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INTRAMOLECULAR ADDITION OF OXYRADICALS TO BENZENE RINGS: A DFT STUDY

Götz Bucher

WestCHEM, School of Chemistry, University of Glasgow, Joseph-Black-Building, Glasgow G12 8QQ, UK; e-Mail: goetz.bucher@gla.ac.uk

Supporting Information

Cartesian coordinates and energies of stationary points optimised

Optimized geometry of radical ap-1a (UM05-2X/6-31G(d))

symmetry c1

C	3.588162000	-0.627827000	-1.379402000
C	2.748964000	0.408626000	-0.979576000
C	2.263304000	0.450728000	0.325001000
C	2.631544000	-0.547435000	1.226554000
C	3.469271000	-1.583245000	0.827649000
C	3.948771000	-1.625815000	-0.479126000
H	3.963455000	-0.653370000	-2.394814000
H	2.469357000	1.194824000	-1.668469000
H	2.265353000	-0.510175000	2.247646000
H	3.751485000	-2.352322000	1.535670000
H	4.603611000	-2.429412000	-0.791302000
C	1.322594000	1.553291000	0.773374000
O	1.281894000	2.634160000	-0.066642000
C	-0.153969000	1.046213000	0.852644000
H	-0.766716000	1.842794000	1.277825000
H	-0.162866000	0.202567000	1.546965000
C	-0.719319000	0.613801000	-0.503745000
H	-0.064115000	-0.139929000	-0.945670000
H	-0.735195000	1.471104000	-1.179867000
C	-2.110643000	0.055305000	-0.336141000
C	-3.227198000	0.890590000	-0.395764000
C	-2.301905000	-1.300249000	-0.062800000
C	-4.506689000	0.383874000	-0.190930000
H	-3.089794000	1.944909000	-0.609962000
C	-3.579221000	-1.811437000	0.143106000
H	-1.440248000	-1.957651000	-0.017388000
C	-4.686023000	-0.969622000	0.079480000
H	-5.362962000	1.044537000	-0.245637000
H	-3.710797000	-2.866499000	0.348580000
H	-5.681189000	-1.366063000	0.236261000
H	1.579609000	1.880620000	1.791359000

E(UM052X+HF-M052X) = -655.712757
E(UM052X+HF-M052X) + ZPE = -655.449101
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.879180
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.882808
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.886388
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.887635

Optimized geometry of radical g-1a (UM05-2X/6-31G(d))

symmetry c1

C	4.540946000	-0.471469000	0.138540000
C	3.289029000	-1.010675000	-0.141269000
C	2.185668000	-0.177131000	-0.308884000
C	2.341979000	1.203202000	-0.205306000
C	3.594148000	1.742562000	0.071134000
C	4.695024000	0.907640000	0.245685000
H	5.394371000	-1.125719000	0.265540000
H	3.168418000	-2.085256000	-0.234029000
H	1.480703000	1.841640000	-0.355515000
H	3.712260000	2.816403000	0.146808000
H	5.668937000	1.330023000	0.458513000
C	0.814238000	-0.779918000	-0.551734000
O	-0.022017000	0.045367000	-1.255768000
C	0.115534000	-1.034523000	0.818600000
H	0.067390000	-0.083047000	1.352404000
H	0.788323000	-1.694355000	1.371587000
C	-1.278863000	-1.659871000	0.694327000
H	-1.521648000	-2.134451000	1.649234000
H	-1.254771000	-2.454377000	-0.056518000
C	-2.363904000	-0.664583000	0.355485000
C	-2.950016000	-0.629326000	-0.909300000
C	-2.799674000	0.245454000	1.321382000
C	-3.948747000	0.293186000	-1.204466000
H	-2.607628000	-1.320003000	-1.670464000
C	-3.795206000	1.171341000	1.030638000
H	-2.357864000	0.221453000	2.312262000
C	-4.374296000	1.196263000	-0.235425000
H	-4.391601000	0.308182000	-2.192420000
H	-4.122918000	1.868204000	1.792033000
H	-5.151905000	1.914212000	-0.463871000

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H        0.908909000     -1.758750000     -1.045867000
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E(UM052X+HF-M052X) = -655.710781
E(UM052X+HF-M052X) + ZPE = -655.447414
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.876648
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.880555
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.884812
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.886418

Optimized geometry of radical 2a (UM05-2X/6-31G(d))

```
symmetry c1
C        0.569355000     -1.150465000     -0.703924000
O       -0.533087000     -0.307562000     -1.028546000
C        0.082281000     -2.003747000      0.474140000
H        0.895613000     -2.397028000      1.082290000
H       -0.514984000     -2.840606000      0.106442000
C       -0.789829000     -1.000274000      1.221759000
H       -0.161090000     -0.310154000      1.790130000
H       -1.514159000     -1.452017000      1.898044000
C       -1.487671000     -0.231471000      0.071915000
C       -2.749819000     -0.918485000     -0.357317000
C       -1.717908000      1.203706000      0.428036000
C       -3.966488000     -0.310316000     -0.341208000
H       -2.646931000     -1.943309000     -0.693068000
C       -2.951698000      1.777035000      0.432897000
H       -0.836405000      1.769579000      0.703330000
C       -4.101967000      1.039156000      0.064088000
H       -4.845254000     -0.859611000     -0.656266000
H       -3.057576000      2.817483000      0.714382000
H       -5.074297000      1.510180000      0.069064000
C        1.811572000     -0.338531000     -0.371666000
C        2.974060000     -0.983615000      0.057433000
C        1.826127000      1.046444000     -0.522428000
C        4.122067000     -0.256520000      0.350719000
H        2.986242000     -2.063684000      0.156431000
C        2.975436000      1.776596000     -0.227199000
H        0.934928000      1.538844000     -0.886207000
C        4.124418000      1.129692000      0.214103000
H        5.014590000     -0.771032000      0.684593000
H        2.972096000      2.852931000     -0.347744000
H        5.017213000      1.697478000      0.443631000
H        0.775096000     -1.763788000     -1.584784000
```

E(UM052X+HF-M052X) = -655.720662
E(UM052X+HF-M052X) + ZPE = -655.456400
E(UM052X+HF-M052X)/6-311++g(d,p) = --655.885980
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.889578
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.893392
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.894792

Optimized geometry of radical 3a (UM05-2X/6-31G(d))

```
symmetry c1
C       -3.076233000      1.802003000     -0.118055000
C       -1.883097000      1.096915000     -0.253735000
C       -1.892345000     -0.296109000     -0.266527000
C       -3.106714000     -0.973528000     -0.151296000
C       -4.297488000     -0.269380000     -0.011771000
C       -4.284570000      1.123227000      0.006025000
H       -3.061515000      2.884965000     -0.115621000
H       -0.940485000      1.614767000     -0.370354000
H       -3.118414000     -2.058361000     -0.174609000
H       -5.234255000     -0.805493000      0.076050000
H       -5.210978000      1.674067000      0.108712000
C       -0.609259000     -1.088310000     -0.346058000
O        0.460443000     -0.286561000     -0.842469000
C       -0.141949000     -1.607567000      1.022042000
H       -0.600468000     -2.563227000      1.276667000
H       -0.403828000     -0.887099000      1.799523000
C        1.367996000     -1.683699000      0.826058000
H        1.634789000     -2.573808000      0.249821000
H        1.942243000     -1.682273000      1.751619000
C        1.655092000     -0.423076000     -0.028075000
```

C	1.808008000	0.792550000	0.838755000
C	2.825057000	-0.619935000	-0.938500000
C	2.938824000	1.548620000	0.855786000
H	0.962851000	1.046346000	1.467621000
C	3.940709000	0.155834000	-0.889116000
H	2.734881000	-1.431648000	-1.649879000
C	4.035173000	1.241678000	0.014477000
H	2.999656000	2.408195000	1.512035000
H	4.764217000	-0.046162000	-1.562824000
H	4.926541000	1.851758000	0.038972000
H	-0.754000000	-1.934880000	-1.028032000

E(UM052X+HF-M052X) = -655.720538
E(UM052X+HF-M052X) + ZPE = -655.456409
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.886100
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.889777
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.893739
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.895211

Optimized geometry for the transition state for the formation of radical 2a (UM05-2X/ 6-31G(d))

symmetry c1

C	0.507399000	-1.160059000	-0.867761000
O	-0.608243000	-0.387597000	-1.171527000
C	0.077924000	-2.141336000	0.233679000
H	0.910430000	-2.691857000	0.673379000
H	-0.622095000	-2.860698000	-0.196720000
C	-0.628871000	-1.255141000	1.257150000
H	0.109525000	-0.642976000	1.779184000
H	-1.160729000	-1.848936000	2.003999000
C	-1.601385000	-0.353289000	0.525251000
C	-2.814469000	-0.912886000	0.014231000
C	-1.590567000	1.051021000	0.778917000
C	-3.853960000	-0.105096000	-0.386070000
H	-2.880486000	-1.988317000	-0.096447000
C	-2.636427000	1.853749000	0.372553000
H	-0.719054000	1.479846000	1.257259000
C	-3.765601000	1.284851000	-0.225687000
H	-4.746625000	-0.542296000	-0.814204000
H	-2.590743000	2.923600000	0.530478000
H	-4.584442000	1.916939000	-0.543128000
H	0.760813000	-1.729976000	-1.774312000
C	1.719565000	-0.329649000	-0.461131000
C	1.663787000	1.061499000	-0.521675000
C	2.907373000	-0.940870000	-0.053337000
C	2.767106000	1.829705000	-0.157249000
H	0.748498000	1.522055000	-0.868677000
C	4.010985000	-0.175709000	0.308735000
H	2.977002000	-2.022956000	-0.025899000
C	3.941816000	1.214613000	0.263416000
H	2.710796000	2.910336000	-0.209025000
H	4.924981000	-0.663769000	0.624138000
H	4.800022000	1.811350000	0.546056000

E(UM052X+HF-M052X) = -655.696389
E(UM052X+HF-M052X) + ZPE = -655.433465
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.863100
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.867375
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.871992
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.873716

Optimized geometry for the transition state for the formation of radical 3a (UM05-2X/ 6-31G(d))

symmetry c1

C	-3.228071000	1.734525000	0.210296000
C	-1.986456000	1.121243000	0.078139000
C	-1.904804000	-0.225777000	-0.270998000
C	-3.075772000	-0.948078000	-0.492801000
C	-4.318102000	-0.336018000	-0.355535000
C	-4.397036000	1.008063000	-0.002923000
H	-3.284051000	2.783412000	0.474953000

H	-1.068925000	1.676222000	0.223464000
H	-3.013594000	-1.992806000	-0.778748000
H	-5.222431000	-0.905654000	-0.530583000
H	-5.362419000	1.487975000	0.097924000
C	-0.556906000	-0.919975000	-0.352820000
O	0.437192000	-0.011403000	-0.712380000
C	-0.167179000	-1.510258000	1.010185000
H	-0.768994000	-2.384402000	1.265993000
H	-0.334856000	-0.748064000	1.775235000
C	1.318026000	-1.828614000	0.877873000
H	1.456226000	-2.678553000	0.204769000
H	1.762943000	-2.093125000	1.840158000
C	2.017364000	-0.616234000	0.297856000
C	2.170059000	0.548344000	1.109439000
C	2.913321000	-0.767900000	-0.800368000
C	3.032648000	1.558907000	0.743522000
H	1.563730000	0.641698000	2.002135000
C	3.773242000	0.247451000	-1.160158000
H	2.864170000	-1.680426000	-1.381302000
C	3.828752000	1.421511000	-0.399940000
H	3.105007000	2.454688000	1.346770000
H	4.412267000	0.134838000	-2.026438000
H	4.504156000	2.217197000	-0.685457000
H	-0.625284000	-1.744931000	-1.080436000

E(UM052X+HF-M052X) = -655.694077
E(UM052X+HF-M052X) + ZPE = -655.431376
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.860872
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.865470
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.870552
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -665.872480

Optimized geometry of radical 4a (UM05-2X/6-31G(d))

symmetry c1

C	0.500334000	0.548977000	0.508035000
O	-0.374107000	-0.566916000	0.447531000
C	0.053356000	1.622395000	-0.490662000
H	0.116790000	1.190324000	-1.492366000
H	0.735903000	2.474394000	-0.444849000
C	-1.389852000	2.056378000	-0.192834000
H	-1.762412000	2.739555000	-0.958454000
H	-1.398962000	2.596464000	0.763794000
C	-2.265483000	0.845157000	-0.085976000
C	-1.720320000	-0.222377000	0.820687000
C	-3.437449000	0.675735000	-0.758447000
C	-2.530362000	-1.476161000	0.831488000
H	-1.663150000	0.186940000	1.847720000
C	-4.190453000	-0.516598000	-0.642397000
H	-3.794522000	1.468626000	-1.406782000
C	-3.701550000	-1.584419000	0.149506000
H	-2.135521000	-2.298062000	1.413919000
H	-5.120795000	-0.623102000	-1.181192000
H	-4.266491000	-2.507131000	0.198475000
C	1.903647000	0.079740000	0.212171000
C	2.990942000	0.823404000	0.670014000
C	2.129723000	-1.056621000	-0.562312000
C	4.290728000	0.439544000	0.357714000
H	2.817775000	1.704322000	1.279510000
C	3.430678000	-1.442931000	-0.871521000
H	1.282451000	-1.635110000	-0.904382000
C	4.513258000	-0.696885000	-0.414957000
H	5.127629000	1.021954000	0.722442000
H	3.598874000	-2.330542000	-1.468848000
H	5.524179000	-1.000870000	-0.655691000
H	0.467928000	0.975532000	1.523390000

E(UM052X+HF-M052X) = -655.725351
E(UM052X+HF-M052X) + ZPE = -655.460511
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.891142
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.894522
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.898219
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -665.899609

Optimized geometry of radical 5a (UM05-2X/6-31G(d))

symmetry c1

C	-3.124340000	-1.669029000	-0.214512000
C	-2.003176000	-1.213655000	0.468009000
C	-1.675536000	0.145586000	0.484745000
C	-2.503921000	1.038462000	-0.195394000
C	-3.630829000	0.584525000	-0.877921000
C	-3.944351000	-0.769374000	-0.891666000
H	-3.359512000	-2.726139000	-0.217260000
H	-1.360230000	-1.907825000	0.994619000
H	-2.280169000	2.097500000	-0.200916000
H	-4.260369000	1.293230000	-1.401386000
H	-4.818797000	-1.121287000	-1.424249000
C	-0.467732000	0.588530000	1.304899000
O	0.550318000	-0.409471000	1.305997000
C	0.133699000	1.941639000	0.916415000
H	0.883986000	2.186056000	1.671319000
H	-0.623644000	2.727304000	0.941924000
C	0.817399000	1.865252000	-0.456907000
H	1.325221000	2.802737000	-0.691868000
H	0.055100000	1.695321000	-1.227024000
C	1.785877000	0.721854000	-0.450770000
C	1.192592000	-0.574492000	0.021602000
C	3.098324000	0.818623000	-0.800012000
C	2.188252000	-1.677970000	0.156226000
H	0.406230000	-0.875733000	-0.692134000
C	3.968535000	-0.294316000	-0.719251000
H	3.486471000	1.773709000	-1.137449000
C	3.486638000	-1.529168000	-0.219633000
H	1.821582000	-2.610932000	0.564154000
H	5.004457000	-0.193283000	-1.008750000
H	4.171067000	-2.363118000	-0.124254000
H	-0.782523000	0.639432000	2.350316000

E(UM052X+HF-M052X) = -655.723476
E(UM052X+HF-M052X) + ZPE = -655.457909
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.888845
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.892209
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.895721
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -665.896994

Optimized geometry for the transition state for the formation of radical 4a (UM05-2X/6-31G(d))

symmetry c1

C	0.495737000	0.608627000	0.499750000
C	0.043665000	1.520140000	-0.650507000
H	0.066893000	0.931632000	-1.571497000
H	0.746047000	2.351007000	-0.760056000
C	-1.384295000	2.040786000	-0.409574000
H	-1.726292000	2.616726000	-1.271778000
H	-1.383933000	2.706582000	0.459316000
C	-2.282986000	0.865426000	-0.162980000
C	-2.115798000	0.159321000	1.060651000
C	-3.103431000	0.333758000	-1.147228000
C	-2.883949000	-1.009608000	1.297203000
H	-1.706568000	0.688563000	1.912801000
C	-3.806954000	-0.847863000	-0.922251000
H	-3.191910000	0.845353000	-2.098658000
C	-3.692115000	-1.518874000	0.304169000
H	-2.800458000	-1.508578000	2.253293000
H	-4.448080000	-1.248451000	-1.696726000
H	-4.255133000	-2.427514000	0.474642000
O	-0.328706000	-0.513082000	0.641965000
C	1.900522000	0.095581000	0.226020000
C	3.008613000	0.755609000	0.752968000
C	2.091135000	-1.012644000	-0.599594000
C	4.296436000	0.321241000	0.451628000
H	2.862372000	1.610822000	1.403734000
C	3.377555000	-1.450350000	-0.895344000

H	1.223950000	-1.530001000	-0.988452000
C	4.483379000	-0.783609000	-0.373324000
H	5.151226000	0.840733000	0.866628000
H	3.517948000	-2.314961000	-1.532366000
H	5.484182000	-1.126415000	-0.603995000
H	0.524328000	1.203902000	1.427873000

E(UM052X+HF-M052X) = -655.695246
E(UM052X+HF-M052X) + ZPE = -655.431901
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.862306
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.866661
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.871512
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -665.873379

Optimized geometry for the transition state for the formation of radical 5a (UM05-2X/6-31G(d))

symmetry c1

C	-0.422763000	0.664933000	1.241875000
C	0.185437000	1.968010000	0.702796000
H	0.982653000	2.254087000	1.392091000
H	-0.548378000	2.776636000	0.692685000
C	0.797880000	1.764096000	-0.696085000
H	1.290309000	2.682116000	-1.023482000
H	0.005001000	1.528698000	-1.411369000
C	1.781066000	0.635479000	-0.610953000
C	1.253258000	-0.672816000	-0.413267000
C	3.148417000	0.840606000	-0.508655000
C	2.149844000	-1.759412000	-0.234475000
H	0.254998000	-0.884295000	-0.775674000
C	4.010705000	-0.229807000	-0.275550000
H	3.544944000	1.844310000	-0.609811000
C	3.504689000	-1.531209000	-0.136930000
H	1.749642000	-2.761086000	-0.150358000
H	5.076677000	-0.056677000	-0.204435000
H	4.185093000	-2.357215000	0.026318000
H	-0.722678000	0.865825000	2.283644000
O	0.543232000	-0.336684000	1.368604000
C	-1.677450000	0.187665000	0.510000000
C	-1.987910000	-1.174568000	0.545847000
C	-2.552434000	1.052731000	-0.149321000
C	-3.136240000	-1.661395000	-0.067899000
H	-1.306101000	-1.841628000	1.058030000
C	-3.703838000	0.567131000	-0.765469000
H	-2.344546000	2.114408000	-0.191711000
C	-3.999618000	-0.790929000	-0.728474000
H	-3.358410000	-2.720797000	-0.030107000
H	-4.367510000	1.253657000	-1.276548000
H	-4.893803000	-1.167655000	-1.208742000

E(UM052X+HF-M052X) = -655.696402
E(UM052X+HF-M052X) + ZPE = -655.432696
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.862865
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.866888
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.871163
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -665.872738

Optimized geometry of radical 6a (UM05-2X/6-31G(d))

symmetry c1

C	1.154553000	1.741799000	1.450286000
C	1.299984000	0.380363000	1.201827000
C	1.857645000	-0.058030000	0.001344000
C	2.281545000	0.881717000	-0.938601000
C	2.132665000	2.242828000	-0.693313000
C	1.564791000	2.674784000	0.502750000
H	0.710493000	2.073875000	2.380248000
H	0.964267000	-0.352604000	1.924359000
H	2.726284000	0.542943000	-1.868921000
H	2.463728000	2.964135000	-1.430132000

H	1.446750000	3.733466000	0.696100000
C	1.933379000	-1.532605000	-0.321076000
O	2.083272000	-2.336390000	0.838424000
C	0.651575000	-2.024863000	-1.023434000
H	0.827051000	-3.068977000	-1.297607000
H	0.530599000	-1.456871000	-1.948432000
C	-0.565864000	-1.943741000	-0.164259000
H	-0.707887000	-2.742572000	0.551620000
C	-1.527817000	-0.907133000	-0.178809000
C	-1.411003000	0.254973000	-0.983922000
C	-2.671307000	-1.006042000	0.656491000
C	-2.379857000	1.242342000	-0.951978000
H	-0.537519000	0.389330000	-1.607619000
C	-3.636254000	-0.016509000	0.677033000
H	-2.779731000	-1.883546000	1.283456000
C	-3.500629000	1.117159000	-0.128344000
H	-2.260380000	2.124289000	-1.569144000
H	-4.499746000	-0.121818000	1.322259000
H	-4.254395000	1.893488000	-0.110075000
H	2.772698000	-1.698248000	-1.009433000
H	2.831192000	-1.988033000	1.339948000

E(UM052X+HF-M052X) = -655.732840
E(UM052X+HF-M052X) + ZPE = -655.469692
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.907992
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.912177
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.916474
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -665.918036

Optimized geometry for the transition state for the formation of radical 6a (UM05-2X/ 6-31G(d))

symmetry c1

C	2.994147000	-1.366259000	-0.963898000
C	2.520240000	-0.060532000	-1.029666000
C	1.877823000	0.517667000	0.067760000
C	1.736690000	-0.219960000	1.239638000
C	2.209603000	-1.528837000	1.306095000
C	2.833765000	-2.106943000	0.205700000
H	3.487950000	-1.805388000	-1.821849000
H	2.644247000	0.512531000	-1.943213000
H	1.247524000	0.239979000	2.087089000
H	2.087159000	-2.097353000	2.219651000
H	3.199220000	-3.124752000	0.258518000
C	1.308585000	1.920075000	-0.042838000
O	0.754652000	2.378841000	1.169141000
C	0.146388000	2.008525000	-1.058336000
H	0.228339000	1.279608000	-1.865250000
H	0.120262000	3.003880000	-1.502746000
C	-1.110525000	1.818253000	-0.191063000
H	-1.802742000	2.657715000	-0.243377000
H	-0.544411000	2.015947000	0.884749000
C	-1.829528000	0.524434000	-0.169549000
C	-1.226962000	-0.687998000	-0.532719000
C	-3.166217000	0.502501000	0.257096000
C	-1.943285000	-1.877756000	-0.473370000
H	-0.194312000	-0.707442000	-0.854608000
C	-3.879875000	-0.685865000	0.318424000
H	-3.643606000	1.433940000	0.539689000
C	-3.268584000	-1.883534000	-0.047389000
H	-1.460238000	-2.803781000	-0.758058000
H	-4.911485000	-0.679119000	0.647050000
H	-3.821916000	-2.812884000	-0.001756000
H	2.113196000	2.613770000	-0.314336000

E(UM052X+HF-M052X) = -655.680436
E(UM052X+HF-M052X) + ZPE = -655.421117
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.849150
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.853106
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.857123
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -665.858559

Optimized geometry of benzaldehyde 7 (M05-2X/6-31G(d))

symmetry cs

C	-0.727440000	-1.722806000	0.000000000
C	-1.032215000	-0.369498000	0.000000000
C	0.000000000	0.571007000	0.000000000
C	1.331209000	0.158070000	0.000000000
C	1.635763000	-1.198963000	0.000000000
C	0.605794000	-2.135790000	0.000000000
H	-1.521245000	-2.458694000	0.000000000
H	-2.054718000	-0.014566000	0.000000000
H	2.122806000	0.899659000	0.000000000
H	2.667552000	-1.525821000	0.000000000
H	0.840983000	-3.192761000	0.000000000
C	-0.321105000	2.016122000	0.000000000
O	-1.445424000	2.461724000	0.000000000
H	0.555982000	2.689538000	0.000000000

E(RM052X+HF-M052X) = -345.528540
E(RM052X+HF-M052X) + ZPE = -345.416289
E(RM052X+HF-M052X)/6-311++g(d,p) = -345.620115
E(RM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -345.623701
E(RM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -345.626998
E(RM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -345.628087

Optimized geometry of radical 8a (UM05-2X/6-31G(d))

symmetry c1

C	-2.820327000	-0.400342000	0.461945000
H	-3.840402000	-0.596565000	0.165237000
H	-2.499562000	-0.721970000	1.442514000
C	-1.954363000	0.505559000	-0.344076000
H	-2.149616000	1.556559000	-0.082762000
H	-2.218577000	0.416923000	-1.403901000
C	-0.473759000	0.236567000	-0.169856000
C	0.014810000	-1.071270000	-0.207860000
C	0.429550000	1.282344000	0.015881000
C	1.374577000	-1.326816000	-0.068368000
H	-0.682731000	-1.889797000	-0.345957000
C	1.791884000	1.031411000	0.155787000
H	0.061963000	2.301726000	0.053990000
C	2.268655000	-0.274703000	0.114012000
H	1.736883000	-2.346876000	-0.101156000
H	2.478585000	1.855913000	0.302161000
H	3.327295000	-0.472413000	0.225089000

E(UM052X+HF-M052X) = -310.162852
E(UM052X+HF-M052X) + ZPE = -310.018244
E(UM052X+HF-M052X)/6-311++g(d,p) = -310.241718
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -310.243297
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -310.244902
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -310.245469

Optimized geometry for the transition state for the formation of radical 8a and benzaldehyde 7 (UM05-2X/6-31G(d))

symmetry c1

C	3.393638000	-0.921128000	-1.408506000
C	2.696890000	0.238161000	-1.088868000
C	2.415541000	0.534419000	0.244638000
C	2.841937000	-0.327342000	1.254338000
C	3.540540000	-1.486250000	0.934581000
C	3.814318000	-1.784600000	-0.398330000
H	3.614846000	-1.151303000	-2.443117000
H	2.368303000	0.933923000	-1.850375000
H	2.628639000	-0.084758000	2.290618000
H	3.873633000	-2.153017000	1.719792000
H	4.359063000	-2.686043000	-0.649166000
C	1.671248000	1.789341000	0.579757000
O	1.402829000	2.643367000	-0.280783000
C	-0.242298000	0.963614000	0.915770000
H	-0.699667000	1.859281000	1.318426000
H	-0.005944000	0.198028000	1.646639000
C	-0.729967000	0.511445000	-0.427076000
H	-0.093724000	-0.288659000	-0.809380000

H	-0.684057000	1.347484000	-1.126358000
C	-2.155222000	0.018200000	-0.273989000
C	-3.226329000	0.908631000	-0.370220000
C	-2.416395000	-1.321225000	0.019554000
C	-4.532585000	0.468088000	-0.186261000
H	-3.031125000	1.950621000	-0.598445000
C	-3.721870000	-1.764874000	0.204164000
H	-1.589812000	-2.019124000	0.095238000
C	-4.783709000	-0.870679000	0.101911000
H	-5.354028000	1.168395000	-0.271552000
H	-3.910268000	-2.808318000	0.423907000
H	-5.800259000	-1.215245000	0.242810000
H	1.707342000	2.066986000	1.648454000

E(UM052X+HF-M052X) = -655.691634
E(UM052X+HF-M052X) + ZPE = -655.431077
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.860926
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.866005
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.870961
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.872682

Optimized geometry of ketone 9a (M05-2X/6-31G(d))

symmetry c1

C	-4.621189000	-0.152297000	0.338432000
C	-3.593869000	0.765419000	0.172285000
C	-2.311103000	0.333963000	-0.176715000
C	-2.070297000	-1.030438000	-0.356060000
C	-3.100215000	-1.950386000	-0.187723000
C	-4.374656000	-1.512446000	0.158811000
H	-5.612838000	0.188002000	0.607835000
H	-3.756542000	1.826470000	0.305583000
H	-1.084100000	-1.384562000	-0.627439000
H	-2.908120000	-3.006287000	-0.328380000
H	-5.175395000	-2.229661000	0.288289000
C	-1.247468000	1.377410000	-0.339161000
O	-1.512700000	2.554275000	-0.189149000
C	0.175598000	0.947518000	-0.630801000
H	0.693870000	1.812587000	-1.043805000
H	0.214058000	0.141370000	-1.365376000
C	0.877150000	0.502768000	0.670645000
H	0.317517000	-0.312956000	1.134054000
H	0.867093000	1.341038000	1.370818000
C	2.294189000	0.064603000	0.397099000
C	3.319483000	1.006116000	0.292266000
C	2.596575000	-1.281847000	0.192528000
C	4.618488000	0.610871000	-0.008303000
H	3.094907000	2.055110000	0.452123000
C	3.894881000	-1.682113000	-0.108847000
H	1.808484000	-2.022636000	0.277705000
C	4.909735000	-0.735636000	-0.210296000
H	5.403781000	1.352774000	-0.081554000
H	4.114008000	-2.731749000	-0.259826000
H	5.921066000	-1.044729000	-0.441814000

E(RM052X+HF-M052X) = -655.183680
E(RM052X+HF-M052X) + ZPE = -655.929872
E(RM052X+HF-M052X)/6-311++g(d,p) = -655.349307
E(RM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.353977
E(RM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.358498
E(RM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.360056

Optimized geometry for the transition state for the formation of ketone 9a and a hydrogen atom (UM05-2X/6-31G(d))

symmetry c1

C	4.542363000	-0.166450000	-0.547418000
C	3.522831000	0.746618000	-0.317340000
C	2.302785000	0.320960000	0.213299000
C	2.115718000	-1.030953000	0.511921000
C	3.137827000	-1.945078000	0.278287000
C	4.351259000	-1.514625000	-0.249855000
H	5.485207000	0.169261000	-0.960018000

H	3.642996000	1.797709000	-0.542596000
H	1.177947000	-1.379222000	0.925308000
H	2.986788000	-2.991715000	0.509523000
H	5.146045000	-2.227474000	-0.429655000
C	1.229400000	1.362961000	0.421588000
O	1.432191000	2.528126000	0.077788000
C	-0.197140000	0.910728000	0.706761000
H	-0.728873000	1.762952000	1.129432000
H	-0.244814000	0.089370000	1.421973000
C	-0.865217000	0.493779000	-0.619960000
H	-0.292588000	-0.315637000	-1.079333000
H	-0.831455000	1.346770000	-1.301129000
C	-2.289019000	0.054034000	-0.391437000
C	-3.318544000	0.994022000	-0.318241000
C	-2.595717000	-1.293101000	-0.196688000
C	-4.625868000	0.596652000	-0.059125000
H	-3.090376000	2.043335000	-0.470566000
C	-3.902225000	-1.695377000	0.063121000
H	-1.803623000	-2.031991000	-0.256697000
C	-4.921282000	-0.750383000	0.132772000
H	-5.414287000	1.337273000	-0.010392000
H	-4.124583000	-2.745411000	0.206524000
H	-5.939014000	-1.061195000	0.331705000
H	1.650084000	1.478248000	2.137506000

E(UM052X+HF-M052X) = -655.667984
E(UM052X+HF-M052X) + ZPE = -655.412634
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.835411
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.839966
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.844453
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.846038

Optimized geometry of ketyl radical 10a (UM05-2X/6-31G(d))

symmetry c1

C	-4.695889000	-0.030942000	0.282580000
C	-3.615770000	0.812192000	0.097051000
C	-2.328867000	0.288534000	-0.189524000
C	-2.193486000	-1.120949000	-0.267424000
C	-3.285754000	-1.949434000	-0.078757000
C	-4.546437000	-1.417251000	0.196675000
H	-5.669013000	0.393269000	0.497822000
H	-3.739041000	1.883572000	0.164607000
H	-1.225860000	-1.561491000	-0.470938000
H	-3.155043000	-3.022646000	-0.143610000
H	-5.396101000	-2.070584000	0.344054000
C	-1.226912000	1.153110000	-0.387241000
O	-1.447316000	2.484678000	-0.170251000
C	0.179593000	0.722053000	-0.629885000
H	0.711016000	1.494427000	-1.199804000
H	0.206920000	-0.176202000	-1.248743000
C	0.953865000	0.456370000	0.684667000
H	0.431816000	-0.325483000	1.240789000
H	0.928114000	1.360096000	1.298304000
C	2.377227000	0.046972000	0.407624000
C	3.398899000	0.995932000	0.353870000
C	2.687964000	-1.286934000	0.136132000
C	4.702047000	0.622626000	0.039678000
H	3.171106000	2.034619000	0.568178000
C	3.988701000	-1.665289000	-0.178755000
H	1.902167000	-2.033824000	0.180084000
C	5.000256000	-0.710017000	-0.228181000
H	5.484303000	1.370745000	0.008108000
H	4.213690000	-2.704977000	-0.381083000
H	6.013991000	-1.002825000	-0.470098000
H	-0.672166000	2.982044000	-0.456727000

E(UM052X+HF-M052X) = -655.739658
E(UM052X+HF-M052X) + ZPE = -655.476095
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.913059
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.917894
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.922937
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.924773

Optimized geometry for the transition state for the formation of ketyl radical 10a (UM05-2X/6-31G(d))

symmetry c1

C	4.470305000	-0.143263000	-0.694122000
C	3.448207000	0.748270000	-0.398726000
C	2.297239000	0.311493000	0.270874000
C	2.196123000	-1.038005000	0.635342000
C	3.222936000	-1.925902000	0.338385000
C	4.363490000	-1.482991000	-0.326137000
H	5.352136000	0.206183000	-1.216270000
H	3.516084000	1.788772000	-0.684728000
H	1.316273000	-1.399206000	1.151825000
H	3.131021000	-2.965820000	0.625307000
H	5.161721000	-2.176702000	-0.557249000
C	1.229225000	1.280912000	0.583963000
O	1.375854000	2.573649000	0.104331000
C	-0.192665000	0.832662000	0.798274000
H	-0.754000000	1.664431000	1.227211000
H	-0.253057000	-0.002515000	1.497985000
C	-0.831607000	0.437357000	-0.549025000
H	-0.260416000	-0.381756000	-0.992417000
H	-0.757776000	1.293442000	-1.223835000
C	-2.271029000	0.027790000	-0.369813000
C	-3.286227000	0.985753000	-0.347804000
C	-2.609602000	-1.311165000	-0.169718000
C	-4.609774000	0.614366000	-0.134946000
H	-3.034190000	2.028947000	-0.505097000
C	-3.932091000	-1.687735000	0.043619000
H	-1.828281000	-2.063645000	-0.188883000
C	-4.936560000	-0.724731000	0.061311000
H	-5.386402000	1.369112000	-0.126642000
H	-4.178118000	-2.731942000	0.191188000
H	-5.966708000	-1.015441000	0.223635000
H	1.587055000	2.248082000	1.294464000

E(UM052X+HF-M052X) = -655.667312
E(UM052X+HF-M052X) + ZPE = -655.408691
E(UM052X+HF-M052X)/6-311++g(d,p) = -655.838907
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -655.843020
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -655.847100
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -655.848535

Optimized geometry of radical ap-1b (UM05-2X/6-31G(d))

symmetry c1

C	4.295294000	-0.968524000	-1.344147000
C	3.599496000	0.169547000	-0.945272000
C	3.103153000	0.266385000	0.352376000
C	3.316744000	-0.780835000	1.248078000
C	4.011256000	-1.918101000	0.850233000
C	4.501500000	-2.014435000	-0.449653000
H	4.679765000	-1.036046000	-2.354210000
H	3.441357000	0.992680000	-1.629584000
H	2.942622000	-0.702740000	2.263966000
H	4.174282000	-2.724860000	1.553821000
H	5.045259000	-2.897403000	-0.760743000
C	2.315766000	1.483791000	0.799130000
O	2.443526000	2.569694000	-0.024931000
C	0.781330000	1.186368000	0.845079000
H	0.278938000	2.057423000	1.269299000
H	0.640075000	0.346121000	1.529109000
C	0.186875000	0.850397000	-0.525798000
H	0.728281000	0.006622000	-0.958835000
H	0.322717000	1.702067000	-1.196340000
C	-1.277960000	0.514026000	-0.399133000
C	-2.244997000	1.525166000	-0.356056000
C	-1.706776000	-0.802351000	-0.267381000
C	-3.586980000	1.229547000	-0.190981000
H	-1.936740000	2.559918000	-0.460256000
C	-3.054236000	-1.122778000	-0.100110000
H	-0.976456000	-1.603523000	-0.299660000
C	-3.999657000	-0.099951000	-0.061278000
H	-4.340119000	2.005862000	-0.162814000

H	-3.345095000	-2.159375000	-0.007656000
H	2.595324000	1.759962000	1.826383000
O	-5.338543000	-0.292082000	0.094414000
C	-5.792232000	-1.625345000	0.221982000
H	-6.871413000	-1.566092000	0.334990000
H	-5.550561000	-2.211676000	-0.668411000
H	-5.359548000	-2.107284000	1.102661000

E(UM052X+HF-M052X) = -770.219936
E(UM052X+HF-M052X) + ZPE = -769.906524
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.420445
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.425008
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.429461
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.431002

Optimized geometry of radical g-1b (UM05-2X/6-31G(d))

symmetry c1

C	-5.301689000	0.006301000	-0.220564000
C	-4.104923000	0.628292000	-0.564440000
C	-2.891322000	-0.026479000	-0.369332000
C	-2.879335000	-1.314077000	0.163065000
C	-4.075440000	-1.936835000	0.504042000
C	-5.288165000	-1.277955000	0.315448000
H	-6.241646000	0.520451000	-0.377106000
H	-4.113579000	1.626056000	-0.990684000
H	-1.930617000	-1.819419000	0.291363000
H	-4.062029000	-2.938983000	0.914068000
H	-6.217954000	-1.765686000	0.579346000
C	-1.587827000	0.683415000	-0.689658000
O	-0.600233000	-0.180574000	-1.087503000
C	-1.064675000	1.391788000	0.595051000
H	-0.952343000	0.633258000	1.372808000
H	-1.863029000	2.071086000	0.904170000
C	0.247926000	2.153945000	0.385821000
H	0.359633000	2.864726000	1.209935000
H	0.181096000	2.744882000	-0.532006000
C	1.466431000	1.264210000	0.332766000
C	2.156106000	1.037975000	-0.852995000
C	1.936499000	0.637997000	1.493331000
C	3.281820000	0.216954000	-0.902068000
H	1.803139000	1.499928000	-1.767299000
C	3.049774000	-0.183204000	1.466957000
H	1.422805000	0.804079000	2.434505000
C	3.730899000	-0.397448000	0.264821000
H	3.786049000	0.065641000	-1.845494000
H	3.420136000	-0.667268000	2.360826000
H	-1.758225000	1.467565000	-1.442833000
O	4.817435000	-1.214461000	0.337099000
C	5.531668000	-1.448945000	-0.860832000
H	5.934318000	-0.518137000	-1.268830000
H	6.350227000	-2.113605000	-0.597414000
H	4.897922000	-1.929909000	-1.610596000

E(UM052X+HF-M052X) = -770.218231
E(UM052X+HF-M052X) + ZPE = -769.921149
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.418423
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.423284
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.428396
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.430278

Optimized geometry of radical 2b (UM05-2X/6-31G(d))

symmetry c1

C	1.481689000	-1.193802000	-0.674465000
O	0.247054000	-0.558909000	-0.990197000
C	1.170673000	-2.103885000	0.522182000
H	2.049828000	-2.329799000	1.124175000
H	0.736647000	-3.043545000	0.174383000
C	0.134366000	-1.266855000	1.264089000
H	0.629444000	-0.461291000	1.812883000
H	-0.485746000	-1.833110000	1.957875000
C	-0.706696000	-0.661987000	0.117137000
C	-1.811876000	-1.581113000	-0.310120000

C	-1.217020000	0.703496000	0.446544000
C	-3.106531000	-1.198131000	-0.386419000
H	-1.523790000	-2.589123000	-0.583284000
C	-2.531753000	1.064347000	0.359432000
H	-0.474042000	1.423787000	0.764939000
C	-3.502021000	0.127527000	-0.051529000
H	-3.880767000	-1.882704000	-0.709166000
H	-2.817672000	2.076789000	0.610149000
C	2.569207000	-0.176738000	-0.368269000
C	3.842276000	-0.612282000	0.008116000
C	2.331301000	1.190737000	-0.484204000
C	4.852085000	0.301973000	0.284229000
H	4.047840000	-1.674984000	0.080504000
C	3.341983000	2.108556000	-0.205462000
H	1.354236000	1.521131000	-0.808975000
C	4.602786000	1.668810000	0.182744000
H	5.833231000	-0.050938000	0.576637000
H	3.143328000	3.169227000	-0.298294000
H	5.387810000	2.382596000	0.398557000
H	1.781827000	-1.775379000	-1.549837000
O	-4.827197000	0.384983000	-0.166698000
C	-5.272070000	1.694305000	0.139833000
H	-6.346752000	1.690610000	-0.020215000
H	-5.058362000	1.947603000	1.181014000
H	-4.806302000	2.430793000	-0.519211000

E(UM052X+HF-M052X) = -770.230051
E(UM052X+HF-M052X) + ZPE = -769.931674
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.429662
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.434288
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.439051
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.440766

Optimized geometry of radical 3b (UM05-2X/6-31G(d))

symmetry c1

C	3.463084000	-2.100796000	-0.063304000
C	2.395338000	-1.219714000	-0.214543000
C	2.628835000	0.150039000	-0.314585000
C	3.939946000	0.625828000	-0.271475000
C	5.005635000	-0.253806000	-0.116840000
C	4.768614000	-1.622202000	-0.011170000
H	3.273789000	-3.164795000	0.008193000
H	1.377864000	-1.582229000	-0.274922000
H	4.125868000	1.691016000	-0.362738000
H	6.019052000	0.126572000	-0.085035000
H	5.596917000	-2.309970000	0.103814000
C	1.487173000	1.134180000	-0.413022000
O	0.282607000	0.487839000	-0.814406000
C	1.171202000	1.814607000	0.928418000
H	1.781582000	2.702895000	1.092613000
H	1.358953000	1.118381000	1.748297000
C	-0.317701000	2.108770000	0.785306000
H	-0.475109000	2.988229000	0.154352000
H	-0.837051000	2.261259000	1.730675000
C	-0.838412000	0.856268000	0.043108000
C	-1.122420000	-0.271901000	0.991161000
C	-2.010085000	1.152919000	-0.834421000
C	-2.313723000	-0.911549000	1.042210000
H	-0.312151000	-0.574800000	1.643782000
C	-3.202304000	0.491582000	-0.760156000
H	-1.860500000	1.929332000	-1.573996000
C	-3.384950000	-0.543483000	0.181126000
H	-2.488293000	-1.726576000	1.733348000
H	-3.999097000	0.764330000	-1.438482000
H	1.737347000	1.897594000	-1.159746000
O	-4.525821000	-1.257278000	0.336331000
C	-5.612472000	-0.957579000	-0.521824000
H	-5.342799000	-1.123195000	-1.567485000
H	-6.412653000	-1.636320000	-0.239842000
H	-5.944569000	0.074803000	-0.388165000

E(UM052X+HF-M052X) = -770.229774
E(UM052X+HF-M052X) + ZPE = -769.931849
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.429601

E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.434271
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.439124
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.440889

Optimized geometry for the transition state for the formation of radical 2b (UM05-2X/6-31G(d))

symmetry c1

C	1.393259000	-1.152107000	-0.922473000
O	0.122751000	-0.641450000	-1.147231000
C	1.247928000	-2.265217000	0.128313000
H	2.203233000	-2.628475000	0.509718000
H	0.717849000	-3.104098000	-0.328601000
C	0.395218000	-1.632666000	1.226181000
H	0.988964000	-0.891857000	1.766235000
H	0.056260000	-2.379230000	1.948419000
C	-0.795021000	-0.951634000	0.585581000
C	-1.865653000	-1.751290000	0.073497000
C	-1.112307000	0.392266000	0.924288000
C	-3.075709000	-1.199957000	-0.246052000
H	-1.687808000	-2.804995000	-0.102684000
C	-2.328858000	0.960586000	0.597545000
H	-0.351968000	0.992752000	1.407643000
C	-3.313347000	0.169817000	-0.008008000
H	-3.876590000	-1.786631000	-0.675561000
H	-2.511884000	2.000324000	0.826884000
H	1.740589000	-1.601649000	-1.865682000
C	2.405028000	-0.094062000	-0.495651000
C	2.028104000	1.244688000	-0.413262000
C	3.726639000	-0.441524000	-0.206025000
C	2.947965000	2.216078000	-0.024604000
H	1.010787000	1.505503000	-0.672938000
C	4.647765000	0.526690000	0.178579000
H	4.043277000	-1.475682000	-0.290831000
C	4.258572000	1.860514000	0.277008000
H	2.641680000	3.253576000	0.035668000
H	5.669042000	0.241560000	0.399938000
H	4.974183000	2.615496000	0.577903000
O	-4.533687000	0.617714000	-0.373267000
C	-4.823833000	1.991557000	-0.172256000
H	-5.827267000	2.143530000	-0.559334000
H	-4.798444000	2.245402000	0.889857000
H	-4.118926000	2.621932000	-0.718612000

E(UM052X+HF-M052X) = -770.207657
E(UM052X+HF-M052X) + ZPE = -769.910737
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.408977
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.414430
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.420136
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.422240

Optimized geometry for the transition state for the formation of radical 3b (UM05-2X/6-31G(d))

symmetry c1

C	3.609553000	-1.996705000	0.499889000
C	2.478169000	-1.212488000	0.300600000
C	2.583898000	0.017386000	-0.347292000
C	3.829918000	0.448016000	-0.798854000
C	4.962995000	-0.334407000	-0.596208000
C	4.855167000	-1.559759000	0.055089000
H	3.519268000	-2.954049000	0.998624000
H	1.500066000	-1.544377000	0.623556000
H	3.911285000	1.398473000	-1.315653000
H	5.926571000	0.008948000	-0.952082000
H	5.734294000	-2.173122000	0.208739000
C	1.363160000	0.906543000	-0.508550000
O	0.208524000	0.136078000	-0.604252000
C	1.203455000	1.828392000	0.709751000
H	1.966446000	2.609182000	0.737831000
H	1.305561000	1.222801000	1.614303000
C	-0.211288000	2.385217000	0.590566000
H	-0.263164000	3.084771000	-0.247948000
H	-0.508191000	2.928094000	1.491390000

C	-1.162751000	1.235565000	0.335783000
C	-1.455590000	0.321741000	1.393927000
C	-2.105085000	1.306771000	-0.723425000
C	-2.501080000	-0.558325000	1.306295000
H	-0.808908000	0.305991000	2.262816000
C	-3.159467000	0.420582000	-0.824612000
H	-1.951168000	2.045356000	-1.500005000
C	-3.354778000	-0.530515000	0.185608000
H	-2.706404000	-1.281300000	2.084202000
H	-3.822700000	0.475293000	-1.675367000
H	1.503503000	1.537830000	-1.402227000
O	-4.346826000	-1.446706000	0.188436000
C	-5.234886000	-1.465219000	-0.917499000
H	-4.694948000	-1.655672000	-1.847408000
H	-5.931064000	-2.276745000	-0.725802000
H	-5.782365000	-0.523210000	-0.994857000

E(UM052X+HF-M052X) = -770.205307
E(UM052X+HF-M052X) + ZPE = -769.908634
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.406739
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.412506
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.418662
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.420965

Optimized geometry of radical 4b (UM05-2X/6-31G(d))

symmetry c1

C	1.330984000	0.664845000	0.496999000
O	0.355632000	-0.353058000	0.651745000
C	0.898445000	1.650298000	-0.595632000
H	0.836251000	1.097214000	-1.535980000
H	1.657401000	2.428237000	-0.709562000
C	-0.468734000	2.260734000	-0.251472000
H	-0.840890000	2.880057000	-1.069609000
H	-0.348398000	2.909588000	0.626798000
C	-1.436188000	1.162210000	0.073563000
C	-0.915687000	0.177066000	1.081498000
C	-2.647757000	1.011925000	-0.509106000
C	-1.838066000	-0.969701000	1.319564000
H	-0.716892000	0.707744000	2.031717000
C	-3.496603000	-0.086078000	-0.189530000
H	-3.005240000	1.721579000	-1.246597000
C	-3.059927000	-1.073724000	0.716883000
H	-1.490160000	-1.737210000	1.997278000
H	-3.685030000	-1.927788000	0.938497000
C	2.653146000	0.020871000	0.157642000
C	3.839186000	0.718862000	0.385344000
C	2.705347000	-1.240716000	-0.431943000
C	5.064190000	0.166231000	0.027834000
H	3.802150000	1.698002000	0.851615000
C	3.931850000	-1.795426000	-0.786388000
H	1.783126000	-1.780709000	-0.596067000
C	5.112799000	-1.094785000	-0.560382000
H	5.978769000	0.715296000	0.213991000
H	3.964639000	-2.778588000	-1.239459000
H	6.065328000	-1.529662000	-0.835882000
H	1.430174000	1.214572000	1.446856000
O	-4.692648000	-0.094948000	-0.828381000
C	-5.562997000	-1.184317000	-0.580366000
H	-6.450934000	-1.000945000	-1.179303000
H	-5.105398000	-2.128942000	-0.884112000
H	-5.838693000	-1.234160000	0.475850000

E(UM052X+HF-M052X) = -770.234079
E(UM052X+HF-M052X) + ZPE = -769.935278
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.434131
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.438470
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.443022
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.444691

Optimized geometry of radical 5b (UM05-2X/6-31G(d))

symmetry c1

C	-3.762564000	-1.809002000	-0.275603000
C	-2.703968000	-1.272087000	0.446294000
C	-2.448484000	0.102672000	0.431732000
C	-3.284717000	0.926756000	-0.321581000
C	-4.348889000	0.390919000	-1.044476000
C	-4.591530000	-0.977428000	-1.025052000
H	-3.942541000	-2.876650000	-0.252473000
H	-2.053733000	-1.912531000	1.029009000
H	-3.115504000	1.995319000	-0.354798000
H	-4.985114000	1.047117000	-1.625343000
H	-5.417170000	-1.393341000	-1.588579000
C	-1.311794000	0.635162000	1.299788000
O	-0.244245000	-0.305489000	1.387667000
C	-0.765555000	2.009686000	0.902274000
H	-0.078022000	2.320206000	1.691812000
H	-1.566829000	2.749605000	0.857430000
C	0.007925000	1.935241000	-0.422937000
H	0.473045000	2.894929000	-0.656230000
H	-0.689599000	1.692989000	-1.233824000
C	1.039741000	0.853791000	-0.308111000
C	0.480416000	-0.465303000	0.141932000
C	2.365177000	1.035620000	-0.509337000
C	1.524624000	-1.506131000	0.360585000
H	-0.252442000	-0.814902000	-0.603602000
C	3.299068000	-0.022312000	-0.317026000
H	2.756705000	1.998455000	-0.817612000
C	2.853420000	-1.281912000	0.132218000
H	1.184149000	-2.466219000	0.724242000
H	3.559300000	-2.082464000	0.306259000
H	-1.687583000	0.699207000	2.324257000
O	4.592223000	0.296077000	-0.576609000
C	5.569322000	-0.708531000	-0.374587000
H	6.522383000	-0.257303000	-0.636998000
H	5.591884000	-1.029917000	0.669630000
H	5.384094000	-1.572057000	-1.018319000

E(UM052X+HF-M052X) = -770.231894
E(UM052X+HF-M052X) + ZPE = -769.932570
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.431482
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.435831
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.440231
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.441795

Optimized geometry for the transition state for the formation of radical 4b (UM05-2X/6-31G(d))

symmetry c1

C	-1.196580000	0.623186000	-0.607641000
C	-1.038706000	1.861324000	0.287786000
H	-1.008532000	1.518853000	1.325626000
H	-1.902828000	2.521308000	0.171014000
C	0.266992000	2.601696000	-0.049052000
H	0.422715000	3.427819000	0.648047000
H	0.191968000	3.023819000	-1.056032000
C	1.404512000	1.628093000	0.022770000
C	1.507307000	0.643652000	-0.995171000
C	2.228439000	1.520457000	1.141072000
C	2.525436000	-0.342159000	-0.936233000
H	1.061182000	0.848916000	-1.960562000
C	3.175280000	0.516003000	1.231375000
H	2.124408000	2.234623000	1.949545000
C	3.320839000	-0.423072000	0.185747000
H	2.625358000	-1.035550000	-1.757661000
H	3.825114000	0.421858000	2.090807000

O	-0.140445000	-0.275923000	-0.441975000
C	-2.482682000	-0.105190000	-0.249259000
C	-3.673855000	0.217565000	-0.896969000
C	-2.492038000	-1.060181000	0.766829000
C	-4.865917000	-0.399436000	-0.529321000
H	-3.666434000	0.953400000	-1.693952000
C	-3.682607000	-1.681792000	1.129515000
H	-1.559613000	-1.315163000	1.252555000
C	-4.872362000	-1.351957000	0.485333000
H	-5.785903000	-0.141591000	-1.039117000
H	-3.681553000	-2.426997000	1.915562000
H	-1.277207000	0.959036000	-1.656021000
H	-5.797623000	-1.837540000	0.768960000
O	4.297685000	-1.345252000	0.381610000
C	4.472552000	-2.322623000	-0.628134000
H	4.766825000	-1.859955000	-1.573729000
H	5.267557000	-2.975942000	-0.279401000
H	3.556989000	-2.900888000	-0.774602000

E(UM052X+HF-M052X) = -770.203850
E(UM052X+HF-M052X) + ZPE = -769.907183
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.405490
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.410663
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.416185
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.418265

Optimized geometry for the transition state for the formation of radical 5b (UM05-2X/6-31G(d))

symmetry c1

C	-1.192150000	0.658468000	1.255300000
C	-0.637279000	1.989621000	0.725008000
H	0.147853000	2.301840000	1.416976000
H	-1.403382000	2.768003000	0.723164000
C	-0.017150000	1.831190000	-0.675569000
H	0.430066000	2.774858000	-0.994212000
H	-0.796732000	1.562930000	-1.393901000
C	1.019966000	0.749593000	-0.602373000
C	0.551594000	-0.584661000	-0.415072000
C	2.364797000	1.023531000	-0.500474000
C	1.504374000	-1.617220000	-0.247224000
H	-0.433452000	-0.843662000	-0.780186000
C	3.288463000	-0.008358000	-0.269034000
H	2.740985000	2.035581000	-0.584805000
C	2.852102000	-1.335658000	-0.139044000
H	1.162000000	-2.640819000	-0.173155000
H	3.556875000	-2.139041000	0.019062000
H	-1.511175000	0.845519000	2.294226000
O	-0.188576000	-0.303660000	1.381942000
C	-2.423629000	0.136523000	0.512672000
C	-2.674867000	-1.238185000	0.529872000
C	-3.334812000	0.970656000	-0.137712000
C	-3.800681000	-1.766469000	-0.091613000
H	-1.964756000	-1.880440000	1.034949000
C	-4.463257000	0.443706000	-0.762366000
H	-3.173566000	2.040883000	-0.165612000
C	-4.700319000	-0.926276000	-0.742931000
H	-3.977110000	-2.834896000	-0.067425000
H	-5.155270000	1.107421000	-1.266071000
O	4.583434000	0.375777000	-0.188373000
C	5.554361000	-0.620083000	0.085857000
H	6.506981000	-0.100598000	0.138533000
H	5.350896000	-1.111940000	1.039667000
H	5.588645000	-1.365411000	-0.712246000
H	-5.576797000	-1.335430000	-1.229304000

E(UM052X+HF-M052X) = -770.206575
E(UM052X+HF-M052X) + ZPE = -769.909176
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.407598

E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.412742
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.417998
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.419894

Optimized geometry of radical 6b (UM05-2X/6-31G(d))

symmetry c1

C	1.343023000	1.907707000	1.435885000
C	1.810302000	0.616503000	1.210954000
C	2.496765000	0.312938000	0.035477000
C	2.720940000	1.320455000	-0.903219000
C	2.251285000	2.610918000	-0.681140000
C	1.558988000	2.906131000	0.490555000
H	0.802832000	2.132431000	2.346892000
H	1.632612000	-0.169790000	1.933290000
H	3.265068000	1.090275000	-1.813574000
H	2.430724000	3.385571000	-1.416254000
H	1.192338000	3.909539000	0.666305000
C	2.938766000	-1.102586000	-0.256867000
O	3.249070000	-1.827842000	0.923215000
C	1.838281000	-1.905288000	-0.979042000
H	2.274833000	-2.876478000	-1.229772000
H	1.608196000	-1.396917000	-1.917985000
C	0.615255000	-2.116628000	-0.150669000
H	0.660944000	-2.907837000	0.586042000
C	-0.575642000	-1.359427000	-0.217353000
C	-0.743704000	-0.226125000	-1.059756000
C	-1.681245000	-1.712971000	0.593568000
C	-1.925890000	0.478650000	-1.085615000
H	0.079592000	0.113387000	-1.673564000
C	-2.874554000	-1.008674000	0.570247000
H	-1.587444000	-2.569003000	1.251379000
C	-3.005646000	0.095908000	-0.276300000
H	-2.048032000	1.346617000	-1.720237000
H	-3.688162000	-1.324542000	1.207748000
H	3.812769000	-1.065352000	-0.920433000
H	3.879537000	-1.301893000	1.431342000
O	-4.125965000	0.860890000	-0.381758000
C	-5.224973000	0.520345000	0.440531000
H	-4.959744000	0.583602000	1.499264000
H	-6.003692000	1.244900000	0.217220000
H	-5.588910000	-0.486039000	0.217145000

E(UM052X+HF-M052X) = -770.240335
E(UM052X+HF-M052X) + ZPE = -769.943509
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.449644
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.454765
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.459965
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.461847

Optimized geometry for the transition state for the formation of radical 6b (UM05-2X/6-31G(d))

symmetry c1

C	-2.683627000	2.334845000	-0.949354000
C	-2.817041000	0.955149000	-1.058233000
C	-2.545777000	0.126670000	0.033301000
C	-2.159973000	0.699698000	1.241840000
C	-2.024943000	2.081926000	1.352091000
C	-2.280874000	2.902285000	0.258320000
H	-2.895510000	2.966987000	-1.802955000
H	-3.130128000	0.516318000	-2.000384000
H	-1.961522000	0.049358000	2.082649000
H	-1.717265000	2.517340000	2.294820000
H	-2.174871000	3.976494000	0.345007000
C	-2.635795000	-1.381267000	-0.116721000
O	-2.388687000	-2.061181000	1.089329000
C	-1.585424000	-1.938082000	-1.105343000
H	-1.314891000	-1.226658000	-1.886401000

H	-1.972397000	-2.837287000	-1.585776000
C	-0.400342000	-2.326001000	-0.201634000
H	-0.142542000	-3.382850000	-0.263066000
H	-1.028800000	-2.275665000	0.850303000
C	0.808994000	-1.481005000	-0.146269000
C	0.808899000	-0.117719000	-0.461404000
C	2.025727000	-2.053571000	0.268013000
C	1.967818000	0.647929000	-0.379613000
H	-0.107597000	0.367082000	-0.770918000
C	3.183288000	-1.307860000	0.356350000
H	2.052834000	-3.107885000	0.519011000
C	3.161911000	0.054073000	0.030849000
H	1.921972000	1.697018000	-0.633681000
H	4.121238000	-1.747840000	0.667647000
H	-3.649071000	-1.648433000	-0.440765000
O	4.345923000	0.705748000	0.142086000
C	4.369851000	2.082404000	-0.190768000
H	5.395603000	2.408117000	-0.041751000
H	4.083567000	2.238833000	-1.233786000
H	3.705345000	2.655689000	0.460163000

E(UM052X+HF-M052X) = -770.189307
E(UM052X+HF-M052X) + ZPE = -769.896393
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.392158
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.397111
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.402015
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.403736

Optimized geometry of radical 8b (UM05-2X/6-31G(d))

symmetry c1

C	-3.709673000	-0.327776000	0.601964000
H	-4.748068000	-0.527909000	0.380299000
H	-3.329959000	-0.601075000	1.576190000
C	-2.885799000	0.517964000	-0.307430000
H	-3.057529000	1.585112000	-0.099693000
H	-3.214808000	0.368318000	-1.342082000
C	-1.401063000	0.243082000	-0.197400000
C	-0.916336000	-1.069874000	-0.239726000
C	-0.478182000	1.272836000	-0.062879000
C	0.438693000	-1.337663000	-0.156481000
H	-1.620062000	-1.889034000	-0.336584000
C	0.893073000	1.025073000	0.022708000
H	-0.828006000	2.298378000	-0.020824000
C	1.353586000	-0.288187000	-0.025293000
H	0.820269000	-2.349641000	-0.189655000
H	1.576237000	1.855358000	0.129633000
O	2.664361000	-0.650394000	0.049965000
C	3.616083000	0.387661000	0.176829000
H	3.456898000	0.959325000	1.095176000
H	4.587633000	-0.097857000	0.215968000
H	3.580217000	1.063474000	-0.681900000

E(UM052X+HF-M052X) = -424.670016
E(UM052X+HF-M052X) + ZPE = -424.492037
E(UM052X+HF-M052X)/6-311++g(d,p) = -424.783060
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -424.785569
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -424.788037
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -424.788893

Optimized geometry for the transition state for the formation of benzaldehyde 7 and radical 8b (UM05-2X/6-31G(d))

symmetry c1

C	4.085404000	-1.179144000	-1.399309000
C	3.541851000	0.051475000	-1.050628000
C	3.272893000	0.338570000	0.287441000
C	3.558664000	-0.605315000	1.273001000

C	4.104413000	-1.835747000	0.924330000
C	4.365693000	-2.123810000	-0.413342000
H	4.296891000	-1.402455000	-2.437468000
H	3.325023000	0.809757000	-1.792221000
H	3.356497000	-0.370735000	2.313336000
H	4.329124000	-2.566390000	1.691038000
H	4.792030000	-3.080881000	-0.686363000
C	2.696127000	1.670609000	0.653609000
O	2.567165000	2.581602000	-0.179520000
C	0.677483000	1.094759000	0.921977000
H	0.335737000	2.030297000	1.348252000
H	0.789672000	0.280016000	1.628961000
C	0.167700000	0.758530000	-0.446187000
H	0.698545000	-0.108174000	-0.843950000
H	0.347557000	1.602157000	-1.114388000
C	-1.314668000	0.461527000	-0.342531000
C	-2.255328000	1.497909000	-0.378608000
C	-1.777158000	-0.836661000	-0.153079000
C	-3.607866000	1.241470000	-0.240228000
H	-1.917270000	2.517712000	-0.525811000
C	-3.136115000	-1.115875000	-0.011721000
H	-1.065982000	-1.654718000	-0.121755000
C	-4.056577000	-0.070041000	-0.054895000
H	2.740556000	1.903344000	1.732720000
H	-4.342395000	2.035032000	-0.275895000
H	-3.456107000	-2.138851000	0.125002000
O	-5.402721000	-0.222647000	0.069331000
C	-5.894135000	-1.536280000	0.253049000
H	-5.499730000	-1.980385000	1.170712000
H	-6.974158000	-1.444707000	0.329788000
H	-5.641824000	-2.174520000	-0.597721000

E(UM052X+HF-M052X) = -770.198983
E(UM052X+HF-M052X) + ZPE = -769.904916
E(UM052X+HF-M052X)/6-311++g(d,p) = -770.402421
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -770.408457
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -770.414299
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -770.416317

Optimized geometry of radical ap-1c (UM05-2X/6-31G(d))

symmetry c1

C	4.563570000	0.215923000	1.463596000
C	3.692555000	-0.743611000	0.954814000
C	3.234819000	-0.646766000	-0.357095000
C	3.663787000	0.411989000	-1.157011000
C	4.533578000	1.371153000	-0.649164000
C	4.984953000	1.274842000	0.664799000
H	4.917113000	0.133162000	2.483732000
H	3.366519000	-1.576680000	1.563522000
H	3.319705000	0.482669000	-2.184044000
H	4.863553000	2.187850000	-1.278889000
H	5.665355000	2.017956000	1.060944000
C	2.259798000	-1.663205000	-0.920152000
O	2.169309000	-2.818996000	-0.190696000
C	0.802508000	-1.098878000	-0.959015000
H	0.165546000	-1.837353000	-1.448613000
H	0.822751000	-0.201345000	-1.581761000
C	0.246340000	-0.762455000	0.427987000
H	0.898297000	-0.034466000	0.915017000
H	0.241776000	-1.663322000	1.045168000
C	-1.152998000	-0.208371000	0.308412000
C	-2.237511000	-1.084184000	0.276191000
C	-1.343318000	1.165716000	0.171821000
C	-3.526529000	-0.571292000	0.107835000
H	-2.061250000	-2.145092000	0.387541000
C	-2.639043000	1.662972000	0.004386000
H	-0.484754000	1.821915000	0.204360000
C	-3.728055000	0.798315000	-0.028364000
H	-4.727493000	1.189880000	-0.152826000
H	2.516089000	-1.898052000	-1.963458000
O	-4.649854000	-1.336888000	0.066917000
O	-2.935092000	2.983584000	-0.131793000
C	-4.491051000	-2.735486000	0.208548000
H	-3.874904000	-3.146533000	-0.595327000
H	-4.043975000	-2.986158000	1.173872000

```
H       -5.490816000     -3.157558000      0.151126000
C       -1.859831000      3.902070000     -0.095704000
H       -1.331752000      3.855127000      0.860054000
H       -1.154518000      3.717372000     -0.910107000
H       -2.303568000      4.886649000     -0.217043000
```

E(UM052X+HF-M052X) = -884.728177
E(UM052X+HF-M052X) + ZPE = -884.397565
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.963205
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.968712
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.974028
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.975854

Optimized geometry of radical g-1c (UM05-2X/6-31G(d))

```
symmetry c1
C       -5.478513000     -0.359541000      0.239771000
C       -4.318212000      0.097456000      0.857889000
C       -3.147979000      0.262312000      0.120790000
C       -3.144697000     -0.024647000     -1.242606000
C       -4.304943000     -0.478544000     -1.861058000
C       -5.472963000     -0.648502000     -1.121775000
H       -6.385688000     -0.482781000      0.817972000
H       -4.322888000      0.331699000      1.917513000
H       -2.233251000      0.124426000     -1.807329000
H       -4.299149000     -0.696187000     -2.921802000
H       -6.375766000     -0.999344000     -1.605466000
C       -1.871580000      0.705564000      0.810714000
O       -1.025079000      1.396419000     -0.016117000
C       -1.084581000     -0.550772000      1.297204000
H       -0.906571000     -1.194519000      0.433516000
H       -1.771147000     -1.073360000      1.967386000
C        0.237195000     -0.224403000      2.010414000
H        0.441454000     -1.020046000      2.731143000
H        0.125732000      0.701269000      2.581028000
C        1.412867000     -0.114763000      1.065831000
C        1.844290000      1.129669000      0.616006000
C        2.038808000     -1.284689000      0.631321000
C        2.902737000      1.199045000     -0.294875000
H        1.330856000      2.016654000      0.953465000
C        3.102632000     -1.197570000     -0.268886000
H        1.691910000     -2.239267000      1.002808000
C        3.535275000      0.041302000     -0.732430000
H        4.355637000      0.101641000     -1.433210000
H       -2.104653000      1.296219000      1.709522000
O        3.782757000     -2.273442000     -0.751312000
O        3.381402000      2.363238000     -0.808881000
C        2.700275000      3.554895000     -0.460442000
H        1.646005000      3.500694000     -0.742785000
H        2.780266000      3.756595000      0.610898000
H        3.189111000      4.351229000     -1.015542000
C        3.366705000     -3.554676000     -0.321487000
H        2.329346000     -3.749402000     -0.606062000
H        4.019369000     -4.265198000     -0.822061000
H        3.472882000     -3.662871000      0.761196000
```

E(UM052X+HF-M052X) = -884.726153
E(UM052X+HF-M052X) + ZPE = -884.395769
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.960644
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.966098
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.971723
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.973765

Optimized geometry of radical 2c (UM05-2X/6-31G(d))

```
symmetry c1
C        1.344191000     -1.496763000     -0.412113000
O        0.266196000     -0.690310000     -0.875460000
C        0.886830000     -2.038044000      0.949774000
H        1.717631000     -2.310438000      1.599282000
H        0.251905000     -2.915798000      0.810977000
C        0.078630000     -0.857229000      1.474626000
H        0.754855000     -0.076627000      1.831771000
H       -0.621524000     -1.107675000      2.270116000
C       -0.657550000     -0.356052000      0.207277000
C       -1.927954000     -1.121863000     -0.015264000
```

C	-0.848600000	1.126914000	0.241251000
C	-3.131409000	-0.501558000	-0.136315000
H	-1.826775000	-2.194685000	-0.094586000
C	-2.075147000	1.699811000	0.115605000
H	0.050377000	1.709400000	0.381440000
C	-3.239981000	0.911011000	-0.066002000
H	-4.203700000	1.385123000	-0.169185000
C	2.633991000	-0.696820000	-0.320197000
C	3.796127000	-1.302880000	0.163229000
C	2.690221000	0.630903000	-0.738595000
C	4.985956000	-0.589471000	0.248586000
H	3.772849000	-2.343150000	0.470267000
C	3.881747000	1.347924000	-0.651395000
H	1.796958000	1.084511000	-1.146177000
C	5.031047000	0.743255000	-0.154378000
H	5.877751000	-1.072847000	0.627676000
H	3.912112000	2.379835000	-0.979381000
H	5.956562000	1.301080000	-0.087391000
H	1.482962000	-2.303925000	-1.136100000
O	-4.324247000	-1.132016000	-0.336902000
O	-2.321300000	3.040197000	0.149963000
C	-1.199421000	3.887082000	0.300207000
H	-0.688329000	3.696920000	1.247897000
H	-0.493871000	3.752243000	-0.524088000
H	-1.584530000	4.903281000	0.290205000
C	-4.287711000	-2.540381000	-0.448792000
H	-3.670855000	-2.850472000	-1.296375000
H	-3.900582000	-2.997070000	0.466384000
H	-5.314791000	-2.857712000	-0.608557000

E(UM052X+HF-M052X) = -884.735290
E(UM052X+HF-M052X) + ZPE = -884.403953
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.969907
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.975141
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.980511
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.982448

Optimized geometry of radical 3c (UM05-2X/6-31G(d))

symmetry c1

C	-3.365358000	0.962910000	-1.531818000
C	-2.274953000	0.150424000	-1.227284000
C	-2.406323000	-0.882109000	-0.300890000
C	-3.646822000	-1.101419000	0.302432000
C	-4.736176000	-0.294177000	-0.005362000
C	-4.596961000	0.744777000	-0.922824000
H	-3.251406000	1.763988000	-2.251965000
H	-1.313331000	0.307893000	-1.696521000
H	-3.759995000	-1.907894000	1.019539000
H	-5.692084000	-0.474152000	0.470722000
H	-5.443612000	1.375717000	-1.162515000
C	-1.231448000	-1.773027000	0.056899000
O	-0.031199000	-1.358203000	-0.589296000
C	-0.933008000	-1.794652000	1.578497000
H	-1.272769000	-2.717525000	2.048208000
H	-1.436342000	-0.963792000	2.074881000
C	0.585867000	-1.631072000	1.634267000
H	1.082753000	-2.596946000	1.518225000
H	0.943466000	-1.158084000	2.547974000
C	0.880896000	-0.775166000	0.381963000
C	0.529838000	0.664260000	0.621232000
C	2.268453000	-0.982339000	-0.128386000
C	1.419201000	1.667567000	0.392650000
H	-0.476798000	0.866231000	0.956543000
C	3.127354000	0.054394000	-0.317324000
H	2.534771000	-2.005628000	-0.349346000
C	2.734829000	1.394027000	-0.059354000
H	3.428862000	2.202224000	-0.230290000
H	-1.441311000	-2.785044000	-0.301250000
O	1.158689000	2.994972000	0.561131000
O	4.409469000	-0.061808000	-0.764283000
C	-0.160016000	3.336866000	0.944153000
H	-0.887988000	2.969112000	0.215752000
H	-0.400326000	2.929258000	1.929968000
H	-0.191306000	4.422581000	0.981502000
C	4.857752000	-1.365890000	-1.076915000

H	4.832680000	-2.010861000	-0.194381000
H	4.247643000	-1.810814000	-1.867326000
H	5.882676000	-1.258189000	-1.421735000

E(UM052X+HF-M052X) = -884.735959
E(UM052X+HF-M052X) + ZPE = -884.404406
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.970677
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.975521
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.980375
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.982096

Optimized geometry for the transition state for the formation of radical 2c (UM05-2X/6-31G(d))

symmetry c1

C	1.116055000	-1.690256000	-0.662670000
O	0.021328000	-0.933588000	-1.058393000
C	0.681932000	-2.448559000	0.598987000
H	1.490170000	-2.990165000	1.091761000
H	-0.089467000	-3.166846000	0.312709000
C	0.091753000	-1.359611000	1.493377000
H	0.900876000	-0.750810000	1.901196000
H	-0.462760000	-1.784360000	2.332762000
C	-0.827864000	-0.482618000	0.662557000
C	-2.137683000	-0.970751000	0.364462000
C	-0.605466000	0.925866000	0.670209000
C	-3.098217000	-0.100232000	-0.102851000
H	-2.321251000	-2.031814000	0.450608000
C	-1.582445000	1.778594000	0.188951000
H	0.360598000	1.285214000	0.991143000
C	-2.825006000	1.273546000	-0.205517000
H	-3.585775000	1.944208000	-0.578193000
H	1.310321000	-2.416170000	-1.467464000
C	2.375157000	-0.853692000	-0.453576000
C	2.395526000	0.473827000	-0.881799000
C	3.527441000	-1.391199000	0.123758000
C	3.535174000	1.255830000	-0.714296000
H	1.504132000	0.871051000	-1.349511000
C	4.667700000	-0.611398000	0.292310000
H	3.543983000	-2.428451000	0.438955000
C	4.673717000	0.717859000	-0.121347000
H	3.537243000	2.284686000	-1.054665000
H	5.552084000	-1.042820000	0.744719000
H	5.560831000	1.324842000	0.009854000
O	-4.356285000	-0.459434000	-0.474797000
O	-1.441716000	3.127275000	0.080256000
C	-4.667918000	-1.838970000	-0.434779000
H	-4.606938000	-2.226528000	0.585721000
H	-5.689237000	-1.926729000	-0.795258000
H	-3.998364000	-2.410313000	-1.082536000
C	-0.184392000	3.672480000	0.436030000
H	-0.253595000	4.738666000	0.237889000
H	0.029135000	3.511029000	1.495822000
H	0.618606000	3.236987000	-0.164876000

E(UM052X+HF-M052X) = -884.711057
E(UM052X+HF-M052X) + ZPE = -884.381177
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.946765
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.952431
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.958287
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.960433

Optimized geometry for the transition state for the formation of radical 3c (UM05-2X/6-31G(d))

symmetry c1

C	-3.932885000	1.174022000	-1.153929000
C	-2.719798000	0.625675000	-0.750346000
C	-2.685796000	-0.630466000	-0.147333000
C	-3.874292000	-1.333909000	0.037905000
C	-5.088737000	-0.783817000	-0.361650000
C	-5.120471000	0.472972000	-0.958856000
H	-3.952124000	2.147244000	-1.629168000
H	-1.784972000	1.146977000	-0.911968000

H	-3.847330000	-2.318243000	0.493578000
H	-6.007066000	-1.338552000	-0.213845000
H	-6.063280000	0.900019000	-1.277046000
C	-1.373318000	-1.203015000	0.358286000
O	-0.303082000	-0.720490000	-0.388965000
C	-1.139309000	-0.792772000	1.822369000
H	-1.788195000	-1.341960000	2.507467000
H	-1.368413000	0.270856000	1.923496000
C	0.340812000	-1.058033000	2.065429000
H	0.525243000	-2.135034000	2.073593000
H	0.673661000	-0.656992000	3.025743000
C	1.136057000	-0.428978000	0.938227000
C	1.182449000	0.994854000	0.861865000
C	2.176104000	-1.184864000	0.325734000
C	2.112978000	1.607058000	0.043392000
H	0.446434000	1.565635000	1.408219000
C	3.096249000	-0.551106000	-0.485909000
H	2.170679000	-2.257078000	0.453493000
C	3.064796000	0.841766000	-0.639559000
H	3.786405000	1.327415000	-1.280618000
H	-1.423917000	-2.303590000	0.315408000
O	2.204178000	2.950000000	-0.153439000
O	4.088116000	-1.180424000	-1.169547000
C	4.136090000	-2.592349000	-1.080768000
H	4.967244000	-2.904003000	-1.707401000
H	4.314093000	-2.915086000	-0.051524000
H	3.209605000	-3.039639000	-1.448835000
C	1.231779000	3.760912000	0.478196000
H	1.300967000	3.683813000	1.566570000
H	1.447639000	4.781200000	0.172982000
H	0.223385000	3.486629000	0.157141000

E(UM052X+HF-M052X) = -884.708373
E(UM052X+HF-M052X) + ZPE = -884.378760
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.944333
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.950433
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.956887
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.959311

Optimized geometry of radical 4c (UM05-2X/6-31G(d))

symmetry c1

C	1.487227000	-0.477074000	-0.779970000
O	0.506300000	0.423102000	-0.291660000
C	1.062268000	-1.927182000	-0.513508000
H	1.005018000	-2.062628000	0.569373000
H	1.823709000	-2.608579000	-0.901761000
C	-0.310201000	-2.207390000	-1.148366000
H	-0.672922000	-3.198868000	-0.869673000
H	-0.197919000	-2.191496000	-2.241202000
C	-1.273043000	-1.141741000	-0.722634000
C	-0.757760000	0.242354000	-0.965932000
C	-2.439694000	-1.383629000	-0.045156000
C	-1.692286000	1.308747000	-0.492445000
H	-0.557656000	0.399171000	-2.040068000
C	-3.242185000	-0.317654000	0.393753000
H	-2.728261000	-2.409020000	0.147065000
C	-2.853670000	1.031570000	0.153402000
H	-3.526533000	1.805194000	0.493838000
C	2.804161000	-0.166711000	-0.110885000
C	3.996514000	-0.567026000	-0.713642000
C	2.844539000	0.466085000	1.130052000
C	5.216522000	-0.341280000	-0.085237000
H	3.968544000	-1.052196000	-1.683844000
C	4.065823000	0.695002000	1.757448000
H	1.917126000	0.785525000	1.584973000
C	5.253387000	0.291590000	1.154373000
H	6.136175000	-0.652116000	-0.565102000
H	4.089517000	1.192518000	2.719132000
H	6.201962000	0.473027000	1.643907000
H	1.593390000	-0.335373000	-1.867303000
O	-1.234438000	2.540155000	-0.804026000

O	-4.418499000	-0.453492000	1.059993000
C	-4.866224000	-1.767428000	1.334376000
H	-5.025890000	-2.329247000	0.410564000
H	-4.153060000	-2.301449000	1.967360000
H	-5.810276000	-1.659207000	1.861686000
C	-2.011340000	3.641213000	-0.370013000
H	-2.110651000	3.637918000	0.718153000
H	-1.478540000	4.532421000	-0.689509000
H	-3.004862000	3.619610000	-0.825743000

E(UM052X+HF-M052X) = -884.743847
E(UM052X+HF-M052X) + ZPE = -884.411235
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.978100
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.983496
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.989273
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.991439

Optimized geometry of radical 5c (UM05-2X/6-31G(d))

symmetry c1

C	3.889038000	1.396077000	-0.596460000
C	2.810210000	1.002043000	0.185856000
C	2.566897000	-0.352109000	0.437660000
C	3.432028000	-1.299358000	-0.110475000
C	4.515725000	-0.904925000	-0.892663000
C	4.748084000	0.443100000	-1.138847000
H	4.058587000	2.448945000	-0.784837000
H	2.128652000	1.736979000	0.596159000
H	3.271204000	-2.355055000	0.066051000
H	5.174909000	-1.655460000	-1.311040000
H	5.588523000	0.749056000	-1.749061000
C	1.406817000	-0.723618000	1.357125000
O	0.361290000	0.240887000	1.282708000
C	0.831706000	-2.131498000	1.162537000
H	0.133098000	-2.305503000	1.983730000
H	1.615927000	-2.887542000	1.233974000
C	0.064231000	-2.238409000	-0.165730000
H	-0.426093000	-3.210618000	-0.248644000
H	0.774490000	-2.149295000	-0.997306000
C	-0.936576000	-1.124658000	-0.226425000
C	-0.324168000	0.219597000	0.006107000
C	-2.290304000	-1.305280000	-0.340256000
C	-1.323597000	1.329795000	0.015705000
H	0.431003000	0.434058000	-0.764773000
C	-3.161093000	-0.203464000	-0.299647000
C	-2.656437000	1.117942000	-0.124384000
H	1.766250000	-0.640237000	2.386042000
H	-3.376406000	1.923356000	-0.123814000
H	-2.675604000	-2.309745000	-0.460333000
O	-4.513465000	-0.277228000	-0.419755000
O	-0.720709000	2.532327000	0.156077000
C	-1.564904000	3.667331000	0.216442000
H	-2.253923000	3.590295000	1.060906000
H	-0.911592000	4.525184000	0.349973000
H	-2.135203000	3.776653000	-0.709787000
C	-5.082018000	-1.559159000	-0.605947000
H	-6.154530000	-1.403555000	-0.688225000
H	-4.708620000	-2.025623000	-1.521207000
H	-4.871441000	-2.210226000	0.246355000

E(UM052X+HF-M052X) = -884.742786
E(UM052X+HF-M052X) + ZPE = -884.409417
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.976334
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.981466
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.986736
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.988637

Optimized geometry for the transition state for the formation of radical 4c (UM05-2X/6-31G(d))

symmetry c1

C	1.496365000	0.041006000	-0.862987000
C	1.120069000	-1.410249000	-1.209711000

H	1.005223000	-1.955986000	-0.269194000
H	1.930048000	-1.877564000	-1.776991000
C	-0.198069000	-1.471680000	-2.002602000
H	-0.488341000	-2.510364000	-2.174014000
H	-0.055171000	-0.997301000	-2.978264000
C	-1.253049000	-0.742300000	-1.222959000
C	-1.131874000	0.661340000	-1.151510000
C	-2.159306000	-1.414143000	-0.413304000
C	-2.041107000	1.387996000	-0.333691000
H	-0.621267000	1.211562000	-1.930468000
C	-3.000038000	-0.679706000	0.426081000
H	-2.189870000	-2.494190000	-0.436481000
C	-2.944376000	0.724856000	0.469322000
H	-3.633730000	1.233566000	1.126077000
O	0.534633000	0.662093000	-0.065190000
C	2.811496000	0.046047000	-0.098548000
C	4.023653000	0.090603000	-0.785433000
C	2.817705000	-0.050086000	1.292675000
C	5.230007000	0.032964000	-0.094132000
H	4.021395000	0.175368000	-1.866986000
C	4.023680000	-0.102249000	1.984573000
H	1.871817000	-0.067824000	1.817265000
C	5.232453000	-0.063451000	1.294572000
H	6.165691000	0.070802000	-0.638230000
H	4.020108000	-0.170900000	3.065610000
H	6.169824000	-0.103003000	1.835214000
H	1.653538000	0.591617000	-1.807241000
O	-1.916900000	2.728409000	-0.411205000
O	-3.920840000	-1.232280000	1.250093000
C	-4.027499000	-2.645657000	1.268058000
H	-4.809278000	-2.875888000	1.986531000
H	-4.308128000	-3.029690000	0.284690000
H	-3.088889000	-3.103971000	1.587331000
C	-2.735635000	3.507800000	0.443654000
H	-2.538525000	3.268050000	1.490740000
H	-2.472550000	4.543306000	0.247657000
H	-3.793895000	3.348094000	0.222820000

E(UM052X+HF-M052X) = -884.716252
E(UM052X+HF-M052X) + ZPE = -884.385433
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.952539
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.958992
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.965966
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.968623

Optimized geometry for the transition state for the formation of radical 5c (UM05-2X/6-31G(d))

symmetry c1

C	1.308552000	-0.937954000	1.250129000
C	0.725782000	-2.256350000	0.709452000
H	-0.063974000	-2.559252000	1.400705000
H	1.477019000	-3.048985000	0.698528000
C	0.107639000	-2.079197000	-0.690646000
H	-0.350352000	-3.015386000	-1.017163000
H	0.892454000	-1.815474000	-1.404767000
C	-0.914247000	-0.983734000	-0.605243000
C	-0.413260000	0.324080000	-0.424397000
C	-2.269362000	-1.247720000	-0.457344000
C	-1.335584000	1.387654000	-0.212050000
H	0.563616000	0.587843000	-0.805156000
C	-3.145740000	-0.191245000	-0.197625000
H	-2.623223000	-2.265757000	-0.537776000
C	-2.681780000	1.131626000	-0.073019000
H	-3.413452000	1.903005000	0.114217000
H	1.628029000	-1.143793000	2.285331000
O	0.326301000	0.042377000	1.380885000
C	2.549992000	-0.441647000	0.505467000
C	2.769697000	0.935045000	0.411842000
C	3.503809000	-1.306900000	-0.035266000
C	3.906923000	1.433641000	-0.214682000
H	2.023772000	1.601432000	0.826577000
C	4.643529000	-0.809277000	-0.662204000
H	3.368831000	-2.379517000	0.029359000
C	4.849369000	0.563155000	-0.755582000

H	4.057094000	2.504316000	-0.281304000
H	5.369561000	-1.496941000	-1.078474000
H	5.734448000	0.950146000	-1.244702000
O	-0.767828000	2.610612000	-0.141845000
O	-4.483916000	-0.332889000	-0.045556000
C	-5.023310000	-1.641024000	-0.125732000
H	-6.092212000	-1.532606000	0.036041000
H	-4.843946000	-2.079444000	-1.110012000
H	-4.598311000	-2.286239000	0.646431000
C	-1.623270000	3.707675000	0.127942000
H	-2.120913000	3.581951000	1.092036000
H	-0.985226000	4.586379000	0.155779000
H	-2.372092000	3.820551000	-0.659787000

E(UM052X+HF-M052X) = -884.717911
E(UM052X+HF-M052X) + ZPE = -884.386780
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.953354
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.959412
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.965629
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.967890

Optimized geometry of radical 6c (UM05-2X/6-31G(d))

symmetry c1

C	1.800304000	0.587261000	2.162755000
C	1.803062000	-0.569270000	1.389483000
C	2.534434000	-0.619125000	0.202817000
C	3.273426000	0.496662000	-0.191093000
C	3.274506000	1.653128000	0.582985000
C	2.533426000	1.700672000	1.761734000
H	1.219676000	0.622109000	3.075781000
H	1.225196000	-1.434761000	1.687218000
H	3.854010000	0.456267000	-1.107036000
H	3.857490000	2.511482000	0.272158000
H	2.531056000	2.599066000	2.365998000
C	2.483616000	-1.842089000	-0.683813000
O	2.339229000	-3.042970000	0.058258000
C	1.291494000	-1.793762000	-1.661097000
H	1.407012000	-2.647559000	-2.334958000
H	1.378528000	-0.886336000	-2.262212000
C	-0.036396000	-1.886349000	-0.987843000
H	-0.359516000	-2.876568000	-0.695952000
C	-0.899017000	-0.806486000	-0.679929000
C	-0.535896000	0.543346000	-0.906008000
C	-2.167939000	-1.095284000	-0.116701000
C	-1.425031000	1.557392000	-0.574922000
H	0.446353000	0.772047000	-1.288715000
C	-3.039531000	-0.061857000	0.195503000
H	-2.432886000	-2.129148000	0.050838000
C	-2.677911000	1.266728000	-0.031962000
H	-3.359960000	2.066174000	0.218202000
H	3.402010000	-1.874564000	-1.284213000
H	3.029036000	-3.053642000	0.733839000
O	-4.278754000	-0.241260000	0.733195000
O	-1.162994000	2.882923000	-0.741171000
C	-4.691904000	-1.570022000	0.981543000
H	-4.725979000	-2.152752000	0.057329000
H	-4.028308000	-2.063365000	1.696576000
H	-5.691278000	-1.499865000	1.403070000
C	0.109281000	3.234465000	-1.250994000
H	0.908145000	2.878590000	-0.595829000
H	0.256197000	2.830114000	-2.256259000
H	0.123824000	4.320709000	-1.292832000

E(UM052X+HF-M052X) = -884.749239
E(UM052X+HF-M052X) + ZPE = -884.418534
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.993090
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.998953
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -885.004812
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -885.006905

Optimized geometry for the transition state for the formation of radical 6c (UM05-2X/6-31G(d))

symmetry c1

C	-3.905913000	0.964323000	-0.720065000
C	-3.254858000	-0.239545000	-0.970434000
C	-2.604287000	-0.924601000	0.059188000
C	-2.617059000	-0.387349000	1.344190000
C	-3.271342000	0.816903000	1.597256000
C	-3.917363000	1.495894000	0.568228000
H	-4.410322000	1.482407000	-1.526459000
H	-3.259624000	-0.654119000	-1.973397000
H	-2.113973000	-0.925941000	2.135318000
H	-3.276902000	1.223302000	2.601145000
H	-4.428262000	2.429716000	0.766783000
C	-1.913799000	-2.248989000	-0.222307000
O	-1.310436000	-2.799558000	0.925252000
C	-0.773473000	-2.142972000	-1.262539000
H	-0.886103000	-1.286234000	-1.927415000
H	-0.743714000	-3.043087000	-1.876992000
C	0.508938000	-2.072376000	-0.412524000
H	1.184382000	-2.909026000	-0.584386000
H	-0.024925000	-2.376772000	0.650569000
C	1.242960000	-0.794755000	-0.281386000
C	0.574632000	0.431140000	-0.363553000
C	2.623570000	-0.836585000	-0.045774000
C	1.299487000	1.614500000	-0.217692000
H	-0.492599000	0.448493000	-0.521768000
C	3.331539000	0.356343000	0.096058000
H	3.117582000	-1.795538000	0.015559000
C	2.673417000	1.580213000	0.008080000
H	3.227540000	2.501524000	0.117413000
H	-2.671597000	-2.965629000	-0.561809000
O	4.670646000	0.427376000	0.318631000
O	0.744850000	2.850884000	-0.282474000
C	5.377594000	-0.791515000	0.448760000
H	5.321225000	-1.380710000	-0.470135000
H	6.411632000	-0.518168000	0.640895000
H	4.994243000	-1.382099000	1.284805000
C	-0.662095000	2.921016000	-0.453425000
H	-0.966609000	2.478783000	-1.405393000
H	-1.184776000	2.414222000	0.359817000
H	-0.909367000	3.979385000	-0.448185000

E(UM052X+HF-M052X) = -884.698488
E(UM052X+HF-M052X) + ZPE = -884.371713
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.935426
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.940698
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.945874
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.947684

Optimized geometry of radical 8c (UM05-2X/6-31G(d))

symmetry c1

C	-1.598808000	3.131207000	0.520760000
H	-2.176166000	4.006918000	0.261720000
H	-1.707030000	2.719203000	1.513998000
C	-0.495253000	2.661216000	-0.363180000
H	0.418703000	3.245388000	-0.178433000
H	-0.756727000	2.854713000	-1.409678000
C	-0.167980000	1.190925000	-0.193623000
C	-1.206922000	0.261819000	-0.144371000
C	1.159128000	0.777049000	-0.109543000
C	-0.904562000	-1.095061000	-0.012024000
H	-2.226791000	0.614580000	-0.206988000
C	1.445148000	-0.585705000	0.021109000
H	1.946657000	1.516233000	-0.144886000
C	0.417867000	-1.520602000	0.070893000
H	0.644403000	-2.571937000	0.175879000
O	-1.841244000	-2.080181000	0.045158000
O	2.705237000	-1.091703000	0.111124000
C	3.782148000	-0.176660000	0.053322000
H	4.686753000	-0.773478000	0.136131000
H	3.788983000	0.366158000	-0.895453000
H	3.739584000	0.537061000	0.880133000
C	-3.199198000	-1.693941000	-0.042255000
H	-3.408026000	-1.196628000	-0.992843000

H	-3.775986000	-2.612908000	0.021500000
H	-3.475721000	-1.031706000	0.782134000

E(UM052X+HF-M052X) = -539.178182
E(UM052X+HF-M052X) + ZPE = -538.966147
E(UM052X+HF-M052X)/6-311++g(d,p) = -539.325646
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -539.329130
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -539.332524
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -539.333691

Optimized geometry for the transition state for the formation of radical 8c (UM05-2X/6-31G(d))

symmetry c1

C	4.378171000	0.478528000	1.548504000
C	3.664135000	-0.609783000	1.061440000
C	3.392026000	-0.708219000	-0.302900000
C	3.844814000	0.279803000	-1.176293000
C	4.560883000	1.367652000	-0.689165000
C	4.825600000	1.468266000	0.674806000
H	4.592381000	0.554956000	2.607078000
H	3.314547000	-1.400026000	1.713558000
H	3.638741000	0.190853000	-2.238278000
H	4.915144000	2.132254000	-1.368893000
H	5.384625000	2.313736000	1.055524000
C	2.629027000	-1.888315000	-0.818852000
O	2.337516000	-2.851088000	-0.090944000
C	0.733339000	-0.985715000	-1.046766000
H	0.261980000	-1.810924000	-1.566445000
H	0.987429000	-0.134021000	-1.668052000
C	0.246976000	-0.708707000	0.343103000
H	0.886426000	0.031448000	0.826812000
H	0.285553000	-1.628557000	0.928121000
C	-1.176425000	-0.192202000	0.251678000
C	-2.235279000	-1.099224000	0.247406000
C	-1.404395000	1.176089000	0.111448000
C	-3.541090000	-0.620943000	0.109932000
H	-2.026457000	-2.154031000	0.358480000
C	-2.716697000	1.637112000	-0.025105000
H	-0.562967000	1.854769000	0.119012000
C	-3.781893000	0.742557000	-0.026777000
H	-4.794408000	1.106163000	-0.128404000
H	2.669853000	-2.011174000	-1.915983000
O	-4.644578000	-1.414538000	0.101531000
O	-3.052126000	2.948032000	-0.159980000
C	-2.001636000	3.895594000	-0.157010000
H	-1.448171000	3.868818000	0.784935000
H	-1.313307000	3.724893000	-0.988641000
H	-2.475097000	4.866905000	-0.272151000
C	-4.448760000	-2.808851000	0.245415000
H	-3.844677000	-3.209257000	-0.572510000
H	-3.971292000	-3.043889000	1.199774000
H	-5.439583000	-3.254009000	0.216026000

E(UM052X+HF-M052X) = -884.707030
E(UM052X+HF-M052X) + ZPE = -884.379327
E(UM052X+HF-M052X)/6-311++g(d,p) = -884.945038
E(UM052X+HF-M052X)/6-311++g(d,p) pcm benzene = -884.951945
E(UM052X+HF-M052X)/6-311++g(d,p) pcm dichloromethane = -884.958568
E(UM052X+HF-M052X)/6-311++g(d,p) pcm acetonitrile = -884.960839