	-1.440328000
H	0.835297000	0.855417000	0.172773000
H	0.668013000	-0.493394000	1.473304000
C	2.203535000	-0.923040000	-0.017402000
H	2.990445000	-0.397259000	0.530272000
H	2.328201000	-1.996772000	0.175396000
H	2.378015000	-0.762940000	-1.086533000
O	-1.984157000	0.658798000	-0.054653000
H	-2.849143000	0.851655000	0.317938000
C	0.922859000	2.222312000	-0.083944000
H	-0.107968000	2.469374000	-0.315217000
H	1.611387000	2.319879000	-0.920382000
H	1.293568000	2.659210000	0.840697000

TS_{γ}(H9)			
C	-1.631928000	0.369586000	0.501139000
C	-0.480758000	-0.600361000	0.729881000
H	-2.348061000	0.291676000	1.331344000
H	-1.251558000	1.400626000	0.478757000
C	0.618497000	-0.509966000	-0.312620000
H	-0.066986000	-0.424361000	1.731087000
H	-0.894992000	-1.619027000	0.741237000
H	0.210263000	-0.477641000	-1.324204000
H	1.160844000	0.671411000	-0.185950000
C	1.746738000	-1.509673000	-0.159562000
H	2.528776000	-1.349837000	-0.906860000
H	2.210311000	-1.442702000	0.830557000
H	1.383958000	-2.538642000	-0.279709000
O	-2.256934000	0.031070000	-0.737772000
H	-2.933597000	0.688106000	-0.922409000
C	1.795529000	1.924197000	-0.025968000
H	1.223347000	2.609151000	-0.647007000
H	1.734443000	2.141038000	1.038111000
H	2.810263000	1.758940000	-0.379987000

rad_{δ}			
C	1.384456000	0.500498000	0.252060000
C	-0.053244000	0.734733000	-0.186233000
H	2.016047000	1.328316000	-0.100173000
H	1.439979000	0.479862000	1.351059000
C	-1.033288000	-0.322201000	0.347142000
H	-0.364402000	1.731413000	0.145736000
H	-0.082275000	0.739693000	-1.281659000
H	-0.636688000	-1.312465000	0.071023000
H	-1.030058000	-0.306107000	1.445267000
C	-2.423499000	-0.158366000	-0.159098000
H	-3.269132000	-0.549266000	0.393363000
H	-2.604924000	0.209967000	-1.162648000
O	1.822544000	-0.740446000	-0.302111000
H	2.704550000	-0.925831000	0.031699000

TS_{δ,(H11)}

C	2.291936000	0.109722000	0.406099000
C	1.055375000	0.878998000	-0.037471000
H	3.180073000	0.749415000	0.302512000
H	2.197535000	-0.165620000	1.467497000
C	-0.254945000	0.099051000	0.171882000
H	1.018262000	1.826511000	0.512885000
H	1.169446000	1.131074000	-1.097590000
H	-0.163173000	-0.866193000	-0.333672000
H	-0.368781000	-0.117376000	1.241805000
C	-1.476625000	0.838329000	-0.331041000
H	-2.541273000	0.084328000	-0.105793000
H	-1.702754000	1.764639000	0.201639000
H	-1.498792000	0.992881000	-1.411621000
O	2.409598000	-1.054160000	-0.412501000
H	3.152009000	-1.573896000	-0.092567000
C	-3.638268000	-0.717790000	0.134769000
H	-4.475198000	-0.187908000	-0.314227000
H	-3.701620000	-0.793075000	1.217957000
H	-3.407352000	-1.661355000	-0.354250000

TS_{δ,(H12)}

C	-1.891577000	-0.810554000	0.132791000
C	-0.513892000	-0.428540000	-0.387614000
H	-2.255993000	-1.697882000	-0.404040000
H	-1.827586000	-1.067074000	1.201209000
C	0.123736000	0.740250000	0.373644000
H	0.134872000	-1.310190000	-0.333810000
H	-0.608547000	-0.167986000	-1.448126000
H	-0.582442000	1.579556000	0.367294000
H	0.250464000	0.461398000	1.428018000
C	1.453666000	1.182575000	-0.199192000
H	1.927971000	2.002988000	0.341503000
H	2.330249000	0.197381000	-0.070498000
H	1.440853000	1.377036000	-1.273750000
O	-2.768328000	0.298217000	-0.071380000
H	-3.621778000	0.082696000	0.314433000
C	3.261157000	-0.814718000	0.092220000
H	3.093831000	-1.497690000	-0.737474000
H	4.223889000	-0.310444000	0.050152000
H	3.042297000	-1.249603000	1.065042000

TS_{δ,(H13)}

C	2.074987000	-0.028945000	0.434073000
C	0.606365000	-0.304667000	0.719966000
H	2.567372000	0.333629000	1.347560000
H	2.576040000	-0.960296000	0.128959000
C	-0.142878000	-0.919230000	-0.468652000
H	0.541044000	-0.973371000	1.587003000
H	0.130654000	0.638361000	1.009725000
H	-0.014313000	-0.271319000	-1.340693000
H	0.335128000	-1.875780000	-0.731116000
C	-1.615556000	-1.148736000	-0.201223000
H	-2.165695000	-1.578200000	-1.039737000
H	-1.834065000	-1.683050000	0.726228000
H	-2.203873000	0.027694000	-0.031448000
O	2.149909000	0.950659000	-0.602572000
H	3.075583000	1.085995000	-0.822759000
C	-2.818551000	1.256836000	0.110941000
H	-3.818001000	1.114762000	-0.293920000
H	-2.808332000	1.460597000	1.179223000
H	-2.207023000	1.944156000	-0.469079000

1-butoxy radical

C	1.516492000	0.416034000	0.198790000
C	0.063999000	0.708919000	-0.187300000
H	2.199324000	1.236143000	-0.093981000
H	1.627039000	0.375205000	1.304238000
C	-0.917278000	-0.343223000	0.337914000
H	-0.206611000	1.704086000	0.187718000
H	0.003143000	0.758568000	-1.280864000
H	-0.566317000	-1.330015000	0.020048000
H	-0.890768000	-0.344889000	1.434977000
C	-2.354571000	-0.122142000	-0.139066000
H	-3.026287000	-0.889040000	0.255641000
H	-2.736711000	0.851724000	0.183174000
H	-2.416999000	-0.156664000	-1.231072000
O	2.020292000	-0.770330000	-0.255239000

TS_{OH,(H15)}

C	0.589130000	0.776201000	0.202402000
C	-0.906502000	0.799649000	-0.138109000
H	1.034597000	1.745425000	-0.065183000
H	0.709611000	0.630486000	1.286918000
C	-1.665413000	-0.455144000	0.305499000
H	-1.340220000	1.688576000	0.337344000
H	-1.011054000	0.935955000	-1.220156000
H	-1.195210000	-1.331911000	-0.147676000
H	-1.557487000	-0.573568000	1.390806000
C	-3.151474000	-0.410790000	-0.059594000
H	-3.669385000	-1.315237000	0.270903000
H	-3.651249000	0.445882000	0.404334000
H	-3.289738000	-0.326806000	-1.142055000
O	1.174448000	-0.277564000	-0.527532000
H	2.332231000	-0.364674000	-0.235009000
C	3.584604000	-0.392646000	0.140250000
H	3.560805000	-0.606418000	1.206081000
H	3.982637000	0.588500000	-0.107056000
H	3.996812000	-1.199312000	-0.461676000

Table 1: Rotational constants and vibrational frequencies of the transition state structures involved in the hydrogen abstraction by CH₃ from the TGt n-butanol conformer, computed at the ROCBS-QB3 level.

Species	I_A, I_B, I_C (GHz)	Frequencies (cm ⁻¹)
TS _{α,(H3)}	5.2485207 1.3877381 1.1713934	<i>i</i> 1466.9, 27.5, 75.6, 79.4, 97.1, 164.5, 242.9, 261.3, 326.7, 341.8, 409.7, 521.0, 527.3, 619.7, 749.6, 860.4, 874.0, 972.7, 1020.5, 1038.5, 1083.8, 1115.5, 1144.4, 1152.7, 1237.9, 1301.7, 1304.1, 1335.7, 1361.9, 1394.4, 1413.5, 1416.9, 1429.8, 1455.3, 1468.7, 1474.9, 1496.9, 1501.1, 1510.9, 2983.8, 3007.9, 3014.7, 3018.4, 3044.4, 3055.3, 3061.8, 3084.1, 3084.8, 3186.6, 3192.4, 3838.2
TS _{α,(H4)}	3.7787066 1.7332805 1.3812121	<i>i</i> 1488.7, 45.6, 69.2, 80.1, 115.4, 163.9, 241.8, 259.8, 321.1, 340.1, 431.4, 504.8, 546.6, 619.6, 749.3, 849.2, 864.9, 969.9, 1005.5, 1043.0, 1090.4, 1112.4, 1152.3, 1164.5, 1233.4, 1276.3, 1325.9, 1334.8, 1353.5, 1399.2, 1414.3, 1419.2, 1428.6, 1456.7, 1468.0, 1473.5, 1498.0, 1501.5, 1512.6, 2981.2, 2996.1, 3016.8, 3026.0, 3034.6, 3054.4, 3061.7, 3084.4, 3086.3, 3185.0, 3191.1, 3837.3
TS _{β,(H6)}	3.1288666 2.0716888 1.3358654	<i>i</i> 1602.5, 33.9, 78.1, 87.2, 104.2, 149.9, 226.9, 246.0, 274.6, 328.2, 430.7, 498.1, 537.4, 607.1, 782.9, 841.8, 923.3, 982.3, 1003.8, 1035.5, 1086.2, 1125.2, 1136.6, 1167.0, 1245.1, 1258.1, 1294.8, 1331.7, 1361.2, 1388.1, 1410.0, 1416.4, 1444.3, 1446.6, 1454.8, 1487.8, 1501.6, 1506.9, 1517.0, 2961.8, 2993.8, 2998.2, 3021.9, 3022.8, 3055.8, 3062.4, 3083.1, 3087.5, 3186.0, 3189.1, 3823.6
TS _{β,(H7)}	3.2735885 2.1423411 1.5347186	<i>i</i> 1608.5, 33.6, 80.4, 87.8, 106.4, 166.6, 219.8, 246.7, 273.4, 343.2, 458.5, 485.0, 545.0, 629.3, 782.2, 847.4, 887.0, 974.4, 1001.3, 1036.7, 1105.8, 1123.0, 1130.6, 1147.1, 1230.3, 1261.1, 1295.3, 1324.7, 1368.6, 1385.2, 1412.6, 1418.0, 1439.7, 1446.1, 1454.1, 1488.8, 1501.7, 1507.2, 1511.8, 2925.1, 2963.8, 2980.8, 3021.8, 3049.8, 3057.5, 3062.2, 3084.7, 3090.6, 3185.2, 3199.3, 3843.4
TS _{γ,(H8)}	3.4876738 2.1714253 1.4400704	<i>i</i> 1621.3, 34.0, 45.9, 120.1, 146.5, 167.6, 222.8, 235.8, 276.6, 330.6, 464.3, 492.2, 551.1, 558.0, 834.0, 843.3, 892.5, 982.4, 987.6, 1050.6, 1101.9, 1120.6, 1126.7, 1161.0, 1227.3, 1261.9, 1312.9, 1323.2, 1365.4, 1407.1, 1410.2, 1411.7, 1442.0, 1452.2, 1457.0, 1465.6, 1493.1, 1496.0, 1521.4, 2958.1, 2971.7, 2991.1, 2995.3, 3026.7, 3043.4, 3054.5, 3058.0, 3083.5, 3181.2, 3211.6, 3839.7
TS _{γ,(H9)}	3.5351552 1.8673954 1.4376871	<i>i</i> 1572.0, 38.7, 49.5, 107.5, 133.4, 167.3, 219.0, 236.8, 283.0, 343.2, 460.1, 496.3, 541.9, 551.2, 819.6, 851.5, 901.5, 971.6, 1007.8, 1053.4, 1095.8, 1122.9, 1131.2, 1157.5, 230.2, 1258.4, 1303.5, 1330.2, 1370.7, 1400.1, 1408.6, 1414.0, 1447.0, 1448.2, 1452.5, 1466.3, 1492.8, 1495.5, 1523.4, 2970.5, 2979.5, 2998.1, 3005.3, 3026.2, 3049.1, 3054.9, 3077.3, 3094.4, 3184.8, 3187.3, 3843.5
TS _{δ,(H11)}	6.8559498 1.1098557 1.0155975	<i>i</i> 1628.2, 29.6, 52.9, 79.4, 94.7, 160.2, 233.1, 275.6, 318.2, 363.4, 461.6, 518.1, 582.1, 681.7, 757.3, 863.8, 879.9, 976.3, 1029.8, 1041.9, 1073.4, 1119.0, 1141.1, 1148.5, 1239.6, 1254.4, 1303.6, 1327.8, 1336.6, 1382.1, 1386.0, 1392.4, 1447.5, 1447.7, 1450.5, 1464.4, 1475.8, 1503.3, 1521.6, 2960.6, 2988.7, 3004.7, 3020.3, 3048.4, 3052.7, 3054.4, 3071.8, 3121.5, 3184.4, 3185.4, 3843.7
TS _{δ,(H12)}	6.7203589 1.2449704 1.1149294	<i>i</i> 1630.8, 39.6, 45.6, 67.3, 137.3, 169.1, 230.2, 277.9, 347.0, 365.7, 466.4, 509.5, 560.4, 689.1, 761.9, 845.3, 898.6, 974.4, 990.0, 1062.5, 1076.1, 1120.9, 1144.0, 1162.4, 1211.6, 1259.9, 1288.3, 1332.2, 1335.6, 1387.9, 1389.9, 1404.6, 1448.0, 1450.4, 1452.6, 1459.4, 1475.6, 1493.0, 1522.5, 2961.0, 2989.6, 2997.8, 3021.6, 3023.7, 3053.3, 3054.7, 3060.7, 3125.0, 3182.4, 3184.1, 3843.3
TS _{δ,(H13)}	4.6161195 1.4447638 1.2611939	<i>i</i> 1634.5, 37.0, 47.9, 71.3, 143.9, 165.6, 231.1, 279.8, 340.9, 369.4, 468.6, 507.2, 563.3, 693.3, 763.9, 847.9, 886.7, 974.0, 998.4, 1058.1, 1080.4, 1123.6, 1142.2, 1157.9, 1215.8, 1254.2, 1294.7, 1323.2, 1339.0, 1386.8, 1389.4, 1405.3, 1447.8, 1449.6, 1453.0, 1460.0, 1475.8, 1493.8, 1522.3, 2959.6, 2965.1, 2989.6, 3018.0, 3048.5, 3053.6, 3054.6, 3067.1, 3123.8, 3183.9, 3185.5, 3843.3
TS _{OH,(H15)}	9.8534862 1.1121587 1.062763	<i>i</i> -1660.3, 33.7, 38.9, 73.4, 118.4, 153.6, 239.5, 257.6, 307.3, 393.5, 469.6, 539.3, 647.9, 750.5, 840.9, 854.0, 974.4, 981.0, 1029.7, 1064.7, 1101.2, 1138.9, 1165.3, 1195.2, 1251.1, 1269.7, 1326.0, 1333.7, 1351.6, 1393.9, 1401.7, 1414.4, 1429.1, 1440.5, 1475.5, 1497.0, 1501.5, 1511.9, 1525.8, 2954.1, 2985.4, 3008.8, 3011.8, 3017.6, 3047.8, 3057.7, 3062.1, 3084.2, 3085.5, 3191.0, 3192.1

Table 2: B3LYP/6-311G(2d,d,p) and MP2 6-311G(d,p) geometrical parameters of transition state structures. MP2 parameters are in brackets.

Site	Bond distances (Å)				L
	B_{react}	B_{react}^{TS}	B_{prod}	B_{prod}^{TS}	
α	1.099 (1.099)	1.283 (1.277)	1.091 (1.090)	1.455 (1.401)	0.51 (0.57)
β	1.096 (1.097)	1.316 (1.308)	1.091 (1.090)	1.398 (1.355)	0.72 (0.80)
γ	1.097 (1.098)	1.306 (1.294)	1.091 (1.090)	1.413 (1.372)	0.65 (0.70)
δ	1.094 (1.095)	1.326 (1.313)	1.091 (1.090)	1.382 (1.348)	0.80 (0.84)
OH	0.961 (0.959)	1.197 (1.262)	1.091 (1.090)	1.308 (1.219)	1.09 (2.35)

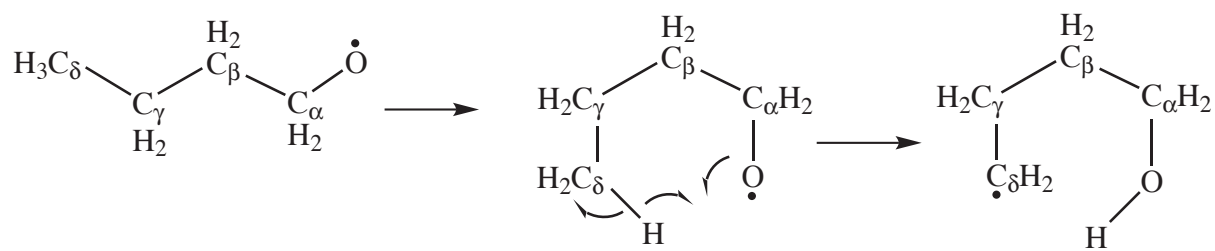


Figure 1: Key post H-abstraction reaction.