Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Atmospheric chemistry of oxazole: The mechanism and kinetic studies on oxidation reaction initiated by OH radicals

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Electronic Supplementary Information

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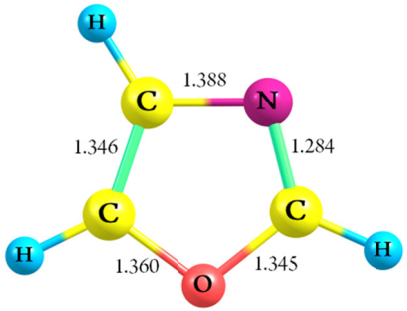
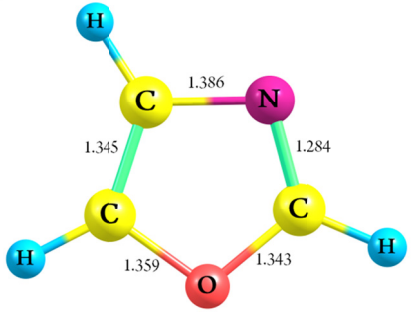
Table S1: Optimize structures of reactants, Pre-reactive complexes, products, and transitions states at M06-2x/ aug-cc-pVTZ and ωB97XD/aug-cc-pVTZ levels.



Oxazole [M06-2x]

6	-0.596128000	-0.958006000	0.000000000
6	0.747760000	-0.876311000	0.000000000
6	0.000000000	1.095687000	0.000000000
1	-1.308232000	-1.761359000	0.000000000
1	1.474977000	-1.668136000	0.000000000
1	-0.165749000	2.159282000	0.000000000
7	1.116500000	0.461873000	0.000000000
8	-1.090786000	0.308611000	0.000000000

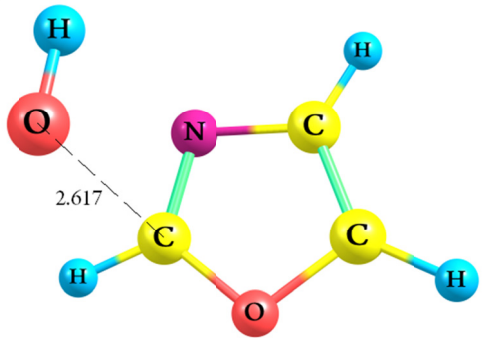
Zero-point correction=	0.059179 (Hartree/Particle)
Thermal correction to Energy=	0.062680
Thermal correction to Enthalpy=	0.063624
Thermal correction to Gibbs Free Energy=	0.033044
Sum of electronic and zero-point Energies=	-246.011529
Sum of electronic and thermal Energies=	-246.008028
Sum of electronic and thermal Enthalpies=	-246.007083
Sum of electronic and thermal Free Energies=	-246.037663



Oxazole [ωB97XD]

6	-0.596049000	-0.956351000	0.000000000
6	0.746766000	-0.875546000	0.000000000
6	0.000000000	1.093744000	0.000000000
1	-1.310086000	-1.757977000	0.000000000
1	1.474018000	-1.667682000	0.000000000
1	-0.162840000	2.157816000	0.000000000
7	1.117214000	0.460010000	0.000000000
8	-1.090737000	0.309586000	0.000000000

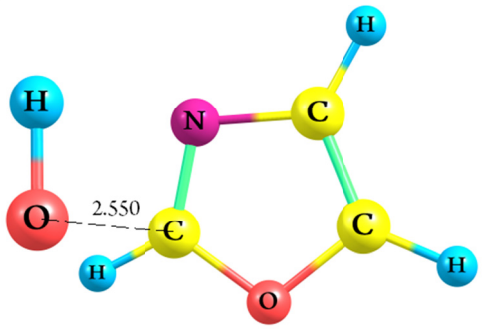
Zero-point correction=	0.059429 (Hartree/Particle)
Thermal correction to Energy=	0.062928
Thermal correction to Enthalpy=	0.063872
Thermal correction to Gibbs Free Energy=	0.033297
Sum of electronic and zero-point Energies=	-246.018359
Sum of electronic and thermal Energies=	-246.014860
Sum of electronic and thermal Enthalpies=	-246.013916
Sum of electronic and thermal Free Energies=	-246.044491



IM1 [M06-2x]

6	-1.323826000	-0.182142000	-0.670959000
6	-0.950557000	1.017070000	-0.185514000
6	0.143602000	-0.458995000	0.858061000
7	0.001608000	0.821365000	0.804851000
8	-0.627732000	-1.138044000	-0.002658000
8	2.266250000	-0.030935000	-0.611510000
1	-2.008624000	-0.514974000	-1.427790000
1	-1.286981000	1.998276000	-0.467333000
1	0.793152000	-1.032643000	1.496598000
1	2.167730000	0.896024000	-0.331620000

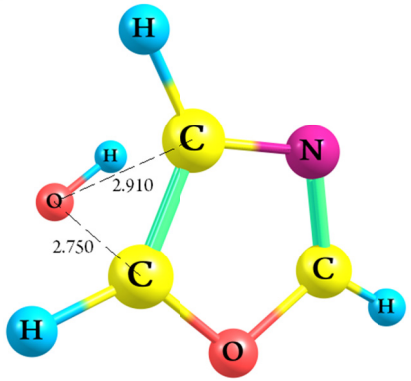
Zero-point correction=	0.070166 (Hartree/Particle)
Thermal correction to Energy=	0.076644
Thermal correction to Enthalpy=	0.077588
Thermal correction to Gibbs Free Energy=	0.038482
Sum of electronic and zero-point Energies=	-321.741970
Sum of electronic and thermal Energies=	-321.735492
Sum of electronic and thermal Enthalpies=	-321.734548
Sum of electronic and thermal Free Energies=	-321.773655



IM1 [ωB97XD]

6	-1.357658000	-0.256124000	-0.619097000
6	-1.014473000	0.983125000	-0.218753000
6	0.195587000	-0.387127000	0.836906000
7	-0.010748000	0.884644000	0.727106000
8	-0.589179000	-1.143759000	0.059696000
8	2.277406000	-0.046020000	-0.595635000
1	-2.065729000	-0.658666000	-1.318396000
1	-1.408669000	1.932149000	-0.535029000
1	0.882695000	-0.895803000	1.489447000
1	2.220392000	0.908795000	-0.432596000

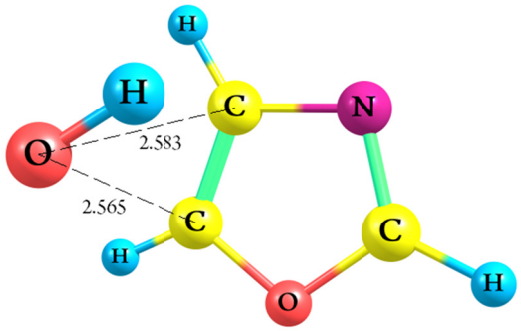
Zero-point correction=	0.070062 (Hartree/Particle)
Thermal correction to Energy=	0.076585
Thermal correction to Enthalpy=	0.077529
Thermal correction to Gibbs Free Energy=	0.038363
Sum of electronic and zero-point Energies=	-321.754459
Sum of electronic and thermal Energies=	-321.747936
Sum of electronic and thermal Enthalpies=	-321.746992
Sum of electronic and thermal Free Energies=	-321.786158



IM$_x$ (x=2,3) [M06-2x]

6	-0.046239000	-0.486922000	0.950119000
6	0.104235000	0.844065000	0.770500000
6	1.230504000	-0.127550000	-0.725968000
1	-0.591253000	-1.099420000	1.642882000
1	-0.318795000	1.654027000	1.337239000
1	1.857214000	-0.414544000	-1.552888000
7	0.929253000	1.056435000	-0.325258000
8	0.683530000	-1.118885000	-0.001640000
8	-2.338019000	-0.079013000	-0.514071000
1	-1.947027000	0.670519000	-0.992637000

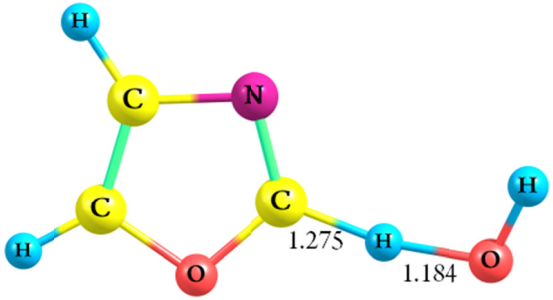
Zero-point correction=	0.069738 (Hartree/Particle)
Thermal correction to Energy=	0.075561
Thermal correction to Enthalpy=	0.076505
Thermal correction to Gibbs Free Energy=	0.038801
Sum of electronic and zero-point Energies=	-321.741909
Sum of electronic and thermal Energies=	-321.736086
Sum of electronic and thermal Enthalpies=	-321.735142
Sum of electronic and thermal Free Energies=	-321.772846



IM$_x$ (x=2,3) [ωB97XD]

6	-0.099207000	0.744972000	0.732443000
6	-0.137036000	-0.602836000	0.862203000
6	1.309361000	-0.145089000	-0.599861000
7	0.778017000	-1.159561000	-0.015778000
8	0.837307000	1.047405000	-0.195350000
8	-2.186404000	0.032292000	-0.576451000
1	-0.620753000	1.561976000	1.192545000
1	-0.745628000	-1.200567000	1.515528000
1	2.071849000	-0.136368000	-1.359417000
1	-1.797521000	-0.727963000	-1.032502000

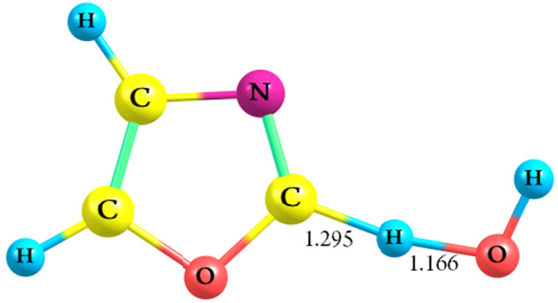
Zero-point correction=	0.070513 (Hartree/Particle)
Thermal correction to Energy=	0.077020
Thermal correction to Enthalpy=	0.077965
Thermal correction to Gibbs Free Energy=	0.038691
Sum of electronic and zero-point Energies=	-321.755047
Sum of electronic and thermal Energies=	-321.748540
Sum of electronic and thermal Enthalpies=	-321.747596
Sum of electronic and thermal Free Energies=	-321.786869



TS1 [M06-2x]

6	0.371065000	-0.012262000	-0.065975000
6	-1.672584000	-0.584800000	0.039120000
6	-1.575445000	0.757016000	0.022464000
1	-2.354781000	1.496829000	0.051937000
1	-2.480263000	-1.290881000	0.081116000
8	2.802284000	-0.097946000	0.014972000
8	-0.403602000	-1.098243000	-0.013861000
7	-0.225437000	1.110975000	-0.040767000
1	1.630204000	-0.204082000	-0.119046000
1	2.855226000	0.831100000	0.288819000

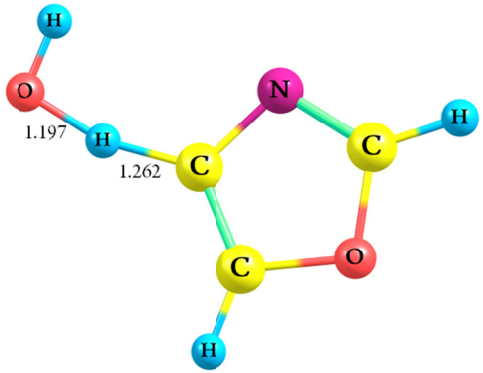
Zero-point correction=	0.063807 (Hartree/Particle)
Thermal correction to Energy=	0.069942
Thermal correction to Enthalpy=	0.070886
Thermal correction to Gibbs Free Energy=	0.032403
Sum of electronic and zero-point Energies=	-321.723173
Sum of electronic and thermal Energies=	-321.717038
Sum of electronic and thermal Enthalpies=	-321.716094
Sum of electronic and thermal Free Energies=	-321.754577



TS1 [ωB97XD]

6	0.365827000	0.008588000	-0.051436000
6	-1.663234000	-0.601713000	0.030948000
6	-1.591174000	0.740892000	0.017517000
1	-2.384361000	1.466370000	0.038647000
1	-2.456918000	-1.323938000	0.061720000
8	2.805785000	-0.099529000	0.007058000
8	-0.384658000	-1.091660000	-0.009558000
7	-0.250110000	1.120221000	-0.031230000
1	1.647115000	-0.169406000	-0.101076000
1	2.907399000	0.828338000	0.257145000

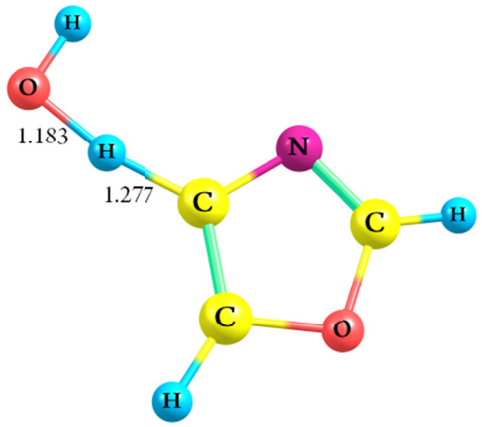
Zero-point correction=	0.063880 (Hartree/Particle)
Thermal correction to Energy=	0.070114
Thermal correction to Enthalpy=	0.071059
Thermal correction to Gibbs Free Energy=	0.031718
Sum of electronic and zero-point Energies=	-321.739428
Sum of electronic and thermal Energies=	-321.733194
Sum of electronic and thermal Enthalpies=	-321.732250
Sum of electronic and thermal Free Energies=	-321.771590



TS2 [M06-2x]

6	-0.523930000	1.129428000	0.000006000
6	-1.439549000	-0.810514000	0.000020000
6	0.410142000	0.161325000	-0.000122000
1	-2.265543000	-1.500507000	0.000061000
1	-0.518886000	2.201770000	0.000041000
8	2.842462000	0.067917000	-0.000009000
7	-0.178156000	-1.072634000	-0.000088000
8	-1.734134000	0.499319000	0.000078000
1	1.665855000	0.289198000	-0.000249000
1	2.819067000	-0.901349000	0.000794000

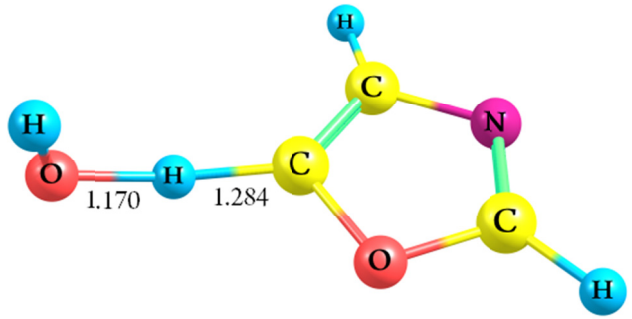
Zero-point correction=	0.064390 (Hartree/Particle)
Thermal correction to Energy=	0.070340
Thermal correction to Enthalpy=	0.071284
Thermal correction to Gibbs Free Energy=	0.033625
Sum of electronic and zero-point Energies=	-321.724662
Sum of electronic and thermal Energies=	-321.718712
Sum of electronic and thermal Enthalpies=	-321.717768
Sum of electronic and thermal Free Energies=	-321.755426



TS2 [ωB97XD**]**

6	0.493547000	1.120068000	0.000106000
6	1.468978000	-0.786337000	0.000033000
6	-0.407401000	0.123092000	-0.000051000
1	2.314132000	-1.452684000	0.000049000
1	0.451133000	2.191740000	0.000191000
8	-2.852739000	0.069540000	-0.000142000
7	0.215778000	-1.088066000	-0.000092000
8	1.723436000	0.530629000	0.000156000
1	-1.680348000	0.230726000	-0.000155000
1	-2.891684000	-0.895610000	-0.000075000

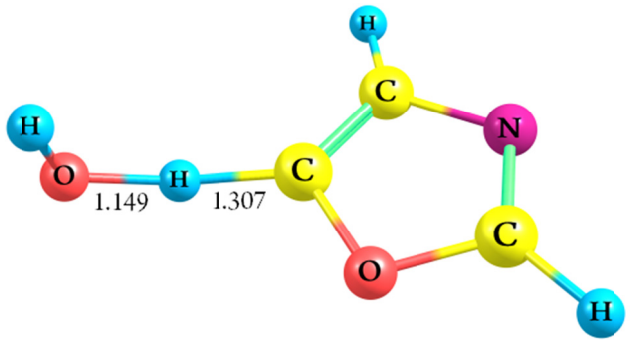
Zero-point correction=	0.064191 (Hartree/Particle)
Thermal correction to Energy=	0.070256
Thermal correction to Enthalpy=	0.071200
Thermal correction to Gibbs Free Energy=	0.033183
Sum of electronic and zero-point Energies=	-321.741386
Sum of electronic and thermal Energies=	-321.735321
Sum of electronic and thermal Enthalpies=	-321.734377
Sum of electronic and thermal Free Energies=	-321.772394



TS3 [M06-2x]

6	-0.390853000	0.150560000	-0.107835000
6	1.553906000	-0.686289000	0.041138000
6	0.502695000	1.154213000	-0.016607000
1	0.343133000	2.216146000	-0.019285000
1	2.271440000	-1.487428000	0.084318000
8	0.253529000	-1.033323000	-0.058470000
7	1.765541000	0.580845000	0.067639000
8	-2.812756000	-0.018864000	-0.031765000
1	-1.668394000	0.114539000	-0.235823000
1	-2.825641000	-0.202578000	0.919021000

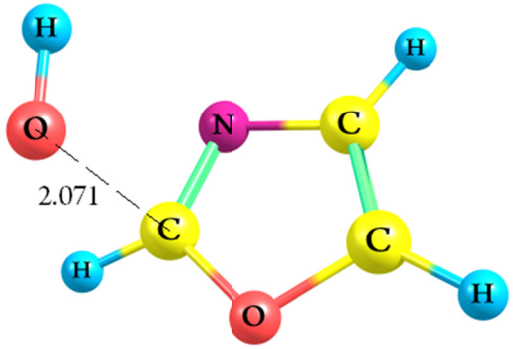
Zero-point correction=	0.064307 (Hartree/Particle)
Thermal correction to Energy=	0.070242
Thermal correction to Enthalpy=	0.071186
Thermal correction to Gibbs Free Energy=	0.033593
Sum of electronic and zero-point Energies=	-321.721477
Sum of electronic and thermal Energies=	-321.715542
Sum of electronic and thermal Enthalpies=	-321.714598
Sum of electronic and thermal Free Energies=	-321.752191



TS3 [ωB97XD]

6	-0.388064000	0.128871000	-0.097902000
6	1.567318000	-0.670659000	0.039203000
6	0.485642000	1.149304000	-0.016394000
1	0.305600000	2.208203000	-0.022103000
1	2.301817000	-1.456314000	0.076179000
8	0.274717000	-1.042527000	-0.047352000
7	1.757373000	0.600886000	0.058393000
8	-2.817801000	-0.025455000	-0.040554000
1	-1.688203000	0.077136000	-0.225855000
1	-2.865529000	-0.136470000	0.916822000

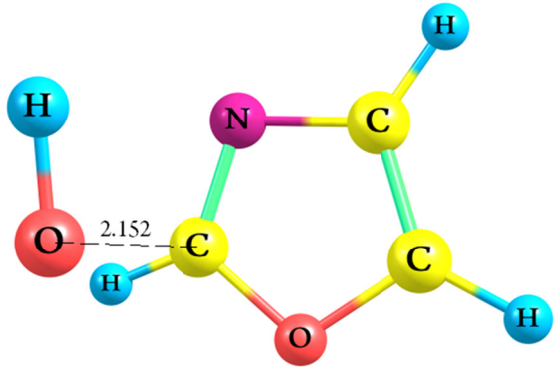
Zero-point correction=	0.064239 (Hartree/Particle)
Thermal correction to Energy=	0.070300
Thermal correction to Enthalpy=	0.071244
Thermal correction to Gibbs Free Energy=	0.033284
Sum of electronic and zero-point Energies=	-321.737826
Sum of electronic and thermal Energies=	-321.731764
Sum of electronic and thermal Enthalpies=	-321.730820
Sum of electronic and thermal Free Energies=	-321.768780



TS4 [M06-2x]

6	-1.290904000	-0.495083000	-0.449492000
6	-1.127628000	0.840630000	-0.275846000
6	0.424971000	-0.145700000	0.775276000
7	-0.046400000	1.054352000	0.537019000
8	-0.328037000	-1.131222000	0.247976000
8	1.934169000	-0.067684000	-0.640916000
1	-1.986957000	-1.103868000	-0.996087000
1	-1.712479000	1.647511000	-0.679949000
1	1.160383000	-0.427210000	1.506988000
1	1.976164000	0.895263000	-0.746192000

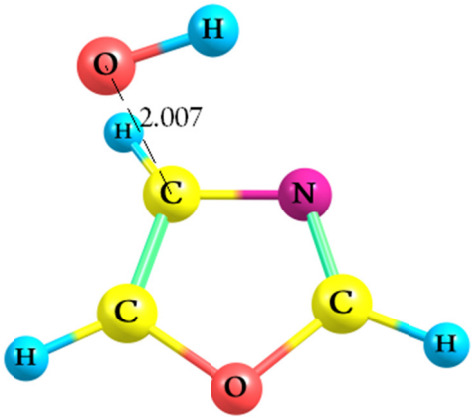
Zero-point correction=	0.070312 (Hartree/Particle)
Thermal correction to Energy=	0.075635
Thermal correction to Enthalpy=	0.076579
Thermal correction to Gibbs Free Energy=	0.040837
Sum of electronic and zero-point Energies=	-321.736867
Sum of electronic and thermal Energies=	-321.731544
Sum of electronic and thermal Enthalpies=	-321.730600
Sum of electronic and thermal Free Energies=	-321.766342



TS4 [ωB97XD**]**

6	-1.310236000	-0.469574000	-0.471247000
6	-1.124289000	0.857164000	-0.276449000
6	0.388419000	-0.172643000	0.784558000
7	-0.048577000	1.038416000	0.552663000
8	-0.365860000	-1.134958000	0.226028000
8	2.010584000	-0.065499000	-0.624900000
1	-2.009365000	-1.057948000	-1.035579000
1	-1.686650000	1.682320000	-0.675922000
1	1.123004000	-0.478200000	1.506541000
1	2.031902000	0.898896000	-0.693881000

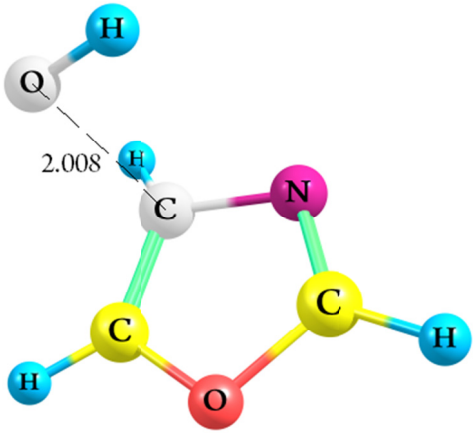
Zero-point correction=	0.070519 (Hartree/Particle)
Thermal correction to Energy=	0.075914
Thermal correction to Enthalpy=	0.076858
Thermal correction to Gibbs Free Energy=	0.040864
Sum of electronic and zero-point Energies=	-321.753036
Sum of electronic and thermal Energies=	-321.747641
Sum of electronic and thermal Enthalpies=	-321.746697
Sum of electronic and thermal Free Energies=	-321.782691



TS5 [M06-2x]

6	0.114307000	1.080330000	0.342159000
6	-0.499179000	-0.067174000	0.792962000
6	1.226638000	-0.627715000	-0.305094000
7	0.291899000	-1.151785000	0.391374000
8	1.188941000	0.724501000	-0.387605000
8	-1.948547000	-0.005155000	-0.594178000
1	-0.133911000	2.123617000	0.391336000
1	-1.239526000	-0.167356000	1.563568000
1	2.033157000	-1.119103000	-0.822503000
1	-1.676760000	-0.842075000	-0.997916000

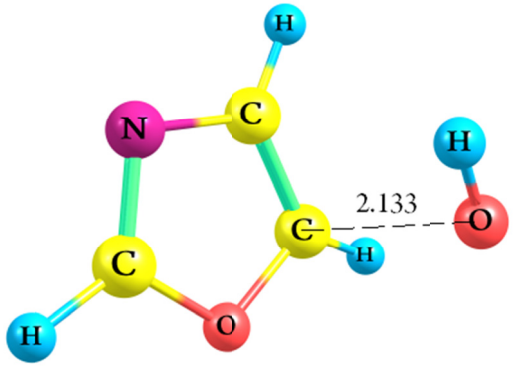
Zero-point correction=	0.070720 (Hartree/Particle)
Thermal correction to Energy=	0.076171
Thermal correction to Enthalpy=	0.077115
Thermal correction to Gibbs Free Energy=	0.040977
Sum of electronic and zero-point Energies=	-321.733282
Sum of electronic and thermal Energies=	-321.727831
Sum of electronic and thermal Enthalpies=	-321.726887
Sum of electronic and thermal Free Energies=	-321.763025



TS5 [ωB97XD]

6	0.121061000	1.077273000	0.337965000
6	-0.499425000	-0.072554000	0.777260000
6	1.237931000	-0.625717000	-0.302726000
7	0.295817000	-1.154568000	0.380729000
8	1.203918000	0.724455000	-0.382662000
8	-1.982147000	-0.001512000	-0.574550000
1	-0.122198000	2.120913000	0.396453000
1	-1.229475000	-0.172644000	1.557519000
1	2.050659000	-1.116513000	-0.810844000
1	-1.701276000	-0.807333000	-1.025530000

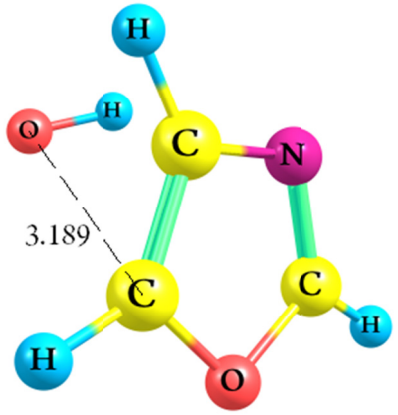
Zero-point correction=	0.070495 (Hartree/Particle)
Thermal correction to Energy=	0.075980
Thermal correction to Enthalpy=	0.076924
Thermal correction to Gibbs Free Energy=	0.040697
Sum of electronic and zero-point Energies=	-321.750429
Sum of electronic and thermal Energies=	-321.744944
Sum of electronic and thermal Enthalpies=	-321.744000
Sum of electronic and thermal Free Energies=	-321.780227



TS6 [M06-2x]

6	-0.406737000	-0.204550000	0.817096000
6	0.073657000	1.033409000	0.480563000
6	1.301744000	-0.398447000	-0.454102000
1	-1.130647000	-0.558336000	1.524812000
1	-0.307034000	1.997966000	0.765630000
1	2.039867000	-0.943469000	-1.017154000
7	1.153210000	0.878553000	-0.360599000
8	0.417198000	-1.120347000	0.254532000
8	-2.013031000	-0.107917000	-0.583341000
1	-1.719977000	0.597612000	-1.179964000

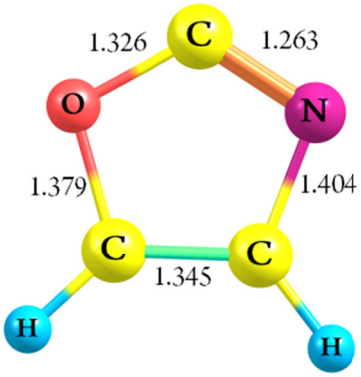
Zero-point correction=	0.070463 (Hartree/Particle)
Thermal correction to Energy=	0.075935
Thermal correction to Enthalpy=	0.076879
Thermal correction to Gibbs Free Energy=	0.040626
Sum of electronic and zero-point Energies=	-321.739076
Sum of electronic and thermal Energies=	-321.733605
Sum of electronic and thermal Enthalpies=	-321.732661
Sum of electronic and thermal Free Energies=	-321.768914



TS6 [ωB97XD**]**

6	-0.545050000	1.146516000	0.059331000
6	0.119714000	0.402011000	0.963746000
6	-0.977304000	-0.918671000	-0.263007000
1	-0.617614000	2.197045000	-0.148811000
1	0.780295000	0.719628000	1.749936000
1	-1.443015000	-1.752523000	-0.759333000
7	-0.170809000	-0.937170000	0.738056000
8	-1.258249000	0.306775000	-0.731782000
8	2.366572000	0.001257000	-0.560118000
1	2.025257000	-0.847349000	-0.233409000

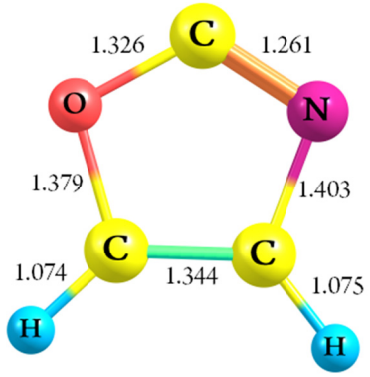
Zero-point correction=	0.070170 (Hartree/Particle)
Thermal correction to Energy=	0.075825
Thermal correction to Enthalpy=	0.076769
Thermal correction to Gibbs Free Energy=	0.039664
Sum of electronic and zero-point Energies=	-321.754198
Sum of electronic and thermal Energies=	-321.748542
Sum of electronic and thermal Enthalpies=	-321.747598
Sum of electronic and thermal Free Energies=	-321.784703



P1 [M06-2x]

6	0.000000000	1.082626000	0.000000000
6	1.069781000	0.268192000	0.000000000
6	-0.627053000	-0.938171000	0.000000000
7	0.629320000	-1.065168000	0.000000000
8	-1.127972000	0.289779000	0.000000000
1	-0.153417000	2.144980000	0.000000000
1	2.115589000	0.517073000	0.000000000

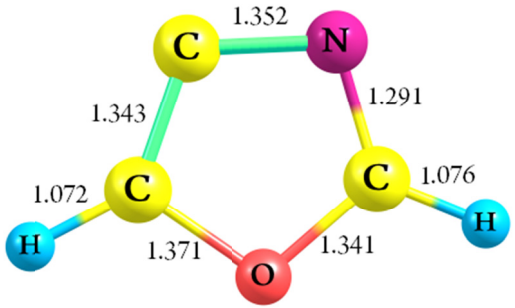
Zero-point correction=	0.046440 (Hartree/Particle)
Thermal correction to Energy=	0.049913
Thermal correction to Enthalpy=	0.050857
Thermal correction to Gibbs Free Energy=	0.019742
Sum of electronic and zero-point Energies=	-245.327971
Sum of electronic and thermal Energies=	-245.324498
Sum of electronic and thermal Enthalpies=	-245.323554
Sum of electronic and thermal Free Energies=	-245.354669



P1 [ωB97XD]

6	0.000000000	1.081160000	0.000000000
6	1.070038000	0.267744000	0.000000000
6	-0.625021000	-0.936708000	0.000000000
7	0.629093000	-1.063942000	0.000000000
8	-1.129605000	0.289339000	0.000000000
1	-0.153182000	2.143738000	0.000000000
1	2.116264000	0.515965000	0.000000000

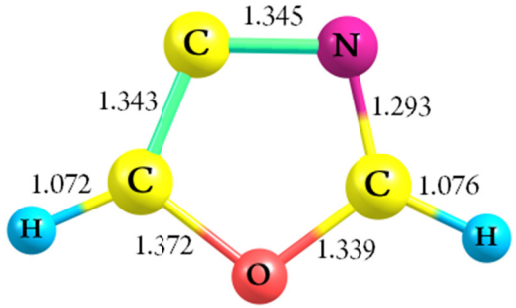
Zero-point correction=	0.046142 (Hartree/Particle)
Thermal correction to Energy=	0.049657
Thermal correction to Enthalpy=	0.050601
Thermal correction to Gibbs Free Energy=	0.019429
Sum of electronic and zero-point Energies=	-245.329437
Sum of electronic and thermal Energies=	-245.325922
Sum of electronic and thermal Enthalpies=	-245.324977
Sum of electronic and thermal Free Energies=	-245.356149



P2 [M06-2x]

6	-0.513477000	-1.039598000	0.000000000
6	0.817270000	-0.862062000	0.000000000
6	0.000000000	1.046167000	0.000000000
1	-0.201368000	2.103548000	0.000000000
7	1.145136000	0.449190000	0.000000000
8	-1.056321000	0.219805000	0.000000000
1	-1.186773000	-1.873356000	0.000000000

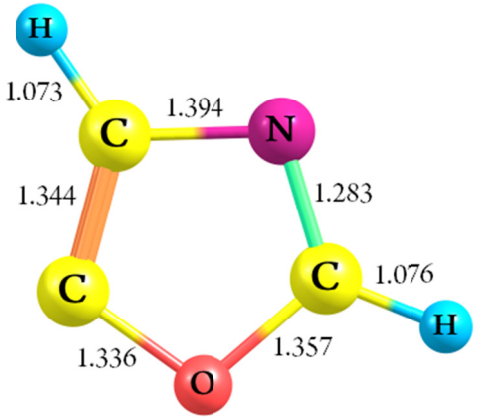
Zero-point correction=	0.046773 (Hartree/Particle)
Thermal correction to Energy=	0.050216
Thermal correction to Enthalpy=	0.051161
Thermal correction to Gibbs Free Energy=	0.020100
Sum of electronic and zero-point Energies=	-245.328187
Sum of electronic and thermal Energies=	-245.324744
Sum of electronic and thermal Enthalpies=	-245.323799
Sum of electronic and thermal Free Energies=	-245.354860



P2 [ωB97XD]

6	-0.513353000	-1.038697000	0.000000000
6	0.817234000	-0.859480000	0.000000000
6	0.000000000	1.044719000	0.000000000
1	-0.197379000	2.102804000	0.000000000
7	1.145151000	0.445134000	0.000000000
8	-1.056704000	0.221655000	0.000000000
1	-1.188337000	-1.871225000	0.000000000

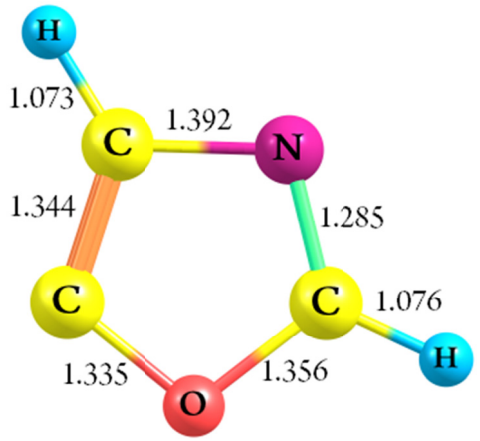
Zero-point correction=	0.046549 (Hartree/Particle)
Thermal correction to Energy=	0.050020
Thermal correction to Enthalpy=	0.050965
Thermal correction to Gibbs Free Energy=	0.019869
Sum of electronic and zero-point Energies=	-245.330085
Sum of electronic and thermal Energies=	-245.326613
Sum of electronic and thermal Enthalpies=	-245.325669
Sum of electronic and thermal Free Energies=	-245.356765



P3 [M06-2x]

6	-0.658904000	-0.957869000	0.000000000
6	0.685023000	-0.966107000	0.000000000
6	0.000000000	1.048719000	0.000000000
1	1.374715000	-1.787871000	0.000000000
1	-0.129154000	2.116885000	0.000000000
7	1.088244000	0.368548000	0.000000000
8	-1.127498000	0.292836000	0.000000000

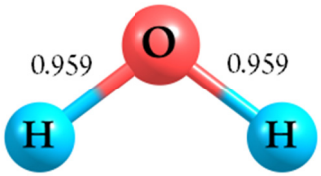
Zero-point correction= 0.046521 (Hartree/Particle)
Thermal correction to Energy= 0.049977
Thermal correction to Enthalpy= 0.050921
Thermal correction to Gibbs Free Energy= 0.019832
Sum of electronic and zero-point Energies= -245.324367
Sum of electronic and thermal Energies= -245.320911
Sum of electronic and thermal Enthalpies= -245.319967
Sum of electronic and thermal Free Energies= -245.351056



P3 [ωB97XD]

6	-0.658761000	-0.953338000	0.000000000
6	0.685577000	-0.968000000	0.000000000
6	0.000000000	1.046894000	0.000000000
1	1.374431000	-1.790673000	0.000000000
1	-0.124167000	2.115696000	0.000000000
7	1.088436000	0.364453000	0.000000000
8	-1.128776000	0.296309000	0.000000000

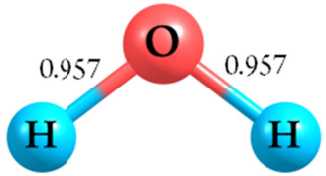
Zero-point correction= 0.046380 (Hartree/Particle)
Thermal correction to Energy= 0.049862
Thermal correction to Enthalpy= 0.050806
Thermal correction to Gibbs Free Energy= 0.019682
Sum of electronic and zero-point Energies= -245.325476
Sum of electronic and thermal Energies= -245.321994
Sum of electronic and thermal Enthalpies= -245.321050
Sum of electronic and thermal Free Energies= -245.352175



H_2O [M06-2x]

8	0.000000000	0.000000000	0.116332000
1	0.000000000	0.762680000	-0.465326000
1	0.000000000	-0.762680000	-0.465326000

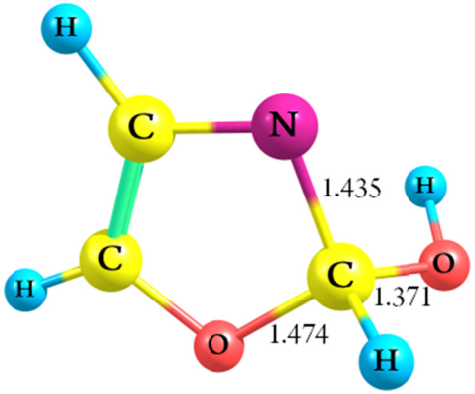
Zero-point correction=	0.021565 (Hartree/Particle)
Thermal correction to Energy=	0.024401
Thermal correction to Enthalpy=	0.025345
Thermal correction to Gibbs Free Energy=	0.003933
Sum of electronic and zero-point Energies=	-76.408527
Sum of electronic and thermal Energies=	-76.405691
Sum of electronic and thermal Enthalpies=	-76.404747
Sum of electronic and thermal Free Energies=	-76.426160



H_2O [ωB97XD**]**

8	0.000000000	0.000000000	0.116406000
1	0.000000000	0.759867000	-0.465625000
1	0.000000000	-0.759867000	-0.465625000

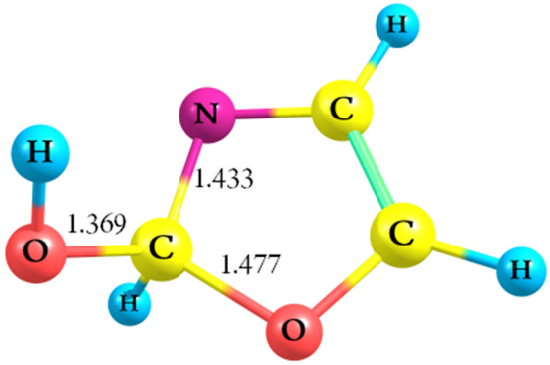
Zero-point correction=	0.021650 (Hartree/Particle)
Thermal correction to Energy=	0.024485
Thermal correction to Enthalpy=	0.025430
Thermal correction to Gibbs Free Energy=	0.004022
Sum of electronic and zero-point Energies=	-76.418273
Sum of electronic and thermal Energies=	-76.415437
Sum of electronic and thermal Enthalpies=	-76.414493
Sum of electronic and thermal Free Energies=	-76.435901



P4 [M06-2x]

6	-1.333810000	-0.644245000	-0.172594000
6	-1.281281000	0.750150000	-0.135028000
6	0.714897000	0.015909000	0.427276000
7	-0.090701000	1.182971000	0.205986000
8	-0.145380000	-1.146123000	0.142366000
8	1.843501000	-0.032429000	-0.349751000
1	-2.130123000	-1.325291000	-0.419028000
1	-2.095436000	1.420026000	-0.367561000
1	1.020442000	-0.091957000	1.468689000
1	1.656221000	0.413956000	-1.182839000

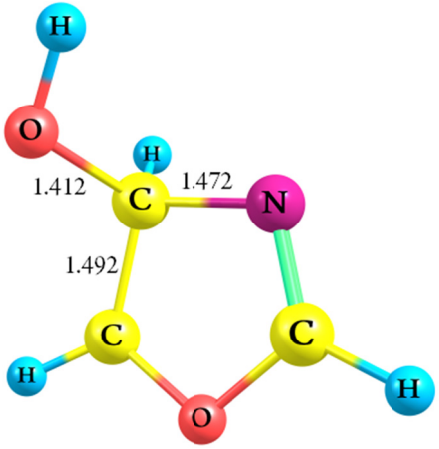
Zero-point correction=	0.074012 (Hartree/Particle)
Thermal correction to Energy=	0.078994
Thermal correction to Enthalpy=	0.079938
Thermal correction to Gibbs Free Energy=	0.045108
Sum of electronic and zero-point Energies=	-321.791099
Sum of electronic and thermal Energies=	-321.786117
Sum of electronic and thermal Enthalpies=	-321.785173
Sum of electronic and thermal Free Energies=	-321.820003



P4 [ωB97XD]

6	-1.334989000	-0.640434000	-0.170613000
6	-1.281892000	0.749652000	-0.134237000
6	0.714758000	0.016607000	0.424396000
7	-0.088529000	1.182469000	0.204141000
8	-0.148168000	-1.148368000	0.139998000
8	1.845468000	-0.033211000	-0.346501000
1	-2.131558000	-1.321177000	-0.417608000
1	-2.093166000	1.423129000	-0.365838000
1	1.016455000	-0.092870000	1.467299000
1	1.662310000	0.411325000	-1.178092000

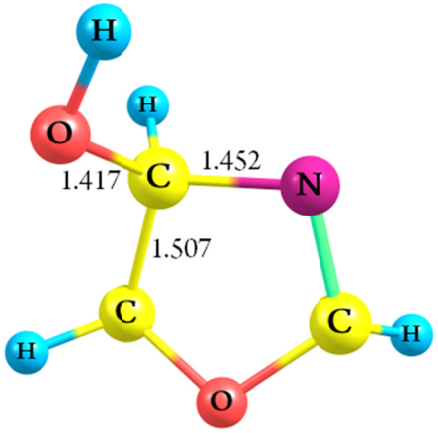
Zero-point correction=	0.073728 (Hartree/Particle)
Thermal correction to Energy=	0.078789
Thermal correction to Enthalpy=	0.079733
Thermal correction to Gibbs Free Energy=	0.044755
Sum of electronic and zero-point Energies=	-321.806060
Sum of electronic and thermal Energies=	-321.801000
Sum of electronic and thermal Enthalpies=	-321.800056
Sum of electronic and thermal Free Energies=	-321.835034



P5 [M06-2x**]**

6	0.205869000	1.140894000	0.247873000
6	-0.746371000	0.012133000	0.459667000
6	1.214522000	-0.731875000	-0.155048000
7	0.099413000	-1.170673000	0.231321000
8	1.383214000	0.621573000	-0.220348000
8	-1.802197000	0.075803000	-0.475379000
1	-0.004190000	2.168127000	0.010307000
1	-1.152344000	-0.028096000	1.474830000
1	2.077475000	-1.311283000	-0.448096000
1	-2.309095000	-0.739955000	-0.405424000

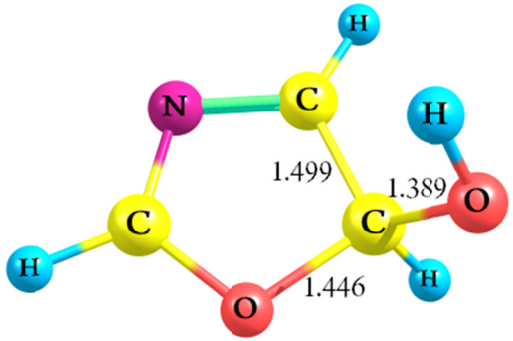
Zero-point correction= 0.073204 (Hartree/Particle)
Thermal correction to Energy= 0.078521
Thermal correction to Enthalpy= 0.079465
Thermal correction to Gibbs Free Energy= 0.044015
Sum of electronic and zero-point Energies= -321.769278
Sum of electronic and thermal Energies= -321.763961
Sum of electronic and thermal Enthalpies= -321.763017
Sum of electronic and thermal Free Energies= -321.798467



P5 [ωB97XD**]**

6	0.206007000	1.136868000	0.235093000
6	-0.744794000	0.010231000	0.450769000
6	1.219419000	-0.730241000	-0.152535000
7	0.099238000	-1.170524000	0.220971000
8	1.389425000	0.620284000	-0.212800000
8	-1.813700000	0.076619000	-0.468362000
1	0.014794000	2.174580000	0.029161000
1	-1.139621000	-0.028956000	1.472451000
1	2.083722000	-1.311174000	-0.437970000
1	-2.343156000	-0.717154000	-0.361111000

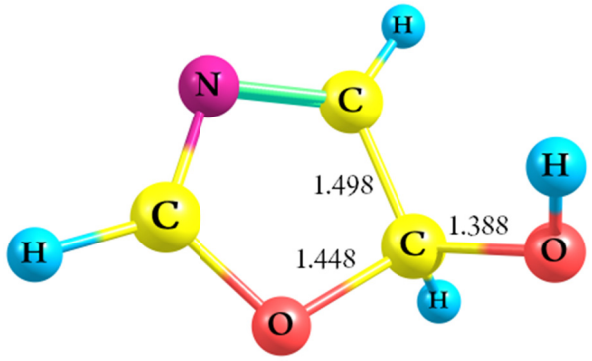
Zero-point correction= 0.07295 (Hartree/Particle)
Thermal correction to Energy= 0.078328
Thermal correction to Enthalpy= 0.079272
Thermal correction to Gibbs Free Energy= 0.043721
Sum of electronic and zero-point Energies= -321.782914
Sum of electronic and thermal Energies= -321.777544
Sum of electronic and thermal Enthalpies= -321.776600
Sum of electronic and thermal Free Energies= -321.812151



P6 [M06-2x]

6	-0.739723000	0.004232000	0.446430000
6	0.190528000	1.150900000	0.186514000
6	1.320921000	-0.592558000	-0.178831000
1	-1.114102000	-0.085220000	1.466513000
1	-0.053839000	2.194992000	0.284248000
1	2.106602000	-1.282778000	-0.438096000
7	1.394644000	0.708264000	-0.210426000
8	0.145681000	-1.114226000	0.209122000
8	-1.860808000	-0.056015000	-0.371488000
1	-1.610503000	0.201641000	-1.265430000

Zero-point correction=	0.073313 (Hartree/Particle)
Thermal correction to Energy=	0.078346
Thermal correction to Enthalpy=	0.079291
Thermal correction to Gibbs Free Energy=	0.044400
Sum of electronic and zero-point Energies=	-321.787995
Sum of electronic and thermal Energies=	-321.782961
Sum of electronic and thermal Enthalpies=	-321.782017
Sum of electronic and thermal Free Energies=	-321.816907



P6 [ωB97XD]

6	-0.739248000	0.006342000	0.443890000
6	0.193060000	1.150641000	0.185649000
6	1.319118000	-0.593763000	-0.178608000
1	-1.113184000	-0.082012000	1.464616000
1	-0.048199000	2.195779000	0.285550000
1	2.102484000	-1.285415000	-0.441015000
7	1.395256000	0.707965000	-0.210570000
8	0.145995000	-1.115231000	0.210123000
8	-1.862330000	-0.055415000	-0.370032000
1	-1.614805000	0.201738000	-1.261474000

Zero-point correction=	0.073228 (Hartree/Particle)
Thermal correction to Energy=	0.078295
Thermal correction to Enthalpy=	0.079239
Thermal correction to Gibbs Free Energy=	0.044302
Sum of electronic and zero-point Energies=	-321.802738
Sum of electronic and thermal Energies=	-321.797671
Sum of electronic and thermal Enthalpies=	-321.796727
Sum of electronic and thermal Free Energies=	-321.831665

Table S2: RRKM rate constants for OH-addition reaction pathways [**4**–**6**] at various *P* and *T*

Table S2a: *T*= 299 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	4.99E-04	1.78E-03	2.40E+09	1.33E+07	8.71E+09	4.92E-14	9.74E-16	6.36E-13	6.86E-13
1.00E+06	4.99E-04	1.78E-03	2.40E+09	1.33E+07	8.71E+09	4.92E-14	9.74E-16	6.36E-13	6.86E-13
1.00E+04	4.99E-04	1.78E-03	2.40E+09	1.33E+07	8.70E+09	4.91E-14	9.74E-16	6.35E-13	6.85E-13
1.00E+02	4.99E-04	1.78E-03	2.23E+09	1.33E+07	7.75E+09	4.56E-14	9.70E-16	5.66E-13	6.13E-13
1.00E+00	4.99E-04	1.78E-03	3.75E+08	9.95E+06	8.34E+08	7.67E-15	7.27E-16	6.09E-14	6.93E-14
1.00E-02	4.99E-04	1.78E-03	5.03E+06	7.25E+05	9.87E+06	1.03E-16	5.29E-17	7.21E-16	8.77E-16
1.00E-04	4.99E-04	1.78E-03	5.05E+04	8.53E+03	9.89E+04	1.03E-18	6.23E-19	7.22E-18	8.88E-18
1.00E-06	4.99E-04	1.78E-03	5.05E+02	8.54E+01	9.89E+02	1.03E-20	6.24E-21	7.22E-20	8.88E-20
1.00E-08	4.99E-04	1.78E-03	5.05E+00	8.54E-01	9.89E+00	1.03E-22	6.24E-23	7.22E-22	8.88E-22
1.00E-10	4.99E-04	1.78E-03	5.05E-02	8.54E-03	9.89E-02	1.03E-24	6.24E-25	7.22E-24	8.88E-24

Table S2b: T= 324 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff} (**4**)	k_{eff} (**5**)	k_{eff} (**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	3.89E-04	1.38E-03	3.61E+09	2.82E+07	1.13E+10	6.13E-14	1.70E-15	6.79E-13	7.42E-13
1.00E+06	3.89E-04	1.38E-03	3.61E+09	2.82E+07	1.13E+10	6.13E-14	1.70E-15	6.79E-13	7.42E-13
1.00E+04	3.89E-04	1.38E-03	3.61E+09	2.82E+07	1.13E+10	6.12E-14	1.70E-15	6.78E-13	7.41E-13
1.00E+02	3.89E-04	1.38E-03	3.29E+09	2.81E+07	9.83E+09	5.59E-14	1.69E-15	5.92E-13	6.50E-13
1.00E+00	3.89E-04	1.38E-03	4.75E+08	1.97E+07	9.17E+08	8.07E-15	1.19E-15	5.52E-14	6.45E-14
1.00E-02	3.89E-04	1.38E-03	6.13E+06	1.21E+06	1.06E+07	1.04E-16	7.29E-17	6.36E-16	8.13E-16
1.00E-04	3.89E-04	1.38E-03	6.15E+04	1.39E+04	1.06E+05	1.04E-18	8.38E-19	6.38E-18	8.26E-18
1.00E-06	3.89E-04	1.38E-03	6.15E+02	1.39E+02	1.06E+03	1.04E-20	8.40E-21	6.38E-20	8.26E-20
1.00E-08	3.89E-04	1.38E-03	6.15E+00	1.39E+00	1.06E+01	1.04E-22	8.40E-23	6.38E-22	8.26E-22
1.00E-10	3.89E-04	1.38E-03	6.15E-02	1.39E-02	1.06E-01	1.04E-24	8.40E-25	6.38E-24	8.26E-24

Table S2c: T= 348 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff} (**4**)	k_{eff} (**5**)	k_{eff} (**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	3.19E-04	1.13E-03	5.05E+09	5.22E+07	1.39E+10	7.36E-14	2.70E-15	7.19E-13	7.96E-13
1.00E+06	3.19E-04	1.13E-03	5.05E+09	5.22E+07	1.39E+10	7.36E-14	2.70E-15	7.19E-13	7.96E-13
1.00E+04	3.19E-04	1.13E-03	5.04E+09	5.22E+07	1.39E+10	7.35E-14	2.70E-15	7.18E-13	7.94E-13
1.00E+02	3.19E-04	1.13E-03	4.52E+09	5.18E+07	1.19E+10	6.59E-14	2.68E-15	6.14E-13	6.83E-13
1.00E+00	3.19E-04	1.13E-03	5.66E+08	3.39E+07	9.74E+08	8.25E-15	1.75E-15	5.03E-14	6.03E-14
1.00E-02	3.19E-04	1.13E-03	7.06E+06	1.80E+06	1.10E+07	1.03E-16	9.28E-17	5.68E-16	7.64E-16
1.00E-04	3.19E-04	1.13E-03	7.08E+04	2.03E+04	1.10E+05	1.03E-18	1.05E-18	5.69E-18	7.77E-18
1.00E-06	3.19E-04	1.13E-03	7.08E+02	2.03E+02	1.10E+03	1.03E-20	1.05E-20	5.69E-20	7.77E-20
1.00E-08	3.19E-04	1.13E-03	7.08E+00	2.03E+00	1.10E+01	1.03E-22	1.05E-22	5.69E-22	7.77E-22
1.00E-10	3.19E-04	1.13E-03	7.08E-02	2.03E-02	1.10E-01	1.03E-24	1.05E-24	5.69E-24	7.77E-24

Table S2d: T= 373 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff} (**4**)	k_{eff} (**5**)	k_{eff} (**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	2.68E-04	9.44E-04	6.82E+09	9.09E+07	1.68E+10	8.69E-14	4.08E-15	7.55E-13	8.46E-13
1.00E+06	2.68E-04	9.44E-04	6.82E+09	9.09E+07	1.68E+10	8.69E-14	4.08E-15	7.55E-13	8.46E-13
1.00E+04	2.68E-04	9.44E-04	6.81E+09	9.09E+07	1.68E+10	8.67E-14	4.08E-15	7.53E-13	8.44E-13
1.00E+02	2.68E-04	9.44E-04	5.99E+09	9.01E+07	1.41E+10	7.63E-14	4.04E-15	6.30E-13	7.11E-13
1.00E+00	2.68E-04	9.44E-04	6.50E+08	5.46E+07	1.01E+09	8.27E-15	2.45E-15	4.55E-14	5.62E-14
1.00E-02	2.68E-04	9.44E-04	7.86E+06	2.50E+06	1.13E+07	1.00E-16	1.12E-16	5.05E-16	7.17E-16
1.00E-04	2.68E-04	9.44E-04	7.88E+04	2.77E+04	1.13E+05	1.00E-18	1.24E-18	5.05E-18	7.30E-18
1.00E-06	2.68E-04	9.44E-04	7.88E+02	2.77E+02	1.13E+03	1.00E-20	1.24E-20	5.05E-20	7.30E-20
1.00E-08	2.68E-04	9.44E-04	7.88E+00	2.77E+00	1.13E+01	1.00E-22	1.24E-22	5.05E-22	7.30E-22
1.00E-10	2.68E-04	9.44E-04	7.88E-02	2.77E-02	1.13E-01	1.00E-24	1.24E-24	5.05E-24	7.30E-24

Table S2e: T= 398 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff} (**4**)	k_{eff} (**5**)	k_{eff} (**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	2.31E-04	8.12E-04	8.87E+09	1.48E+08	1.98E+10	9.99E-14	5.84E-15	7.85E-13	8.91E-13
1.00E+06	2.31E-04	8.12E-04	8.87E+09	1.48E+08	1.98E+10	9.99E-14	5.84E-15	7.85E-13	8.91E-13
1.00E+04	2.31E-04	8.12E-04	8.86E+09	1.48E+08	1.98E+10	9.97E-14	5.84E-15	7.83E-13	8.89E-13
1.00E+02	2.31E-04	8.12E-04	7.62E+09	1.46E+08	1.62E+10	8.58E-14	5.78E-15	6.40E-13	7.32E-13
1.00E+00	2.31E-04	8.12E-04	7.20E+08	8.14E+07	1.04E+09	8.11E-15	3.22E-15	4.10E-14	5.24E-14
1.00E-02	2.31E-04	8.12E-04	8.49E+06	3.25E+06	1.13E+07	9.56E-17	1.29E-16	4.49E-16	6.73E-16
1.00E-04	2.31E-04	8.12E-04	8.51E+04	3.55E+04	1.13E+05	9.58E-19	1.41E-18	4.49E-18	6.86E-18
1.00E-06	2.31E-04	8.12E-04	8.51E+02	3.56E+02	1.13E+03	9.58E-21	1.41E-20	4.49E-20	6.86E-20
1.00E-08	2.31E-04	8.12E-04	8.51E+00	3.56E+00	1.13E+01	9.58E-23	1.41E-22	4.49E-22	6.86E-22
1.00E-10	2.31E-04	8.12E-04	8.51E-02	3.56E-02	1.13E-01	9.58E-25	1.41E-24	4.49E-24	6.86E-24

Table S2f: T= 423 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff} (**4**)	k_{eff} (**5**)	k_{eff} (**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	2.04E-04	7.14E-04	1.12E+10	2.26E+08	2.29E+10	1.14E-13	8.06E-15	8.17E-13	9.39E-13
1.00E+06	2.04E-04	7.14E-04	1.12E+10	2.26E+08	2.29E+10	1.14E-13	8.06E-15	8.17E-13	9.39E-13
1.00E+04	2.04E-04	7.14E-04	1.12E+10	2.26E+08	2.28E+10	1.14E-13	8.06E-15	8.15E-13	9.37E-13
1.00E+02	2.04E-04	7.14E-04	9.38E+09	2.23E+08	1.82E+10	9.56E-14	7.95E-15	6.50E-13	7.54E-13
1.00E+00	2.04E-04	7.14E-04	7.77E+08	1.14E+08	1.05E+09	7.92E-15	4.06E-15	3.73E-14	4.93E-14
1.00E-02	2.04E-04	7.14E-04	8.95E+06	4.01E+06	1.13E+07	9.13E-17	1.43E-16	4.03E-16	6.38E-16
1.00E-04	2.04E-04	7.14E-04	8.97E+04	4.33E+04	1.13E+05	9.15E-19	1.54E-18	4.03E-18	6.49E-18
1.00E-06	2.04E-04	7.14E-04	8.97E+02	4.33E+02	1.13E+03	9.15E-21	1.55E-20	4.03E-20	6.50E-20
1.00E-08	2.04E-04	7.14E-04	8.97E+00	4.33E+00	1.13E+01	9.15E-23	1.55E-22	4.03E-22	6.50E-22
1.00E-10	2.04E-04	7.14E-04	8.97E-02	4.33E-02	1.13E-01	9.15E-25	1.55E-24	4.03E-24	6.50E-24

Table S2g: T= 449 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff} (**4**)	k_{eff} (**5**)	k_{eff} (**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	1.82E-04	6.37E-04	1.38E+10	3.34E+08	2.61E+10	1.34E-13	1.13E-14	8.86E-13	1.03E-12
1.00E+06	1.82E-04	6.37E-04	1.38E+10	3.34E+08	2.61E+10	1.34E-13	1.13E-14	8.86E-13	1.03E-12
1.00E+04	1.82E-04	6.37E-04	1.38E+10	3.34E+08	2.60E+10	1.34E-13	1.13E-14	8.84E-13	1.03E-12
1.00E+02	1.82E-04	6.37E-04	1.13E+10	3.28E+08	2.02E+10	1.10E-13	1.11E-14	6.87E-13	8.07E-13
1.00E+00	1.82E-04	6.37E-04	8.21E+08	1.53E+08	1.04E+09	7.96E-15	5.18E-15	3.55E-14	4.86E-14
1.00E-02	1.82E-04	6.37E-04	9.28E+06	4.77E+06	1.12E+07	9.00E-17	1.62E-16	3.79E-16	6.31E-16
1.00E-04	1.82E-04	6.37E-04	9.29E+04	5.08E+04	1.12E+05	9.01E-19	1.73E-18	3.79E-18	6.42E-18
1.00E-06	1.82E-04	6.37E-04	9.29E+02	5.09E+02	1.12E+03	9.01E-21	1.73E-20	3.79E-20	6.42E-20
1.00E-08	1.82E-04	6.37E-04	9.29E+00	5.09E+00	1.12E+01	9.01E-23	1.73E-22	3.79E-22	6.42E-22
1.00E-10	1.82E-04	6.37E-04	9.29E-02	5.09E-02	1.12E-01	9.01E-25	1.73E-24	3.79E-24	6.42E-24

Table S2h: T= 468 K.

P	Equilibrium constants (bar^{-1})		Unimolecular rate constants (s^{-1})			Effective rate constants ($cm^3\ molecule^{-1}\ s^{-1}$)			
	$K_{P(1)}$	$K_{P(X),x=2,3}$	k_2 (**4**)	k_2 (**5**)	k_2 (**6**)	k_{eff} (**4**)	k_{eff} (**5**)	k_{eff} (**6**)	k_{eff} [(**4**)+(**5**)+(**6**)]
1.00E+08	1.70E-04	5.92E-04	1.59E+10	4.32E+08	2.85E+10	1.50E-13	1.42E-14	9.35E-13	1.10E-12
1.00E+06	1.70E-04	5.92E-04	1.59E+10	4.32E+08	2.85E+10	1.50E-13	1.42E-14	9.35E-13	1.10E-12
1.00E+04	1.70E-04	5.92E-04	1.59E+10	4.32E+08	2.84E+10	1.50E-13	1.42E-14	9.32E-13	1.10E-12
1.00E+02	1.70E-04	5.92E-04	1.27E+10	4.24E+08	2.16E+10	1.20E-13	1.39E-14	7.10E-13	8.44E-13
1.00E+00	1.70E-04	5.92E-04	8.44E+08	1.83E+08	1.04E+09	7.97E-15	6.02E-15	3.41E-14	4.81E-14
1.00E-02	1.70E-04	5.92E-04	9.42E+06	5.28E+06	1.10E+07	8.89E-17	1.73E-16	3.62E-16	6.24E-16
1.00E-04	1.70E-04	5.92E-04	9.44E+04	5.59E+04	1.10E+05	8.90E-19	1.84E-18	3.62E-18	6.35E-18
1.00E-06	1.70E-04	5.92E-04	9.44E+02	5.59E+02	1.10E+03	8.91E-21	1.84E-20	3.62E-20	6.35E-20
1.00E-08	1.70E-04	5.92E-04	9.44E+00	5.59E+00	1.10E+01	8.91E-23	1.84E-22	3.62E-22	6.35E-22
1.00E-10	1.70E-04	5.92E-04	9.44E-02	5.59E-02	1.10E-01	8.91E-25	1.84E-24	3.62E-24	6.35E-24

Table S3: Effective rate coefficients k_{eff} (in cm^3 $molecule^{-1}$ s^{-1}), regioselectivity, and branching ratios (%) for the OH-addition pathways [**4**–**6**] at different *P* and *T* using RRKM theory.

Table S3a: *T*= 299 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	*R*(**4**)	*R*(**5**)	*R*(**6**)	Log*P*	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	4.92E-14	9.74E-16	6.36E-13	7.16	0.14	92.70	8	0.8539	-13.308	-15.011	-12.196
1.00E+06	4.92E-14	9.74E-16	6.36E-13	7.16	0.14	92.70	6	0.8539	-13.308	-15.011	-12.196
1.00E+04	4.91E-14	9.74E-16	6.35E-13	7.17	0.14	92.69	4	0.8538	-13.309	-15.011	-12.197
1.00E+02	4.56E-14	9.70E-16	5.66E-13	7.44	0.16	92.40	2	0.8480	-13.341	-15.013	-12.247
1.00E+00	7.67E-15	7.27E-16	6.09E-14	11.07	1.05	87.88	0	0.7577	-14.115	-15.139	-13.215
1.00E-02	1.03E-16	5.29E-17	7.21E-16	11.75	6.04	82.22	-2	0.6443	-15.987	-16.276	-15.142
1.00E-04	1.03E-18	6.23E-19	7.22E-18	11.65	7.01	81.34	-4	0.6268	-17.985	-18.206	-17.141
1.00E-06	1.03E-20	6.24E-21	7.22E-20	11.65	7.02	81.33	-6	0.6266	-19.985	-20.205	-19.141
1.00E-08	1.03E-22	6.24E-23	7.22E-22	11.65	7.02	81.33	-8	0.6266	-21.985	-22.205	-21.141
1.00E-10	1.03E-24	6.24E-25	7.22E-24	11.65	7.02	81.33	-10	0.6266	-23.985	-24.205	-23.141

Table S3b: T= 324 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	R(**4**)	R(**5**)	R(**6**)	Log$P$	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	6.13E-14	1.70E-15	6.79E-13	8.26	0.23	91.51	8	0.8303	-13.213	-14.770	-12.168
1.00E+06	6.13E-14	1.70E-15	6.79E-13	8.26	0.23	91.51	6	0.8303	-13.213	-14.770	-12.168
1.00E+04	6.12E-14	1.70E-15	6.78E-13	8.26	0.23	91.51	4	0.8302	-13.213	-14.770	-12.169
1.00E+02	5.59E-14	1.69E-15	5.92E-13	8.60	0.26	91.14	2	0.8227	-13.253	-14.772	-12.228
1.00E+00	8.07E-15	1.19E-15	5.52E-14	12.52	1.84	85.64	0	0.7128	-14.093	-14.926	-13.258
1.00E-02	1.04E-16	7.29E-17	6.36E-16	12.79	8.97	78.24	-2	0.5649	-15.983	-16.137	-15.196
1.00E-04	1.04E-18	8.38E-19	6.38E-18	12.64	10.15	77.21	-4	0.5442	-17.981	-18.077	-17.195
1.00E-06	1.04E-20	8.40E-21	6.38E-20	12.64	10.16	77.20	-6	0.5439	-19.981	-20.076	-19.195
1.00E-08	1.04E-22	8.40E-23	6.38E-22	12.64	10.16	77.20	-8	0.5439	-21.981	-22.076	-21.195
1.00E-10	1.04E-24	8.40E-25	6.38E-24	12.64	10.16	77.20	-10	0.5439	-23.981	-24.076	-23.195

Table S3c: T= 348 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	R(**4**)	R(**5**)	R(**6**)	Log$P$	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	7.36E-14	2.70E-15	7.19E-13	9.25	0.34	90.41	8	0.8082	-13.133	-14.569	-12.143
1.00E+06	7.36E-14	2.70E-15	7.19E-13	9.25	0.34	90.41	6	0.8082	-13.133	-14.569	-12.143
1.00E+04	7.35E-14	2.70E-15	7.18E-13	9.25	0.34	90.41	4	0.8081	-13.134	-14.569	-12.144
1.00E+02	6.59E-14	2.68E-15	6.14E-13	9.66	0.39	89.95	2	0.7991	-13.181	-14.572	-12.212
1.00E+00	8.25E-15	1.75E-15	5.03E-14	13.68	2.91	83.41	0	0.6682	-14.083	-14.756	-13.298
1.00E-02	1.03E-16	9.28E-17	5.68E-16	13.47	12.15	74.38	-2	0.4877	-15.988	-16.032	-15.245
1.00E-04	1.03E-18	1.05E-18	5.69E-18	13.28	13.46	73.25	-4	0.4651	-17.986	-17.980	-17.245
1.00E-06	1.03E-20	1.05E-20	5.69E-20	13.28	13.48	73.24	-6	0.4648	-19.986	-19.980	-19.245
1.00E-08	1.03E-22	1.05E-22	5.69E-22	13.28	13.48	73.24	-8	0.4648	-21.986	-21.980	-21.245
1.00E-10	1.03E-24	1.05E-24	5.69E-24	13.28	13.48	73.24	-10	0.4648	-23.986	-23.980	-23.245

Table S3d: T= 373 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	R(**4**)	R(**5**)	R(**6**)	Log$P$	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	8.69E-14	4.08E-15	7.55E-13	10.27	0.48	89.24	8	0.7849	-13.061	-14.389	-12.122
1.00E+06	8.69E-14	4.08E-15	7.55E-13	10.27	0.48	89.25	6	0.7849	-13.061	-14.389	-12.122
1.00E+04	8.67E-14	4.08E-15	7.53E-13	10.28	0.48	89.24	4	0.7848	-13.062	-14.390	-12.123
1.00E+02	7.63E-14	4.04E-15	6.30E-13	10.74	0.57	88.69	2	0.7739	-13.118	-14.393	-12.201
1.00E+00	8.27E-15	2.45E-15	4.55E-14	14.72	4.36	80.92	0	0.6184	-14.082	-14.611	-13.342
1.00E-02	1.00E-16	1.12E-16	5.05E-16	13.96	15.64	70.40	-2	0.4080	-16.000	-15.950	-15.297
1.00E-04	1.00E-18	1.24E-18	5.05E-18	13.75	17.02	69.23	-4	0.3847	-17.999	-17.906	-17.297
1.00E-06	1.00E-20	1.24E-20	5.05E-20	13.75	17.04	69.22	-6	0.3843	-19.999	-19.905	-19.297
1.00E-08	1.00E-22	1.24E-22	5.05E-22	13.75	17.04	69.22	-8	0.3843	-21.999	-21.905	-21.297
1.00E-10	1.00E-24	1.24E-24	5.05E-24	13.75	17.04	69.22	-10	0.3843	-23.999	-23.905	-23.297

Table S3e: T= 398 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	R(**4**)	R(**5**)	R(**6**)	Log$P$	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	9.99E-14	5.84E-15	7.85E-13	11.22	0.66	88.13	8	0.7625	-13.000	-14.233	-12.105
1.00E+06	9.99E-14	5.84E-15	7.85E-13	11.22	0.66	88.13	6	0.7625	-13.000	-14.233	-12.105
1.00E+04	9.97E-14	5.84E-15	7.83E-13	11.22	0.66	88.12	4	0.7624	-13.001	-14.234	-12.106
1.00E+02	8.58E-14	5.78E-15	6.40E-13	11.73	0.79	87.48	2	0.7496	-13.066	-14.238	-12.194
1.00E+00	8.11E-15	3.22E-15	4.10E-14	15.48	6.15	78.37	0	0.5673	-14.091	-14.492	-13.387
1.00E-02	9.56E-17	1.29E-16	4.49E-16	14.21	19.13	66.66	-2	0.3333	-16.019	-15.890	-15.348
1.00E-04	9.58E-19	1.41E-18	4.49E-18	13.98	20.51	65.52	-4	0.3103	-18.019	-17.852	-17.348
1.00E-06	9.58E-21	1.41E-20	4.49E-20	13.97	20.52	65.50	-6	0.3100	-20.018	-19.852	-19.348
1.00E-08	9.58E-23	1.41E-22	4.49E-22	13.97	20.52	65.50	-8	0.3100	-22.018	-21.852	-21.348
1.00E-10	9.58E-25	1.41E-24	4.49E-24	13.97	20.52	65.50	-10	0.3100	-24.018	-23.852	-23.348

Table S3f: T= 423 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	R(**4**)	R(**5**)	R(**6**)	Log$P$	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	1.14E-13	8.06E-15	8.17E-13	12.14	0.86	87.00	8	0.7401	-12.943	-14.094	-12.088
1.00E+06	1.14E-13	8.06E-15	8.17E-13	12.14	0.86	87.00	6	0.7401	-12.943	-14.094	-12.088
1.00E+04	1.14E-13	8.06E-15	8.15E-13	12.14	0.86	87.00	4	0.7399	-12.944	-14.094	-12.089
1.00E+02	9.56E-14	7.95E-15	6.50E-13	12.69	1.06	86.26	2	0.7251	-13.019	-14.100	-12.187
1.00E+00	7.92E-15	4.06E-15	3.73E-14	16.06	8.24	75.71	0	0.5142	-14.101	-14.391	-13.428
1.00E-02	9.13E-17	1.43E-16	4.03E-16	14.32	22.46	63.22	-2	0.2644	-16.039	-15.844	-15.395
1.00E-04	9.15E-19	1.54E-18	4.03E-18	14.09	23.78	62.13	-4	0.2426	-18.039	-17.811	-17.394
1.00E-06	9.15E-21	1.55E-20	4.03E-20	14.09	23.80	62.11	-6	0.2423	-20.039	-19.811	-19.394
1.00E-08	9.15E-23	1.55E-22	4.03E-22	14.09	23.80	62.11	-8	0.2423	-22.039	-21.811	-21.394
1.00E-10	9.15E-25	1.55E-24	4.03E-24	14.09	23.80	62.11	-10	0.2423	-24.039	-23.811	-23.394

Table S3g: T= 449 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	R(**4**)	R(**5**)	R(**6**)	Log$P$	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	1.34E-13	1.13E-14	8.86E-13	12.99	1.10	85.91	8	0.7182	-12.873	-13.945	-12.052
1.00E+06	1.34E-13	1.13E-14	8.86E-13	12.99	1.10	85.91	6	0.7182	-12.873	-13.945	-12.052
1.00E+04	1.34E-13	1.13E-14	8.84E-13	13.00	1.10	85.90	4	0.7180	-12.874	-13.945	-12.054
1.00E+02	1.10E-13	1.11E-14	6.87E-13	13.56	1.38	85.05	2	0.7011	-12.961	-13.953	-12.163
1.00E+00	7.96E-15	5.18E-15	3.55E-14	16.38	10.65	72.97	0	0.4594	-14.099	-14.286	-13.450
1.00E-02	9.00E-17	1.62E-16	3.79E-16	14.27	25.67	60.06	-2	0.2012	-16.046	-15.791	-15.422
1.00E-04	9.01E-19	1.73E-18	3.79E-18	14.04	26.90	59.06	-4	0.1811	-18.045	-17.763	-17.421
1.00E-06	9.01E-21	1.73E-20	3.79E-20	14.04	26.92	59.04	-6	0.1809	-20.045	-19.762	-19.421
1.00E-08	9.01E-23	1.73E-22	3.79E-22	14.04	26.92	59.04	-8	0.1808	-22.045	-21.762	-21.421
1.00E-10	9.01E-25	1.73E-24	3.79E-24	14.04	26.92	59.04	-10	0.1808	-24.045	-23.762	-23.421

Table S3h: T= 468 K.

P	Effective rate constants			Branching ratios			Regioselectivity				
	k_{eff}(**4**)	k_{eff}(**5**)	k_{eff}(**6**)	R(**4**)	R(**5**)	R(**6**)	Log$P$	{R(**6**)–[R(**4**)+R(**5**)]/ [R(**4**)+R(**5**)+R(**6**)]}	logk_{eff}(**4**)	logk_{eff}(**5**)	logk_{eff}(**6**)
1.00E+08	1.50E-13	1.42E-14	9.35E-13	13.64	1.29	85.07	8	0.7013	-12.824	-13.847	-12.029
1.00E+06	1.50E-13	1.42E-14	9.35E-13	13.64	1.29	85.07	6	0.7013	-12.824	-13.847	-12.029
1.00E+04	1.50E-13	1.42E-14	9.32E-13	13.65	1.30	85.05	4	0.7011	-12.825	-13.848	-12.030
1.00E+02	1.20E-13	1.39E-14	7.10E-13	14.22	1.65	84.13	2	0.6826	-12.921	-13.856	-12.149
1.00E+00	7.97E-15	6.02E-15	3.41E-14	16.56	12.52	70.92	0	0.4184	-14.099	-14.220	-13.467
1.00E-02	8.89E-17	1.73E-16	3.62E-16	14.25	27.79	57.97	-2	0.1593	-16.051	-15.761	-15.442
1.00E-04	8.90E-19	1.84E-18	3.62E-18	14.03	28.94	57.03	-4	0.1407	-18.050	-17.736	-17.441
1.00E-06	8.91E-21	1.84E-20	3.62E-20	14.03	28.95	57.02	-6	0.1405	-20.050	-19.736	-19.441
1.00E-08	8.91E-23	1.84E-22	3.62E-22	14.03	28.95	57.02	-8	0.1404	-22.050	-21.736	-21.441
1.00E-10	8.91E-25	1.84E-24	3.62E-24	14.03	28.95	57.02	-10	0.1404	-24.050	-23.736	-23.441