

Quenching of triplet benzophenone by benzene and diphenyl ether – a DFT study

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Supporting Information

Cartesian coordinates and energies of stationary points optimized

Benzene (B3lyp/cc-pVTZ)

C	0.000000000	1.390738000	0.000000000
C	1.204414000	0.695369000	0.000000000
C	1.204414000	-0.695369000	0.000000000
C	0.000000000	-1.390738000	0.000000000
C	-1.204414000	-0.695369000	0.000000000
C	-1.204414000	0.695369000	0.000000000
H	0.000000000	2.472808000	0.000000000
H	2.141515000	1.236404000	0.000000000
H	2.141515000	-1.236404000	0.000000000
H	0.000000000	-2.472808000	0.000000000
H	-2.141515000	-1.236404000	0.000000000
H	-2.141515000	1.236404000	0.000000000

E (RB+HF-LYP) = -232.3333656

E (RB+HF-LYP + ZPE) = -232.232987

No vibrational mode with imaginary frequency

Benzene M052X (M05-2X/cc-pVTZ)

C	0.000000000	1.386456000	0.000000000
C	1.200706000	0.693228000	0.000000000
C	1.200706000	-0.693228000	0.000000000
C	0.000000000	-1.386456000	0.000000000
C	-1.200706000	-0.693228000	0.000000000
C	-1.200706000	0.693228000	0.000000000
H	0.000000000	2.465282000	0.000000000
H	2.134997000	1.232641000	0.000000000
H	2.134997000	-1.232641000	0.000000000
H	0.000000000	-2.465282000	0.000000000
H	-2.134997000	-1.232641000	0.000000000
H	-2.134997000	1.232641000	0.000000000

E (M052X+HF-M052X) = -232.306648

E (M052X+HF-M052X) + ZPE = -232.204286

No vibrational mode with imaginary frequency

Benzophenone singlet (B3lyp/cc-pVTZ)

H	-2.303579000	1.931893000	-0.991235000
C	-2.422388000	0.960224000	-0.533172000
C	-2.692085000	-1.511436000	0.709093000
C	-1.299304000	0.342727000	0.025465000
C	-3.659745000	0.337525000	-0.492937000
C	-3.797518000	-0.899883000	0.130422000
C	-1.446233000	-0.898703000	0.649054000
H	-4.519989000	0.817062000	-0.940469000
H	-4.765199000	-1.382265000	0.169128000
H	-0.592876000	-1.375396000	1.109883000
H	-2.798773000	-2.464953000	1.208685000
C	0.000010000	1.088386000	0.000105000
C	1.299314000	0.342687000	-0.025359000
C	3.797503000	-0.899949000	-0.130617000
C	1.446111000	-0.898835000	-0.648773000
C	2.422491000	0.960244000	0.533018000
C	3.659843000	0.337551000	0.492607000
C	2.691965000	-1.511578000	-0.708980000

H	0.592685000	-1.375581000	-1.109417000
H	2.303763000	1.931980000	0.990964000
H	4.520192000	0.817144000	0.939877000
H	2.798520000	-2.465178000	-1.208444000
H	4.765191000	-1.382312000	-0.169412000
O	0.000035000	2.306730000	0.000110000

E (RB+HF-LYP) = -576.8332682

E (RB+HF-LYP + ZPE = -576.642044

No vibrational mode with imaginary frequency

Benzophenone singlet (M05-2X/cc-pVTZ)

H	2.292795000	1.930158000	0.982790000
C	2.408607000	0.959030000	0.528526000
C	2.651320000	-1.510871000	-0.710264000
C	1.289458000	0.349189000	-0.028520000
C	3.636362000	0.325040000	0.489243000
C	3.758236000	-0.910326000	-0.132027000
C	1.415391000	-0.887118000	-0.651807000
H	4.500050000	0.793152000	0.934142000
H	4.717854000	-1.401691000	-0.170025000
H	0.554615000	-1.348668000	-1.108892000
H	2.750106000	-2.462822000	-1.207421000
C	0.000001000	1.099159000	0.000004000
C	-1.289457000	0.349190000	0.028522000
C	-3.758237000	-0.910323000	0.132021000
C	-1.415396000	-0.887113000	0.651817000
C	-2.408603000	0.959028000	-0.528535000
C	-3.636358000	0.325039000	-0.489256000
C	-2.651325000	-1.510864000	0.710270000
H	-0.554623000	-1.348661000	1.108911000
H	-2.292787000	1.930153000	-0.982804000
H	-4.500043000	0.793148000	-0.934165000
H	-2.750115000	-2.462812000	1.207432000
H	-4.717856000	-1.401687000	0.170016000
O	0.000001000	2.310672000	0.000006000

E (M052X+HF-M052X) = -576.7862892

E (M052X+HF-M052X) + ZPE = -576.591108

No vibrational mode with imaginary frequency

Benzophenone triplet (UB3lyp/cc-pVTZ)

H	2.280541000	2.010233000	0.860459000
C	2.427858000	1.023183000	0.446941000
C	2.786667000	-1.540373000	-0.570825000
C	1.304353000	0.297012000	-0.015969000
C	3.693317000	0.465590000	0.405536000
C	3.884562000	-0.819767000	-0.094130000
C	1.518794000	-0.992086000	-0.551943000
H	4.537379000	1.032876000	0.775031000
H	4.873935000	-1.255077000	-0.120119000
H	0.687849000	-1.544607000	-0.965141000
H	2.929197000	-2.534093000	-0.974823000
C	0.000075000	0.913522000	0.000357000
C	-1.304291000	0.297050000	0.016270000
C	-3.884605000	-0.819552000	0.093372000
C	-1.519158000	-0.991809000	0.552857000

C	-2.427452000	1.023054000	-0.447535000
C	-3.692996000	0.465529000	-0.406716000
C	-2.787006000	-1.540009000	0.571168000
H	-0.688402000	-1.544019000	0.966831000
H	-2.279805000	2.009976000	-0.861296000
H	-4.536772000	1.032717000	-0.777013000
H	-2.929922000	-2.533510000	0.975571000
H	-4.874004000	-1.254822000	0.118931000
O	-0.000087000	2.236532000	0.000658000

E (UB+HF-LYP) = -576.7309276

E (UB+HF-LYP + ZPE = -576.543080

No vibrational mode with imaginary frequency

Benzophenone triplet (UM05-2X/cc-pVTZ)

H	2.284397000	2.019687000	0.824242000
C	2.418317000	1.026117000	0.427585000
C	2.749595000	-1.546672000	-0.553637000
C	1.297151000	0.306222000	-0.019295000
C	3.675195000	0.456553000	0.389386000
C	3.849970000	-0.833683000	-0.091243000
C	1.489384000	-0.986840000	-0.532609000
H	4.524379000	1.018835000	0.745057000
H	4.832369000	-1.276899000	-0.114478000
H	0.650392000	-1.528477000	-0.937317000
H	2.880550000	-2.541644000	-0.949604000
C	-0.000023000	0.922584000	0.000181000
C	-1.297229000	0.306391000	0.019434000
C	-3.849971000	-0.833699000	0.090965000
C	-1.489501000	-0.986696000	0.532840000
C	-2.418314000	1.026211000	-0.427535000
C	-3.675190000	0.456511000	-0.389611000
C	-2.749611000	-1.546611000	0.553666000
H	-0.650452000	-1.528118000	0.937749000
H	-2.284456000	2.019854000	-0.824037000
H	-4.524313000	1.018795000	-0.745438000
H	-2.880602000	-2.541550000	0.949696000
H	-4.832343000	-1.276977000	0.113958000
O	0.000181000	2.252271000	-0.000074000

E (UM052X+HF-M052X) = -576.6770612

E (UM052X+HF-M052X) + ZPE = -576.485237

No vibrational mode with imaginary frequency

Singlet biradical ¹5 (UM05-2X/cc-pVTZ)

H	-1.192910000	2.136245000	-0.411907000
C	-0.163238000	2.432274000	-0.303258000
C	2.496024000	3.186661000	-0.096512000
C	0.170346000	3.765140000	-0.170634000
C	0.832148000	1.438460000	-0.305430000
C	2.174961000	1.851064000	-0.222451000
C	1.498629000	4.153429000	-0.057882000
H	-0.610955000	4.509262000	-0.161773000
H	2.963311000	1.120757000	-0.296623000
H	1.755405000	5.195951000	0.041453000
H	3.532916000	3.480459000	-0.042360000
C	0.457287000	0.063161000	-0.444352000

C	1.290919000	-1.083422000	-0.156459000
C	2.814323000	-3.370787000	0.390480000
C	1.083337000	-2.276285000	-0.864562000
C	2.266450000	-1.074733000	0.850291000
C	3.018036000	-2.203531000	1.114226000
C	1.839393000	-3.401026000	-0.596518000
H	0.337169000	-2.292087000	-1.643428000
H	2.405653000	-0.186591000	1.444970000
H	3.757480000	-2.178464000	1.899459000
H	1.672029000	-4.304568000	-1.161815000
H	3.402972000	-4.249687000	0.600238000
O	-0.786934000	-0.176575000	-0.918764000
C	-1.711400000	-0.930470000	-0.005554000
H	-1.126018000	-1.791011000	0.326614000
C	-2.862777000	-1.365232000	-0.826202000
H	-2.647596000	-1.995343000	-1.674839000
C	-2.080976000	-0.061952000	1.133848000
H	-1.276475000	0.297025000	1.757787000
C	-4.130144000	-0.978591000	-0.548471000
H	-4.939531000	-1.314574000	-1.178014000
C	-3.366637000	0.306173000	1.374647000
H	-3.587638000	0.956550000	2.206912000
C	-4.413896000	-0.139829000	0.550538000
H	-5.427035000	0.165653000	0.748969000

E (UM052X+HF-M052X) = -809.0000889

E (UM052X+HF-M052X) + ZPE = -808.704530

No vibrational mode with imaginary frequency

TS for decay of ¹5 (UM05-2X/cc-pVTZ)

H	-1.418399000	1.963663000	-0.385776000
C	-0.426516000	2.372299000	-0.291279000
C	2.136082000	3.417632000	-0.131139000
C	-0.241062000	3.732678000	-0.144995000
C	0.673525000	1.497288000	-0.324568000
C	1.962978000	2.056044000	-0.267144000
C	1.037538000	4.265521000	-0.055078000
H	-1.099983000	4.384977000	-0.109640000
H	2.825058000	1.417642000	-0.366647000
H	1.178932000	5.329072000	0.053515000
H	3.134447000	3.825231000	-0.097208000
C	0.450321000	0.086831000	-0.469718000
C	1.407888000	-0.958075000	-0.170546000
C	3.160406000	-3.066020000	0.408583000
C	1.312157000	-2.183297000	-0.845786000
C	2.390161000	-0.825681000	0.820910000
C	3.254738000	-1.866276000	1.100955000
C	2.181094000	-3.219531000	-0.562314000
H	0.560259000	-2.293881000	-1.611363000
H	2.447194000	0.085814000	1.393205000
H	3.997793000	-1.747275000	1.874160000
H	2.098500000	-4.149383000	-1.103078000
H	3.837928000	-3.875231000	0.629975000
O	-0.756456000	-0.293290000	-0.914063000
C	-1.615061000	-1.129585000	0.068332000
H	-0.909489000	-1.883465000	0.415719000
C	-2.701391000	-1.718642000	-0.730841000
H	-2.422809000	-2.413422000	-1.507316000
C	-2.069747000	-0.238144000	1.144769000

H	-1.313174000	0.198771000	1.778746000
C	-3.998591000	-1.378157000	-0.535063000
H	-4.764295000	-1.814791000	-1.157474000
C	-3.383717000	0.082307000	1.308710000
H	-3.670990000	0.769824000	2.089160000
C	-4.368510000	-0.468656000	0.477001000
H	-5.403089000	-0.202446000	0.611795000

E (UM052X+HF-M052X) = -808.9999414

E (UB UM052X+HF-M052X) + ZPE = -808.704952

One vibrational mode with imaginary frequency

TS for formation of ³5 (UB3lyp/cc-pVTZ)

H	0.094933000	-2.622302000	-0.025066000
C	-0.968701000	-2.449414000	-0.084773000
C	-3.704082000	-1.990435000	-0.257020000
C	-1.852707000	-3.511672000	-0.050537000
C	-1.432590000	-1.114423000	-0.190324000
C	-2.831143000	-0.920210000	-0.299978000
C	-3.227610000	-3.295965000	-0.127533000
H	-1.469908000	-4.520130000	0.041077000
H	-3.221411000	0.076543000	-0.441523000
H	-3.916435000	-4.129166000	-0.097297000
H	-4.768245000	-1.811170000	-0.341511000
C	-0.484218000	-0.028858000	-0.243384000
C	-0.817104000	1.374630000	-0.070768000
C	-1.403954000	4.119134000	0.250228000
C	-0.163452000	2.360929000	-0.840341000
C	-1.771294000	1.814807000	0.869602000
C	-2.055809000	3.161426000	1.024220000
C	-0.456775000	3.705267000	-0.683383000
H	0.551952000	2.047026000	-1.587499000
H	-2.266087000	1.090072000	1.500381000
H	-2.784060000	3.469251000	1.763439000
H	0.048362000	4.437005000	-1.300864000
H	-1.629158000	5.169542000	0.374026000
O	0.748733000	-0.394713000	-0.628681000
C	2.230058000	0.405032000	0.324321000
H	1.640790000	1.266590000	0.597212000
C	3.171080000	0.542337000	-0.742284000
H	3.030621000	1.334072000	-1.464012000
C	2.488483000	-0.576623000	1.330797000
H	1.826961000	-0.634278000	2.183751000
C	4.208148000	-0.351484000	-0.871580000
H	4.896042000	-0.268504000	-1.702099000
C	3.529346000	-1.457899000	1.187986000
H	3.701887000	-2.221995000	1.933848000
C	4.387453000	-1.363210000	0.079014000
H	5.203108000	-2.065082000	-0.029988000

E (UB+HF-LYP) = -809.0473334

E (UB+HF-LYP + ZPE = -808.758177

One vibrational mode with imaginary frequency

TS for formation of ³5 (UM05-2X/cc-pVTZ)

H	0.041258000	-2.612329000	-0.015742000
C	-1.014521000	-2.408392000	-0.081756000

C	-3.725968000	-1.855919000	-0.259616000
C	-1.934328000	-3.435884000	-0.035065000
C	-1.436022000	-1.070091000	-0.203187000
C	-2.817099000	-0.820803000	-0.314876000
C	-3.295445000	-3.170785000	-0.114432000
H	-1.589960000	-4.453328000	0.068962000
H	-3.163144000	0.187453000	-0.472026000
H	-4.011123000	-3.976319000	-0.074423000
H	-4.779841000	-1.641667000	-0.348468000
C	-0.453334000	-0.022485000	-0.261570000
C	-0.739618000	1.381468000	-0.081489000
C	-1.245029000	4.123544000	0.243878000
C	-0.048954000	2.341096000	-0.839850000
C	-1.684216000	1.836487000	0.851089000
C	-1.930551000	3.186776000	1.006698000
C	-0.302635000	3.689219000	-0.679318000
H	0.663827000	2.001480000	-1.575120000
H	-2.200070000	1.120044000	1.470360000
H	-2.654167000	3.513556000	1.737528000
H	0.228864000	4.407300000	-1.284759000
H	-1.440564000	5.176374000	0.369369000
O	0.756146000	-0.425813000	-0.670671000
C	2.270471000	0.432694000	0.388195000
H	1.672951000	1.296006000	0.623332000
C	3.187924000	0.499243000	-0.682894000
H	3.122485000	1.318325000	-1.380413000
C	2.411102000	-0.588634000	1.355603000
H	1.748360000	-0.598729000	2.206059000
C	4.111223000	-0.503676000	-0.859377000
H	4.785902000	-0.480228000	-1.699941000
C	3.336347000	-1.582733000	1.170637000
H	3.422038000	-2.386920000	1.883833000
C	4.178129000	-1.551765000	0.055087000
H	4.899156000	-2.340656000	-0.089726000

E (UM052X+HF-M052X)= -808.9712245

E (UM052X+HF-M052X) + ZPE = -808.676448

One vibrational mode with imaginary frequency

Triplet biradical ³5 (UB3lyp/cc-pVTZ)

H	0.266056000	-2.576407000	-0.270006000
C	-0.805299000	-2.457279000	-0.220778000
C	-3.565136000	-2.150554000	-0.133513000
C	-1.625406000	-3.568992000	-0.169375000
C	-1.345547000	-1.148393000	-0.211620000
C	-2.755992000	-1.030492000	-0.185916000
C	-3.011054000	-3.429475000	-0.117297000
H	-1.182515000	-4.556583000	-0.170206000
H	-3.211400000	-0.053150000	-0.238029000
H	-3.648985000	-4.301831000	-0.076844000
H	-4.640411000	-2.028154000	-0.120345000
C	-0.474972000	-0.009782000	-0.276784000
C	-0.859186000	1.377573000	-0.076073000
C	-1.547918000	4.087894000	0.291723000
C	-0.291667000	2.392400000	-0.873688000
C	-1.774955000	1.769458000	0.919877000
C	-2.111661000	3.101971000	1.096791000
C	-0.635062000	3.721796000	-0.693734000
H	0.399663000	2.115948000	-1.657341000

H	-2.197709000	1.021807000	1.575416000
H	-2.810119000	3.375284000	1.876881000
H	-0.194943000	4.477718000	-1.330970000
H	-1.813277000	5.126746000	0.432711000
O	0.793763000	-0.273127000	-0.723275000
C	1.935287000	0.242198000	0.051676000
H	1.620062000	1.211223000	0.458764000
C	3.066787000	0.443563000	-0.899216000
H	2.880959000	1.081123000	-1.752695000
C	2.260120000	-0.686634000	1.177363000
H	1.471632000	-0.889123000	1.890056000
C	4.278814000	-0.145884000	-0.715792000
H	5.072380000	0.033422000	-1.429944000
C	3.486691000	-1.256204000	1.311490000
H	3.677709000	-1.924375000	2.141728000
C	4.521440000	-0.997538000	0.383297000
H	5.489091000	-1.462385000	0.506437000

E(UB+HF-LYP) = -809.0613053

E (UB+HF-LYP + ZPE = -808.770864

No vibrational mode with imaginary frequency

Triplet biradical ³5 (M05-2X/cc-pVTZ)

H	0.636245000	-2.434573000	-0.343995000
C	-0.437675000	-2.469829000	-0.265387000
C	-3.204185000	-2.546119000	-0.106590000
C	-1.092527000	-3.680650000	-0.177900000
C	-1.156308000	-1.259564000	-0.253672000
C	-2.560802000	-1.328975000	-0.192831000
C	-2.478188000	-3.730553000	-0.089219000
H	-0.520315000	-4.595466000	-0.180540000
H	-3.141313000	-0.423474000	-0.250842000
H	-2.986193000	-4.679190000	-0.021589000
H	-4.282186000	-2.574589000	-0.068346000
C	-0.455706000	-0.016918000	-0.353395000
C	-1.010996000	1.296352000	-0.110633000
C	-2.018455000	3.872190000	0.340766000
C	-0.569108000	2.388448000	-0.872338000
C	-1.957260000	1.533249000	0.895816000
C	-2.453618000	2.804575000	1.113338000
C	-1.071221000	3.655552000	-0.651057000
H	0.155468000	2.217406000	-1.653204000
H	-2.275631000	0.716966000	1.524252000
H	-3.175232000	2.966579000	1.898937000
H	-0.727876000	4.478914000	-1.257931000
H	-2.408370000	4.862578000	0.513362000
O	0.816820000	-0.085727000	-0.844259000
C	1.864353000	0.487476000	-0.004534000
H	1.473620000	1.435137000	0.378416000
C	3.036758000	0.745735000	-0.881380000
H	2.865969000	1.364735000	-1.747889000
C	2.161780000	-0.423030000	1.137663000
H	1.337632000	-0.669815000	1.789939000
C	4.260297000	0.228359000	-0.618704000
H	5.084483000	0.447991000	-1.279616000
C	3.400368000	-0.923398000	1.354694000
H	3.571622000	-1.579969000	2.193864000
C	4.476276000	-0.605368000	0.497571000
H	5.454827000	-1.012614000	0.686016000

E (UM052X+HF-M052X) = -808.9980506
 E (UM052X+HF-M052X) + ZPE = -808.702015
 No vibrational mode with imaginary frequency

Triplet biradical ³**11** (B3lyp/cc-pVTZ)

C	-1.228029000	0.310395000	-0.292160000
C	-2.442423000	-0.332777000	-0.712952000
C	-4.793626000	-1.645293000	-1.572833000
C	-2.506504000	-1.742693000	-0.811001000
C	-3.595858000	0.393797000	-1.093171000
C	-4.744639000	-0.254254000	-1.509331000
C	-3.661608000	-2.379723000	-1.225958000
H	-1.636128000	-2.325089000	-0.551164000
H	-3.571851000	1.472861000	-1.091610000
H	-5.607082000	0.330410000	-1.802045000
H	-3.682114000	-3.460510000	-1.280466000
H	-5.694595000	-2.147207000	-1.898376000
O	-0.087561000	-0.450920000	-0.436512000
C	0.739851000	-0.852822000	0.712893000
C	1.080520000	-2.290433000	0.456037000
H	1.619731000	-2.509853000	-0.452544000
C	0.040338000	-0.638330000	2.019591000
H	-0.139326000	0.387290000	2.302355000
C	0.706582000	-3.282383000	1.305578000
H	0.962040000	-4.306773000	1.067039000
C	-0.311783000	-1.671479000	2.827964000
H	-0.820048000	-1.462638000	3.760290000
C	-0.005188000	-3.007062000	2.493098000
H	-0.294505000	-3.812782000	3.152334000
O	1.895768000	-0.015508000	0.776177000
C	2.921461000	-0.075365000	-0.143428000
C	5.126834000	-0.018433000	-1.849518000
C	4.195926000	0.165003000	0.366532000
C	2.745145000	-0.281081000	-1.511462000
C	3.854269000	-0.257280000	-2.351714000
C	5.290513000	0.197157000	-0.484906000
H	4.306129000	0.325459000	1.429795000
H	1.757929000	-0.447093000	-1.913164000
H	3.712490000	-0.418685000	-3.412302000
H	6.275390000	0.385922000	-0.078587000
H	5.980559000	0.003262000	-2.512750000
C	-1.089195000	1.700982000	0.099200000
C	0.083269000	2.420328000	-0.204298000
C	-2.099464000	2.374269000	0.817105000
C	0.223972000	3.746657000	0.168385000
H	0.874255000	1.931521000	-0.751166000
C	-1.948211000	3.698673000	1.192917000
H	-2.990443000	1.837627000	1.108805000
C	-0.788801000	4.397385000	0.867206000
H	1.130239000	4.277965000	-0.090947000
H	-2.734641000	4.186235000	1.754172000
H	-0.673784000	5.432088000	1.160364000

E (UB+HF-LYP) = -1115.4275588
 E (UB+HF-LYP + ZPE = -1115.052943
 No vibrational mode with imaginary frequency

Triplet biradical ³**11** (M05-2X/cc-pVTZ)

C	-1.147050000	0.416108000	-0.356209000
C	-2.443833000	-0.089151000	-0.689595000
C	-4.960048000	-1.134615000	-1.361792000
C	-2.655568000	-1.477468000	-0.765813000
C	-3.524193000	0.759089000	-0.994189000
C	-4.760128000	0.239478000	-1.320105000
C	-3.896741000	-1.985803000	-1.089706000
H	-1.834502000	-2.144765000	-0.561876000
H	-3.373461000	1.825547000	-1.009669000
H	-5.571138000	0.909599000	-1.559481000
H	-4.038864000	-3.054618000	-1.131958000
H	-5.927889000	-1.535886000	-1.616486000
O	-0.102305000	-0.452876000	-0.553868000
C	0.609908000	-1.000729000	0.592671000
C	0.905801000	-2.418581000	0.224561000
H	1.539292000	-2.579649000	-0.630561000
C	-0.196824000	-0.871588000	1.841694000
H	-0.327178000	0.130377000	2.215275000
C	0.367637000	-3.459376000	0.901815000
H	0.585459000	-4.466056000	0.580888000
C	-0.712593000	-1.946916000	2.478973000
H	-1.304343000	-1.800375000	3.368759000
C	-0.465261000	-3.256630000	2.020601000
H	-0.887442000	-4.100021000	2.539430000
O	1.782124000	-0.240303000	0.832706000
C	2.848660000	-0.254370000	-0.033884000
C	5.132192000	-0.143553000	-1.611088000
C	4.090946000	-0.056763000	0.552893000
C	2.739715000	-0.388300000	-1.412330000
C	3.889508000	-0.338742000	-2.188218000
C	5.225718000	0.002020000	-0.234714000
H	4.140183000	0.049333000	1.624658000
H	1.775149000	-0.518495000	-1.871737000
H	3.802331000	-0.446447000	-3.258342000
H	6.186928000	0.157041000	0.229995000
H	6.017562000	-0.102009000	-2.225070000
C	-0.839901000	1.759982000	0.073896000
C	0.400990000	2.333145000	-0.234730000
C	-1.742030000	2.509362000	0.844207000
C	0.711505000	3.612180000	0.183618000
H	1.110249000	1.770308000	-0.818014000
C	-1.421875000	3.786201000	1.263872000
H	-2.680107000	2.067447000	1.139178000
C	-0.197105000	4.348368000	0.931256000
H	1.668367000	4.037418000	-0.075699000
H	-2.125811000	4.341283000	1.864238000
H	0.050079000	5.345322000	1.259663000

E (UM052X+HF-M052X) = -1115.3527543
 E (UM052X+HF-M052X) + ZPE = -1114.970885
 No vibrational mode with imaginary frequency

TS for cleavage of triplet biradical ³**11** into **12** and **13** (UB3lyp/cc-pVTZ)

C	-1.666001000	0.210726000	-0.411565000
C	-2.899280000	-0.500101000	-0.224440000
C	-5.306771000	-1.944165000	0.107927000
C	-2.918959000	-1.915371000	-0.232070000

C	-4.142276000	0.161033000	-0.076538000
C	-5.315904000	-0.551054000	0.089654000
C	-4.098493000	-2.616328000	-0.061912000
H	-1.994956000	-2.455648000	-0.368949000
H	-4.183379000	1.237841000	-0.130789000
H	-6.250984000	-0.015678000	0.190206000
H	-4.077986000	-3.698305000	-0.062848000
H	-6.227479000	-2.496099000	0.238825000
O	-0.659159000	-0.530423000	-1.016668000
C	0.438912000	-0.996854000	-0.318312000
C	0.980509000	-2.203714000	-0.919593000
H	0.839072000	-2.323146000	-1.983785000
C	0.446036000	-0.932284000	1.131261000
H	-0.068410000	-0.113762000	1.610563000
C	1.693757000	-3.093328000	-0.169282000
H	2.145764000	-3.954655000	-0.642503000
C	1.170812000	-1.840018000	1.851999000
H	1.228317000	-1.741183000	2.927762000
C	1.822321000	-2.915049000	1.221026000
H	2.392930000	-3.620834000	1.807553000
O	1.602821000	0.206037000	-0.816371000
C	2.883128000	0.193419000	-0.411316000
C	5.584639000	0.329187000	0.321936000
C	3.272966000	0.855582000	0.764230000
C	3.872148000	-0.408455000	-1.206022000
C	5.208368000	-0.333641000	-0.843039000
C	4.611406000	0.924352000	1.120110000
H	2.512780000	1.329453000	1.368999000
H	3.569633000	-0.908501000	-2.115492000
H	5.961491000	-0.790322000	-1.472156000
H	4.899846000	1.449546000	2.021527000
H	6.627824000	0.386938000	0.602159000
C	-1.434372000	1.624154000	-0.200755000
C	-0.529667000	2.332973000	-1.016352000
C	-2.084672000	2.336344000	0.829165000
C	-0.316191000	3.687705000	-0.828696000
H	-0.000456000	1.803760000	-1.792201000
C	-1.858021000	3.690055000	1.014591000
H	-2.743366000	1.812552000	1.506382000
C	-0.979201000	4.377817000	0.182632000
H	0.375014000	4.210494000	-1.476436000
H	-2.360512000	4.209124000	1.820255000
H	-0.805611000	5.435593000	0.327396000

E (UB+HF-LYP) = -1115.4183317

E (UB+HF-LYP + ZPE = -1115.045384

One vibrational mode with imaginary frequency

TS for cleavage of triplet biradical ³**11** into **12** and **13** (UM05-2X/cc-pVTZ)

C	-1.662666000	0.190230000	-0.536633000
C	-2.905920000	-0.409957000	-0.174604000
C	-5.338698000	-1.630249000	0.510513000
C	-3.025754000	-1.811522000	-0.121620000
C	-4.053616000	0.359487000	0.095809000
C	-5.245132000	-0.246055000	0.435578000
C	-4.222380000	-2.405042000	0.222856000
H	-2.167557000	-2.423100000	-0.347238000
H	-4.008906000	1.431336000	-0.001865000

H	-6.114000000	0.363801000	0.628542000
H	-4.287895000	-3.481112000	0.266703000
H	-6.272491000	-2.098683000	0.776640000
O	-0.773952000	-0.639024000	-1.194800000
C	0.302697000	-1.141971000	-0.514853000
C	0.907807000	-2.275536000	-1.153234000
H	0.715965000	-2.407575000	-2.204926000
C	0.358395000	-1.065432000	0.913049000
H	-0.221852000	-0.312425000	1.419488000
C	1.771641000	-3.065270000	-0.452621000
H	2.290644000	-3.868472000	-0.951002000
C	1.237669000	-1.862685000	1.586955000
H	1.354567000	-1.744077000	2.652417000
C	1.978935000	-2.844725000	0.915207000
H	2.679570000	-3.454770000	1.460084000
O	1.552253000	0.085397000	-1.054356000
C	2.718165000	0.142356000	-0.423505000
C	5.196128000	0.350078000	0.842920000
C	2.860496000	0.909753000	0.741795000
C	3.838915000	-0.523431000	-0.936915000
C	5.066228000	-0.412877000	-0.308571000
C	4.089883000	1.014553000	1.360907000
H	1.991562000	1.428426000	1.118185000
H	3.718408000	-1.100340000	-1.840032000
H	5.926541000	-0.918414000	-0.719319000
H	4.193259000	1.618514000	2.249292000
H	6.154587000	0.435488000	1.330193000
C	-1.279514000	1.569082000	-0.345262000
C	-0.424437000	2.199752000	-1.258017000
C	-1.717853000	2.295645000	0.771028000
C	-0.046705000	3.514602000	-1.070393000
H	-0.059083000	1.641901000	-2.102160000
C	-1.329021000	3.609006000	0.955410000
H	-2.336857000	1.811205000	1.509489000
C	-0.496887000	4.227099000	0.032756000
H	0.607113000	3.986209000	-1.787029000
H	-1.666186000	4.147720000	1.827200000
H	-0.194034000	5.252034000	0.177243000

E (UM052X+HF-M052X) = -1115.3363873

E (UM052X+HF-M052X) + ZPE = -1114.956020

One vibrational mode with imaginary frequency

Triplet biradical ³15 (UB3lyp/cc-pVTZ)

H	-3.197523000	-2.175671000	-0.676755000
C	-3.293334000	-1.690990000	0.284959000
C	-3.589997000	-0.420705000	2.733813000
C	-4.112321000	-2.241500000	1.256726000
C	-2.606832000	-0.480545000	0.509816000
C	-2.771361000	0.136979000	1.764470000
C	-4.268440000	-1.611072000	2.488228000
H	-4.639718000	-3.163756000	1.050528000
H	-2.227752000	1.044730000	1.983981000
H	-4.906704000	-2.043223000	3.246775000
H	-3.690308000	0.070765000	3.692724000
C	-1.747760000	0.076013000	-0.523505000
C	-1.633052000	1.463309000	-0.868935000
C	-1.383288000	4.177869000	-1.616132000
C	-0.621635000	1.892613000	-1.762419000

C	-2.533008000	2.445898000	-0.390113000
C	-2.401277000	3.773219000	-0.754276000
C	-0.502509000	3.222531000	-2.120607000
H	0.059690000	1.158891000	-2.164433000
H	-3.353889000	2.153235000	0.246855000
H	-3.108469000	4.499867000	-0.375766000
H	0.283574000	3.521095000	-2.802300000
H	-1.286425000	5.217095000	-1.899407000
O	-1.098590000	-0.787936000	-1.364907000
C	-0.236500000	-1.831008000	-0.778509000
H	-0.783100000	-2.231682000	0.084045000
C	1.058653000	-1.252740000	-0.309143000
H	1.013612000	-0.478285000	0.441780000
C	-0.094771000	-2.897175000	-1.810165000
H	-1.006135000	-3.328964000	-2.199242000
C	2.244832000	-1.694488000	-0.797452000
C	1.126516000	-3.303446000	-2.256309000
H	1.192323000	-4.083402000	-3.003743000
C	2.312029000	-2.725644000	-1.773771000
H	3.281610000	-3.039876000	-2.130190000
O	3.478720000	-1.224890000	-0.408434000
C	3.567102000	-0.181714000	0.501328000
C	3.911463000	1.891711000	2.307902000
C	3.870607000	-0.470353000	1.824749000
C	3.436597000	1.131762000	0.068653000
C	3.608159000	2.167626000	0.978874000
C	4.044179000	0.572958000	2.727319000
H	3.975745000	-1.501940000	2.130466000
H	3.207140000	1.330977000	-0.968624000
H	3.507500000	3.191989000	0.646543000
H	4.285491000	0.352890000	3.758614000
H	4.047959000	2.701213000	3.011873000

E (UB+HF-LYP) = -1115.431211

E (UB+HF-LYP + ZPE = -1115.056425

No vibrational mode with imaginary frequency

Triplet biradical ³15 (M05-2X/cc-pVTZ)

H	-3.394644000	1.822609000	-0.662596000
C	-3.268008000	0.781047000	-0.913461000
C	-2.939853000	-1.900157000	-1.527153000
C	-4.084962000	0.181754000	-1.852852000
C	-2.280736000	0.042816000	-0.247123000
C	-2.122078000	-1.308223000	-0.582931000
C	-3.929190000	-1.162482000	-2.162197000
H	-4.849857000	0.762960000	-2.344059000
H	-1.325054000	-1.876380000	-0.129382000
H	-4.565479000	-1.627616000	-2.898207000
H	-2.793595000	-2.938441000	-1.781044000
C	-1.415109000	0.707834000	0.704357000
C	-0.845288000	0.129758000	1.877132000
C	0.353539000	-0.982990000	4.160435000
C	0.205892000	0.791863000	2.542302000
C	-1.307427000	-1.083788000	2.422072000
C	-0.709499000	-1.628795000	3.539632000
C	0.795044000	0.235985000	3.659045000
H	0.551022000	1.736628000	2.156301000
H	-2.155362000	-1.577310000	1.977144000
H	-1.083445000	-2.557924000	3.941424000

H	1.607436000	0.754494000	4.144580000
H	0.817841000	-1.414146000	5.032683000
O	-1.120093000	2.019006000	0.474765000
C	-0.392058000	2.303603000	-0.779848000
H	-1.142346000	2.314747000	-1.572353000
C	0.617879000	1.246065000	-1.058560000
H	0.263415000	0.267415000	-1.335249000
C	0.187100000	3.659596000	-0.581817000
H	-0.505885000	4.472947000	-0.441901000
C	1.937773000	1.493107000	-0.929942000
C	1.527293000	3.856190000	-0.498377000
H	1.913516000	4.846080000	-0.312444000
C	2.429416000	2.789854000	-0.638721000
H	3.492929000	2.931090000	-0.552985000
O	2.913954000	0.544714000	-1.113115000
C	2.537497000	-0.786630000	-1.076149000
C	1.888666000	-3.468576000	-1.022459000
C	2.713984000	-1.549698000	-2.213975000
C	2.043798000	-1.342355000	0.093225000
C	1.716836000	-2.687416000	0.112423000
C	2.390899000	-2.898470000	-2.180847000
H	3.103398000	-1.082006000	-3.103779000
H	1.909954000	-0.724712000	0.967580000
H	1.329529000	-3.121657000	1.021275000
H	2.529920000	-3.500708000	-3.064841000
H	1.637368000	-4.517195000	-1.000594000

E (UM052X+HF-M052X) = -1115.35295

E (UM052X+HF-M052X) + ZPE = -1114.970679

No vibrational mode with imaginary frequency

Triplet biradical ³**14** (UB3lyp/cc-pVTZ)

H	-0.820938000	1.622592000	-1.878151000
C	-0.376681000	2.317594000	-1.184209000
C	0.778054000	4.116227000	0.593189000
C	-0.922263000	3.576669000	-1.016919000
C	0.768066000	1.911724000	-0.452142000
C	1.338569000	2.863314000	0.431568000
C	-0.359265000	4.487099000	-0.123386000
H	-1.797497000	3.855202000	-1.589812000
H	2.238860000	2.615905000	0.972956000
H	-0.790926000	5.470565000	0.003743000
H	1.239738000	4.819316000	1.274490000
C	1.339023000	0.615186000	-0.652776000
C	2.528302000	0.116195000	0.044398000
C	4.846039000	-0.821789000	1.331341000
C	2.626694000	0.113688000	1.443346000
C	3.622666000	-0.364872000	-0.693538000
C	4.766381000	-0.821135000	-0.058712000
C	3.769546000	-0.354060000	2.077119000
H	1.787815000	0.454725000	2.033830000
H	3.568084000	-0.358157000	-1.773138000
H	5.602602000	-1.173041000	-0.648881000
H	3.816618000	-0.359891000	3.158278000
H	5.737448000	-1.182538000	1.826727000
O	0.879182000	-0.080429000	-1.742026000
C	0.299750000	-1.444916000	-1.572039000
H	-0.118767000	-1.580270000	-2.573974000
C	-0.816862000	-1.451502000	-0.575014000

C	1.322612000	-2.490413000	-1.285175000
H	2.107557000	-2.609318000	-2.018316000
C	1.298108000	-3.249316000	-0.158645000
H	2.082182000	-3.974486000	0.015238000
C	-0.793933000	-2.214320000	0.560001000
H	-1.610794000	-2.153263000	1.264471000
C	0.266871000	-3.105657000	0.794532000
H	0.275773000	-3.696703000	1.698804000
O	-1.845047000	-0.641481000	-0.953615000
C	-3.001135000	-0.575652000	-0.181366000
C	-5.364051000	-0.351639000	1.241654000
C	-4.022205000	-1.488406000	-0.407842000
C	-3.143583000	0.450558000	0.741284000
C	-4.333663000	0.557550000	1.452924000
C	-5.206687000	-1.371972000	0.309744000
H	-3.884770000	-2.270688000	-1.141218000
H	-2.337160000	1.155887000	0.881777000
H	-4.454582000	1.357922000	2.170440000
H	-6.008113000	-2.077373000	0.135949000
H	-6.288326000	-0.262035000	1.795904000

E (UB+HF-LYP) = -1115.4280401

E (UB+HF-LYP + ZPE = -1115.052690

No vibrational mode with imaginary frequency

Triplet biradical ³**14** (UM05-2X/cc-pVTZ)

H	-1.000758000	1.414846000	-2.279674000
C	-0.891435000	2.102088000	-1.459557000
C	-0.601316000	3.862046000	0.665335000
C	-1.802176000	3.119498000	-1.274203000
C	0.187367000	1.926746000	-0.567169000
C	0.322402000	2.853203000	0.488647000
C	-1.675862000	4.001052000	-0.206102000
H	-2.624489000	3.226225000	-1.964599000
H	1.166875000	2.782030000	1.153709000
H	-2.394702000	4.791843000	-0.062968000
H	-0.477139000	4.556539000	1.481874000
C	1.107442000	0.859810000	-0.755750000
C	2.233786000	0.561171000	0.123996000
C	4.416732000	-0.054977000	1.752114000
C	2.073796000	0.415089000	1.501743000
C	3.507949000	0.392186000	-0.424215000
C	4.588703000	0.093535000	0.382615000
C	3.156478000	0.106477000	2.307470000
H	1.087886000	0.511205000	1.930188000
H	3.634249000	0.505147000	-1.489653000
H	5.568265000	-0.023794000	-0.054471000
H	3.013749000	-0.018969000	3.369563000
H	5.259482000	-0.294459000	2.381518000
O	1.003961000	0.153817000	-1.920275000
C	0.739600000	-1.293235000	-1.795430000
H	0.341829000	-1.514228000	-2.786491000
C	-0.317748000	-1.545585000	-0.776685000
C	1.978045000	-2.072826000	-1.532004000
H	2.761500000	-1.989415000	-2.268033000
C	2.144215000	-2.821756000	-0.415813000
H	3.077135000	-3.338637000	-0.253967000
C	-0.114373000	-2.290126000	0.342585000
H	-0.909530000	-2.407190000	1.060845000

C	1.122988000	-2.924650000	0.548342000
H	1.280432000	-3.502093000	1.442872000
O	-1.491274000	-0.947415000	-1.115092000
C	-2.534104000	-0.994606000	-0.200444000
C	-4.649841000	-1.059544000	1.560670000
C	-3.484824000	-1.989598000	-0.324287000
C	-2.619697000	-0.026821000	0.783787000
C	-3.687943000	-0.065948000	1.665978000
C	-4.548576000	-2.017812000	0.564220000
H	-3.382352000	-2.722144000	-1.109047000
H	-1.866570000	0.743888000	0.837717000
H	-3.769680000	0.687091000	2.433892000
H	-5.297873000	-2.788585000	0.475423000
H	-5.479454000	-1.083016000	2.249193000

E (UM052X+HF-M052X) = -1115.3536284

E (UM052X+HF-M052X) + ZPE = -1114.970867

No vibrational mode with imaginary frequency

Triplet biradical ³**16** (UB3lyp/cc-pVTZ)

H	-1.428597000	-2.480002000	-0.207785000
C	-2.507517000	-2.497571000	-0.203802000
C	-5.285263000	-2.542760000	-0.232592000
C	-3.182136000	-3.703720000	-0.165344000
C	-3.208584000	-1.268041000	-0.239506000
C	-4.622378000	-1.329860000	-0.272247000
C	-4.575311000	-3.740644000	-0.171459000
H	-2.618319000	-4.626997000	-0.130455000
H	-5.194822000	-0.418818000	-0.359102000
H	-5.099041000	-4.686379000	-0.140932000
H	-6.367021000	-2.557555000	-0.264336000
C	-2.486594000	-0.028388000	-0.291349000
C	-3.054077000	1.299456000	-0.125412000
C	-4.107816000	3.898592000	0.175673000
C	-4.052138000	1.576910000	0.829332000
C	-2.593481000	2.372579000	-0.915590000
C	-3.116145000	3.646581000	-0.768779000
C	-4.568087000	2.854765000	0.973593000
H	-4.399136000	0.785757000	1.478322000
H	-1.840919000	2.181772000	-1.667724000
H	-2.754666000	4.447846000	-1.400115000
H	-5.327050000	3.040956000	1.722235000
H	-4.513096000	4.894610000	0.290781000
O	-1.179121000	-0.133030000	-0.684385000
C	4.924424000	-0.461597000	0.283961000
C	7.375358000	0.594403000	-0.477948000
C	5.199409000	0.880153000	0.528782000
C	5.864943000	-1.280199000	-0.328736000
C	7.090954000	-0.747177000	-0.706506000
C	6.427044000	1.401942000	0.140787000
H	4.464619000	1.500738000	1.021644000
H	5.625960000	-2.320747000	-0.497283000
H	7.823584000	-1.383715000	-1.184173000
H	6.644445000	2.444294000	0.332085000
H	8.329683000	1.006825000	-0.774902000
C	-0.137777000	0.539540000	0.127120000
H	-0.593894000	1.463825000	0.496752000
C	0.254479000	-0.335710000	1.272862000
H	-0.516575000	-0.588561000	1.987940000

C	0.995640000	0.847325000	-0.791084000
H	0.777190000	1.466360000	-1.650171000
C	2.247994000	0.353099000	-0.604150000
C	1.513622000	-0.814918000	1.421791000
H	1.770391000	-1.461669000	2.250311000
C	2.534802000	-0.473919000	0.503788000
H	3.032415000	0.586200000	-1.310322000
O	3.753703000	-1.059442000	0.712901000

E (UB+HF-LYP) = -1115.4337012

E (UB+HF-LYP + ZPE = -1115.058587

No vibrational mode with imaginary frequency

Triplet biradical ³**16** (UM05-2X/cc-pVTZ)

H	-1.345560000	-2.410492000	-0.367982000
C	-2.417208000	-2.454223000	-0.266693000
C	-5.179132000	-2.552531000	-0.049851000
C	-3.059558000	-3.669566000	-0.153701000
C	-3.145992000	-1.249981000	-0.252172000
C	-4.548410000	-1.330938000	-0.161799000
C	-4.442564000	-3.730506000	-0.035600000
H	-2.479468000	-4.579427000	-0.159157000
H	-5.138130000	-0.431160000	-0.216643000
H	-4.940727000	-4.682738000	0.052206000
H	-6.255836000	-2.589795000	0.011398000
C	-2.458526000	-0.002488000	-0.378136000
C	-3.022648000	1.308482000	-0.140818000
C	-4.045357000	3.880482000	0.298681000
C	-3.947962000	1.550006000	0.883637000
C	-2.609376000	2.394255000	-0.927272000
C	-3.119206000	3.659310000	-0.711940000
C	-4.451640000	2.819477000	1.095620000
H	-4.243446000	0.739707000	1.530635000
H	-1.900738000	2.219269000	-1.721776000
H	-2.798360000	4.477440000	-1.337962000
H	-5.156205000	2.985326000	1.895718000
H	-4.441116000	4.869331000	0.466870000
O	-1.192997000	-0.064143000	-0.886961000
C	4.841168000	-0.494653000	0.292083000
C	7.254440000	0.737639000	-0.247448000
C	5.000559000	0.849235000	0.590636000
C	5.872657000	-1.230543000	-0.263273000
C	7.081327000	-0.608477000	-0.529342000
C	6.211973000	1.460361000	0.312541000
H	4.186581000	1.399621000	1.035260000
H	5.712946000	-2.275336000	-0.475106000
H	7.888202000	-1.178598000	-0.962098000
H	6.342391000	2.505863000	0.543524000
H	8.195239000	1.219621000	-0.458750000
C	-0.138432000	0.530773000	-0.064185000
H	-0.541243000	1.472918000	0.315680000
C	0.188670000	-0.377227000	1.072399000
H	-0.613372000	-0.615977000	1.753877000
C	1.016499000	0.788214000	-0.965319000
H	0.828643000	1.403279000	-1.830836000
C	2.242174000	0.260177000	-0.748927000
C	1.424256000	-0.892929000	1.251964000
H	1.642128000	-1.555376000	2.075113000
C	2.473111000	-0.570389000	0.367282000

H	3.052462000	0.459760000	-1.432346000
O	3.678083000	-1.170483000	0.595983000

E (UM052X+HF-M052X) = -1115.352270

E (UM052X+HF-M052X) + ZPE = -1114.969715

No vibrational mode with imaginary frequency

TS for formation of biradical ³**11** (UB3lyp/cc-pVTZ)

H	-3.183974000	1.767716000	0.781348000
C	-2.319590000	2.335476000	0.468946000
C	-0.071613000	3.811206000	-0.218341000
C	-2.273937000	3.694960000	0.730463000
C	-1.238921000	1.672788000	-0.151158000
C	-0.107172000	2.450706000	-0.474599000
C	-1.153879000	4.448026000	0.384016000
H	-3.114326000	4.170939000	1.219605000
H	0.734934000	1.966156000	-0.944965000
H	-1.123201000	5.509998000	0.586844000
H	0.805967000	4.382083000	-0.493992000
C	-1.223853000	0.239257000	-0.417142000
C	-2.388596000	-0.546220000	-0.746206000
C	-4.600217000	-2.180297000	-1.425498000
C	-2.303959000	-1.962089000	-0.718954000
C	-3.619409000	0.013049000	-1.173554000
C	-4.696584000	-0.788666000	-1.496946000
C	-3.389761000	-2.754599000	-1.043114000
H	-1.363583000	-2.412013000	-0.443706000
H	-3.709565000	1.082859000	-1.282863000
H	-5.620043000	-0.329582000	-1.826192000
H	-3.293883000	-3.832383000	-1.003146000
H	-5.447832000	-2.801765000	-1.680612000
O	-0.046785000	-0.383551000	-0.498037000
C	1.104939000	-0.578692000	1.128378000
C	1.268986000	-2.009346000	1.024109000
H	2.023055000	-2.402419000	0.360996000
C	0.193157000	-0.071154000	2.120423000
H	0.157322000	0.996711000	2.269315000
C	0.464190000	-2.838382000	1.750322000
H	0.576636000	-3.909809000	1.655140000
C	-0.610804000	-0.932708000	2.819753000
H	-1.323057000	-0.538846000	3.531312000
C	-0.502380000	-2.317086000	2.634988000
H	-1.139719000	-2.988776000	3.192290000
O	2.123129000	0.265282000	0.847547000
C	3.129712000	-0.034848000	-0.063987000
C	5.240703000	-0.437185000	-1.811540000
C	4.425948000	0.242638000	0.351865000
C	2.867549000	-0.500746000	-1.347873000
C	3.937036000	-0.703698000	-2.213608000
C	5.481082000	0.039976000	-0.527515000
H	4.590212000	0.614774000	1.353248000
H	1.847517000	-0.679318000	-1.653299000
H	3.742191000	-1.064341000	-3.214712000
H	6.491510000	0.254191000	-0.206464000
H	6.063325000	-0.594231000	-2.495592000

E (UB+HF-LYP) = -1115.416311

E (UB+HF-LYP + ZPE = -1115.043049

One vibrational mode with imaginary frequency

TS for formation of biradical ³**11** (UM05-2X/cc-pVTZ)

H	-2.994731000	1.903651000	0.812447000
C	-2.079333000	2.379846000	0.498640000
C	0.309669000	3.591318000	-0.206098000
C	-1.871242000	3.716543000	0.778660000
C	-1.094017000	1.617302000	-0.148805000
C	0.110519000	2.253159000	-0.486092000
C	-0.677718000	4.335081000	0.426237000
H	-2.639872000	4.278782000	1.286791000
H	0.876645000	1.680276000	-0.981946000
H	-0.519025000	5.378710000	0.646404000
H	1.240528000	4.059827000	-0.486560000
C	-1.245359000	0.201302000	-0.407837000
C	-2.486970000	-0.441087000	-0.726181000
C	-4.876895000	-1.790119000	-1.346617000
C	-2.572559000	-1.848138000	-0.658056000
C	-3.628869000	0.261748000	-1.165975000
C	-4.798556000	-0.403712000	-1.458202000
C	-3.751131000	-2.502376000	-0.955388000
H	-1.693483000	-2.399170000	-0.371425000
H	-3.574767000	1.328626000	-1.305355000
H	-5.657504000	0.156510000	-1.794816000
H	-3.793496000	-3.579002000	-0.887139000
H	-5.795672000	-2.303862000	-1.579916000
O	-0.164205000	-0.574214000	-0.467522000
C	1.171168000	-0.606895000	1.208988000
C	1.333644000	-2.015960000	1.109384000
H	2.167025000	-2.415635000	0.557981000
C	0.164271000	-0.073972000	2.053158000
H	0.134707000	0.993634000	2.191917000
C	0.406333000	-2.828534000	1.690912000
H	0.500755000	-3.898645000	1.596772000
C	-0.759998000	-0.917278000	2.621685000
H	-1.559521000	-0.509270000	3.217857000
C	-0.663531000	-2.288259000	2.423928000
H	-1.397212000	-2.946863000	2.859249000
O	2.148298000	0.252439000	0.872049000
C	3.123011000	-0.095607000	-0.053356000
C	5.140194000	-0.622389000	-1.852969000
C	4.433314000	0.160095000	0.305882000
C	2.793898000	-0.601201000	-1.299876000
C	3.819168000	-0.866260000	-2.194979000
C	5.444109000	-0.106073000	-0.602739000
H	4.640316000	0.564923000	1.283302000
H	1.758460000	-0.771349000	-1.548016000
H	3.577381000	-1.259488000	-3.169683000
H	6.469255000	0.090200000	-0.331155000
H	5.928759000	-0.828861000	-2.558754000

E (UM052X+HF-M052X) = -1115.327871

E (UM052X+HF-M052X) + ZPE = -1114.947356

One vibrational mode with imaginary frequency

TS for formation of biradical ³**15** (UB3lyp/cc-pVTZ)

H	-3.015713000	-2.229372000	-0.821905000
C	-3.284934000	-1.783721000	0.125221000
C	-4.032573000	-0.603363000	2.521787000

C	-4.173717000	-2.429808000	0.968374000
C	-2.750255000	-0.520268000	0.454748000
C	-3.147293000	0.051005000	1.680801000
C	-4.555389000	-1.847130000	2.174398000
H	-4.581487000	-3.390147000	0.679615000
H	-2.730193000	1.001462000	1.981540000
H	-5.246788000	-2.354120000	2.833503000
H	-4.309064000	-0.145436000	3.462749000
C	-1.809427000	0.130897000	-0.444417000
C	-1.778422000	1.547808000	-0.716792000
C	-1.672620000	4.305217000	-1.337989000
C	-0.679029000	2.107336000	-1.414192000
C	-2.839992000	2.421421000	-0.377239000
C	-2.776597000	3.769977000	-0.673174000
C	-0.631836000	3.456740000	-1.711958000
H	0.125814000	1.453375000	-1.713132000
H	-3.724172000	2.026456000	0.099952000
H	-3.603971000	4.412107000	-0.399392000
H	0.223927000	3.855756000	-2.241872000
H	-1.631740000	5.360614000	-1.570441000
O	-0.987500000	-0.599916000	-1.206655000
C	-0.010595000	-2.019892000	-0.329213000
H	-0.738973000	-2.084502000	0.464239000
C	1.247742000	-1.427693000	-0.015832000
H	1.324465000	-0.768852000	0.834776000
C	-0.079445000	-2.990775000	-1.379008000
H	-1.013133000	-3.501353000	-1.560759000
C	2.324734000	-1.667153000	-0.827088000
C	1.020913000	-3.217978000	-2.177730000
H	0.963273000	-3.916997000	-3.000686000
C	2.217290000	-2.553996000	-1.927154000
H	3.090622000	-2.713256000	-2.543537000
O	3.575644000	-1.144116000	-0.647988000
C	3.795134000	-0.144482000	0.292478000
C	4.403871000	1.848620000	2.116067000
C	4.602136000	-0.439476000	1.381566000
C	3.292075000	1.135655000	0.097420000
C	3.597573000	2.130242000	1.017917000
C	4.907189000	0.565386000	2.293044000
H	4.986354000	-1.442919000	1.499385000
H	2.671090000	1.345185000	-0.761819000
H	3.205569000	3.127616000	0.872545000
H	5.538454000	0.341845000	3.142467000
H	4.641314000	2.627379000	2.827693000

E (UB+HF-LYP) = -1115.418136

E (UB+HF-LYP + ZPE = -1115.044553

One vibrational mode with imaginary frequency

TS for formation of biradical ³**15** (UM05-2X/cc-pVTZ)

H	-0.498099000	3.635773000	-0.730040000
C	-0.154697000	3.262557000	0.222651000
C	0.804497000	2.319982000	2.642707000
C	-0.244480000	4.049579000	1.356193000
C	0.419857000	1.987195000	0.279411000
C	0.899153000	1.528830000	1.512944000
C	0.232544000	3.583353000	2.573004000
H	-0.678048000	5.035534000	1.288794000
H	1.311635000	0.533529000	1.580839000

H	0.158969000	4.196650000	3.456974000
H	1.167036000	1.943038000	3.586569000
C	0.479942000	1.160952000	-0.916049000
C	1.635008000	0.414977000	-1.313660000
C	3.858919000	-1.107909000	-2.112055000
C	1.535993000	-0.528519000	-2.358102000
C	2.897597000	0.601142000	-0.713814000
C	3.980790000	-0.156605000	-1.103140000
C	2.630356000	-1.276733000	-2.739769000
H	0.583562000	-0.664204000	-2.843698000
H	3.019081000	1.356183000	0.044995000
H	4.936393000	0.002645000	-0.627520000
H	2.527306000	-2.001735000	-3.532567000
H	4.710994000	-1.696367000	-2.412253000
O	-0.515609000	1.186189000	-1.808422000
C	-2.374580000	1.212295000	-0.968244000
H	-2.259333000	2.250381000	-0.714136000
C	-2.189820000	0.248200000	0.043565000
H	-1.716950000	0.516997000	0.974331000
C	-3.088647000	0.864224000	-2.141623000
H	-3.273124000	1.619192000	-2.887538000
C	-2.573031000	-1.052386000	-0.189757000
C	-3.483566000	-0.431490000	-2.338268000
H	-4.001616000	-0.712919000	-3.240951000
C	-3.211866000	-1.404813000	-1.371451000
H	-3.499105000	-2.433858000	-1.515342000
O	-2.386326000	-2.027725000	0.760181000
C	-1.103632000	-2.182350000	1.256127000
C	1.416529000	-2.604824000	2.303539000
C	-0.971267000	-2.508601000	2.593947000
C	0.003740000	-2.066113000	0.433486000
C	1.265803000	-2.278017000	0.964321000
C	0.295669000	-2.721768000	3.112531000
H	-1.856298000	-2.591551000	3.203939000
H	-0.114676000	-1.809708000	-0.606756000
H	2.127221000	-2.179721000	0.320870000
H	0.405521000	-2.976429000	4.155085000
H	2.400150000	-2.770081000	2.713381000

E (UM052X+HF-M052X) = -1115.329248

E (UM052X+HF-M052X) + ZPE = -1114.947774

One vibrational mode with imaginary frequency

TS for formation of biradical ³**14** (UB3lyp/cc-pVTZ)

H	-1.361370000	-2.592738000	0.374072000
C	-2.257614000	-2.391086000	-0.192227000
C	-4.559425000	-1.856305000	-1.653680000
C	-3.089805000	-3.425905000	-0.577224000
C	-2.563975000	-1.045638000	-0.515000000
C	-3.733710000	-0.813468000	-1.279187000
C	-4.251299000	-3.172258000	-1.304947000
H	-2.835728000	-4.442673000	-0.305506000
H	-3.972457000	0.190839000	-1.595854000
H	-4.900567000	-3.983977000	-1.603742000
H	-5.446046000	-1.647581000	-2.238716000
C	-1.663460000	0.009436000	-0.119424000
C	-1.992613000	1.425102000	-0.133591000
C	-2.578801000	4.188545000	-0.150714000
C	-3.262772000	1.907570000	0.244208000

C	-1.023714000	2.378938000	-0.513569000
C	-1.316634000	3.732726000	-0.524268000
C	-3.546536000	3.263190000	0.234473000
H	-4.017975000	1.207523000	0.572542000
H	-0.047837000	2.035068000	-0.826460000
H	-0.557769000	4.438947000	-0.836222000
H	-4.527369000	3.603403000	0.541003000
H	-2.803915000	5.246319000	-0.157137000
O	-0.408223000	-0.394727000	0.127713000
C	0.489219000	0.397002000	1.652325000
H	0.180669000	1.400923000	1.410749000
C	1.820320000	0.015459000	1.280984000
C	-0.109383000	-0.265954000	2.763439000
H	-1.066697000	0.086213000	3.119722000
C	0.495044000	-1.360670000	3.322470000
H	0.020942000	-1.891141000	4.136564000
C	2.419944000	-1.095041000	1.847227000
H	3.402621000	-1.407645000	1.527141000
C	1.752720000	-1.786276000	2.854646000
H	2.226569000	-2.648108000	3.304514000
O	2.401525000	0.816238000	0.354111000
C	3.429545000	0.333537000	-0.449628000
C	5.453215000	-0.482564000	-2.147286000
C	4.652077000	0.986130000	-0.410273000
C	3.193841000	-0.714699000	-1.330607000
C	4.216977000	-1.121183000	-2.177292000
C	5.666198000	0.571573000	-1.266961000
H	4.794911000	1.807007000	0.278263000
H	2.220126000	-1.184232000	-1.352319000
H	4.042510000	-1.933246000	-2.870131000
H	6.623033000	1.075349000	-1.243850000
H	6.243784000	-0.801299000	-2.812591000

E (UB+HF-LYP) = -1115.4226572

E (UB+HF-LYP + ZPE = -1115.048787

One vibrational mode with imaginary frequency

TS for formation of biradical ³**14** (UM05-2X/cc-pVTZ)

H	-1.269002000	-2.555082000	0.356689000
C	-2.168556000	-2.343304000	-0.196877000
C	-4.476923000	-1.769106000	-1.621604000
C	-3.030531000	-3.359196000	-0.556322000
C	-2.454015000	-1.004215000	-0.529315000
C	-3.621767000	-0.745533000	-1.273234000
C	-4.194272000	-3.083245000	-1.262886000
H	-2.797728000	-4.376536000	-0.280786000
H	-3.832668000	0.260780000	-1.595812000
H	-4.866059000	-3.879594000	-1.540665000
H	-5.365459000	-1.546894000	-2.192461000
C	-1.532368000	0.029380000	-0.148050000
C	-1.834667000	1.442316000	-0.154630000
C	-2.356567000	4.200771000	-0.167979000
C	-3.095436000	1.941239000	0.206658000
C	-0.838842000	2.366571000	-0.512267000
C	-1.100833000	3.722588000	-0.520226000
C	-3.348315000	3.299458000	0.197137000
H	-3.864077000	1.253176000	0.521304000
H	0.133238000	1.996401000	-0.799715000
H	-0.323639000	4.412093000	-0.811999000

H	-4.322834000	3.659993000	0.488394000
H	-2.558303000	5.260002000	-0.174105000
O	-0.280381000	-0.389113000	0.073558000
C	0.507042000	0.486898000	1.764859000
H	0.213373000	1.488947000	1.507859000
C	1.801688000	0.058738000	1.394678000
C	-0.213762000	-0.250424000	2.725445000
H	-1.168228000	0.123192000	3.059152000
C	0.271413000	-1.454172000	3.160696000
H	-0.291152000	-2.051555000	3.859350000
C	2.289323000	-1.157486000	1.832704000
H	3.254726000	-1.506842000	1.505934000
C	1.515650000	-1.908076000	2.701959000
H	1.893467000	-2.856325000	3.050606000
O	2.482034000	0.893981000	0.576936000
C	3.362652000	0.343634000	-0.344353000
C	5.106103000	-0.631906000	-2.234763000
C	4.653350000	0.831776000	-0.381949000
C	2.915971000	-0.616771000	-1.236035000
C	3.802226000	-1.104940000	-2.181038000
C	5.526895000	0.337636000	-1.339067000
H	4.953630000	1.587284000	0.325909000
H	1.890583000	-0.951537000	-1.181056000
H	3.468392000	-1.850750000	-2.885013000
H	6.537389000	0.712073000	-1.381347000
H	5.788363000	-1.013536000	-2.977440000

E (UM052X+HF-M052X) = -1115.331024

E (UM052X+HF-M052X) + ZPE = -1114.949672

One vibrational mode with imaginary frequency

TS for formation of biradical ³**16** (UB3lyp/cc-pVTZ)

H	1.063429000	2.378895000	0.522287000
C	2.081371000	2.558092000	0.211324000
C	4.695386000	3.007942000	-0.612867000
C	2.592166000	3.843012000	0.197762000
C	2.875062000	1.449735000	-0.173185000
C	4.194637000	1.719465000	-0.608518000
C	3.904455000	4.082958000	-0.205780000
H	1.964349000	4.668891000	0.507620000
H	4.813711000	0.910610000	-0.966779000
H	4.301719000	5.088871000	-0.213152000
H	5.708532000	3.182316000	-0.952088000
C	2.302995000	0.123106000	-0.168778000
C	3.071236000	-1.107402000	-0.260512000
C	4.503555000	-3.537206000	-0.447622000
C	4.321565000	-1.272871000	0.371644000
C	2.563433000	-2.207722000	-0.984801000
C	3.269780000	-3.395070000	-1.078589000
C	5.019626000	-2.465396000	0.278231000
H	4.725951000	-0.464296000	0.963705000
H	1.621307000	-2.096480000	-1.502522000
H	2.862011000	-4.214106000	-1.657469000
H	5.970455000	-2.565443000	0.785833000
H	5.052331000	-4.466343000	-0.518573000
O	0.966607000	0.090624000	-0.211226000
C	-4.755622000	0.227830000	0.298225000
C	-6.760144000	0.258737000	-1.609544000
C	-5.967197000	-0.388274000	0.574072000

C	-4.531592000	0.869528000	-0.913725000
C	-5.541207000	0.877330000	-1.867943000
C	-6.970923000	-0.369392000	-0.387646000
H	-6.112425000	-0.867099000	1.532088000
H	-3.584914000	1.357092000	-1.099637000
H	-5.374953000	1.375975000	-2.813168000
H	-7.918174000	-0.847790000	-0.178909000
H	-7.543042000	0.271800000	-2.355136000
C	0.064064000	-1.198637000	0.925490000
H	0.953057000	-1.799065000	1.034726000
C	-0.332593000	-0.369427000	2.020738000
H	0.405606000	-0.090014000	2.758923000
C	-0.956870000	-1.656467000	0.039224000
H	-0.701400000	-2.374263000	-0.726499000
C	-2.237487000	-1.167713000	0.119191000
C	-1.606847000	0.112276000	2.105134000
H	-1.913728000	0.773435000	2.903241000
C	-2.564611000	-0.258669000	1.136582000
H	-2.994165000	-1.491276000	-0.579413000
O	-3.804741000	0.266087000	1.312012000

E (UB+HF-LYP) = -1115.423078

E (UB+HF-LYP + ZPE = -1115.049048

One vibrational mode with imaginary frequency

TS for formation of biradical ³16 (UM05-2X/cc-pVTZ)

1	0.929363000	2.333701000	0.631183000
6	1.926664000	2.542195000	0.281005000
6	4.494169000	3.053265000	-0.629450000
6	2.418645000	3.831685000	0.286093000
6	2.721204000	1.469439000	-0.166538000
6	4.012164000	1.761333000	-0.644874000
6	3.706567000	4.099079000	-0.159627000
1	1.795852000	4.637008000	0.644477000
1	4.619041000	0.968988000	-1.051216000
1	4.089066000	5.107182000	-0.151436000
1	5.487070000	3.253173000	-1.002046000
6	2.174349000	0.137774000	-0.169728000
6	2.962151000	-1.067023000	-0.292515000
6	4.437565000	-3.443922000	-0.545766000
6	4.231655000	-1.196488000	0.292510000
6	2.451063000	-2.167422000	-1.000533000
6	3.180607000	-3.333142000	-1.126411000
6	4.953828000	-2.367018000	0.164024000
1	4.629845000	-0.378747000	0.871863000
1	1.487329000	-2.070411000	-1.474680000
1	2.773402000	-4.158740000	-1.689976000
1	5.923058000	-2.446296000	0.632007000
1	5.004555000	-4.355880000	-0.642522000
8	0.843093000	0.082090000	-0.192992000
6	-4.585885000	0.266885000	0.297183000
6	-6.445805000	0.297278000	-1.732443000
6	-5.804371000	-0.352086000	0.491712000
6	-4.277727000	0.908657000	-0.889648000
6	-5.216572000	0.916728000	-1.907217000
6	-6.738326000	-0.331930000	-0.533166000
1	-6.006515000	-0.833088000	1.434978000
1	-3.317217000	1.386405000	-1.004493000
1	-4.988122000	1.413087000	-2.836856000

1	-7.694351000	-0.810511000	-0.391700000
1	-7.173746000	0.310105000	-2.527600000
6	0.054608000	-1.409297000	1.044177000
1	0.984920000	-1.948059000	1.067457000
6	-0.281289000	-0.550925000	2.113771000
1	0.472022000	-0.297655000	2.842099000
6	-0.955775000	-1.803916000	0.147110000
1	-0.726778000	-2.526850000	-0.618714000
6	-2.207897000	-1.243048000	0.206257000
6	-1.524542000	0.008019000	2.183205000
1	-1.800382000	0.700642000	2.961432000
6	-2.482058000	-0.315769000	1.211385000
1	-2.971387000	-1.514340000	-0.503001000
8	-3.686466000	0.288934000	1.353697000

E (UM052X+HF-M052X) = -1115.328813

E (UM052X+HF-M052X) + ZPE = -1114.947663

One vibrational mode with imaginary frequency

Diphenyl ether **9** (B3LYP/cc-pVTZ)

O	0.000000000	0.000000000	1.171921000
C	0.000000000	1.201501000	0.495209000
C	-0.735419000	2.237679000	1.060328000
C	0.759420000	1.417448000	-0.651302000
C	-0.712837000	3.495548000	0.472074000
H	-1.310191000	2.043983000	1.955086000
C	0.767328000	2.678954000	-1.233944000
H	1.338320000	0.610651000	-1.077223000
C	0.033866000	3.721664000	-0.678866000
H	-1.285626000	4.299792000	0.914294000
H	1.359143000	2.846691000	-2.124049000
H	0.047237000	4.701047000	-1.136783000
C	0.000000000	-1.201501000	0.495209000
C	-0.759420000	-1.417448000	-0.651302000
C	0.735419000	-2.237679000	1.060328000
C	-0.767328000	-2.678954000	-1.233944000
H	-1.338320000	-0.610651000	-1.077223000
C	0.712837000	-3.495548000	0.472074000
H	1.310191000	-2.043983000	1.955086000
C	-0.033866000	-3.721664000	-0.678866000
H	-1.359143000	-2.846691000	-2.124049000
H	1.285626000	-4.299792000	0.914294000
H	-0.047237000	-4.701047000	-1.136783000

E (RB+HF-LYP) = -538.7033531

E (RB+HF-LYP) + ZPE = -538.518445

No vibrational mode with imaginary frequency

Diphenyl ether **9** (M05-2X/cc-pVTZ)

O	0.000000000	0.000000000	1.227975000
C	0.000000000	1.186713000	0.529897000
C	-0.757922000	2.223020000	1.047009000
C	0.775613000	1.369515000	-0.604491000
C	-0.741511000	3.457267000	0.418327000
H	-1.343022000	2.046017000	1.934997000
C	0.776978000	2.606430000	-1.227752000
H	1.366794000	0.553246000	-0.987627000

C	0.020776000	3.653195000	-0.722496000
H	-1.331070000	4.265959000	0.820751000
H	1.379211000	2.752780000	-2.110738000
H	0.028740000	4.613496000	-1.212246000
C	0.000000000	-1.186713000	0.529897000
C	-0.775613000	-1.369515000	-0.604491000
C	0.757922000	-2.223020000	1.047009000
C	-0.776978000	-2.606430000	-1.227752000
H	-1.366794000	-0.553246000	-0.987627000
C	0.741511000	-3.457267000	0.418327000
H	1.343022000	-2.046017000	1.934997000
C	-0.020776000	-3.653195000	-0.722496000
H	-1.379211000	-2.752780000	-2.110738000
H	1.331070000	-4.265959000	0.820751000
H	-0.028740000	-4.613496000	-1.212246000

E (M052X+HF-M052X) = -538.659057

E (M052X+HF-M052X) + ZPE = -538.470562

No vibrational mode with imaginary frequency

Diphenylphenoxymethyl **12** (UB3LYP/cc-pVTZ)

H	1.121462000	-2.571195000	-0.183047000
C	1.993210000	-1.940445000	-0.097135000
C	4.246735000	-0.327753000	0.097812000
C	1.835806000	-0.536290000	-0.174508000
C	3.238882000	-2.509790000	0.091432000
C	4.375917000	-1.711507000	0.197706000
C	3.005965000	0.253930000	-0.088647000
H	3.327088000	-3.586388000	0.156343000
H	5.348640000	-2.160852000	0.343914000
H	2.937637000	1.324578000	-0.206314000
H	5.125418000	0.301701000	0.150378000
C	0.532758000	0.027726000	-0.378442000
C	0.127808000	1.406255000	-0.214122000
C	-0.717433000	4.078942000	0.085979000
C	-0.910826000	1.938470000	-1.006339000
C	0.713045000	2.253927000	0.749109000
C	0.296084000	3.566805000	0.891410000
C	-1.318384000	3.252806000	-0.860039000
H	-1.378438000	1.312081000	-1.751516000
H	1.473274000	1.864720000	1.409994000
H	0.755580000	4.192004000	1.645692000
H	-2.108807000	3.638478000	-1.490325000
H	-1.040087000	5.104828000	0.199999000
O	-0.385683000	-0.842461000	-0.931542000
C	-1.585202000	-1.119070000	-0.305417000
C	-4.026094000	-1.833972000	0.816928000
C	-2.577290000	-1.678333000	-1.105514000
C	-1.801463000	-0.919062000	1.053474000
C	-3.026563000	-1.277417000	1.605084000
C	-3.793126000	-2.034678000	-0.540130000
H	-2.378965000	-1.829609000	-2.157530000
H	-1.024493000	-0.492298000	1.670391000
H	-3.194277000	-1.121523000	2.662528000
H	-4.562134000	-2.469854000	-1.164447000
H	-4.975395000	-2.110254000	1.254442000

E (UB+HF-LYP) = -808.521445

E (UB+HF-LYP + ZPE = -808.239949

No vibrational mode with imaginary frequency

Diphenylphenoxymethyl **12** (UM05-2X/cc-pVTZ)

H	1.205065000	-2.520222000	-0.165004000
C	2.052445000	-1.859146000	-0.088309000
C	4.232223000	-0.154951000	0.084468000
C	1.851187000	-0.473357000	-0.216065000
C	3.312950000	-2.369829000	0.142745000
C	4.410320000	-1.523796000	0.238836000
C	2.975916000	0.367602000	-0.143737000
H	3.443949000	-3.435405000	0.249753000
H	5.394128000	-1.927079000	0.418050000
H	2.859158000	1.425818000	-0.307938000
H	5.082932000	0.507318000	0.126711000
C	0.533803000	0.030868000	-0.452113000
C	0.064528000	1.376597000	-0.251579000
C	-0.919085000	3.969843000	0.141658000
C	-1.021594000	1.856746000	-0.998923000
C	0.626607000	2.221400000	0.717457000
C	0.141217000	3.500661000	0.904966000
C	-1.498969000	3.137494000	-0.805962000
H	-1.472658000	1.217792000	-1.740623000
H	1.422131000	1.853541000	1.344557000
H	0.582208000	4.131111000	1.661264000
H	-2.328089000	3.490746000	-1.398791000
H	-1.296176000	4.968895000	0.291261000
O	-0.344768000	-0.867833000	-1.005714000
C	-1.515266000	-1.166246000	-0.339799000
C	-3.892600000	-1.887337000	0.874029000
C	-2.535562000	-1.709932000	-1.103083000
C	-1.664123000	-0.983505000	1.024666000
C	-2.861002000	-1.345719000	1.623206000
C	-3.722464000	-2.070575000	-0.490471000
H	-2.379059000	-1.843750000	-2.161600000
H	-0.857867000	-0.564599000	1.605309000
H	-2.982813000	-1.202713000	2.685486000
H	-4.518189000	-2.494151000	-1.082914000
H	-4.819760000	-2.165544000	1.348246000

E (UM052X+HF-M052X) = -808.4617829

E (UM052X+HF-M052X) + ZPE = -808.174908

No vibrational mode with imaginary frequency

Phenoxy **13** (UB3LYP/cc-pVTZ)

C	0.000000000	0.000000000	-1.777730000
C	0.000000000	1.220667000	-1.082911000
C	0.000000000	1.235525000	0.288148000
C	0.000000000	0.000000000	1.044925000
C	0.000000000	-1.235525000	0.288148000
C	0.000000000	-1.220667000	-1.082911000
H	0.000000000	0.000000000	-2.859271000
H	0.000000000	2.148816000	-1.638805000
H	0.000000000	2.157421000	0.853204000
H	0.000000000	-2.157421000	0.853204000
H	0.000000000	-2.148816000	-1.638805000
O	0.000000000	0.000000000	2.295558000

E (UB+HF-LYP) = -306.9391297

E (UB+HF-LYP + ZPE = -306.847708
No vibrational mode with imaginary frequency

Phenoxy **13** (UM05-2X/cc-pVTZ)

C	0.000000000	0.000000000	-1.769153000
C	0.000000000	1.219145000	-1.077929000
C	0.000000000	1.233723000	0.287765000
C	0.000000000	0.000000000	1.039579000
C	0.000000000	-1.233723000	0.287765000
C	0.000000000	-1.219145000	-1.077929000
H	0.000000000	0.000000000	-2.847046000
H	0.000000000	2.144050000	-1.632647000
H	0.000000000	2.149959000	0.855500000
H	0.000000000	-2.149959000	0.855500000
H	0.000000000	-2.144050000	-1.632647000
O	0.000000000	0.000000000	2.282595000

E (UM052X+HF-M052X) = -306.9028071
E (UM052X+HF-M052X) + ZPE = -306.809771
No vibrational mode with imaginary frequency