Supporting Information

Mechanistic insights of degradation of O-Anisidine carcinogenic pollutant initiated by OH radial attack: Theoretical investigations

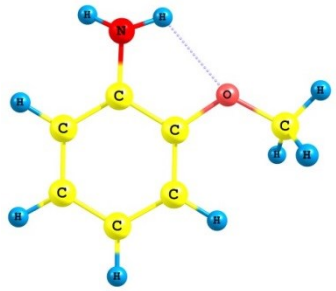
Mohamed A. Abdel-Rahman[1], Mohamed F. Shibl[2,**], Safwat Abdel-Azeim[3], Safinaz H. El-demerdash[1], Nessreen Al-Hashimi[2], and Ahmed M. El-Nahas[1,*]

[1]Chemistry Department, Faculty of Science, Menoufia University, Shebin El-Kom, Egypt

[2]Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University, P.O. Box 2713, Doha, Qatar

[3]Center for Integrative Petroleum Research (CIPR), College of Petroleum Engineering and Geosciences, King Fahd University of Petroleum and Minerals (KFUPM), Dhahran 31261, Saudi Arabia

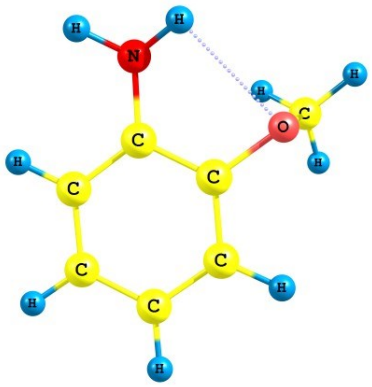
Table S1. Optimized structures of reactants, products, and transition states at M06-2X/6-311++G(2df,2p) and electronic energies at ROCBS-QB3.



O-AND (trans form)

6	1.333947000	-1.688116000	0.004515000
6	-0.027647000	-1.387770000	-0.000011000
6	2.262801000	-0.665106000	0.005905000
1	-0.750681000	-2.189873000	0.003347000
1	3.320806000	-0.887426000	0.011167000
6	-0.446660000	-0.069542000	-0.005372000
6	1.840562000	0.659521000	-0.001525000
1	2.565352000	1.464254000	-0.009776000
6	0.490196000	0.978673000	-0.009241000
1	1.652723000	-2.720725000	0.008300000
6	-2.741620000	-0.665370000	0.003255000
1	-3.697346000	-0.149558000	0.005558000
1	-2.670389000	-1.292732000	-0.888364000
1	-2.666153000	-1.294414000	0.893590000
7	0.033929000	2.289207000	-0.074850000
1	0.660104000	2.983022000	0.297811000
1	-0.923018000	2.415657000	0.212325000
8	-1.749797000	0.334201000	0.000605000

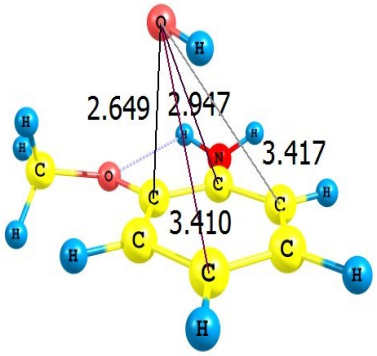
Zero-point correction= 0.151105 (Hartree/Particle)
Thermal correction to Energy= 0.159218
Thermal correction to Enthalpy= 0.160162
Thermal correction to Gibbs Free Energy= 0.118760
Sum of electronic and zero-point Energies= -401.943619
Sum of electronic and thermal Energies= -401.935505
Sum of electronic and thermal Enthalpies= -401.934561
Sum of electronic and thermal Free Energies= -401.975963
Electronic energy at ROCBS-QB3= -401.577273



O-AND (gauche form)

6	1.844477000	-1.282227000	0.011319000
6	0.488411000	-1.447800000	-0.240865000
6	2.342368000	-0.004901000	0.224464000
1	0.063120000	-2.426689000	-0.421632000
1	3.396061000	0.140557000	0.420043000
6	-0.352230000	-0.351446000	-0.276299000
6	1.501001000	1.097004000	0.183668000
1	1.896826000	2.091820000	0.347562000
6	0.140158000	0.942065000	-0.069346000
1	2.501684000	-2.139576000	0.035280000
6	-2.480447000	-0.676308000	0.619400000
1	-3.517108000	-0.738664000	0.297696000
1	-2.200429000	-1.598597000	1.133045000
1	-2.354680000	0.167568000	1.302216000
7	-0.747983000	2.013639000	-0.075883000
1	-0.330625000	2.908984000	-0.271292000
1	-1.578315000	1.843575000	-0.623499000
8	-1.692884000	-0.500347000	-0.550286000

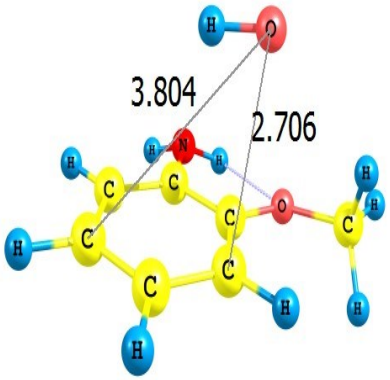
Zero-point correction= 0.150923 (Hartree/Particle)
Thermal correction to Energy= 0.159162
Thermal correction to Enthalpy= 0.160106
Thermal correction to Gibbs Free Energy= 0.118214
Sum of electronic and zero-point Energies= -401.940781
Sum of electronic and thermal Energies= -401.932542
Sum of electronic and thermal Enthalpies= -401.931598
Sum of electronic and thermal Free Energies= -401.973491
Electronic energy at ROCBS-QB3= -401.574688



IMx

6	1.369851000	-1.637217000	-0.389840000
6	0.014059000	-1.331530000	-0.480211000
6	2.293254000	-0.618617000	-0.220166000
1	-0.708023000	-2.126059000	-0.594433000
1	3.347721000	-0.845677000	-0.145824000
6	-0.411406000	-0.014035000	-0.395247000
6	1.871309000	0.703968000	-0.148116000
1	2.593078000	1.500389000	-0.017188000
6	0.523930000	1.029648000	-0.235965000
1	1.691791000	-2.666838000	-0.450343000
7	0.066306000	2.333000000	-0.202230000
1	0.663950000	2.990429000	0.269777000
1	-0.907776000	2.426684000	0.038383000
8	-0.363456000	-0.327285000	2.233331000
1	0.525159000	-0.665390000	2.029639000
8	-1.706469000	0.386761000	-0.449713000
6	-2.697939000	-0.610054000	-0.318926000
1	-2.703282000	-1.276516000	-1.183972000
1	-2.536474000	-1.187191000	0.594290000
1	-3.649238000	-0.089612000	-0.262835000

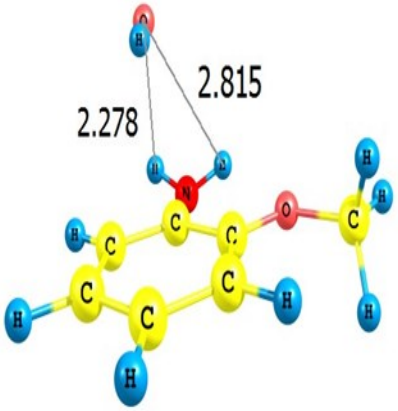
Zero-point correction= 0.162226 (Hartree/Particle)
Thermal correction to Energy= 0.173314
Thermal correction to Enthalpy= 0.174258
Thermal correction to Gibbs Free Energy= 0.124938
Sum of electronic and zero-point Energies= -477.673495
Sum of electronic and thermal Energies= -477.662408
Sum of electronic and thermal Enthalpies= -477.661464
Sum of electronic and thermal Free Energies= -477.710784
Electronic energy at ROCBS-QB3= -477.245274



IMy

6	0.026530000	-1.163646000	-0.654759000
6	-1.306122000	-1.575643000	-0.608681000
6	0.361292000	0.149020000	-0.357181000
1	-1.553900000	-2.601710000	-0.839536000
6	-2.290844000	-0.673039000	-0.258547000
6	-0.639202000	1.076996000	-0.001885000
6	-1.956116000	0.645141000	0.045157000
1	0.797400000	-1.872868000	-0.915123000
8	0.746556000	-1.271274000	1.951822000
1	-0.183330000	-0.994579000	2.006441000
7	-0.263180000	2.363578000	0.349247000
1	-0.964150000	3.074623000	0.226958000
1	0.656049000	2.636647000	0.042630000
1	-3.325723000	-0.983159000	-0.216076000
1	-2.726538000	1.350893000	0.330010000
8	1.618998000	0.655386000	-0.378528000
6	2.688374000	-0.258252000	-0.506807000
1	3.599915000	0.323456000	-0.407774000
1	2.640021000	-1.010696000	0.282775000
1	2.674614000	-0.744009000	-1.485165000

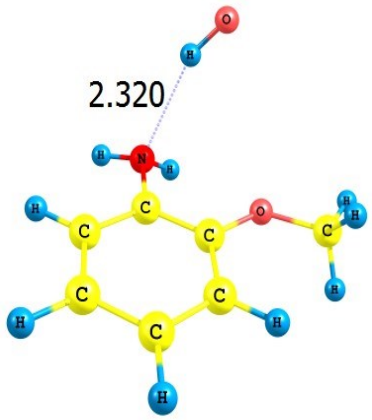
Zero-point correction= 0.161614 (Hartree/Particle)
Thermal correction to Energy= 0.172983
Thermal correction to Enthalpy= 0.173927
Thermal correction to Gibbs Free Energy= 0.123513
Sum of electronic and zero-point Energies= -477.673231
Sum of electronic and thermal Energies= -477.661863
Sum of electronic and thermal Enthalpies= -477.660918
Sum of electronic and thermal Free Energies= -477.711332
Electronic energy at ROCBS-QB3= -477.244602



IMz

6	-0.287425000	2.322377000	0.336243000
6	-1.159822000	1.234439000	0.303149000
6	1.026356000	2.163447000	-0.060441000
1	-2.184167000	1.361964000	0.620008000
1	1.710046000	3.000252000	-0.034985000
6	-0.713666000	-0.000765000	-0.130647000
6	1.477854000	0.921662000	-0.496611000
1	2.505433000	0.791454000	-0.813072000
6	0.621022000	-0.171187000	-0.546236000
1	-0.646667000	3.283011000	0.676096000
7	1.026769000	-1.411266000	-1.006071000
1	2.016441000	-1.597689000	-1.006825000
1	0.449635000	-2.192543000	-0.740626000
8	2.422699000	-1.789154000	1.226164000
1	1.973117000	-0.938781000	1.370084000
8	-1.472398000	-1.129153000	-0.193322000
6	-2.816909000	-1.036056000	0.218727000
1	-3.367915000	-0.324764000	-0.400310000
1	-3.243492000	-2.027013000	0.098134000
1	-2.886683000	-0.734080000	1.266156000

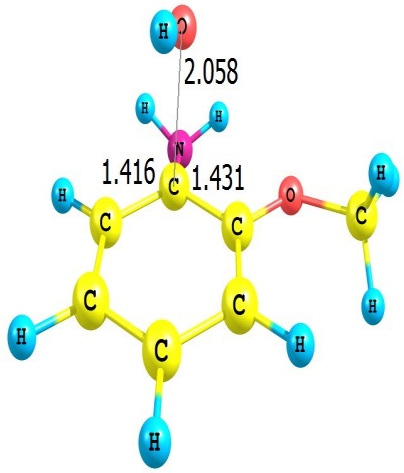
Zero-point correction= 0.162121 (Hartree/Particle)
Thermal correction to Energy= 0.173313
Thermal correction to Enthalpy= 0.174258
Thermal correction to Gibbs Free Energy= 0.123501
Sum of electronic and zero-point Energies= -477.671449
Sum of electronic and thermal Energies= -477.660257
Sum of electronic and thermal Enthalpies= -477.659313
Sum of electronic and thermal Free Energies= -477.710069
Electronic energy at ROCBS-QB3= -477.243318



IMt

6	2.041673000	1.301112000	0.363649000
6	0.694905000	1.467109000	0.047108000
6	2.611745000	0.042352000	0.329425000
1	0.250851000	2.451082000	0.077526000
1	3.655839000	-0.091337000	0.574453000
6	-0.069951000	0.368820000	-0.302314000
6	1.839577000	-1.061330000	-0.018545000
1	2.278177000	-2.051454000	-0.036631000
6	0.499697000	-0.912850000	-0.332542000
1	2.633980000	2.162871000	0.636323000
7	-0.347927000	-2.002440000	-0.597650000
1	0.144353000	-2.847157000	-0.845600000
1	-1.072153000	-1.786114000	-1.269259000
8	-2.342226000	-0.974816000	1.415207000
1	-1.708194000	-1.557605000	0.951709000
8	-1.387869000	0.406189000	-0.638273000
6	-2.112444000	1.576935000	-0.319731000
1	-1.988388000	1.824492000	0.735816000
1	-1.793932000	2.417043000	-0.940137000
1	-3.155497000	1.351390000	-0.518424000

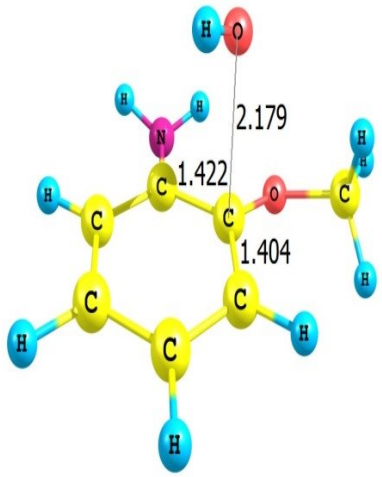
Zero-point correction= 0.163020 (Hartree/Particle)
Thermal correction to Energy= 0.173726
Thermal correction to Enthalpy= 0.174670
Thermal correction to Gibbs Free Energy= 0.126084
Sum of electronic and zero-point Energies= -477.673413
Sum of electronic and thermal Energies= -477.662707
Sum of electronic and thermal Enthalpies= -477.661763
Sum of electronic and thermal Free Energies= -477.710348
Electronic energy at ROCBS-QB3= -477.246685



TS1

6	0.520275000	-0.197088000	-0.217849000
6	0.158999000	-1.521439000	-0.035555000
6	-0.480364000	0.818763000	-0.335129000
1	0.916344000	-2.280773000	0.085262000
6	-1.185366000	-1.875633000	-0.012533000
6	-1.835074000	0.408211000	-0.367219000
1	-1.457440000	-2.912174000	0.127975000
6	-2.179186000	-0.909743000	-0.183454000
1	-3.220427000	-1.198773000	-0.178330000
1	-2.591389000	1.168360000	-0.511295000
7	-0.104305000	2.070265000	-0.772661000
1	-0.768759000	2.787039000	-0.521618000
1	0.827319000	2.318650000	-0.471678000
8	-0.335739000	1.143055000	1.691752000
1	-0.798976000	0.394798000	2.091317000
8	1.779142000	0.259219000	-0.291988000
6	2.827490000	-0.631831000	0.028745000
1	2.691038000	-1.035654000	1.033272000
1	2.881454000	-1.448002000	-0.693924000
1	3.743104000	-0.050955000	-0.012505000

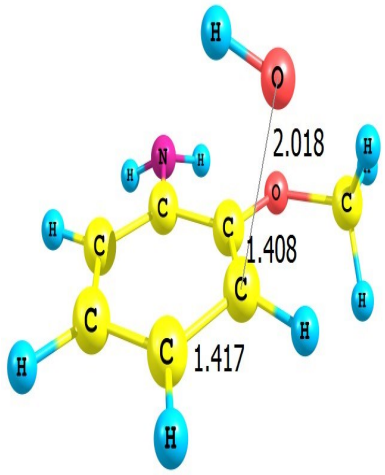
Zero-point correction= 0.162610 (Hartree/Particle)
Thermal correction to Energy= 0.172755
Thermal correction to Enthalpy= 0.173699
Thermal correction to Gibbs Free Energy= 0.127004
Sum of electronic and zero-point Energies= -477.667508
Sum of electronic and thermal Energies= -477.657363
Sum of electronic and thermal Enthalpies= -477.656418
Sum of electronic and thermal Free Energies= -477.703114
Electronic energy at ROCBS-QB3= -477.245642



TS2

6	-0.084569000	-1.421612000	-0.289003000
6	-1.433633000	-1.678616000	-0.168764000
6	0.385448000	-0.098330000	-0.291351000
1	-1.786068000	-2.699506000	-0.139981000
6	-2.341387000	-0.619065000	-0.089676000
6	-0.541093000	0.979776000	-0.245586000
1	-3.399407000	-0.822446000	0.000758000
6	-1.901755000	0.689271000	-0.132326000
1	-2.606857000	1.508907000	-0.083397000
8	0.618610000	0.141302000	1.862022000
1	-0.179039000	-0.297741000	2.188212000
7	-0.061212000	2.253113000	-0.349592000
1	0.921252000	2.356736000	-0.149439000
1	-0.646843000	2.987415000	0.010043000
8	1.657332000	0.258385000	-0.559161000
6	2.666552000	-0.689646000	-0.263057000
1	2.531182000	-1.065276000	0.751362000
1	2.653927000	-1.511161000	-0.981782000
1	3.612094000	-0.162198000	-0.343622000
1	0.623333000	-2.234688000	-0.349328000

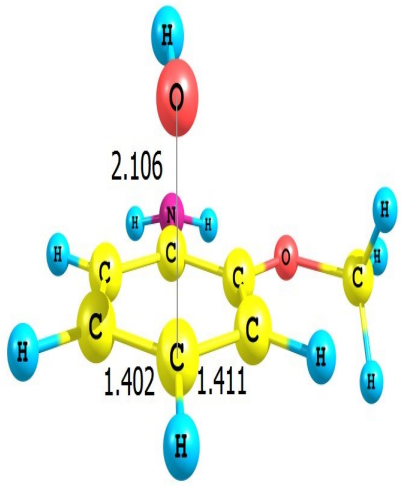
Zero-point correction= 0.162471 (Hartree/Particle)
Thermal correction to Energy= 0.172585
Thermal correction to Enthalpy= 0.173529
Thermal correction to Gibbs Free Energy= 0.127234
Sum of electronic and zero-point Energies= -477.671374
Sum of electronic and thermal Energies= -477.661261
Sum of electronic and thermal Enthalpies= -477.660317
Sum of electronic and thermal Free Energies= -477.706612
Electronic energy at ROCBS-QB3= -477.246358



TS3

6	-1.999788000	0.588798000	0.035241000
6	-0.718209000	1.105895000	0.064047000
6	-2.235376000	-0.759857000	-0.278448000
6	0.358390000	0.244046000	-0.227900000
6	-1.191996000	-1.603042000	-0.548682000
6	0.139787000	-1.125385000	-0.469276000
1	0.935884000	-1.726678000	-0.876623000
1	-1.358336000	-2.642648000	-0.788700000
8	0.794549000	-1.720684000	1.344453000
1	0.010207000	-1.451090000	1.841792000
1	-3.252819000	-1.123829000	-0.307700000
1	-2.831648000	1.243857000	0.261585000
8	1.572109000	0.818725000	-0.204921000
6	2.710247000	0.000229000	-0.425670000
1	3.571928000	0.645417000	-0.287648000
1	2.727952000	-0.817544000	0.292651000
1	2.709658000	-0.389204000	-1.445619000
7	-0.444381000	2.420467000	0.417318000
1	0.467374000	2.749319000	0.143672000
1	-1.181131000	3.080697000	0.233244000

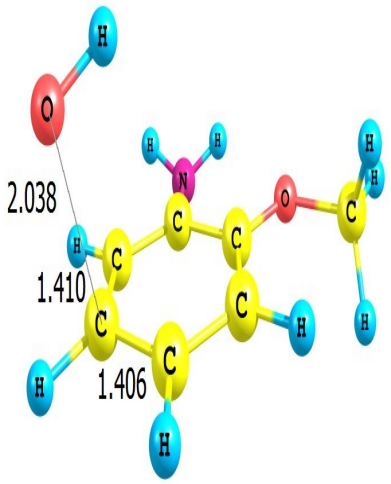
Zero-point correction= 0.162978 (Hartree/Particle)
Thermal correction to Energy= 0.173055
Thermal correction to Enthalpy= 0.174000
Thermal correction to Gibbs Free Energy= 0.127671
Sum of electronic and zero-point Energies= -477.665716
Sum of electronic and thermal Energies= -477.655639
Sum of electronic and thermal Enthalpies= -477.654695
Sum of electronic and thermal Free Energies= -477.701023
Electronic energy at ROCBS-QB3= -477.243482



TS4

6	0.277243000	1.257831000	0.034996000
6	0.694683000	-0.085893000	-0.134887000
6	-1.060467000	1.580830000	-0.195949000
6	-0.203219000	-1.053370000	-0.508003000
6	-1.965725000	0.608669000	-0.571465000
1	0.109080000	-2.078810000	-0.632084000
6	-1.565200000	-0.730063000	-0.685795000
1	-2.227874000	-1.458007000	-1.123517000
1	-3.000192000	0.868540000	-0.742515000
8	-2.410362000	-1.408050000	1.119977000
1	-1.961921000	-0.756528000	1.676503000
1	-1.377649000	2.608353000	-0.071395000
7	1.195611000	2.182149000	0.457674000
1	2.165816000	1.925798000	0.392071000
1	0.980747000	3.154818000	0.328483000
8	2.021097000	-0.287544000	0.097923000
6	2.508152000	-1.604772000	-0.035284000
1	2.001790000	-2.279115000	0.658179000
1	2.375481000	-1.969084000	-1.056271000
1	3.566762000	-1.565637000	0.201955000

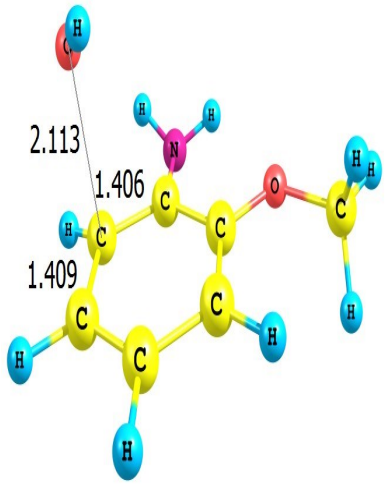
Zero-point correction= 0.162471 (Hartree/Particle)
Thermal correction to Energy= 0.172778
Thermal correction to Enthalpy= 0.173722
Thermal correction to Gibbs Free Energy= 0.126417
Sum of electronic and zero-point Energies= -477.666309
Sum of electronic and thermal Energies= -477.656002
Sum of electronic and thermal Enthalpies= -477.655057
Sum of electronic and thermal Free Energies= -477.702362
Electronic energy at ROCBS-QB3= -477.242265



TS5

6	0.794586000	-0.083668000	-0.097650000
6	0.169465000	-1.300237000	-0.337379000
6	0.065472000	1.131969000	-0.151622000
1	0.734365000	-2.219427000	-0.304722000
6	-1.186451000	-1.336472000	-0.619693000
6	-1.280715000	1.079635000	-0.430534000
1	-1.678313000	-2.280457000	-0.799973000
6	-1.943234000	-0.151576000	-0.611063000
1	-2.946969000	-0.155670000	-1.004136000
1	-1.847731000	2.000011000	-0.477727000
7	0.753890000	2.323493000	0.021044000
1	0.199147000	3.102105000	0.334682000
1	1.640070000	2.240975000	0.491660000
8	-2.843128000	-0.525792000	1.178510000
1	-2.036724000	-0.553326000	1.711293000
8	2.106698000	0.063356000	0.199548000
6	2.908758000	-1.097266000	0.256712000
1	2.551751000	-1.780782000	1.029441000
1	2.919639000	-1.610173000	-0.706623000
1	3.911683000	-0.762528000	0.501703000

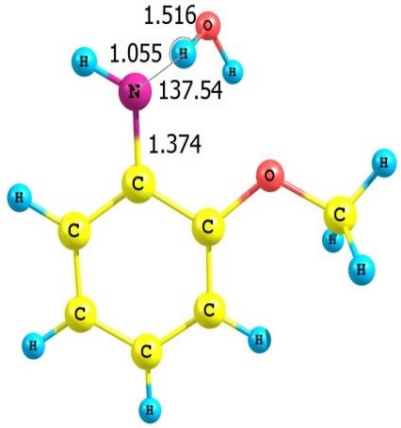
Zero-point correction= 0.162528 (Hartree/Particle)
Thermal correction to Energy= 0.172826
Thermal correction to Enthalpy= 0.173770
Thermal correction to Gibbs Free Energy= 0.126474
Sum of electronic and zero-point Energies= -477.663061
Sum of electronic and thermal Energies= -477.652763
Sum of electronic and thermal Enthalpies= -477.651819
Sum of electronic and thermal Free Energies= -477.699115
Electronic energy at ROCBS-QB3= -477.240588



TS6

6	-0.635109000	1.432878000	0.063183000
6	0.618844000	2.053249000	-0.093215000
6	-0.763432000	0.073588000	-0.109760000
1	0.695485000	3.123391000	0.035648000
6	1.723076000	1.309296000	-0.417148000
6	0.363306000	-0.713211000	-0.435554000
1	2.687543000	1.777659000	-0.550082000
6	1.617459000	-0.088501000	-0.555985000
1	2.438056000	-0.655187000	-0.967958000
8	2.290844000	-0.905392000	1.273208000
1	1.926490000	-0.212512000	1.840928000
7	0.221908000	-2.058401000	-0.621073000
1	-0.638635000	-2.455996000	-0.280548000
1	1.045314000	-2.602521000	-0.415628000
8	-1.920104000	-0.632369000	0.018745000
6	-3.088216000	0.087160000	0.341303000
1	-2.986675000	0.586772000	1.307355000
1	-3.315315000	0.828917000	-0.427534000
1	-3.892563000	-0.640078000	0.392119000
1	-1.494545000	2.033697000	0.320638000

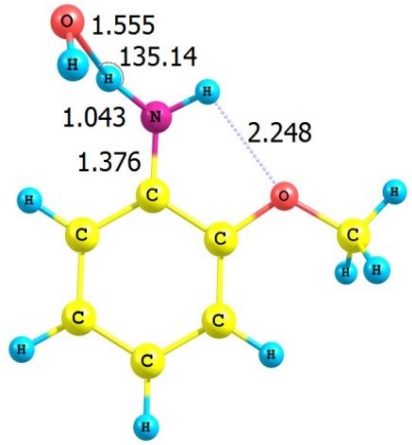
Zero-point correction= 0.162735 (Hartree/Particle)
Thermal correction to Energy= 0.172972
Thermal correction to Enthalpy= 0.173916
Thermal correction to Gibbs Free Energy= 0.126724
Sum of electronic and zero-point Energies= -477.669094
Sum of electronic and thermal Energies= -477.658857
Sum of electronic and thermal Enthalpies= -477.657912
Sum of electronic and thermal Free Energies= -477.705105
Electronic energy at ROCBS-QB3= -477.244963



TS7

6	-2.413725000	0.692611000	0.325746000
6	-2.555808000	-0.678550000	0.185017000
6	-1.163936000	1.287748000	0.174242000
1	-3.524245000	-1.142072000	0.309323000
1	-1.062399000	2.355724000	0.295866000
6	-1.450832000	-1.459908000	-0.110069000
6	-0.059017000	0.510369000	-0.129854000
6	-0.192982000	-0.885253000	-0.290248000
1	-3.269824000	1.308988000	0.561101000
7	0.899450000	-1.626072000	-0.671594000
1	1.868911000	-1.299618000	-0.414188000
1	0.798407000	-2.622653000	-0.540097000
8	2.799725000	-1.390736000	0.778808000
1	2.526984000	-0.578167000	1.228153000
8	1.204024000	0.977649000	-0.274188000
6	1.410562000	2.370184000	-0.172334000
1	0.839855000	2.904858000	-0.934400000
1	1.129564000	2.738165000	0.816922000
1	2.472058000	2.531290000	-0.332998000
1	-1.551012000	-2.532526000	-0.220477000

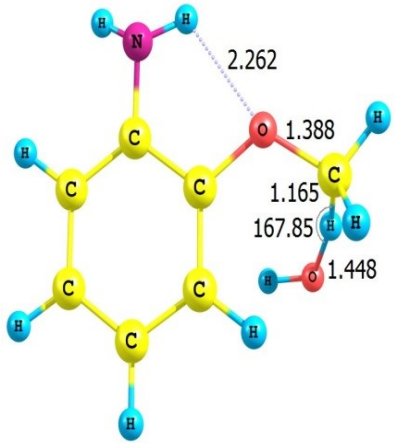
Zero-point correction= 0.159753 (Hartree/Particle)
Thermal correction to Energy= 0.170087
Thermal correction to Enthalpy= 0.171031
Thermal correction to Gibbs Free Energy= 0.123234
Sum of electronic and zero-point Energies= -477.667911
Sum of electronic and thermal Energies= -477.657577
Sum of electronic and thermal Enthalpies= -477.656633
Sum of electronic and thermal Free Energies= -477.704431
Electronic energy at ROCBS-QB3= -477.237833



TS8

6	-0.998155000	2.188242000	0.257446000
6	-1.549822000	0.909358000	0.238867000
6	0.341997000	2.376911000	-0.040464000
1	-2.594269000	0.774282000	0.476197000
1	0.769318000	3.369333000	-0.021666000
6	-0.756053000	-0.180285000	-0.076466000
6	1.137868000	1.290230000	-0.366043000
1	2.186394000	1.418354000	-0.602059000
6	0.606332000	0.002310000	-0.390926000
1	-1.625260000	3.031861000	0.509136000
6	-2.536582000	-1.725333000	0.177798000
1	-3.193215000	-1.211819000	-0.527661000
1	-2.671148000	-2.798462000	0.083088000
1	-2.782040000	-1.415204000	1.195781000
7	1.375421000	-1.081335000	-0.749150000
1	2.395829000	-1.027703000	-0.539933000
1	0.963079000	-1.982358000	-0.553477000
8	3.266834000	-1.162437000	0.740931000
1	2.763267000	-0.709686000	1.431722000
8	-1.181009000	-1.468545000	-0.116975000

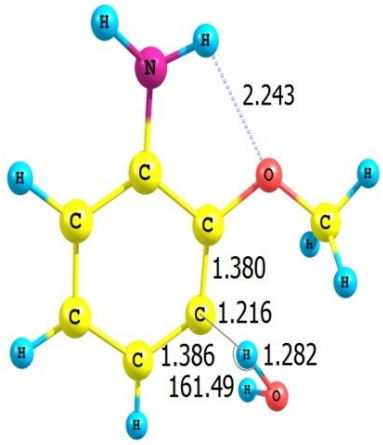
Zero-point correction= 0.159917 (Hartree/Particle)
Thermal correction to Energy= 0.170464
Thermal correction to Enthalpy= 0.171408
Thermal correction to Gibbs Free Energy= 0.122689
Sum of electronic and zero-point Energies= -477.669597
Sum of electronic and thermal Energies= -477.659050
Sum of electronic and thermal Enthalpies= -477.658105
Sum of electronic and thermal Free Energies= -477.706825
Electronic energy at ROCBS-QB3= -477.24019



TS9

6	0.987176000	1.909325000	0.375153000
6	-0.134149000	1.099113000	0.538697000
6	2.182438000	1.350189000	-0.039359000
1	-1.069095000	1.536798000	0.857469000
1	3.057213000	1.971555000	-0.171209000
6	-0.046911000	-0.259995000	0.284968000
6	2.268817000	-0.013767000	-0.288430000
1	3.206504000	-0.451932000	-0.606900000
6	1.164356000	-0.840727000	-0.131064000
1	0.913358000	2.968709000	0.573471000
6	-2.342520000	-0.633963000	0.706634000
1	-2.701514000	0.095027000	-0.127519000
1	-3.039189000	-1.466179000	0.727434000
1	-2.351848000	-0.073671000	1.643161000
7	1.228808000	-2.211726000	-0.317166000
1	1.957823000	-2.535661000	-0.929929000
1	0.342568000	-2.667479000	-0.461538000
8	-2.848024000	1.042197000	-1.212951000
1	-1.906598000	1.202596000	-1.388888000
8	-1.087741000	-1.137038000	0.391079000

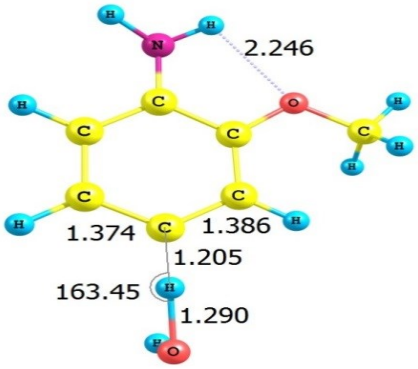
Zero-point correction= 0.158330 (Hartree/Particle)
Thermal correction to Energy= 0.168395
Thermal correction to Enthalpy= 0.169339
Thermal correction to Gibbs Free Energy= 0.122279
Sum of electronic and zero-point Energies= -477.665511
Sum of electronic and thermal Energies= -477.655447
Sum of electronic and thermal Enthalpies= -477.654502
Sum of electronic and thermal Free Energies= -477.701562
Electronic energy at ROCBS-QB3= -477.23484



TS10

6	-0.008122000	1.965700000	-0.093342000
6	0.623692000	0.732165000	-0.081054000
6	-1.391594000	1.996720000	-0.048030000
1	1.838100000	0.761285000	-0.143820000
1	-1.913642000	2.943192000	-0.065850000
6	-0.065602000	-0.461549000	-0.010149000
6	-2.113011000	0.811036000	0.022313000
6	-1.474760000	-0.421595000	0.041733000
1	0.573999000	2.874339000	-0.152132000
8	3.058922000	1.083051000	0.076004000
1	2.942776000	1.578597000	0.899746000
1	-3.194482000	0.835240000	0.068162000
7	-2.167038000	-1.617520000	0.159779000
1	-3.113081000	-1.607348000	-0.182910000
1	-1.645722000	-2.435682000	-0.111343000
8	0.472404000	-1.705423000	-0.010451000
6	1.881390000	-1.807323000	-0.096986000
1	2.359868000	-1.350625000	0.769015000
1	2.106311000	-2.868768000	-0.130629000
1	2.252567000	-1.319534000	-1.000021000

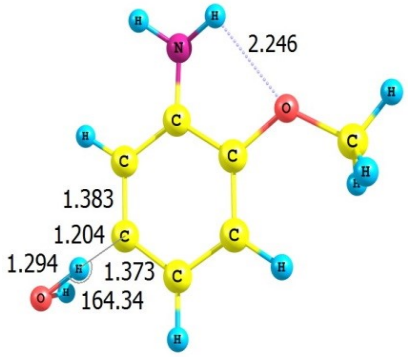
Zero-point correction= 0.156851 (Hartree/Particle)
Thermal correction to Energy= 0.167405
Thermal correction to Enthalpy= 0.168349
Thermal correction to Gibbs Free Energy= 0.120539
Sum of electronic and zero-point Energies= -477.658570
Sum of electronic and thermal Energies= -477.648016
Sum of electronic and thermal Enthalpies= -477.647072
Sum of electronic and thermal Free Energies= -477.694882
Electronic energy at ROCBS-QB3= -477.227123



TS11

6	-1.434816000	-1.453426000	-0.083099000
6	-1.594054000	-0.089887000	-0.128123000
6	-0.140056000	-1.963943000	-0.011804000
1	-2.701251000	0.376455000	-0.225440000
1	0.018511000	-3.034741000	0.021116000
6	-0.525277000	0.791588000	-0.079170000
6	0.962531000	-1.122031000	0.027210000
1	-0.698278000	1.856946000	-0.111130000
6	0.756487000	0.270987000	-0.009387000
1	-2.286132000	-2.118357000	-0.111700000
8	-3.847124000	0.906797000	0.038315000
1	-3.844269000	0.799286000	1.000341000
7	2.257911000	-1.601621000	0.156298000
1	2.412017000	-2.535093000	-0.185969000
1	2.978538000	-0.949382000	-0.107654000
8	1.895975000	1.014524000	0.018821000
6	1.759064000	2.417408000	-0.011567000
1	1.193324000	2.773644000	0.851940000
1	2.764881000	2.824521000	0.021496000
1	1.263201000	2.743325000	-0.928522000

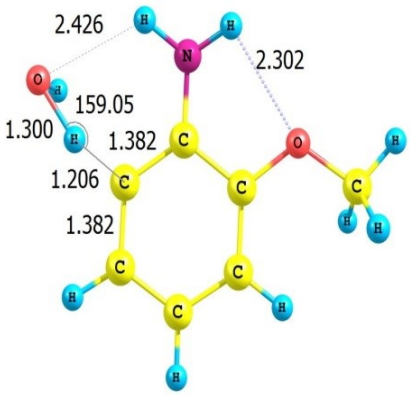
Zero-point correction= 0.156672 (Hartree/Particle)
Thermal correction to Energy= 0.167330
Thermal correction to Enthalpy= 0.168274
Thermal correction to Gibbs Free Energy= 0.119741
Sum of electronic and zero-point Energies= -477.658705
Sum of electronic and thermal Energies= -477.648047
Sum of electronic and thermal Enthalpies= -477.647102
Sum of electronic and thermal Free Energies= -477.695636
Electronic energy at ROCBS-QB3= -477.227823



TS12

6	1.033525000	-1.407489000	-0.093592000
6	1.735933000	-0.227812000	-0.123239000
6	-0.361314000	-1.337203000	-0.039226000
1	2.935957000	-0.264656000	-0.207699000
1	-0.937430000	-2.250500000	-0.029577000
6	1.128787000	1.013437000	-0.073168000
6	-0.996657000	-0.109001000	-0.000601000
6	-0.257348000	1.090411000	-0.013989000
1	1.534610000	-2.363828000	-0.122613000
8	4.203380000	-0.273897000	0.051875000
1	4.154854000	-0.302453000	1.018442000
7	-0.932031000	2.296696000	0.083287000
1	-0.448580000	3.098801000	-0.284222000
1	-1.907151000	2.258458000	-0.165785000
1	1.718779000	1.920954000	-0.084942000
8	-2.347158000	0.066433000	0.044992000
6	-3.156134000	-1.087103000	0.062739000
1	-3.008086000	-1.685132000	-0.839315000
1	-2.945179000	-1.700150000	0.941668000
1	-4.184093000	-0.740088000	0.102551000

Zero-point correction= 0.156616 (Hartree/Particle)
Thermal correction to Energy= 0.167308
Thermal correction to Enthalpy= 0.168252
Thermal correction to Gibbs Free Energy= 0.119571
Sum of electronic and zero-point Energies= -477.658656
Sum of electronic and thermal Energies= -477.647964
Sum of electronic and thermal Enthalpies= -477.647020
Sum of electronic and thermal Free Energies= -477.695701
Electronic energy at ROCBS-QB3= -477.227502

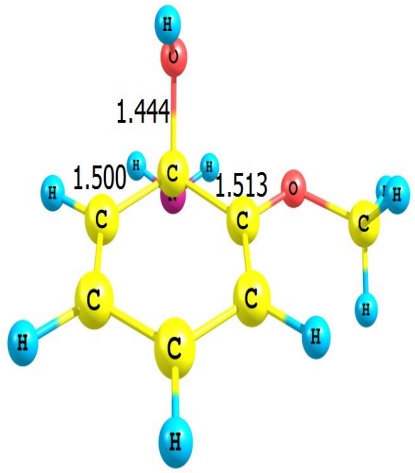


TS13

6	-1.197102000	1.782555000	-0.042655000
6	-1.414008000	0.417960000	-0.084636000
6	0.111368000	2.232425000	0.009437000
1	-2.531480000	-0.024680000	-0.182333000
1	0.322701000	3.291950000	0.031107000
6	-0.407938000	-0.528378000	-0.045408000
6	1.164491000	1.317064000	0.025205000
6	0.915487000	-0.043721000	-0.003601000

1	-2.026538000	2.474665000	-0.066268000
8	-3.548364000	-0.808478000	0.019063000
1	-3.509352000	-0.845819000	0.986616000
1	2.180527000	1.680714000	0.060964000
7	-0.653041000	-1.885962000	0.000671000
1	-1.566888000	-2.166999000	-0.319498000
1	0.109913000	-2.472662000	-0.293584000
8	1.867772000	-1.016287000	0.004012000
6	3.216107000	-0.607982000	0.045653000
1	3.424450000	-0.036662000	0.952870000
1	3.811456000	-1.515844000	0.045230000
1	3.470804000	-0.004351000	-0.828375000

Zero-point correction= 0.157187 (Hartree/Particle)
Thermal correction to Energy= 0.167641
Thermal correction to Enthalpy= 0.168585
Thermal correction to Gibbs Free Energy= 0.120864
Sum of electronic and zero-point Energies= -477.660838
Sum of electronic and thermal Energies= -477.650385
Sum of electronic and thermal Enthalpies= -477.649440
Sum of electronic and thermal Free Energies= -477.697161
Electronic energy at ROCBS-QB3= -477.230151

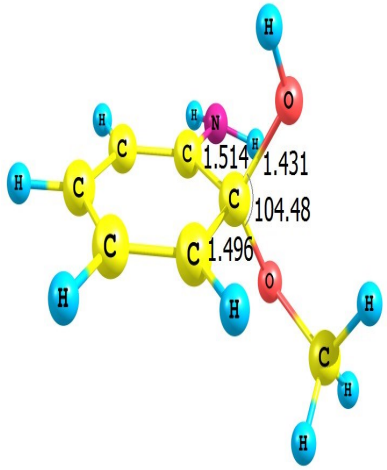


P1

6	-0.554808000	0.203474000	-0.017600000
6	-0.292547000	1.541193000	0.018116000
6	0.531645000	-0.848758000	-0.006258000
1	-1.101325000	2.255539000	0.060337000
6	1.035794000	2.009249000	-0.019173000
6	1.893968000	-0.239116000	-0.153551000
1	1.227589000	3.071155000	0.011612000
6	2.110694000	1.095658000	-0.120046000
1	3.121330000	1.476569000	-0.182284000
1	2.710443000	-0.945190000	-0.239798000
7	0.283098000	-1.793725000	-1.060878000
1	0.981403000	-2.526809000	-1.026864000
1	-0.627686000	-2.217552000	-0.926553000
8	0.470498000	-1.556814000	1.251043000
1	0.737921000	-0.953674000	1.951605000

8	-1.773769000	-0.355095000	-0.029588000
6	-2.896485000	0.500454000	-0.023092000
1	-2.914793000	1.106864000	0.884569000
1	-2.889433000	1.153630000	-0.897750000
1	-3.770531000	-0.142101000	-0.050734000

Zero-point correction= 0.165273 (Hartree/Particle)
Thermal correction to Energy= 0.175029
Thermal correction to Enthalpy= 0.175973
Thermal correction to Gibbs Free Energy= 0.130282
Sum of electronic and zero-point Energies= -477.694433
Sum of electronic and thermal Energies= -477.684677
Sum of electronic and thermal Enthalpies= -477.683733
Sum of electronic and thermal Free Energies= -477.729424
Electronic energy at ROCBS-QB3= -477.273915

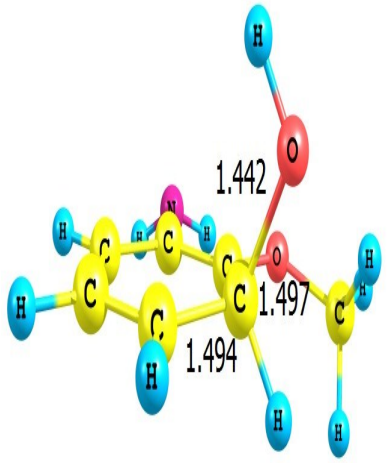


P2

6	0.438811000	-0.040303000	0.232632000
6	-0.099703000	-1.436259000	0.214390000
6	-0.627132000	0.990993000	-0.069916000
1	0.609148000	-2.222727000	0.435778000
6	-1.406393000	-1.712138000	-0.003384000
6	-1.943691000	0.643607000	-0.279905000
1	-1.742486000	-2.740582000	0.021772000
6	-2.352526000	-0.686426000	-0.256537000
1	-3.388017000	-0.937703000	-0.430240000
1	-2.663156000	1.430391000	-0.471913000
7	-0.178645000	2.272286000	-0.065823000
1	-0.761034000	2.998744000	-0.443085000
1	0.816966000	2.412712000	-0.115712000
8	1.042264000	0.239309000	1.499654000
1	0.440202000	-0.058486000	2.186888000
8	1.460458000	0.203906000	-0.705574000
6	2.553623000	-0.692937000	-0.675306000
1	2.915561000	-0.838784000	0.342789000
1	2.284796000	-1.655040000	-1.115545000
1	3.338825000	-0.239465000	-1.274456000

Zero-point correction= 0.164729 (Hartree/Particle)
Thermal correction to Energy= 0.174749

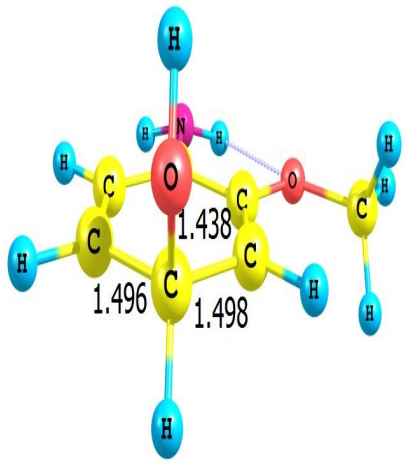
Thermal correction to Enthalpy= 0.175693
Thermal correction to Gibbs Free Energy= 0.129348
Sum of electronic and zero-point Energies= -477.703118
Sum of electronic and thermal Energies= -477.693098
Sum of electronic and thermal Enthalpies= -477.692154
Sum of electronic and thermal Free Energies= -477.738499
Electronic energy at ROCBS-QB3= -477.279965



P3

6	0.343883000	0.282688000	-0.080767000
6	0.236466000	-1.203938000	-0.217210000
6	-0.750847000	1.115061000	0.066620000
1	0.833126000	-1.542761000	-1.071077000
6	-1.177042000	-1.660660000	-0.377559000
6	-2.035359000	0.574657000	-0.016442000
1	-1.322266000	-2.718119000	-0.549971000
6	-2.220175000	-0.813125000	-0.254512000
1	-3.230364000	-1.192317000	-0.337265000
1	-2.890739000	1.224543000	0.106789000
7	-0.552043000	2.469844000	0.346532000
1	-1.277362000	3.074583000	-0.004177000
1	0.370438000	2.800751000	0.110219000
8	0.872685000	-1.863321000	0.895829000
1	0.326991000	-1.700241000	1.671728000
8	1.559198000	0.871430000	0.005674000
6	2.702060000	0.157221000	-0.438810000
1	2.823019000	-0.772393000	0.114033000
1	2.632438000	-0.049726000	-1.508749000
1	3.550045000	0.810482000	-0.257194000

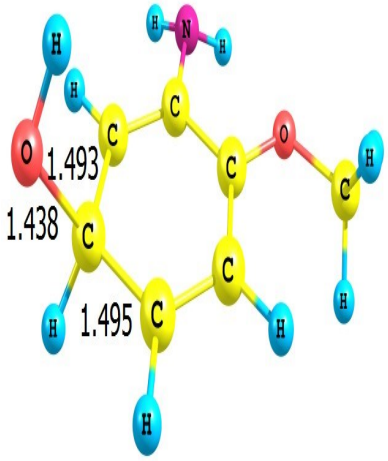
Zero-point correction= 0.165306 (Hartree/Particle)
Thermal correction to Energy= 0.175251
Thermal correction to Enthalpy= 0.176196
Thermal correction to Gibbs Free Energy= 0.130158
Sum of electronic and zero-point Energies= -477.691138
Sum of electronic and thermal Energies= -477.681192
Sum of electronic and thermal Enthalpies= -477.680248
Sum of electronic and thermal Free Energies= -477.726285
Electronic energy at ROCBS-QB3= -477.269597



P4

6	0.687039000	-0.127292000	-0.075846000
6	-0.273262000	-1.052568000	-0.292624000
6	0.377673000	1.268943000	0.029103000
1	-0.033280000	-2.101581000	-0.379324000
6	-1.725534000	-0.696884000	-0.378725000
6	-0.969005000	1.671547000	-0.104599000
1	-2.153858000	-1.109494000	-1.297762000
6	-1.964157000	0.778979000	-0.324049000
1	-2.988779000	1.109583000	-0.424593000
1	-1.194966000	2.729084000	-0.027659000
7	1.385717000	2.158022000	0.306470000
1	1.227358000	3.126529000	0.087679000
1	2.326864000	1.827649000	0.171625000
8	-2.481341000	-1.371891000	0.641990000
1	-2.162160000	-1.049462000	1.490155000
8	2.019001000	-0.386631000	0.049985000
6	2.425068000	-1.733435000	-0.039835000
1	1.955540000	-2.334148000	0.741740000
1	2.172346000	-2.152517000	-1.016056000
1	3.502702000	-1.739362000	0.092548000

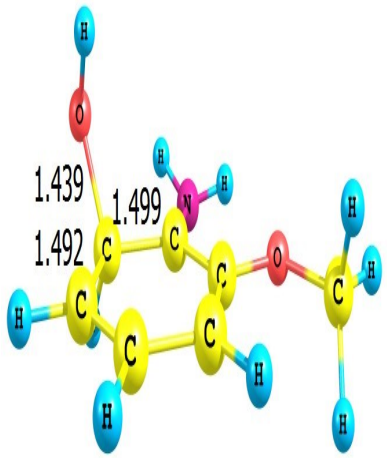
Zero-point correction= 0.165654 (Hartree/Particle)
Thermal correction to Energy= 0.175549
Thermal correction to Enthalpy= 0.176493
Thermal correction to Gibbs Free Energy= 0.130368
Sum of electronic and zero-point Energies= -477.697965
Sum of electronic and thermal Energies= -477.688070
Sum of electronic and thermal Enthalpies= -477.687126
Sum of electronic and thermal Free Energies= -477.733251
Electronic energy at ROCBS-QB3= -477.275488



P5

6	0.839376000	-0.090914000	-0.038335000
6	0.225596000	-1.348267000	-0.150386000
6	0.050260000	1.110789000	-0.089459000
1	0.827431000	-2.244468000	-0.100625000
6	-1.121449000	-1.456961000	-0.318727000
6	-1.288262000	1.024091000	-0.271424000
1	-1.588308000	-2.429633000	-0.389556000
6	-2.028175000	-0.269418000	-0.365385000
1	-2.617593000	-0.298533000	-1.288843000
1	-1.883802000	1.928088000	-0.311700000
7	0.721864000	2.314250000	0.105330000
1	0.247445000	3.125877000	-0.254154000
1	1.702353000	2.292165000	-0.123227000
8	-3.042175000	-0.367799000	0.649343000
1	-2.599894000	-0.287225000	1.499686000
8	2.167911000	0.109012000	0.109912000
6	3.011198000	-1.021587000	0.167622000
1	2.756685000	-1.653689000	1.020223000
1	2.944045000	-1.605804000	-0.752070000
1	4.021437000	-0.642618000	0.285480000

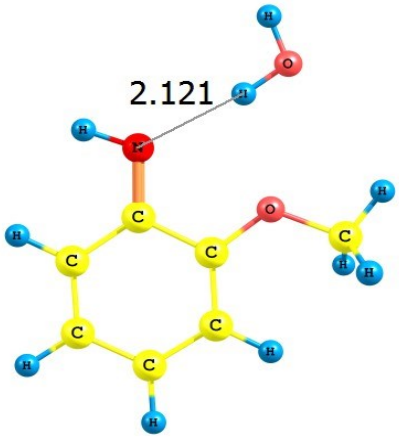
Zero-point correction= 0.165405 (Hartree/Particle)
Thermal correction to Energy= 0.175334
Thermal correction to Enthalpy= 0.176278
Thermal correction to Gibbs Free Energy= 0.129984
Sum of electronic and zero-point Energies= -477.692157
Sum of electronic and thermal Energies= -477.682228
Sum of electronic and thermal Enthalpies= -477.681284
Sum of electronic and thermal Free Energies= -477.727578
Electronic energy at ROCBS-QB3= -477.270087



P6

6	-0.814672000	0.049566000	-0.058132000
6	-0.730700000	1.429219000	0.019331000
6	0.325730000	-0.732214000	-0.210729000
1	-1.610247000	2.037863000	0.151704000
6	0.553528000	2.049252000	-0.051948000
6	1.698770000	-0.141869000	-0.320514000
1	0.601155000	3.127948000	0.022016000
6	1.692453000	1.345610000	-0.209709000
1	2.653689000	1.837383000	-0.271613000
1	2.133613000	-0.455498000	-1.278834000
7	0.245898000	-2.089201000	-0.312559000
1	1.077496000	-2.603778000	-0.069849000
1	-0.633209000	-2.517598000	-0.073820000
8	2.582488000	-0.757730000	0.633514000
1	2.364759000	-0.394754000	1.497982000
8	-1.976400000	-0.668391000	0.023350000
6	-3.172452000	0.054138000	0.200934000
1	-3.153721000	0.623835000	1.132758000
1	-3.347616000	0.735554000	-0.634385000
1	-3.971861000	-0.679790000	0.241650000

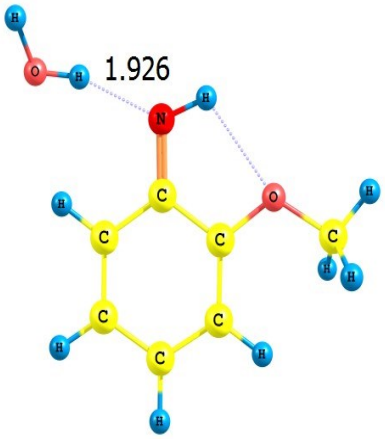
Zero-point correction= 0.165842 (Hartree/Particle)
Thermal correction to Energy= 0.175650
Thermal correction to Enthalpy= 0.176594
Thermal correction to Gibbs Free Energy= 0.130582
Sum of electronic and zero-point Energies= -477.698776
Sum of electronic and thermal Energies= -477.688967
Sum of electronic and thermal Enthalpies= -477.688023
Sum of electronic and thermal Free Energies= -477.734035
Electronic energy at ROCBS-QB3= -477.276139



P7---H_2O

6	2.483334000	0.909387000	0.001700000
6	2.800078000	-0.456872000	0.001100000
6	1.161691000	1.340126000	0.000693000
1	3.835257000	-0.767561000	0.001806000
1	0.940465000	2.396820000	0.001014000
6	1.799143000	-1.390338000	-0.000306000
6	0.134370000	0.410379000	-0.000892000
6	0.420451000	-1.009939000	-0.001097000
1	3.277343000	1.643039000	0.002884000
7	-0.599856000	-1.842093000	-0.001769000
1	-2.565117000	-1.044744000	-0.000848000
1	-0.262599000	-2.803788000	-0.002055000
8	-3.501644000	-0.794420000	0.000590000
1	-3.983751000	-1.621302000	0.019506000
1	2.027220000	-2.448969000	-0.000694000
8	-1.159000000	0.702832000	-0.002308000
6	-1.578986000	2.051434000	-0.000456000
1	-2.663325000	2.013650000	-0.000884000
1	-1.221261000	2.566212000	0.893209000
1	-1.220572000	2.568939000	-0.892269000

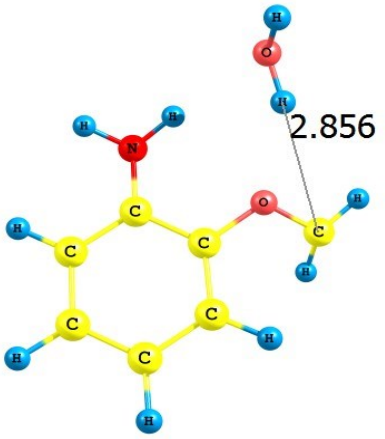
Zero-point correction= 0.162213 (Hartree/Particle)
Thermal correction to Energy= 0.173709
Thermal correction to Enthalpy= 0.174653
Thermal correction to Gibbs Free Energy= 0.122715
Sum of electronic and zero-point Energies= -477.713422
Sum of electronic and thermal Energies= -477.701926
Sum of electronic and thermal Enthalpies= -477.700982
Sum of electronic and thermal Free Energies= -477.752920
Electronic energy at ROCBS-QB3= -477.291938



P8---H_2O

6	-0.846888000	2.221254000	-0.000831000
6	-1.595553000	1.045135000	-0.002549000
6	0.552161000	2.189381000	0.006492000
1	-2.673524000	1.101320000	-0.009035000
1	1.110086000	3.114875000	0.006321000
6	-0.950634000	-0.176010000	0.003221000
6	1.211316000	0.988328000	0.012619000
1	2.292156000	0.926331000	0.017854000
6	0.493898000	-0.248026000	0.011943000
1	-1.363757000	3.170848000	-0.005858000
7	1.156037000	-1.387353000	0.015650000
1	3.070636000	-1.188297000	-0.039019000
1	0.508293000	-2.173214000	0.009340000
8	3.966207000	-0.809736000	-0.083961000
1	4.512331000	-1.360261000	0.477382000
8	-1.568738000	-1.368134000	0.001724000
6	-2.981897000	-1.389995000	-0.009496000
1	-3.384071000	-0.899517000	0.878613000
1	-3.369756000	-0.901710000	-0.905120000
1	-3.268836000	-2.436347000	-0.010528000

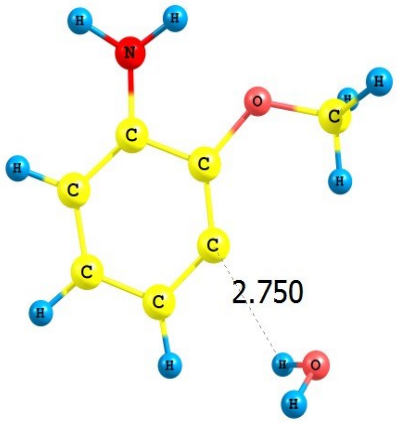
Zero-point correction= 0.162988 (Hartree/Particle)
Thermal correction to Energy= 0.173991
Thermal correction to Enthalpy= 0.174935
Thermal correction to Gibbs Free Energy= 0.125176
Sum of electronic and zero-point Energies= -477.716124
Sum of electronic and thermal Energies= -477.705121
Sum of electronic and thermal Enthalpies= -477.704176
Sum of electronic and thermal Free Energies= -477.753936
Electronic energy at ROCBS-QB3= -477.296430



P9---H_2O

6	2.450819000	0.835324000	0.434576000
6	1.150294000	1.309297000	0.319386000
6	2.704223000	-0.507647000	0.202108000
1	0.916591000	2.347041000	0.514812000
1	3.710745000	-0.893086000	0.288529000
6	0.129217000	0.446486000	-0.031751000
6	1.673100000	-1.369552000	-0.136505000
1	1.877804000	-2.416987000	-0.319761000
6	0.359387000	-0.916577000	-0.261452000
1	3.248678000	1.509301000	0.710044000
1	-2.723171000	-0.046966000	0.707224000
7	-0.666978000	-1.751120000	-0.660420000
1	-0.474361000	-2.734613000	-0.570794000
1	-1.605038000	-1.505363000	-0.375107000
8	-3.310015000	-0.811272000	0.696307000
1	-3.523722000	-0.997073000	1.611693000
8	-1.181501000	0.869844000	-0.152074000
6	-1.413536000	2.134671000	-0.589046000
1	-2.462660000	2.369760000	-0.660257000
1	-0.684913000	2.565235000	-1.261198000

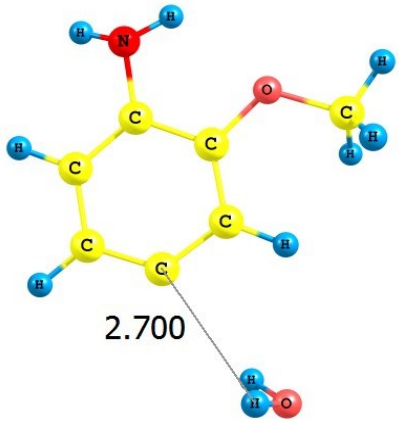
Zero-point correction= 0.161463 (Hartree/Particle)
Thermal correction to Energy= 0.173102
Thermal correction to Enthalpy= 0.174046
Thermal correction to Gibbs Free Energy= 0.123444
Sum of electronic and zero-point Energies= -477.703398
Sum of electronic and thermal Energies= -477.691758
Sum of electronic and thermal Enthalpies= -477.690814
Sum of electronic and thermal Free Energies= -477.741417
Electronic energy at ROCBS-QB3= -477.277420



P10---H_2O

6	0.071551000	1.990858000	0.054693000
6	-0.479016000	0.733245000	0.047668000
6	1.461085000	2.047115000	0.018182000
1	-4.225689000	1.550391000	-0.147251000
1	1.960355000	3.006284000	0.021205000
6	0.205942000	-0.450956000	0.012015000
6	2.213276000	0.879219000	-0.024386000
6	1.612976000	-0.376192000	-0.029862000
1	-0.530533000	2.887823000	0.087033000
8	-3.756877000	0.718809000	-0.060065000
1	-2.822278000	0.943307000	-0.107642000
1	3.293667000	0.935534000	-0.060678000
7	2.336881000	-1.553796000	-0.122689000
1	3.281027000	-1.516977000	0.223253000
1	1.834181000	-2.383009000	0.150498000
8	-0.339620000	-1.690251000	0.025895000
6	-1.756586000	-1.737959000	0.052975000
1	-2.176623000	-1.271209000	-0.839443000
1	-2.028806000	-2.788172000	0.082049000
1	-2.146861000	-1.227849000	0.935450000

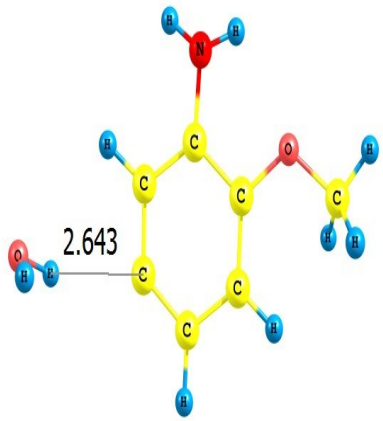
Zero-point correction= 0.161621 (Hartree/Particle)
Thermal correction to Energy= 0.173895
Thermal correction to Enthalpy= 0.174839
Thermal correction to Gibbs Free Energy= 0.121884
Sum of electronic and zero-point Energies= -477.678908
Sum of electronic and thermal Energies= -477.666634
Sum of electronic and thermal Enthalpies= -477.665690
Sum of electronic and thermal Free Energies= -477.718644
Electronic energy at ROCBS-QB3= -477.250630



P11---H_2O

6	-0.494162000	-2.175029000	0.004882000
6	-1.267829000	-1.052114000	0.002260000
6	0.890071000	-1.977988000	-0.001698000
1	-3.710637000	-0.189355000	-0.757453000
1	1.556252000	-2.832145000	-0.009670000
6	-0.802710000	0.243139000	-0.001739000
6	1.437208000	-0.702579000	-0.008571000
1	-1.483868000	1.082162000	0.001344000
6	0.576545000	0.413144000	-0.005838000
1	-0.910252000	-3.172492000	0.009631000
8	-4.069922000	0.272716000	0.003962000
1	-3.708066000	-0.204967000	0.754449000
7	2.809523000	-0.486079000	-0.074249000
1	3.378686000	-1.222064000	0.309516000
1	3.100805000	0.433798000	0.215532000
8	1.205622000	1.618178000	0.000698000
6	0.397011000	2.774300000	0.002562000
1	1.074975000	3.622070000	0.004996000
1	-0.231695000	2.812288000	-0.889292000
1	-0.235261000	2.808867000	0.892268000

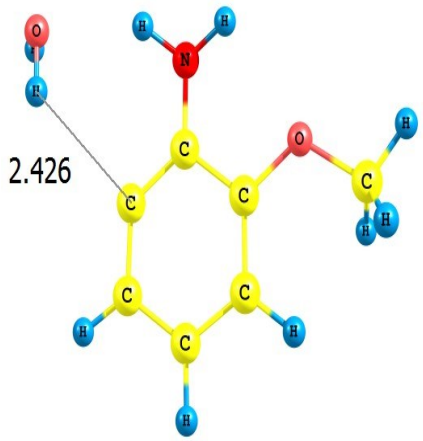
Zero-point correction= 0.161821 (Hartree/Particle)
Thermal correction to Energy= 0.174055
Thermal correction to Enthalpy= 0.174999
Thermal correction to Gibbs Free Energy= 0.121870
Sum of electronic and zero-point Energies= -477.677043
Sum of electronic and thermal Energies= -477.664809
Sum of electronic and thermal Enthalpies= -477.663865
Sum of electronic and thermal Free Energies= -477.716993
Electronic energy at ROCBS-QB3= -477.249055



P12---H_2O

6	0.616357000	-1.794719000	0.010120000
6	1.532870000	-0.785499000	0.016124000
6	-0.730741000	-1.405170000	0.001490000
1	4.076505000	-0.254972000	-0.794657000
1	-1.499292000	-2.164131000	0.001540000
6	1.255861000	0.559104000	0.010247000
6	-1.072443000	-0.064626000	-0.004259000
6	-0.084155000	0.941959000	-0.003618000
1	0.889454000	-2.839860000	0.013401000
8	4.519703000	0.066881000	-0.005973000
1	4.045526000	-0.356991000	0.713641000
7	-0.476390000	2.266281000	-0.067145000
1	0.186652000	2.941328000	0.273838000
1	-1.429231000	2.445406000	0.204562000
1	2.040686000	1.305834000	0.010572000
8	-2.351031000	0.411030000	-0.003004000
6	-3.398288000	-0.530857000	-0.006409000
1	-3.362188000	-1.162887000	0.883969000
1	-4.322962000	0.038144000	-0.009020000
1	-3.356555000	-1.160285000	-0.898179000

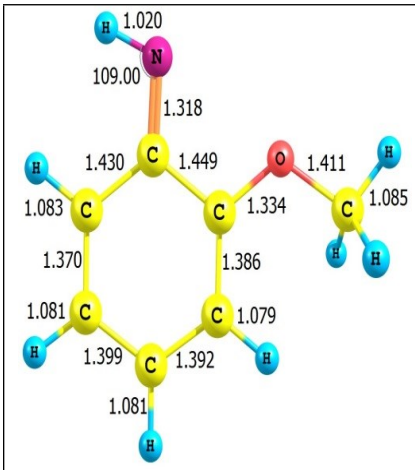
Zero-point correction= 0.161679 (Hartree/Particle)
Thermal correction to Energy= 0.173982
Thermal correction to Enthalpy= 0.174926
Thermal correction to Gibbs Free Energy= 0.121247
Sum of electronic and zero-point Energies= -477.677314
Sum of electronic and thermal Energies= -477.665012
Sum of electronic and thermal Enthalpies= -477.664068
Sum of electronic and thermal Free Energies= -477.717747
Electronic energy at ROCBS-QB3= -477.248650



P13---H_2O

6	0.770669000	2.103161000	-0.079560000
6	1.221128000	0.810705000	-0.163499000
6	-0.602331000	2.277889000	0.038144000
1	3.396522000	-0.008890000	0.530174000
1	-1.021293000	3.271713000	0.108724000
6	0.461526000	-0.334393000	-0.153006000
6	-1.444202000	1.166669000	0.067007000
6	-0.929275000	-0.116820000	-0.024395000
1	1.445197000	2.947885000	-0.102199000
8	3.830942000	-0.842568000	0.321618000
1	4.264262000	-0.690048000	-0.520892000
1	-2.509187000	1.314694000	0.162953000
7	0.957689000	-1.613186000	-0.304127000
1	1.930407000	-1.731415000	-0.058443000
1	0.339431000	-2.344151000	0.006507000
8	-1.670499000	-1.258264000	0.003912000
6	-3.067900000	-1.128169000	0.132503000
1	-3.488323000	-0.570450000	-0.707162000
1	-3.470380000	-2.136532000	0.134698000
1	-3.331690000	-0.628107000	1.067126000

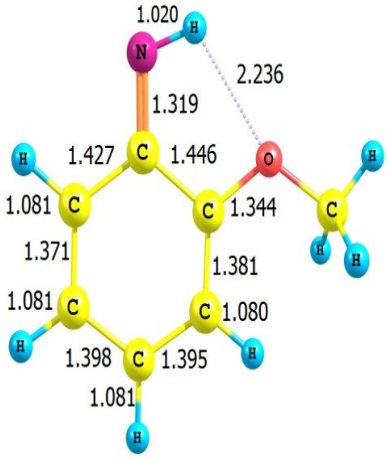
Zero-point correction= 0.162517 (Hartree/Particle)
Thermal correction to Energy= 0.174448
Thermal correction to Enthalpy= 0.175392
Thermal correction to Gibbs Free Energy= 0.123075
Sum of electronic and zero-point Energies= -477.679917
Sum of electronic and thermal Energies= -477.667987
Sum of electronic and thermal Enthalpies= -477.667043
Sum of electronic and thermal Free Energies= -477.719359
Electronic energy at ROCBS-QB3= -477.252944



P7

6	2.220895000	-0.741594000	-0.000078000
6	1.891876000	0.588412000	-0.000174000
6	1.207082000	-1.705648000	0.000049000
1	2.663357000	1.348757000	-0.000285000
1	1.462189000	-2.756457000	0.000126000
6	0.532738000	1.034067000	-0.000127000
6	-0.134312000	-1.334078000	0.000055000
1	-0.893987000	-2.100724000	0.000117000
6	-0.488100000	0.005932000	-0.000049000
1	3.257514000	-1.048509000	-0.000104000
8	-1.745152000	0.451904000	-0.000138000
6	-2.793743000	-0.492058000	0.000425000
1	-2.755891000	-1.121217000	-0.891368000
1	-2.755237000	-1.120893000	0.892416000
1	-3.713929000	0.083142000	0.000652000
7	0.156111000	2.297058000	-0.000125000
1	0.985800000	2.891061000	-0.000189000

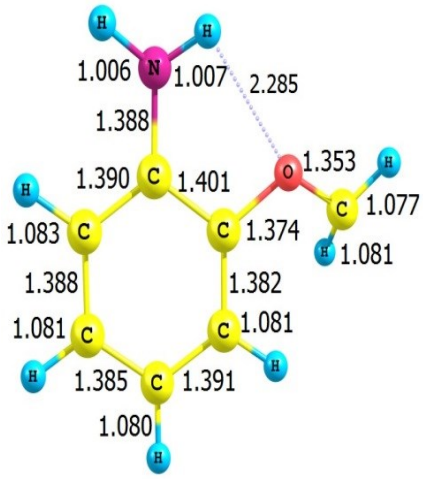
Zero-point correction= 0.137813 (Hartree/Particle)
Thermal correction to Energy= 0.145505
Thermal correction to Enthalpy= 0.146450
Thermal correction to Gibbs Free Energy= 0.105077
Sum of electronic and zero-point Energies= -401.298012
Sum of electronic and thermal Energies= -401.290320
Sum of electronic and thermal Enthalpies= -401.289376
Sum of electronic and thermal Free Energies= -401.330749
Electronic energy at ROCBS-QB3= -400.919054



P8

6	-2.262553000	-0.650092000	0.000022000
6	-1.882857000	0.667363000	-0.000062000
6	-1.289664000	-1.654291000	0.000071000
1	-2.605657000	1.471660000	-0.000108000
1	-1.587326000	-2.693881000	0.000136000
6	-0.508274000	1.050698000	-0.000134000
6	0.069108000	-1.339318000	0.000061000
1	0.797523000	-2.136280000	0.000106000
6	0.467473000	-0.016642000	-0.000019000
1	-3.310368000	-0.916016000	0.000045000
8	1.747066000	0.394332000	-0.000043000
6	2.764796000	-0.584686000	0.000194000
1	2.702615000	-1.211064000	0.892211000
1	2.702833000	-1.211268000	-0.891695000
1	3.705573000	-0.043601000	0.000247000
7	-0.193129000	2.331131000	-0.000178000
1	0.822004000	2.429670000	-0.000144000

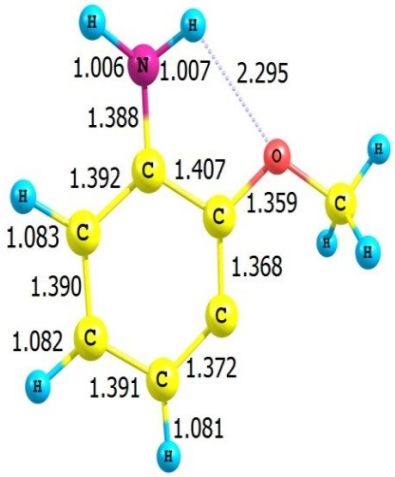
Zero-point correction= 0.137871 (Hartree/Particle)
Thermal correction to Energy= 0.145565
Thermal correction to Enthalpy= 0.146509
Thermal correction to Gibbs Free Energy= 0.105139
Sum of electronic and zero-point Energies= -401.302651
Sum of electronic and thermal Energies= -401.294957
Sum of electronic and thermal Enthalpies= -401.294013
Sum of electronic and thermal Free Energies= -401.335384
Electronic energy at ROCBS-QB3= -400.924244



P9

6	2.261245000	-0.506882000	0.060945000
6	1.732959000	0.776537000	0.079103000
6	1.425243000	-1.606776000	-0.037289000
1	2.387691000	1.635311000	0.159558000
1	1.831987000	-2.607283000	-0.063930000
6	0.360256000	0.985830000	0.005821000
6	0.049816000	-1.418101000	-0.116781000
1	-0.618933000	-2.260056000	-0.227368000
6	-0.470966000	-0.138002000	-0.086884000
1	3.332361000	-0.642139000	0.119661000
8	-1.813554000	0.138529000	-0.184583000
6	-2.708124000	-0.813118000	0.169067000
1	-3.730075000	-0.508170000	0.018870000
1	-2.427294000	-1.496024000	0.959115000
7	-0.202554000	2.252173000	0.079479000
1	-1.144275000	2.321301000	-0.270246000
1	0.392272000	3.006690000	-0.219243000

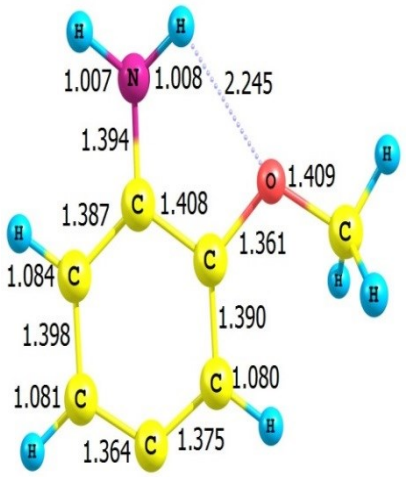
Zero-point correction= 0.136622 (Hartree/Particle)
Thermal correction to Energy= 0.144866
Thermal correction to Enthalpy= 0.145810
Thermal correction to Gibbs Free Energy= 0.103552
Sum of electronic and zero-point Energies= -401.293949
Sum of electronic and thermal Energies= -401.285705
Sum of electronic and thermal Enthalpies= -401.284761
Sum of electronic and thermal Free Energies= -401.327020
Electronic energy at ROCBS-QB3= -400.909498



P10

6	-1.306108000	-1.734395000	0.004148000
6	0.013526000	-1.357768000	-0.003648000
6	-2.237716000	-0.700957000	0.008562000
1	-3.295040000	-0.928877000	0.015571000
6	0.479144000	-0.071643000	-0.008938000
6	-1.821671000	0.625307000	-0.000300000
1	-2.555454000	1.421273000	-0.006520000
6	-0.472186000	0.965494000	-0.011014000
1	-1.609494000	-2.771748000	0.005907000
6	2.713991000	-0.774340000	0.007498000
1	3.703783000	-0.328037000	0.022698000
1	2.573223000	-1.399640000	0.892113000
1	2.597676000	-1.391696000	-0.885985000
7	-0.029384000	2.279174000	-0.074035000
1	-0.656738000	2.968151000	0.306115000
1	0.930573000	2.413400000	0.200581000
8	1.787909000	0.294096000	-0.001259000

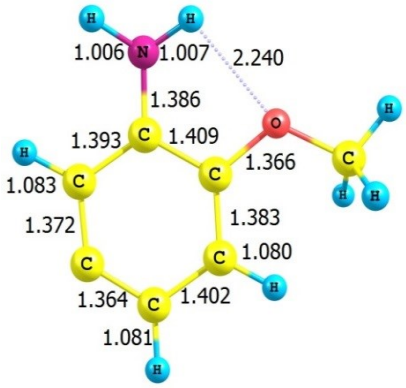
Zero-point correction= 0.137676 (Hartree/Particle)
Thermal correction to Energy= 0.146073
Thermal correction to Enthalpy= 0.147017
Thermal correction to Gibbs Free Energy= 0.104034
Sum of electronic and zero-point Energies= -401.271874
Sum of electronic and thermal Energies= -401.263477
Sum of electronic and thermal Enthalpies= -401.262533
Sum of electronic and thermal Free Energies= -401.305516
Electronic energy at ROCBS-QB3= -400.886939



P11

6	-2.255995000	-0.863095000	0.005999000
6	-1.906544000	0.490843000	-0.003273000
6	-1.229841000	-1.761156000	0.005817000
1	-2.681080000	1.248441000	-0.013935000
6	-0.578707000	0.891768000	-0.009885000
6	0.107524000	-1.440149000	0.001689000
1	0.872284000	-2.203360000	0.006863000
6	0.432031000	-0.088187000	-0.004800000
1	-3.294072000	-1.165088000	0.010805000
8	1.701473000	0.403495000	0.001764000
6	2.760049000	-0.526472000	0.002018000
1	2.728305000	-1.158082000	0.892881000
1	2.727975000	-1.156353000	-0.889806000
1	3.678001000	0.053539000	0.001923000
7	-0.210121000	2.233942000	-0.077960000
1	0.734217000	2.417926000	0.221152000
1	-0.877667000	2.876114000	0.316326000

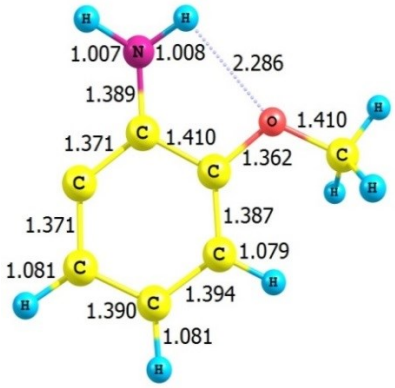
Zero-point correction= 0.138312 (Hartree/Particle)
Thermal correction to Energy= 0.146340
Thermal correction to Enthalpy= 0.147285
Thermal correction to Gibbs Free Energy= 0.105448
Sum of electronic and zero-point Energies= -401.269162
Sum of electronic and thermal Energies= -401.261134
Sum of electronic and thermal Enthalpies= -401.260189
Sum of electronic and thermal Free Energies= -401.302026
Electronic energy at ROCBS-QB3= -400.885599



P12

6	-2.218139000	-0.789197000	0.005452000
6	-1.936844000	0.553890000	-0.001638000
6	-1.296826000	-1.794462000	0.005018000
1	-2.715141000	1.307144000	-0.009706000
1	-1.568688000	-2.840324000	0.008729000
6	-0.597574000	0.938541000	-0.008847000
6	0.050440000	-1.405951000	0.001336000
1	0.819145000	-2.165045000	0.005891000
6	0.391546000	-0.065262000	-0.004446000
8	1.671283000	0.411893000	0.001977000
6	2.717568000	-0.529937000	0.001226000
1	2.679922000	-1.162699000	0.891372000
1	2.679067000	-1.159672000	-0.890794000
1	3.642689000	0.038885000	0.001303000
7	-0.206555000	2.266470000	-0.072444000
1	0.744754000	2.441249000	0.208121000
1	-0.867149000	2.934299000	0.287757000

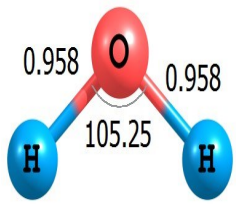
Zero-point correction= 0.138201 (Hartree/Particle)
Thermal correction to Energy= 0.146237
Thermal correction to Enthalpy= 0.147181
Thermal correction to Gibbs Free Energy= 0.105343
Sum of electronic and zero-point Energies= -401.269720
Sum of electronic and thermal Energies= -401.261684
Sum of electronic and thermal Enthalpies= -401.260740
Sum of electronic and thermal Free Energies= -401.302578
Electronic energy at ROCBS-QB3= -400.885555



P13

6	-2.360438000	-0.486668000	0.009072000
6	-1.791824000	0.760380000	0.002785000
6	-1.489347000	-1.569575000	0.002442000
1	-1.875777000	-2.579241000	0.003528000
6	-0.451402000	1.049141000	-0.010178000
6	-0.111774000	-1.357804000	-0.003632000
1	0.552866000	-2.208393000	-0.003550000
6	0.405459000	-0.070955000	-0.007334000
1	-3.432549000	-0.626315000	0.017532000
8	1.731625000	0.239161000	0.000433000
6	2.654503000	-0.826342000	0.005995000
1	2.531184000	-1.448987000	0.895234000
1	2.544387000	-1.445074000	-0.887452000
1	3.642280000	-0.375207000	0.013746000
7	0.077621000	2.331799000	-0.079259000
1	1.031887000	2.402623000	0.236239000
1	-0.521684000	3.055650000	0.281180000

Zero-point correction= 0.138220 (Hartree/Particle)
Thermal correction to Energy= 0.146408
Thermal correction to Enthalpy= 0.147352
Thermal correction to Gibbs Free Energy= 0.104963
Sum of electronic and zero-point Energies= -401.269414
Sum of electronic and thermal Energies= -401.261226
Sum of electronic and thermal Enthalpies= -401.260282
Sum of electronic and thermal Free Energies= -401.302670
Electronic energy at ROCBS-QB3= -400.885994

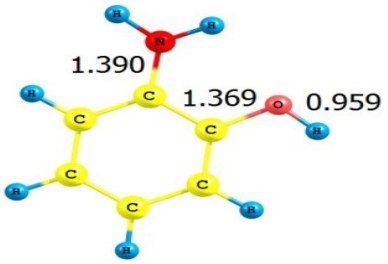


H_2O

8	0.000000000	0.000000000	0.116345000
1	0.000000000	0.761603000	-0.465380000
1	0.000000000	-0.761603000	-0.465380000

Zero-point correction= 0.021671 (Hartree/Particle)
Thermal correction to Energy= 0.024506

Thermal correction to Enthalpy= 0.025450
Thermal correction to Gibbs Free Energy= 0.004040
Sum of electronic and zero-point Energies= -76.403226
Sum of electronic and thermal Energies= -76.400390
Sum of electronic and thermal Enthalpies= -76.399446
Sum of electronic and thermal Free Energies= -76.420857
Electronic energy at ROCBS-QB3= -76.358593

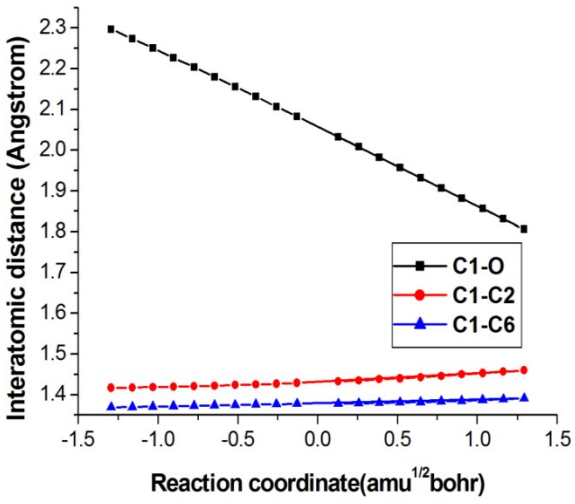


2AP

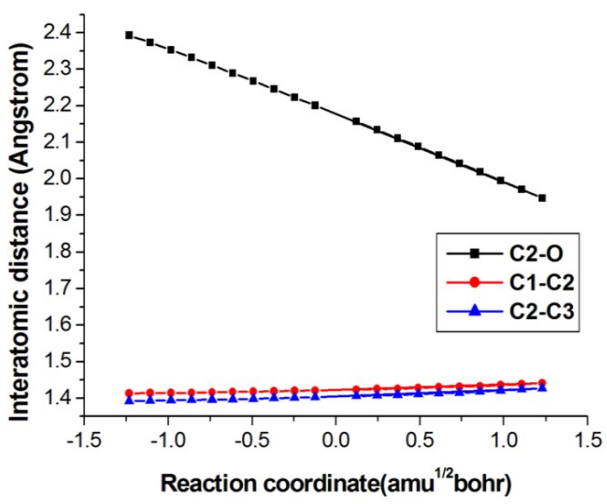
6	1.925318000	0.627841000	0.005752000
6	0.741536000	1.358222000	0.001471000
6	1.869559000	-0.755643000	0.004727000
1	0.764633000	2.442009000	0.006387000
1	2.780477000	-1.337567000	0.009419000
6	-0.478247000	0.710150000	-0.005061000
6	0.641875000	-1.405198000	-0.003470000
1	0.597818000	-2.487245000	-0.011892000
6	-0.548967000	-0.688515000	-0.009607000
1	2.875514000	1.141935000	0.010880000
7	-1.793838000	-1.303438000	-0.074390000
1	-1.833309000	-2.235913000	0.302155000
1	-2.564623000	-0.723703000	0.217197000
8	-1.679616000	1.366160000	0.000718000
1	-1.533155000	2.314132000	0.017968000

Zero-point correction= 0.122481 (Hartree/Particle)
Thermal correction to Energy= 0.129377
Thermal correction to Enthalpy= 0.130322
Thermal correction to Gibbs Free Energy= 0.091969
Sum of electronic and zero-point Energies= -362.680413
Sum of electronic and thermal Energies= -362.673516
Sum of electronic and thermal Enthalpies= -362.672572
Sum of electronic and thermal Free Energies= -362.710924
Electronic energy at ROCBS-QB3= -362.338295

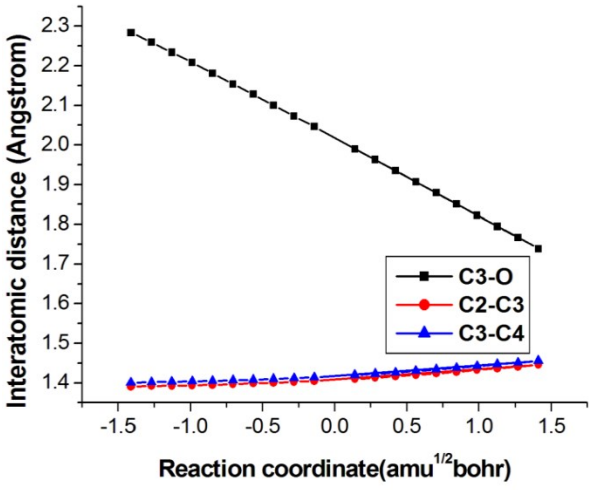
Table S2. Variation of bond distances along the reaction coordinates for OH reaction with O-AND.



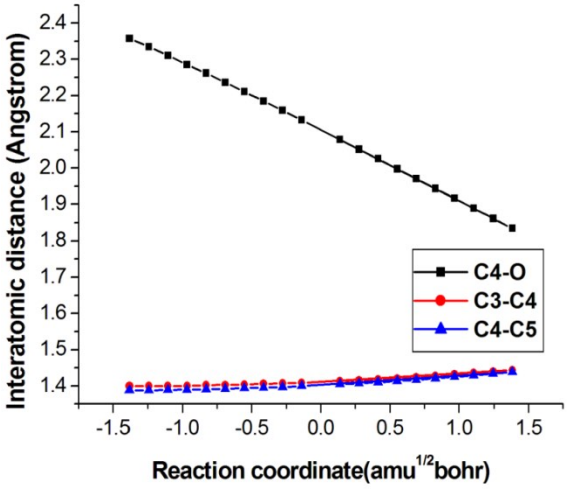
TS1



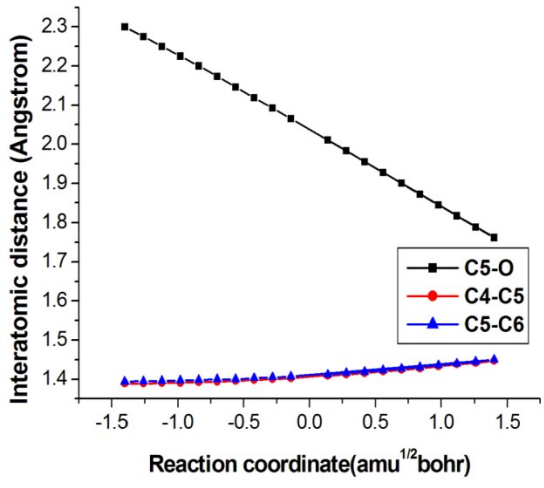
TS2



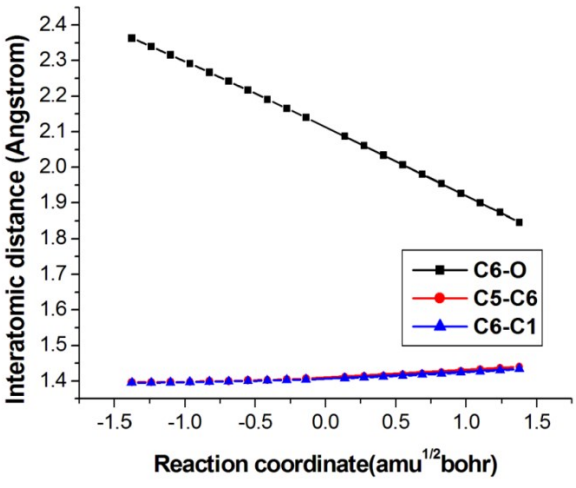
TS3



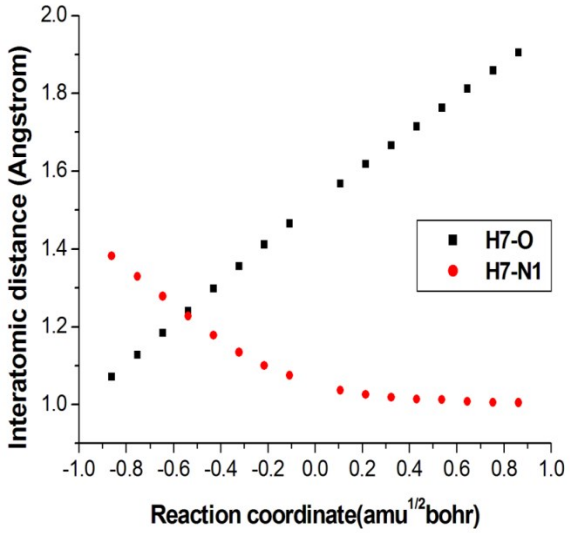
TS4



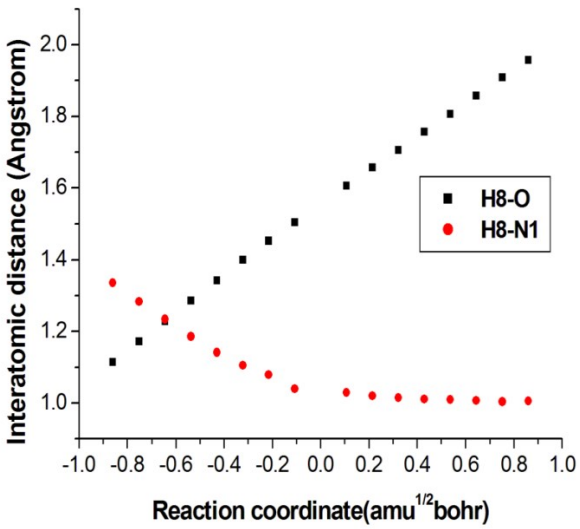
TS5



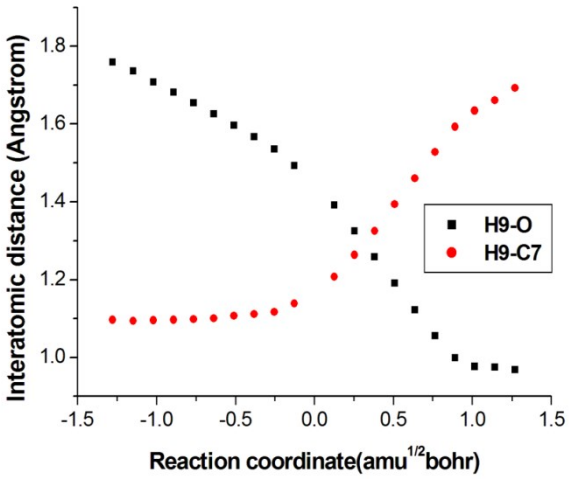
TS6



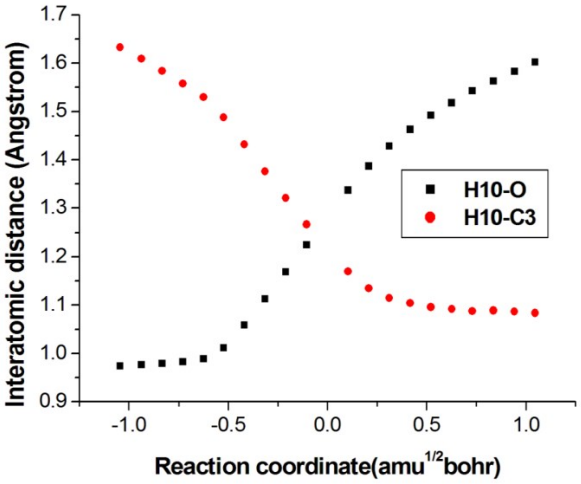
TS7



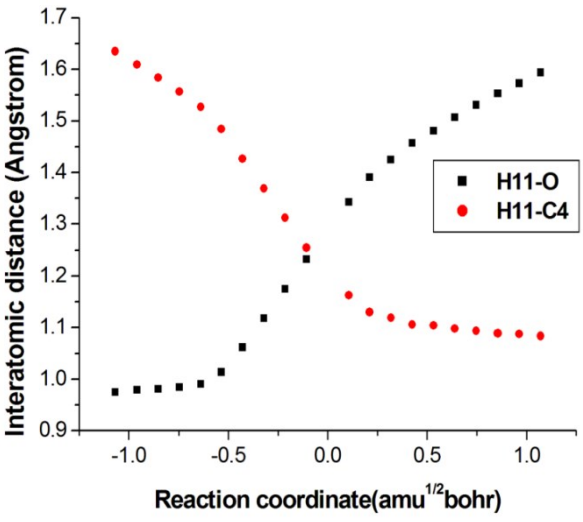
TS8



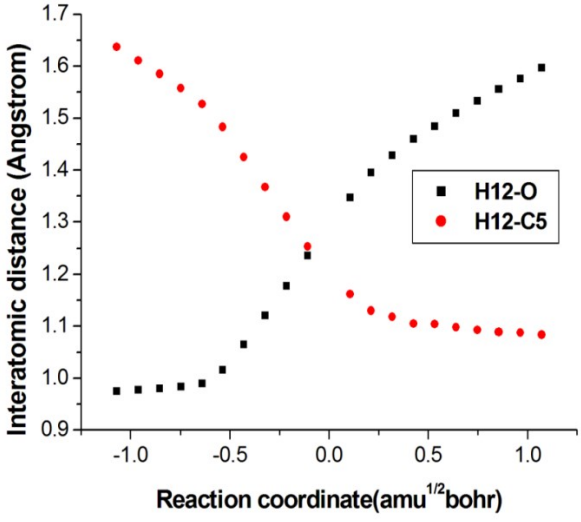
TS9



TS10



TS11



TS12

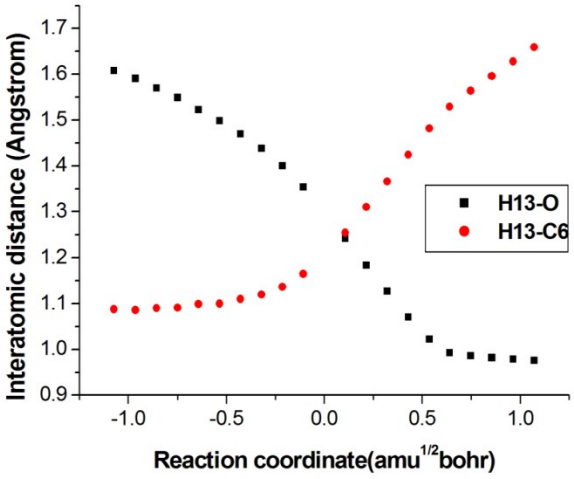
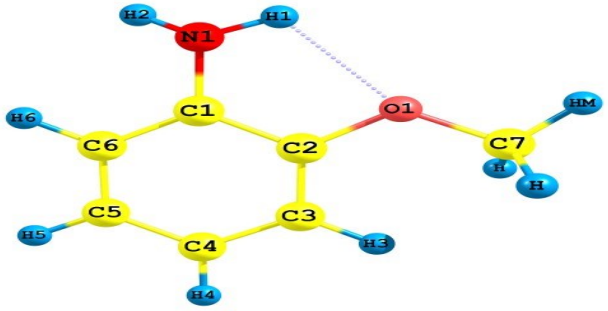
 Interatomic distance (Angstrom) 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 -1.0 -0.5 0.0 0.5 1.0 Reaction coordinate(amu^1/2bohr) H13-O H13-C6	
TS13	

Table S3. Geometrical parameters (bond lengths and bond angles) of O-AND obtained at different levels.



Interatomic distance (Å)	B3LYP/6-31G(d)[a]	B3LYP/6-311++G(d,p) [a]	M06-2X/6-311++G(2df,2p)
C1-C2	1.416	1.413	1.406
C2-C3	1.392	1.390	1.383
C3-C4	1.401	1.399	1.394
C4-C5	1.391	1.389	1.382
C5-C6	1.398	1.395	1.390
C1-C6	1.398	1.396	1.387
C2-O	1.376	1.374	1.364
C7-O	1.416	1.420	1.408
C1-N	1.397	1.394	1.389
N-H1	1.012	1.010	1.007
N-H2	1.012	1.009	1.006
C3-H3	1.086	1.084	1.080
C4-H4	1.086	1.084	1.080
C5-H5	1.086	1.084	1.080
C6-H6	1.086	1.084	1.080
C-H (meth.	1.096	1.093	1.093
Bond angle			
C1-C2-C3	120.6	120.6	120.6
C2-C3-C4	120.1	120.2	120.1
C3-C4-C5	119.8	119.7	119.8
C4-C5-C6	120.1	120.1	120.1
C5-C6-C1	121.0	121.1	121.0
C6-C1-C2	118.3	118.3	118.5
N-C1-C2	119.2	119.3	119.0
N-C1-C6	122.4	122.3	122.5
C1-N-HN1	113.5	114.7	114.6
C1-N-HN2	114.5	115.7	115.4
H-N-H	112.3	113.5	113.5
H_{met}-C-H_{meta}	109.3	109.4	109.4
C2-O-C7	118.1	118.5	117.6
C1-C2-O	114.2	114.4	114.6
C3-C2-O	125.1	125.0	124.8

.

Table S4. Calculated excitation energies (eV), wavelengths (nm), and oscillator strength (f, in a.u.) using TDDFT/6-311++G(2df,2p)//M06-2X/6-311++G(2df,2p) level of theory

Structure	Contributions	Excitation energy (eV)	Wavelength (nm)	Oscillator Strength (f, in a.u.)
P1	Homo→Lumo + 2 (43%)	5.4299	228.34	0.0013
P2	Homo→Lumo + 3 (40%)	4.7289	262.18	0.0328
P3	Homo→Lumo + 5 (52%)	5.5254	224.39	0.0207
P4	Homo→Lumo + 5 (45%)	4.8550	255.38	0.0450
P5	Homo→Lumo + 2 (52%)	5.3328	232.50	0.0029
P6	Homo→Lumo + 3 (43%)	5.1897	238.91	0.0495
P7---H_2O	Homo-4→Lumo+2 (52%)	5.3226	232.94	0.0325
P8---H_2O	Homo-4→Lumo+2 (45%)	5.5215	224.55	0.0058
P9---H_2O	Homo-5→Lumo + 1 (61%)	4.7701	259.92	0.0003
P10---H_2O	Homo→Lumo + 5 (70%)	4.8616	255.03	0.0021
P11---H_2O	Homo→Lumo + 5 (73%)	5.0225	246.86	0.0120
P12---H_2O	Homo→Lumo + 3 (75%)	5.1067	242.78	0.0183
P13---H_2O	Homo→Lumo + 6 (65%)	5.0921	243.48	0.0031

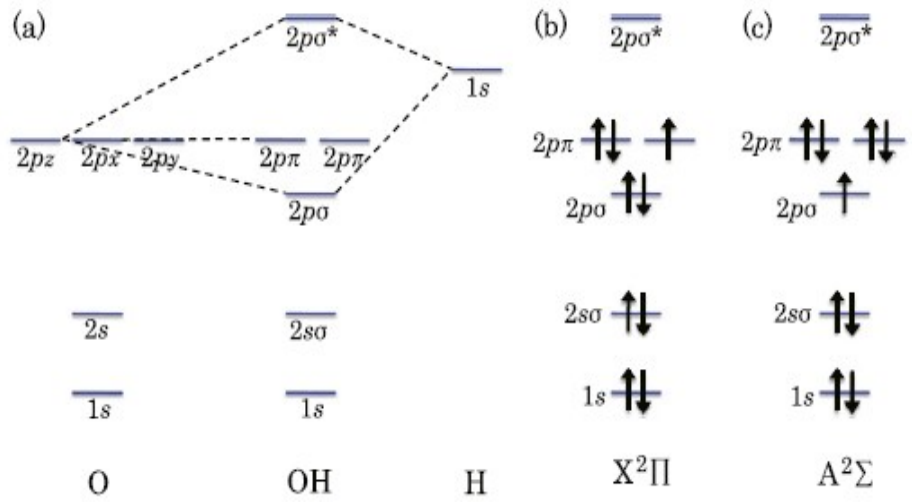
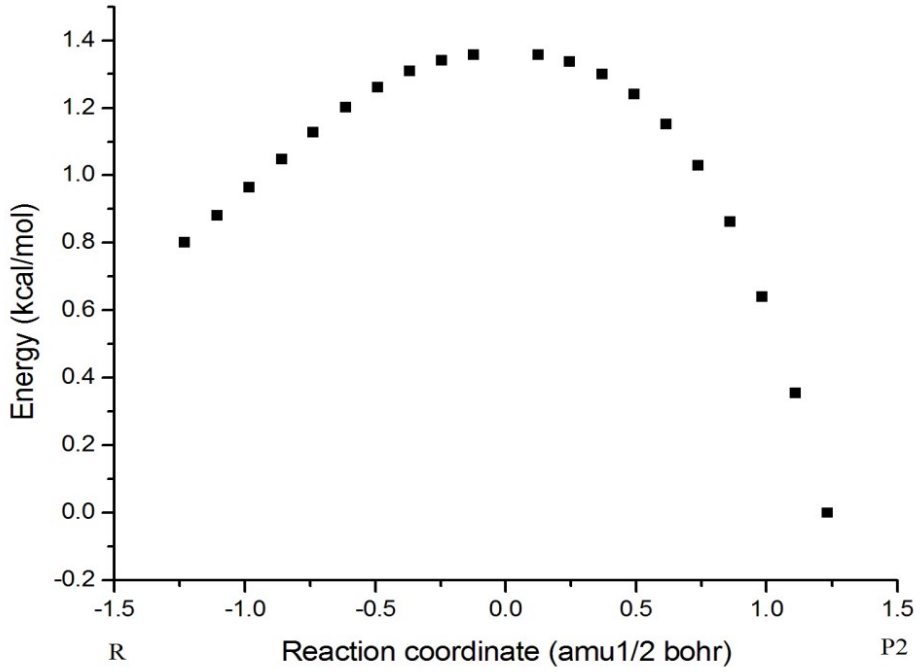
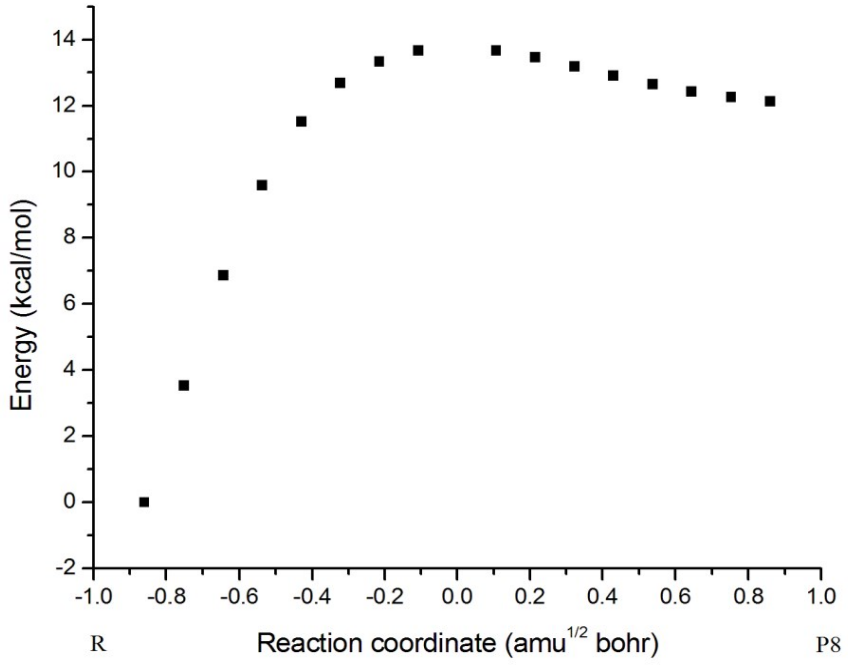


Fig S1. (a) Energy level diagram of electrons in O, H atoms and OH molecule. (b) Electronic configuration in the ground state $X^2\Pi$, and (c) in the first excited $A^2\Sigma$ state.



(a)



(b)

Fig S2. Relative energies (kcal/mol) vs. IRC for main OH addition reaction (a) P2 and H abstraction reaction (b) P8.