Supplementary Information for

Comment on "Atmospheric chemistry of oxazole: the mechanism and kinetic studies on oxidation reaction initiated by OH radicals" by A. Shiroudi, M. A. Abdel-Rahman, A. M. El-Nahas and M. Altarawneh, New Journal of Chemistry, 2021, 45, 2237

Tam V.-T. Mai[a] and Lam K. Huynh[b*]

[a] University of Science, Ho Chi Minh City, 227 Nguyen Van Cu, Ward 4, District 5, Ho Chi Minh City, Vietnam.

[b] International University, International University, Block 6, Linh Trung Ward, Thu Duc City, Ho Chi Minh City, Vietnam.

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Table S1: Optimized geometries, electronic energies at 0 K ($E_{elec}^{0\,K}$), zero-point energy (ZPE) corrections and harmonic wavenumbers of the species involved with the lowest-energy conformer of a given species, calculated at the M06-2X/aug-cc-pVTZ level of theory for the title reaction. See Figure 1 (in the main text) for the notations.

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
OH ($C_{\infty v}$)	8	0.000000000	0.000000000	0.107999000	-75.733789	0.008530	3742.0378 (3737.8) [1]		
	1	0.000000000	0.000000000	-0.863995000					
H_2O (C_{2v})	8	0.000000000	0.000000000	0.116332000	-76.4300922	0.021565	1615.7190	3873.1681	3977.2474
	1	0.000000000	0.762680000	-0.465326000			(1595.0; 3657.0 [2]; 3756.0 [1])		
	1	0.000000000	-0.762680000	-0.465326000					
H ($D_{\infty h}$)	1	1.216198000	-1.008264000	0.000000000	-0.498207	0.00000	/		
Oxazole (C_s)	6	-0.596128000	-0.958006000	0.000000000	-246.070729	0.059464	636.7748	672.7995	797.9645
	6	0.747760000	-0.876311000	0.000000000			885.0241	915.1526	921.4602
	6	0.000000000	1.095687000	0.000000000			940.2646	1100.3657	1123.0928
	1	-1.308232000	-1.761359000	0.000000000			1148.6577	1204.8602	1283.0508
	1	1.474977000	-1.668136000	0.000000000			1385.5414	1562.3750	1615.3641
	1	-0.165749000	2.159282000	0.000000000			3291.0473	3292.7571	3325.3136
	7	1.116500000	0.461873000	0.000000000					
	8	-1.090786000	0.308611000	0.000000000					
RC1 (C_1)	6	1.721018000	0.652095000	-0.000185000	-321.815627	0.070739	27.5531	50.3706	153.0587
	6	0.450760000	1.094129000	-0.000136000			510.7275	604.3560	639.0300
	6	0.388414000	-1.022099000	0.000211000			678.2631	804.2877	892.7808
	1	2.687245000	1.119458000	-0.000366000			918.5816	929.0307	949.0072
	1	0.079310000	2.102595000	-0.000290000			1100.2549	1129.7351	1150.9743
	1	0.130025000	-2.066867000	0.000377000			1218.1618	1284.9065	1386.9349
	7	-0.398388000	-0.004735000	0.000176000			1566.5702	1621.7838	3296.5116
	8	1.690153000	-0.708408000	0.000036000			3297.5241	3327.8663	3512.5079
	8	-3.330448000	0.023028000	-0.000080000					
	1	-2.346666000	0.016248000	0.000063000					
RC2 (C_1)	6	0.224094000	1.102852000	0.369204000	-321.812220	0.070274	53.9898	71.2194	150.1954
	6	0.012462000	0.023123000	1.149561000			259.4291	449.3223	635.3024
	6	1.017457000	-0.635940000	-0.587052000			673.6946	805.8382	886.2231
	7	0.529133000	-1.097161000	0.509567000			914.2190	922.8671	940.5613
	8	0.878578000	0.690491000	-0.744723000			1103.1085	1125.8072	1146.7449
	8	-2.185761000	-0.093976000	-0.505972000			1205.7007	1283.5438	1383.9629

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	1	-0.010112000	2.147786000	0.443259000			1559.0111	1605.5523	3294.1852
	1	-0.473599000	-0.036909000	2.106496000			3295.8570	3328.1194	3752.1552
	1	1.515339000	-1.173458000	-1.375499000					
	1	-1.802171000	-0.969628000	-0.325938000					
TS0	6	-0.637384000	1.129986000	-0.059036000	-321.812101	0.070026	-32.4625	56.4346	125.7412
(C_1)	6	0.056556000	0.550071000	0.938871000			317.6213	390.8075	635.1652
	6	-0.860792000	-0.993363000	-0.175961000			675.0909	801.4452	886.6854
	1	-0.799240000	2.140678000	-0.382178000			912.1490	922.3681	940.5829
	1	0.657439000	1.007438000	1.703789000			1100.6451	1126.4619	1142.5448
	1	-1.225847000	-1.914209000	-0.597014000			1207.1946	1283.1028	1383.0511
	7	-0.097859000	-0.829433000	0.845859000			1562.6880	1609.5644	3294.1036
	8	-1.235502000	0.145588000	-0.778971000			3296.4685	3328.8373	3739.0516
	8	2.319901000	0.009408000	-0.568089000					
	1	2.027188000	-0.788014000	-0.092371000					
Abstraction channels									
TS1	6	0.371146000	-0.027998000	0.000282000	-321.787013	0.064025	-1791.7503	56.3438	91.7093
(C_1)	6	-1.683252000	-0.570740000	-0.000161000			190.9498	407.0605	573.4561
	6	-1.566071000	0.769227000	-0.000095000			632.7030	779.9621	795.0320
	1	-2.335034000	1.520218000	-0.000215000			803.0743	903.4646	913.3530
	1	-2.502027000	-1.265040000	-0.000323000			954.5022	1101.3714	1129.3270
	8	2.805860000	-0.101460000	-0.000087000			1145.3307	1204.1924	1352.4921
	8	-0.420420000	-1.102868000	0.000054000			1446.5832	1577.6847	1629.5329
	7	-0.209339000	1.103553000	0.000165000			3295.7156	3325.8193	3794.0470
	1	1.628687000	-0.235600000	0.000515000					
	1	2.859283000	0.867245000	-0.001024000					
TS2	6	-0.525092000	1.129596000	0.000002000	-321.789082	0.064520	-1686.9089	95.4286	96.0232
(C_1)	6	-1.438270000	-0.811567000	0.000002000			198.8532	408.2293	597.8720
	6	0.410019000	0.162859000	-0.000016000			663.8153	755.9093	798.5073
	1	-2.263275000	-1.502609000	0.000009000			828.3227	887.9882	933.3386
	1	-0.521261000	2.202028000	0.000005000			943.6355	1095.9607	1168.5822
	8	2.841865000	0.067907000	-0.000004000			1192.2362	1250.4411	1353.0413
	7	-0.176584000	-1.071905000	-0.000013000			1478.1242	1558.4704	1587.4050
	8	-1.734618000	0.498182000	0.000011000			3294.8700	3333.3309	3800.5794
	1	1.665818000	0.291247000	-0.000029000					

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	1	2.816887000	-0.901363000	0.000127000					
TS3	6	-0.391273000	0.145365000	-0.109589000	-321.785808	0.064256	-1638.7196	81.8274	110.8762
(C_1)	6	1.557207000	-0.682257000	0.043018000			152.3471	381.7764	596.9248
	6	0.497606000	1.153111000	-0.018862000			670.3165	724.1507	873.8520
	1	0.333426000	2.214340000	-0.023530000			884.0732	894.7077	931.5417
	1	2.278242000	-1.479977000	0.086803000			972.7428	1098.6327	1152.2258
	8	0.258429000	-1.035586000	-0.057219000			1160.6057	1249.6285	1332.9311
	7	1.762918000	0.585819000	0.067566000			1379.5567	1530.1026	1604.9189
	8	-2.813057000	-0.023775000	-0.031743000			3296.2529	3311.0102	3813.9707
	1	-1.668365000	0.103898000	-0.238738000					
	1	-2.827947000	-0.161409000	0.926801000					
P1	6	0.000000000	1.082554000	0.000000000	-245.374418	0.046487	618.0690	624.0449	788.3333
(C_s)	6	1.069772000	0.268097000	0.000000000			892.0394	901.4470	932.6202
	6	-0.627104000	-0.938299000	0.000000000			1075.6487	1106.8643	1126.6834
	7	0.629358000	-1.064984000	0.000000000			1192.8102	1337.1069	1569.8687
	8	-1.128026000	0.289785000	0.000000000			1618.3726	3294.5008	3327.0308
	1	-0.152655000	2.145003000	0.000000000					
	1	2.115349000	0.517495000	0.000000000					
P2	6	-0.513485000	-1.038813000	0.000000000	-245.374966	0.046846	618.8719	671.8595	786.7383
(C_s)	6	0.817335000	-0.861849000	0.000000000			879.8643	885.1457	938.6087
	6	0.000000000	1.045727000	0.000000000			1079.2258	1159.8451	1200.5114
	1	-0.201129000	2.102719000	0.000000000			1258.3242	1359.7499	1528.3098
	7	1.145408000	0.448895000	0.000000000			1560.2032	3295.8400	3339.8907
	8	-1.056682000	0.219661000	0.000000000					
	1	-1.186373000	-1.872656000	0.000000000					
P3	6	-0.658840000	-0.957892000	0.000000000	-245.370901	0.046664	589.6886	671.1587	857.7760
(C_s)	6	0.685069000	-0.965838000	0.000000000			865.2341	892.0553	935.1308
	6	0.000000000	1.048585000	0.000000000			1084.2179	1120.5949	1151.3254
	1	1.375111000	-1.787347000	0.000000000			1246.2106	1353.1233	1502.7057
	1	-0.128668000	2.116711000	0.000000000			1596.3059	3297.9591	3319.7053
	7	1.088346000	0.368522000	0.000000000					
	8	-1.127780000	0.292732000	0.000000000					
Addition channels									
TS4	6	-1.291409000	-0.494564000	-0.449208000	-321.807206	0.070611	-514.0005	148.1643	188.9194
(C_1)	6	-1.127195000	0.841057000	-0.275618000			272.9454	609.9035	637.0587

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	6	0.425509000	-0.146229000	0.774611000			715.3770	808.4276	870.9678
	7	-0.045876000	1.054233000	0.536914000			915.5789	923.6861	934.7299
	8	-0.328286000	-1.131315000	0.247748000			1108.6563	1119.9676	1169.5641
	8	1.933297000	-0.067970000	-0.641284000			1193.5030	1276.5411	1344.6938
	1	-1.988979000	-1.102886000	-0.994199000			1501.4839	1549.3957	3287.0272
	1	-1.711942000	1.648337000	-0.679036000			3303.6364	3320.3071	3794.1098
	1	1.160540000	-0.427646000	1.506332000					
	1	1.980004000	0.895263000	-0.741918000					
TS5 (C_1)	6	0.111160000	1.079124000	0.343664000	-321.803989	0.070584	-468.2233	121.6401	155.7664
	6	-0.498930000	-0.070781000	0.792978000			222.6002	557.3184	645.1855
	6	1.228288000	-0.624971000	-0.305915000			774.6482	818.8873	901.8642
	7	0.295102000	-1.152547000	0.389930000			909.1226	927.1083	939.2520
	8	1.186774000	0.727406000	-0.386693000			1094.5937	1100.9099	1126.6484
	8	-1.949152000	-0.006632000	-0.593209000			1185.6024	1283.5110	1381.0300
	1	-0.139208000	2.121583000	0.396279000			1491.9882	1616.2212	3292.2872
	1	-1.238563000	-0.173531000	1.563702000			3304.9067	3325.7505	3805.8382
	1	2.036202000	-1.112586000	-0.824342000					
	1	-1.668219000	-0.834054000	-1.010296000					
TS6 (C_1)	6	-0.408062000	-0.206921000	0.815751000	-321.809542	0.070523	-343.3531	122.4405	146.0179
	6	0.071357000	1.032397000	0.481862000			222.0139	598.2260	653.7705
	6	1.302513000	-0.396420000	-0.453517000			700.0912	848.3477	883.7214
	1	-1.131740000	-0.561841000	1.522877000			904.3972	920.1868	940.0978
	1	-0.312203000	1.995929000	0.766204000			1105.7141	1111.5498	1162.0219
	1	2.041615000	-0.939468000	-1.016888000			1192.9180	1284.1521	1368.2273
	7	1.151909000	0.880210000	-0.358369000			1500.7400	1577.7509	3291.9071
	8	0.418182000	-1.120836000	0.253082000			3294.6426	3334.8318	3792.2030
	8	-2.011063000	-0.106988000	-0.583468000					
	1	-1.712839000	0.592171000	-1.185104000					
TS7 (C_1)	6	-1.391033000	-0.639498000	-0.043468000	-321.798411	0.066377	-1078.6398	312.7456	335.1122
	6	-1.369854000	0.709842000	-0.052079000			440.6915	551.7050	581.8007
	6	0.628672000	0.044293000	0.078788000			635.5599	738.0695	774.4055
	7	-0.064401000	1.151760000	-0.027464000			820.7407	910.5592	934.2361
	8	-0.100444000	-1.084610000	-0.018868000			989.7768	1117.3518	1148.1358
	8	1.935645000	-0.114947000	-0.133129000			1180.8259	1218.1048	1327.3126
	1	-2.163274000	-1.384419000	-0.047656000			1485.0498	1572.4475	1583.9125

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	1	-2.200998000	1.391307000	-0.074865000			3291.4649	3330.8298	3855.4808
	1	0.595760000	0.075979000	1.800613000					
	1	2.331003000	0.763445000	-0.169307000					
TS8	6	0.178657000	1.111341000	-0.029601000	-321.788855	0.066080	-1134.4803	241.8096	303.5017
(C_1)	6	-0.674120000	0.038664000	0.080231000			417.6370	549.4946	609.2550
	6	1.291066000	-0.727023000	-0.042415000			622.3695	686.1156	746.4252
	7	0.079286000	-1.136499000	-0.023188000			817.1797	907.6352	929.2475
	8	1.445098000	0.609625000	-0.032374000			1004.8741	1093.9471	1160.2885
	8	-1.998296000	0.053928000	-0.181412000			1213.3088	1276.0044	1331.2930
	1	0.050009000	2.175143000	0.001884000			1389.2319	1599.8983	1630.3736
	1	-0.768234000	0.026850000	1.762436000			3289.1703	3333.9681	3852.6267
	1	2.190813000	-1.317850000	-0.073175000					
	1	-2.375638000	-0.774964000	0.132173000					
TS9	6	-0.653368000	0.087736000	0.033999000	-321.793757	0.065624	-812.1535	214.2445	300.6564
(C_1)	6	0.218617000	1.138402000	-0.031872000			411.2220	498.9767	525.6702
	6	1.360670000	-0.637670000	-0.024474000			661.1747	691.8485	735.6612
	1	-0.702640000	0.105928000	1.859805000			846.8297	871.2586	934.6531
	1	-0.009863000	2.188238000	-0.018899000			997.8421	1139.6751	1170.7092
	1	2.126290000	-1.393791000	-0.012067000			1211.8113	1277.3117	1292.8493
	7	1.502729000	0.641106000	-0.031278000			1382.8292	1569.6335	1647.9333
	8	0.080261000	-1.062322000	-0.040842000			3294.9385	3303.3981	3824.5681
	8	-1.967284000	0.014399000	-0.201937000					
	1	-2.392219000	-0.535535000	0.466411000					
P4	6	-1.385670000	-0.634986000	-0.000608000	-321.310927	0.064331	307.5991	426.7563	457.2223
(C_s)	6	-1.361527000	0.706528000	0.000622000			629.3045	740.2670	743.6521
	6	0.632343000	0.050057000	0.000062000			784.2251	907.7183	935.5118
	7	-0.038324000	1.145455000	-0.000525000			1003.9828	1108.2961	1145.8017
	8	-0.080345000	-1.073955000	0.000442000			1185.6279	1237.3139	1320.6971
	8	1.948400000	-0.115533000	-0.000029000			1520.1798	1613.1542	1686.2423
	1	-2.148968000	-1.388533000	-0.001136000			3292.6002	3335.1537	3856.6423
	1	-2.186761000	1.395426000	0.000994000					
	1	2.348675000	0.761240000	0.000052000					
P5	6	0.165343000	1.109716000	-0.000019000	-321.303968	0.064038	309.6683	338.3939	424.4395
(C_s)	6	-0.678771000	0.056906000	-0.000013000			643.2671	703.6299	706.5179
	6	1.268681000	-0.730927000	-0.000039000			767.8086	888.3554	944.6532

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	7	0.038620000	-1.117065000	0.000040000			1027.9925	1096.5891	1170.2003
	8	1.434885000	0.591574000	0.000037000			1232.9816	1279.6055	1352.2901
	8	-2.021713000	0.061855000	-0.000032000			1415.2086	1583.6906	1725.8241
	1	0.054792000	2.175418000	-0.000023000			3294.4556	3340.1582	3863.8566
	1	2.154071000	-1.342802000	-0.000009000					
	1	-2.316088000	-0.854767000	0.000133000					
P6 (C_s)	6	0.657225000	0.122127000	0.000006000	-321.300660	0.063365	112.0359	311.4878	426.1972
	6	-0.216009000	1.147916000	0.000014000			668.7776	695.4818	707.5113
	6	-1.336165000	-0.655643000	-0.000003000			825.0641	835.4580	939.7754
	1	-0.020825000	2.203239000	0.000028000			1013.3539	1118.7507	1135.7609
	1	-2.071285000	-1.440501000	0.000009000			1182.5671	1278.9314	1301.8749
	7	-1.501205000	0.610709000	-0.000012000			1440.2541	1610.0760	1723.4487
	8	-0.027955000	-1.042646000	-0.000010000			3302.8473	3314.6731	3869.6214
	8	1.990403000	0.059764000	-0.000058000					
	1	2.270649000	-0.861053000	0.000484000					

Frequencies in the parentheses ("( )") are taken from experimental studies.

Table S2: Calculated overall rate constants, k_{tot}, of the oxazole + OH → products over the range of temperature 299 – 468 K at different pressures, including the HIR treatments, Eckart quantum tunneling effects. Units are in cm^3/molecule/s.

T (K)	0.76 Torr	7.6 Torr	76 Torr	100 Torr	750 Torr	760 Torr	7600 Torr	76000 Torr
299	8.72E-12	9.39E-12	9.62E-12	9.65E-12	1.07E-11	1.07E-11	1.56E-11	4.60E-11
324	7.57E-12	8.37E-12	8.55E-12	8.57E-12	9.30E-12	9.31E-12	1.23E-11	2.72E-11
348	6.56E-12	7.50E-12	7.67E-12	7.71E-12	8.22E-12	8.21E-12	1.02E-11	1.79E-11
373	5.60E-12	6.65E-12	6.87E-12	6.88E-12	7.24E-12	7.25E-12	8.63E-12	1.28E-11
398	4.73E-12	5.92E-12	6.15E-12	6.16E-12	6.42E-12	6.43E-12	7.41E-12	1.02E-11
423	3.93E-12	5.25E-12	5.49E-12	5.52E-12	5.70E-12	5.69E-12	6.39E-12	8.38E-12
449	3.25E-12	4.62E-12	4.91E-12	4.92E-12	5.07E-12	5.09E-12	5.61E-12	7.10E-12
468	2.83E-12	4.21E-12	4.51E-12	4.54E-12	4.66E-12	4.65E-12	5.11E-12	6.36E-12

Table S3: Comparison of the zero-point energy corrected relative energies (in kcal·mol^{-1}) of all species involved in the title reaction calculated at the same methods, M06-2X/aug-cc-pVTZ and ROCBS-QB3//M06-2X/aug-cc-pVTZ, by this work and Shiroudi *et al.* [3] (0 K). The numbers are relative to the energies of oxazole + OH. See Fig. 1 for the species notations.

Species	M06-2X/aug-cc-pVTZ		ROCBS-QB3//M06-2X/aug-cc-pVTZ	
	This work	Shiroudi *et al.* [3]	This work	Shiroudi *et al.* [3]
RC1	-5.3	-3.3	-5.4	-2.3
RC2	-3.5	-3.5	-2.3	-2.3
TS0	-3.5	N/A	-2.6	N/A
TS1	8.5	8.3	8.7	8.4
TS2	7.5	7.4	7.6	7.4
TS3	9.4	9.4	8.8	8.9
TS4	-0.1	-0.2	-0.8	-1.0
TS5	2.0	2.0	0.5	0.6
TS6	-1.6	-1.6	-2.2	-2.3
TS7	2.8	N/A	4.3	N/A
TS8	8.6	N/A	9.0	N/A
TS9	5.3	N/A	6.3	N/A
I1	-34.3	-34.1	-34.3	-34.1
I2	-20.6	-20.3	-20.1	-19.9
I3	-32.3	-32.1	-32.4	-32.3
P1 + H_2O	0.0	0.2	1.0	1.1
P2 + H_2O	-0.1	0.0	0.8	1.0
P3 + H_2O	2.4	2.4	3.2	3.3
P4 + H	-5.2	N/A	-3.3	N/A
P5 + H	-1.0	N/A	0.4	N/A
P6 + H	0.6	N/A	2.4	N/A
MAD (kcal/mol)	**0.25**		**0.35**	

Table S4: Calculated overall rate constants, k_{tot}, of the oxazole + OH → products over the range of temperature 299 – 468 K at P = 100 Torr with and without HIR treatments based on M06-2X/aug-cc-pVTZ level of theory. Units are in cm^3/molecule/s.

T (K)	Oxazole + OH → products ($k_{\_tot}$)		HIR factor
	With HIR	Without HIR	
299	9.65E-12	6.30E-12	1.53
324	8.57E-12	5.60E-12	1.53
348	7.71E-12	5.03E-12	1.53
373	6.88E-12	4.50E-12	1.53
398	6.16E-12	4.03E-12	1.53
423	5.52E-12	3.62E-12	1.52
449	4.92E-12	3.24E-12	1.52
468	4.54E-12	3.00E-12	1.51

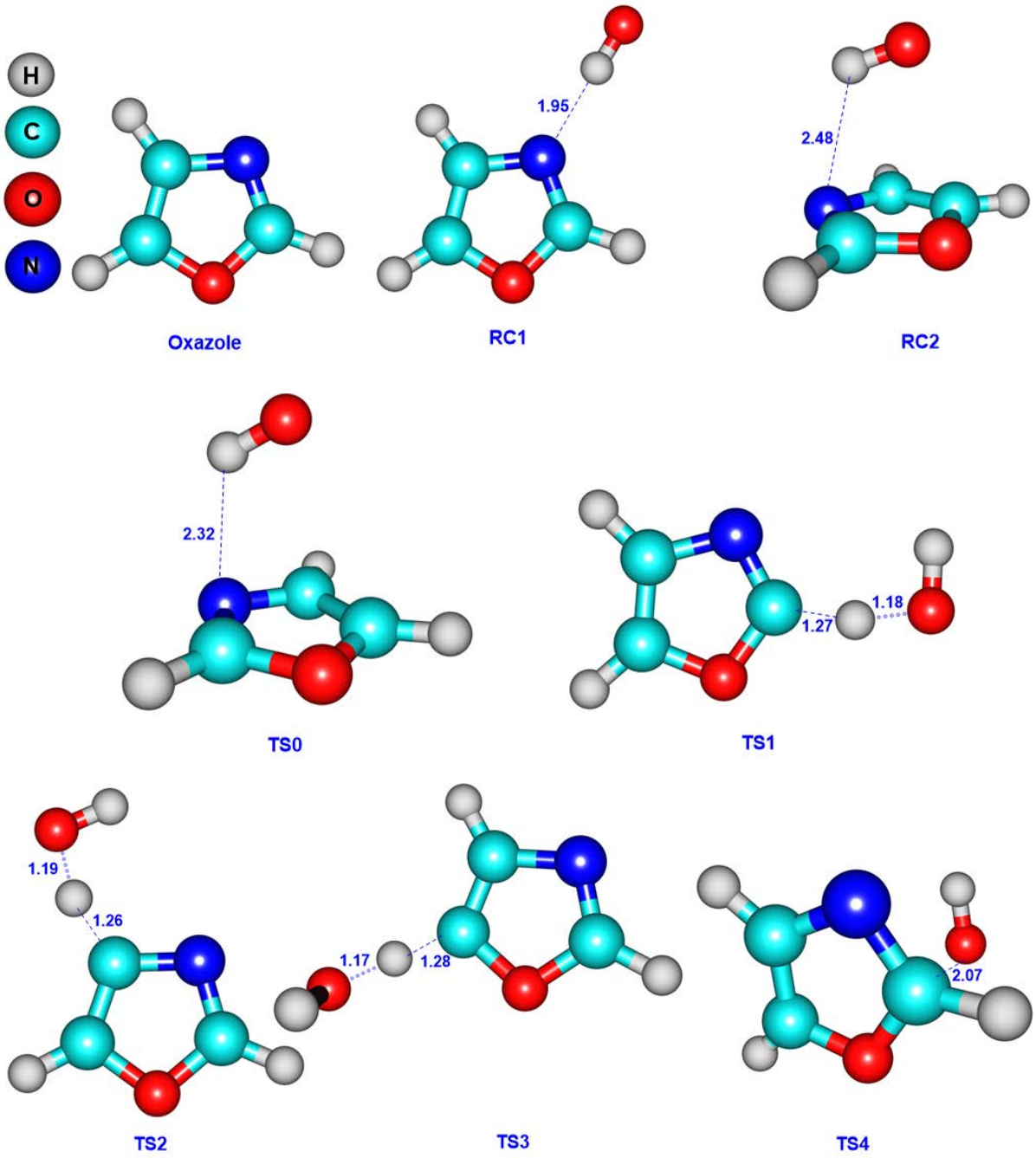
Table S5: The calculated Eckart tunneling factor via tight transition state channels over the wide range of temperature 299 – 468 K, based on the M06-2X/aug-cc-pVTZ level of theory.

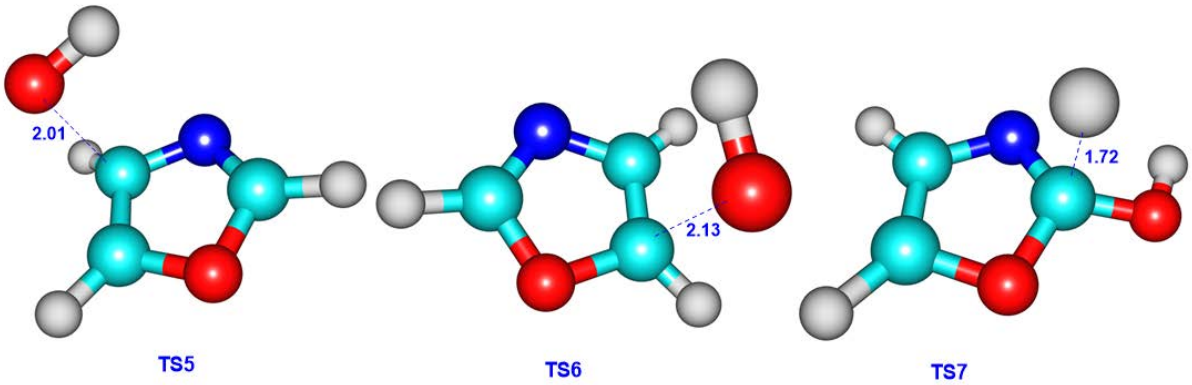
T (K)	via TS1	via TS2	via TS3	via TS4	via TS5	via TS6	via TS7	via TS8	via TS9
299	30.0	18.7	16.9	1.3	1.3	1.1	3.6	4.4	1.9
324	17.6	11.9	10.9	1.3	1.2	1.1	2.9	3.4	1.7
348	11.8	8.5	7.8	1.2	1.2	1.1	2.5	2.8	1.6
373	8.5	6.4	5.9	1.2	1.2	1.1	2.2	2.5	1.5
398	6.5	5.1	4.8	1.2	1.1	1.1	2.0	2.2	1.4
423	5.2	4.3	4.0	1.1	1.1	1.1	1.8	2.0	1.4
449	4.3	3.6	3.4	1.1	1.1	1.1	1.7	1.8	1.3
468	3.9	3.3	3.1	1.1	1.1	1.1	1.6	1.7	1.3

Table S6: Individual rate constants for Oxazole + OH → Products (cm^3/molecule/s) at different pressures (0.76, 7.6, 76, 100, 750, 760, 7600, and 76000 Torr). ("Unc." stands for the uncertainty).

P = 0.76 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	4.93E-13	4.10E-03	1.06E-14	1.90E-01	8.21E-12	2.40E-04	8.00E-17	2.50E+01	1.20E-16	1.70E+01	4.00E-17	5.00E+01
324	4.77E-13	4.20E-03	1.15E-14	1.70E-01	7.08E-12	2.80E-04	2.20E-16	9.10E+00	1.60E-16	1.20E+01	2.00E-17	1.00E+02
348	4.56E-13	4.40E-03	1.41E-14	1.40E-01	6.09E-12	3.30E-04	3.20E-16	6.20E+00	5.40E-16	3.70E+00	2.00E-17	1.00E+02
373	4.38E-13	4.60E-03	1.41E-14	1.40E-01	5.15E-12	3.90E-04	6.40E-16	3.10E+00	9.20E-16	2.20E+00	4.00E-17	5.00E+01
398	4.18E-13	4.80E-03	1.34E-14	1.50E-01	4.30E-12	4.70E-04	6.20E-16	3.20E+00	1.34E-15	1.50E+00	6.00E-17	3.30E+01
423	4.06E-13	4.90E-03	1.28E-14	1.60E-01	3.51E-12	5.70E-04	1.42E-15	1.40E+00	1.94E-15	1.00E+00	2.20E-16	9.10E+00
449	3.80E-13	5.30E-03	1.19E-14	1.70E-01	2.85E-12	7.00E-04	2.34E-15	8.50E-01	2.70E-15	7.40E-01	3.80E-16	5.30E+00
468	3.65E-13	5.50E-03	1.16E-14	1.70E-01	2.44E-12	8.20E-04	3.28E-15	6.10E-01	3.96E-15	5.10E-01	5.00E-16	4.00E+00
P = 7.6 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	4.75E-13	4.20E-03	1.19E-14	1.70E-01	8.90E-12	2.20E-04	8.00E-17	2.50E+01	1.00E-16	2.00E+01	2.00E-17	1.00E+02
324	4.48E-13	4.50E-03	1.40E-14	1.40E-01	7.91E-12	2.50E-04	1.60E-16	1.20E+01	2.60E-16	7.70E+00	2.00E-17	1.00E+02
348	4.25E-13	4.70E-03	1.55E-14	1.30E-01	7.06E-12	2.80E-04	2.80E-16	7.10E+00	4.60E-16	4.30E+00	4.00E-17	5.00E+01
373	4.07E-13	4.90E-03	1.72E-14	1.20E-01	6.23E-12	3.20E-04	5.80E-16	3.40E+00	9.00E-16	2.20E+00	1.20E-16	1.70E+01
398	3.84E-13	5.20E-03	1.84E-14	1.10E-01	5.52E-12	3.60E-04	7.80E-16	2.60E+00	1.38E-15	1.40E+00	1.80E-16	1.10E+01
423	3.74E-13	5.30E-03	1.92E-14	1.00E-01	4.86E-12	4.10E-04	1.42E-15	1.40E+00	2.14E-15	9.30E-01	1.60E-16	1.20E+01
449	3.61E-13	5.50E-03	2.05E-14	9.70E-02	4.24E-12	4.70E-04	2.20E-15	9.10E-01	3.50E-15	5.70E-01	4.20E-16	4.80E+00
468	3.44E-13	5.80E-03	2.06E-14	9.70E-02	3.84E-12	5.20E-04	2.92E-15	6.80E-01	4.44E-15	4.50E-01	3.80E-16	5.30E+00
P = 76 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	4.76E-13	4.20E-03	1.08E-14	1.90E-01	9.13E-12	2.20E-04	1.20E-16	1.70E+01	1.00E-16	2.00E+01	2.00E-17	1.00E+02
324	4.43E-13	4.50E-03	1.25E-14	1.60E-01	8.09E-12	2.50E-04	1.40E-16	1.40E+01	2.20E-16	9.10E+00	2.00E-17	1.00E+02
348	4.17E-13	4.80E-03	1.56E-14	1.30E-01	7.23E-12	2.80E-04	4.00E-16	5.00E+00	3.40E-16	5.90E+00	2.00E-17	1.00E+02
373	3.94E-13	5.10E-03	1.73E-14	1.20E-01	6.45E-12	3.10E-04	5.40E-16	3.70E+00	8.40E-16	2.40E+00	6.00E-17	3.30E+01
398	3.70E-13	5.40E-03	2.01E-14	1.00E-01	5.76E-12	3.50E-04	8.40E-16	2.40E+00	1.28E-15	1.60E+00	2.00E-17	1.00E+02
423	3.50E-13	5.70E-03	1.92E-14	1.00E-01	5.12E-12	3.90E-04	1.28E-15	1.60E+00	1.76E-15	1.10E+00	1.40E-16	1.40E+01
449	3.27E-13	6.10E-03	2.19E-14	9.10E-02	4.56E-12	4.40E-04	2.12E-15	9.40E-01	3.20E-15	6.20E-01	3.40E-16	5.90E+00
468	3.14E-13	6.40E-03	2.28E-14	8.80E-02	4.16E-12	4.80E-04	2.68E-15	7.50E-01	4.36E-15	4.60E-01	5.20E-16	3.80E+00
P = 100 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	4.78E-13	4.20E-03	1.14E-14	1.80E-01	9.16E-12	2.20E-04	2.00E-17	1.00E+02	8.00E-17	2.50E+01	2.00E-17	1.00E+02
324	4.40E-13	4.50E-03	1.42E-14	1.40E-01	8.12E-12	2.50E-04	1.20E-16	1.70E+01	3.80E-16	5.30E+00	2.00E-17	1.00E+02
348	4.18E-13	4.80E-03	1.65E-14	1.20E-01	7.28E-12	2.70E-04	2.80E-16	7.10E+00	5.20E-16	3.80E+00	2.00E-17	1.00E+02
373	3.95E-13	5.10E-03	1.72E-14	1.20E-01	6.47E-12	3.10E-04	4.00E-16	5.00E+00	4.80E-16	4.20E+00	8.00E-17	2.50E+01
398	3.68E-13	5.40E-03	1.94E-14	1.00E-01	5.77E-12	3.50E-04	1.08E-15	1.90E+00	1.46E-15	1.40E+00	1.00E-16	2.00E+01
423	3.46E-13	5.80E-03	2.11E-14	9.50E-02	5.14E-12	3.90E-04	1.38E-15	1.40E+00	2.44E-15	8.20E-01	1.20E-16	1.70E+01
449	3.23E-13	6.20E-03	2.20E-14	9.10E-02	4.57E-12	4.40E-04	2.60E-15	7.70E-01	3.46E-15	5.80E-01	3.40E-16	5.90E+00
468	3.13E-13	6.40E-03	2.34E-14	8.50E-02	4.20E-12	4.80E-04	3.46E-15	5.80E-01	4.52E-15	4.40E-01	4.40E-16	4.50E+00
P = 750 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	4.88E-13	4.10E-03	1.24E-14	1.60E-01	1.01E-11	2.00E-04	8.01E-17	2.50E+01	1.40E-16	1.40E+01	2.00E-17	1.00E+02
324	4.46E-13	4.50E-03	1.42E-14	1.40E-01	8.80E-12	2.30E-04	8.00E-17	2.50E+01	3.00E-16	6.70E+00	2.00E-17	1.00E+02
348	4.18E-13	4.80E-03	1.54E-14	1.30E-01	7.77E-12	2.60E-04	3.00E-16	6.70E+00	5.20E-16	3.80E+00	2.00E-17	1.00E+02
373	3.93E-13	5.10E-03	1.71E-14	1.20E-01	6.81E-12	2.90E-04	4.60E-16	4.30E+00	9.40E-16	2.10E+00	1.00E-16	2.00E+01
398	3.73E-13	5.40E-03	1.95E-14	1.00E-01	6.02E-12	3.30E-04	6.80E-16	2.90E+00	1.38E-15	1.40E+00	6.00E-17	3.30E+01
423	3.46E-13	5.80E-03	2.21E-14	9.00E-02	5.33E-12	3.80E-04	1.68E-15	1.20E+00	1.86E-15	1.10E+00	2.60E-16	7.70E+00

449	3.23E-13	6.20E-03	2.27E-14	8.80E-02	4.71E-12	4.20E-04	2.24E-15	8.90E-01	3.08E-15	6.50E-01	4.00E-16	5.00E+00
468	3.11E-13	6.40E-03	2.44E-14	8.20E-02	4.32E-12	4.60E-04	3.34E-15	6.00E-01	3.88E-15	5.20E-01	5.00E-16	4.00E+00
P = 760 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	4.82E-13	4.10E-03	1.22E-14	1.60E-01	1.01E-11	2.00E-04	1.00E-16	2.00E+01	8.00E-17	2.50E+01	2.00E-17	1.00E+02
324	4.46E-13	4.50E-03	1.32E-14	1.50E-01	8.81E-12	2.30E-04	1.40E-16	1.40E+01	1.80E-16	1.10E+01	2.00E-17	1.00E+02
348	4.22E-13	4.70E-03	1.60E-14	1.20E-01	7.76E-12	2.60E-04	3.60E-16	5.60E+00	5.60E-16	3.60E+00	8.00E-17	2.50E+01
373	3.98E-13	5.00E-03	1.83E-14	1.10E-01	6.82E-12	2.90E-04	4.00E-16	5.00E+00	7.40E-16	2.70E+00	6.00E-17	3.30E+01
398	3.72E-13	5.40E-03	1.96E-14	1.00E-01	6.03E-12	3.30E-04	9.20E-16	2.20E+00	1.58E-15	1.30E+00	1.60E-16	1.20E+01
423	3.44E-13	5.80E-03	2.14E-14	9.40E-02	5.32E-12	3.80E-04	1.22E-15	1.60E+00	2.20E-15	9.10E-01	1.20E-16	1.70E+01
449	3.30E-13	6.10E-03	2.29E-14	8.70E-02	4.73E-12	4.20E-04	2.18E-15	9.20E-01	3.66E-15	5.50E-01	2.00E-16	1.00E+01
468	3.08E-13	6.50E-03	2.49E-14	8.00E-02	4.31E-12	4.60E-04	3.54E-15	5.60E-01	4.44E-15	4.50E-01	5.40E-16	3.70E+00
P = 7600 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	5.05E-13	4.00E-03	1.34E-14	1.50E-01	1.25E-11	1.60E-04	4.00E-17	5.00E+01	1.40E-16	1.40E+01	2.00E-17	1.00E+02
324	4.71E-13	4.20E-03	1.60E-14	1.20E-01	1.07E-11	1.90E-04	1.60E-16	1.20E+01	2.00E-16	1.00E+01	2.00E-17	1.00E+02
348	4.44E-13	4.50E-03	1.81E-14	1.10E-01	9.21E-12	2.20E-04	3.00E-16	6.70E+00	5.80E-16	3.40E+00	2.00E-17	1.00E+02
373	4.22E-13	4.70E-03	2.05E-14	9.80E-02	7.92E-12	2.50E-04	3.80E-16	5.30E+00	8.80E-16	2.30E+00	4.00E-17	5.00E+01
398	3.94E-13	5.10E-03	2.27E-14	8.80E-02	6.84E-12	2.90E-04	8.60E-16	2.30E+00	1.22E-15	1.60E+00	8.00E-17	2.50E+01
423	3.66E-13	5.50E-03	2.23E-14	9.00E-02	5.92E-12	3.40E-04	1.22E-15	1.60E+00	1.80E-15	1.10E+00	1.80E-16	1.10E+01
449	3.39E-13	5.90E-03	2.54E-14	7.90E-02	5.19E-12	3.90E-04	2.14E-15	9.30E-01	3.22E-15	6.20E-01	2.20E-16	9.10E+00
468	3.30E-13	6.10E-03	2.66E-14	7.50E-02	4.72E-12	4.20E-04	3.00E-15	6.70E-01	4.06E-15	4.90E-01	3.40E-16	5.90E+00
P = 76000 Torr												
T (K)	I1	Unc. (%)	I2	Unc. (%)	I3	Unc. (%)	P1 + H_2O	Unc. (%)	P2 + H_2O	Unc. (%)	P3 + H_2O	Unc. (%)
299	5.24E-13	3.80E-03	1.85E-14	1.10E-01	1.28E-11	1.60E-04	8.00E-17	2.50E+01	1.60E-16	1.20E+01	2.00E-17	1.00E+02
324	5.21E-13	3.80E-03	2.22E-14	9.00E-02	1.16E-11	1.70E-04	1.40E-16	1.40E+01	3.40E-16	5.90E+00	2.00E-17	1.00E+02
348	5.07E-13	3.90E-03	2.84E-14	7.10E-02	1.03E-11	1.90E-04	2.40E-16	8.30E+00	3.20E-16	6.20E+00	6.00E-17	3.30E+01
373	4.89E-13	4.10E-03	2.99E-14	6.70E-02	8.98E-12	2.20E-04	4.80E-16	4.20E+00	6.40E-16	3.10E+00	2.00E-17	1.00E+02
398	4.68E-13	4.30E-03	3.37E-14	5.90E-02	7.81E-12	2.60E-04	7.80E-16	2.60E+00	1.08E-15	1.90E+00	1.00E-16	2.00E+01
423	4.49E-13	4.50E-03	3.70E-14	5.40E-02	6.88E-12	2.90E-04	1.38E-15	1.40E+00	1.68E-15	1.20E+00	8.00E-17	2.50E+01
449	4.24E-13	4.70E-03	4.02E-14	5.00E-02	6.09E-12	3.30E-04	2.46E-15	8.10E-01	3.54E-15	5.60E-01	3.60E-16	5.60E+00
468	4.08E-13	4.90E-03	4.15E-14	4.80E-02	5.55E-12	3.60E-04	3.28E-15	6.10E-01	3.90E-15	5.10E-01	4.80E-16	4.20E+00

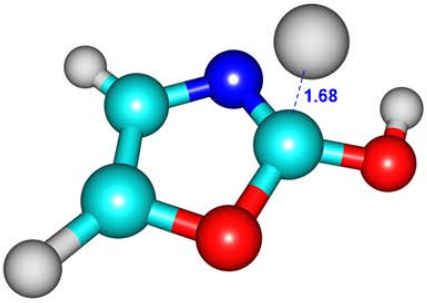

H
C
O
N
1.95
2.48
2.32
1.18
1.27
1.19
1.26
1.17
1.28
2.07
Oxazole
RC1
RC2
TS0
TS1
TS2
TS3
TS4



TS5

TS6

TS7



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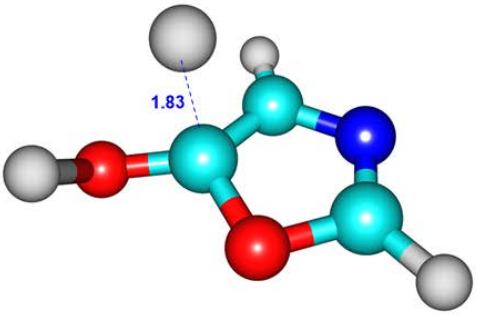
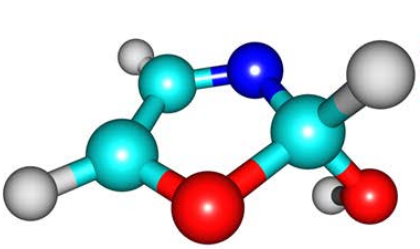
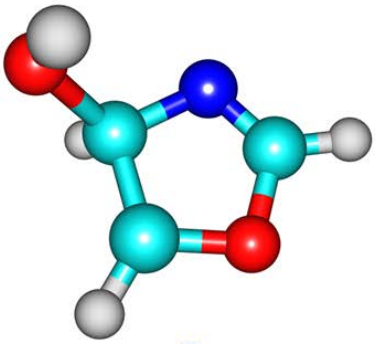


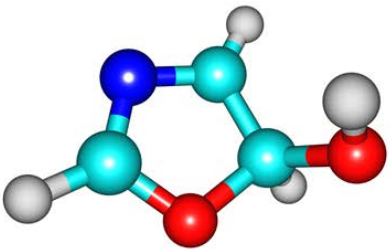
TS9



I1



I2



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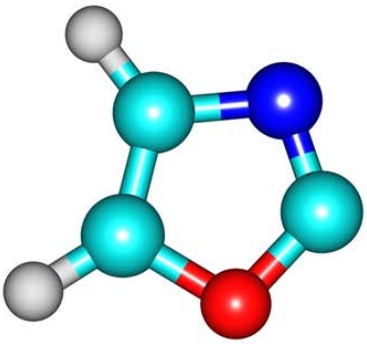
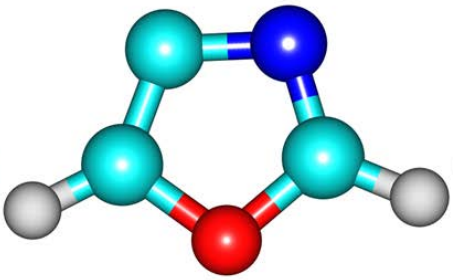


P1



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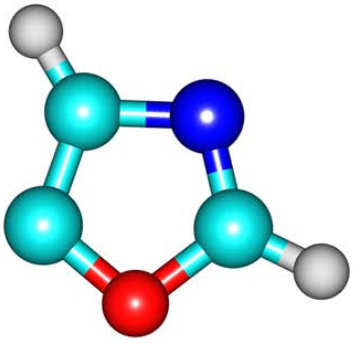


P3

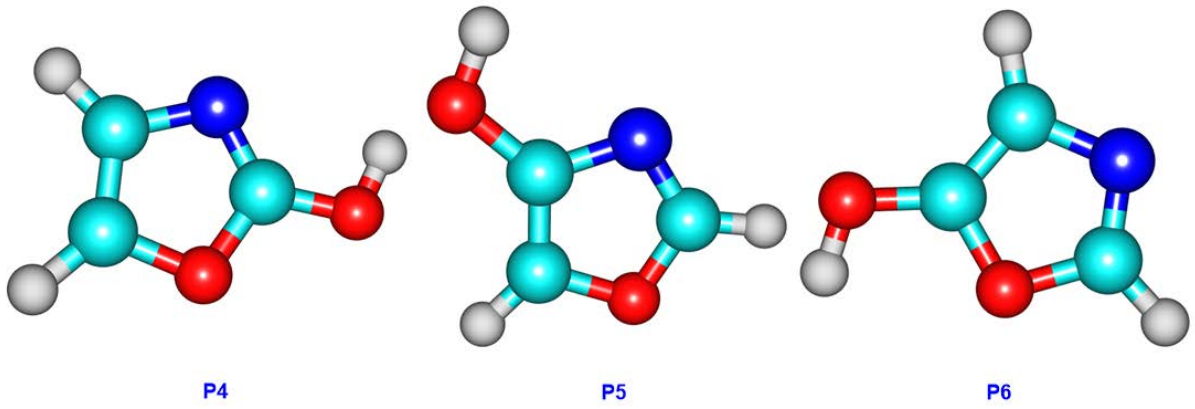


Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the oxazole + OH reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths are in Å.

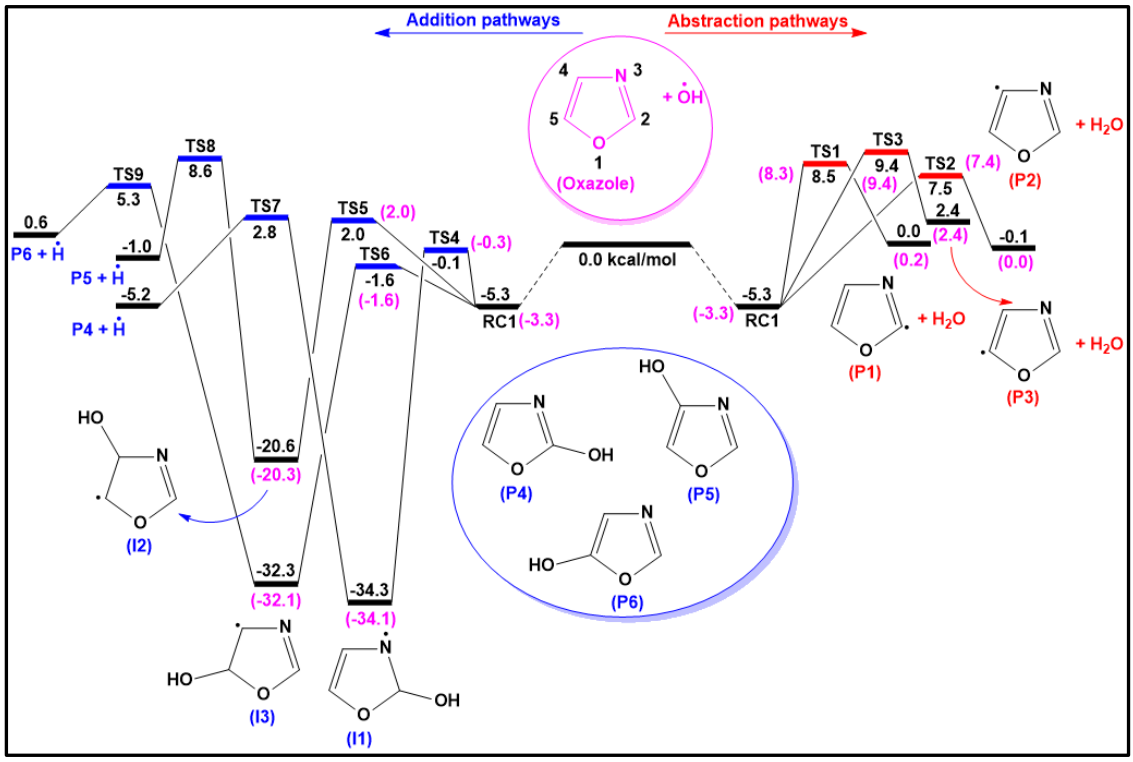


Figure S2: The M06-2X/aug-cc-pVTZ ZPE-corrected energy profiles (0 K) used for the RC1 rate model. Numbers in parentheses, "( )", are suggested by Shiroudi *et al.*[3] at the same level. Units are in kcal/mol.

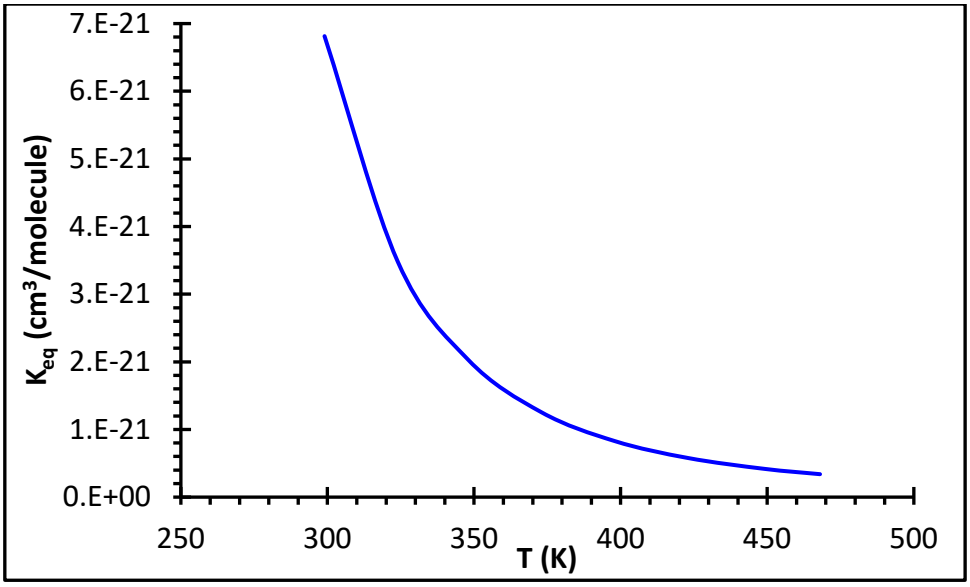
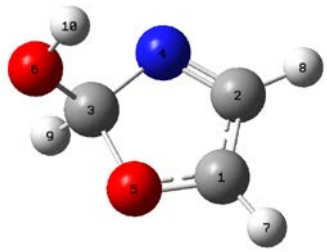
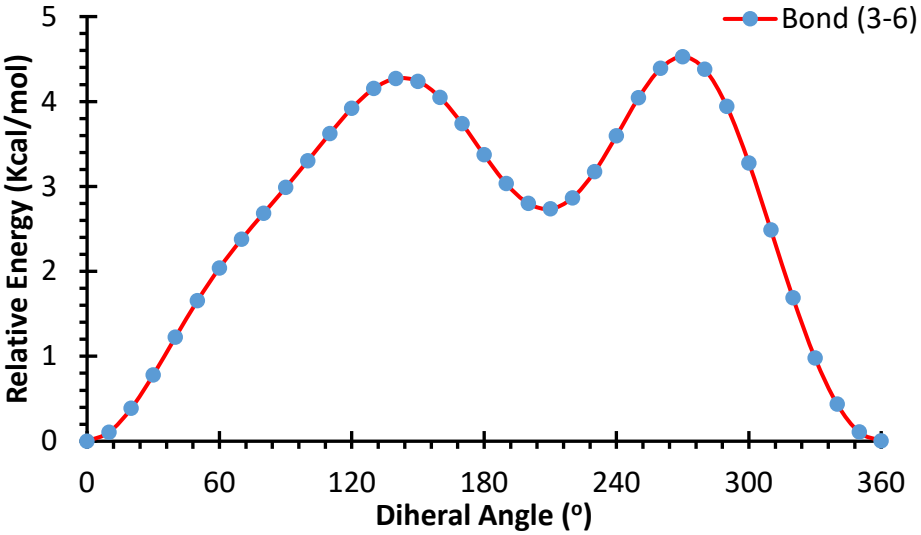
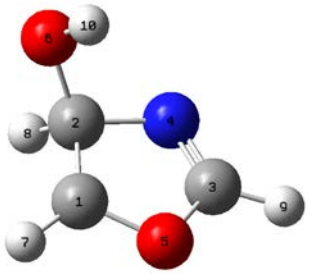
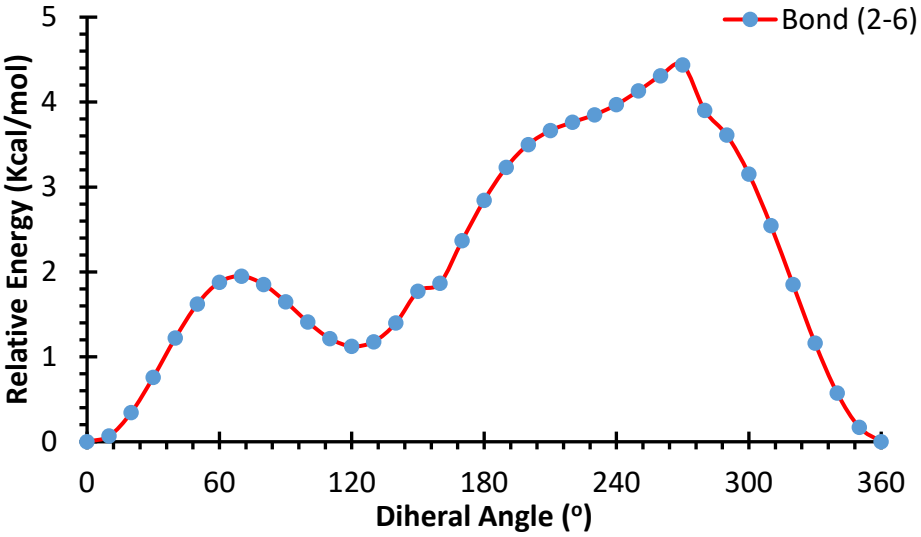
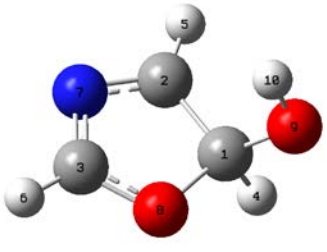
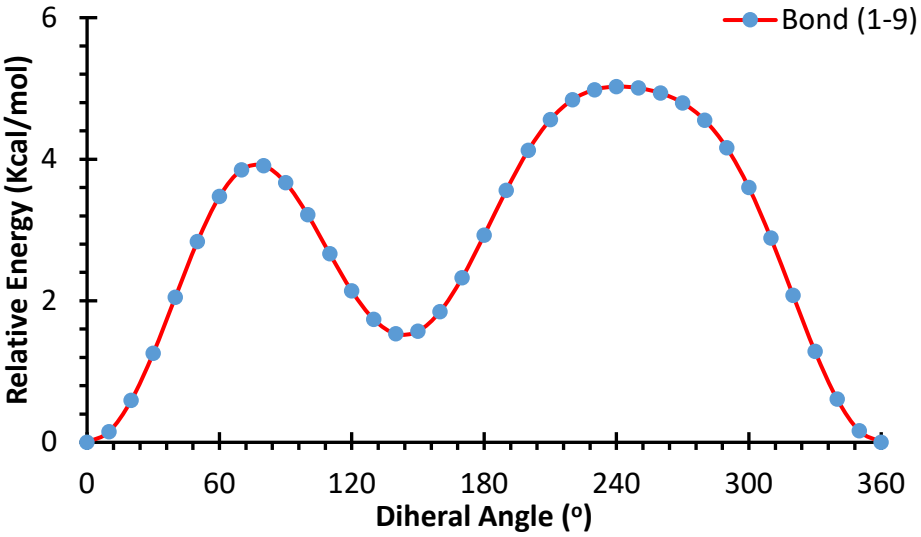
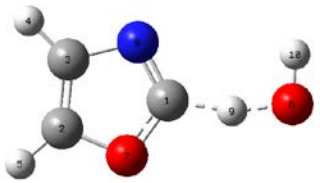
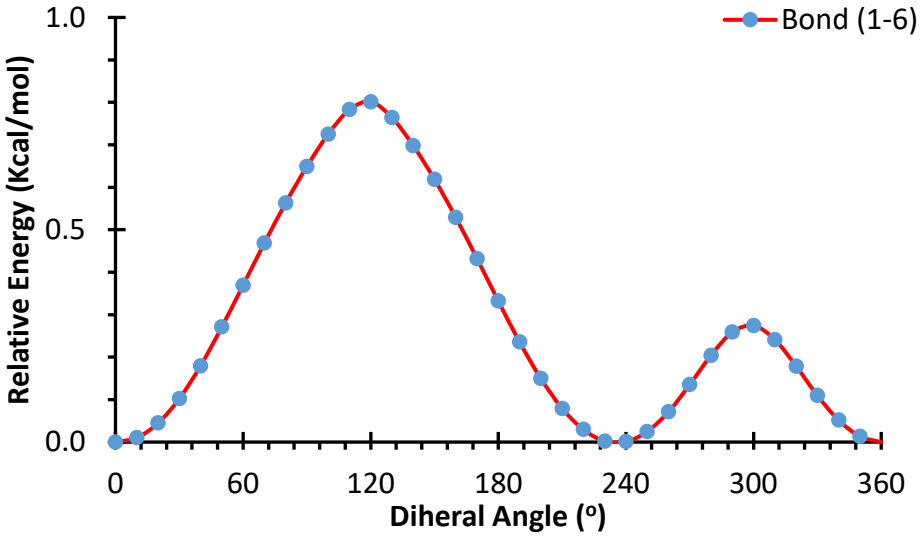
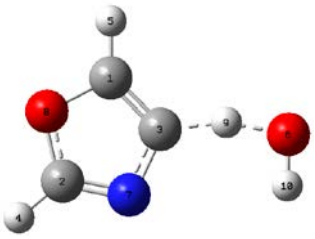
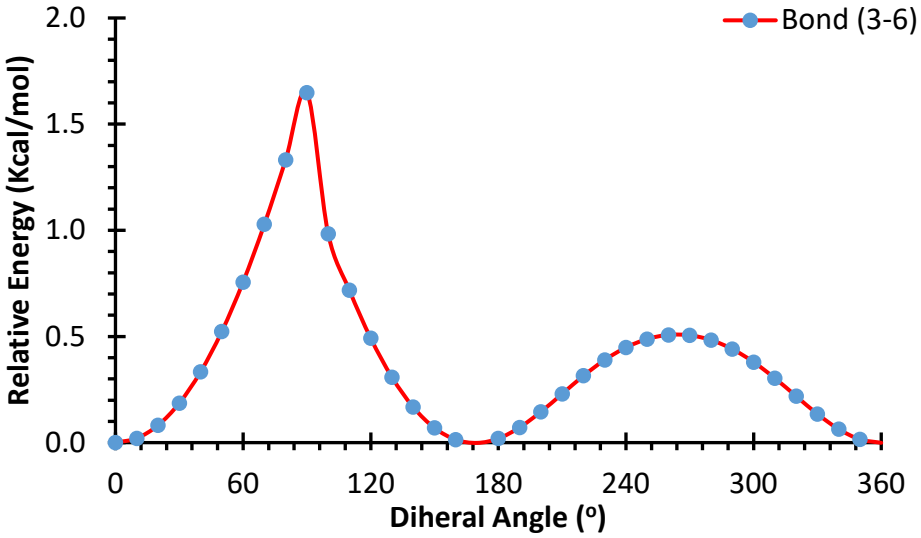
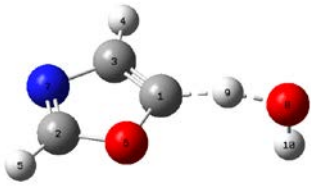
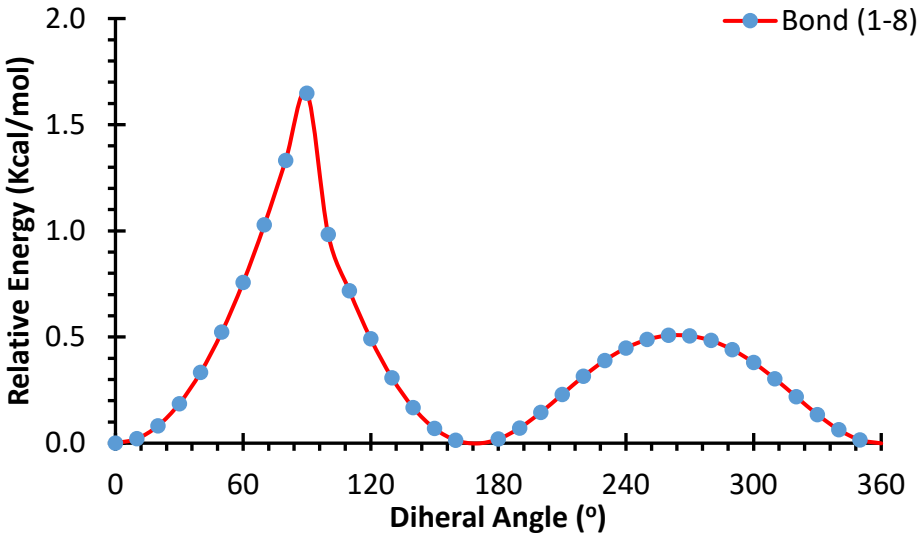
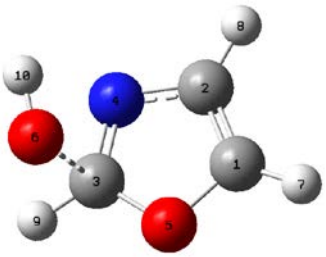
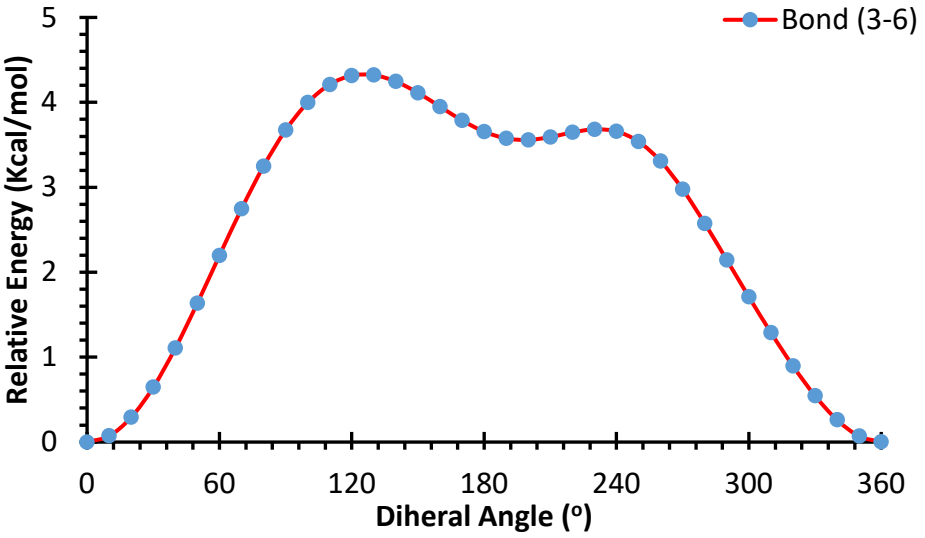
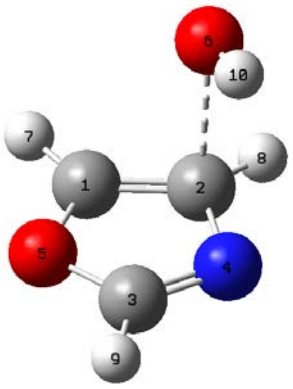
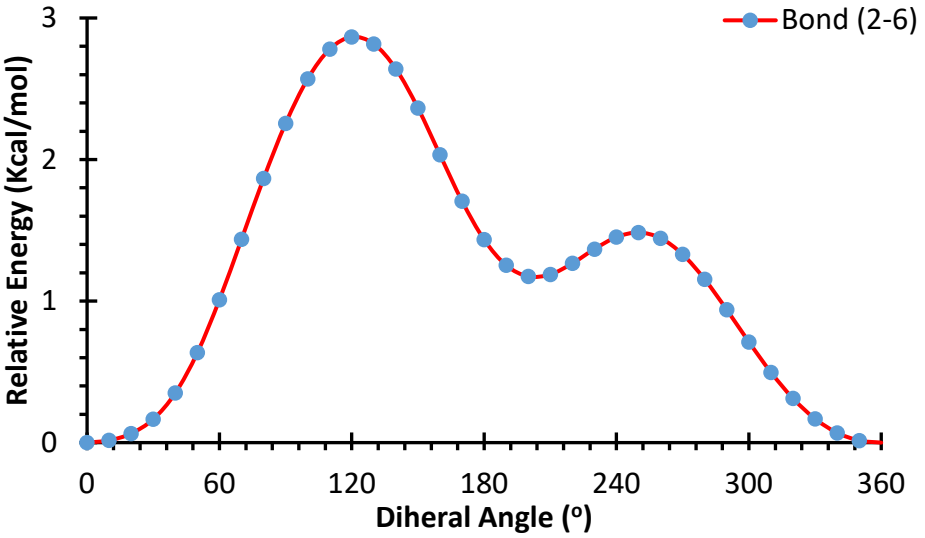
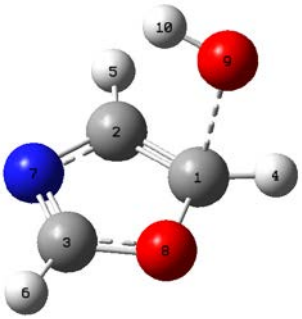
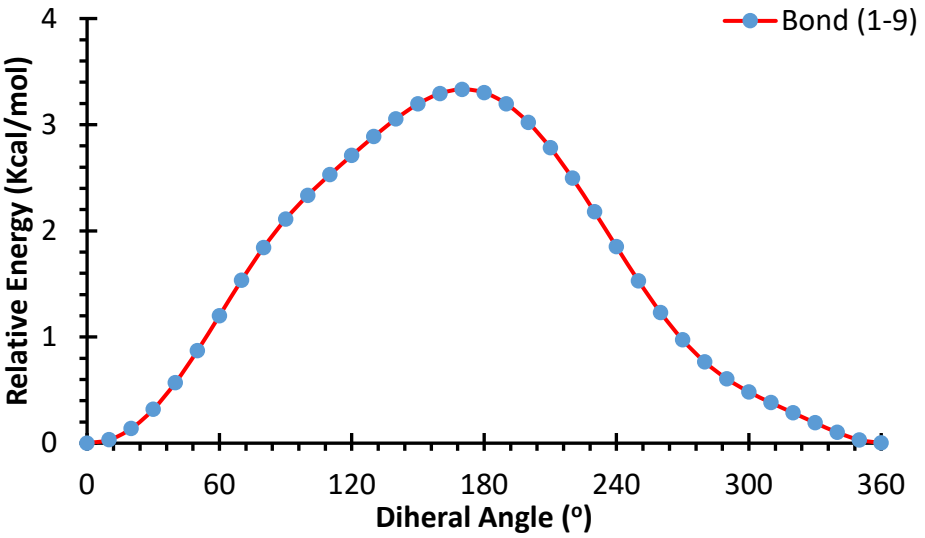
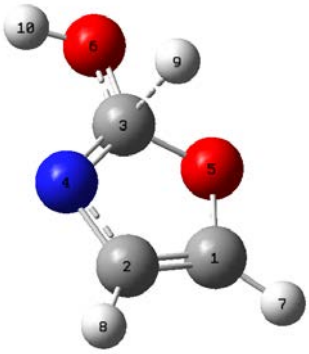
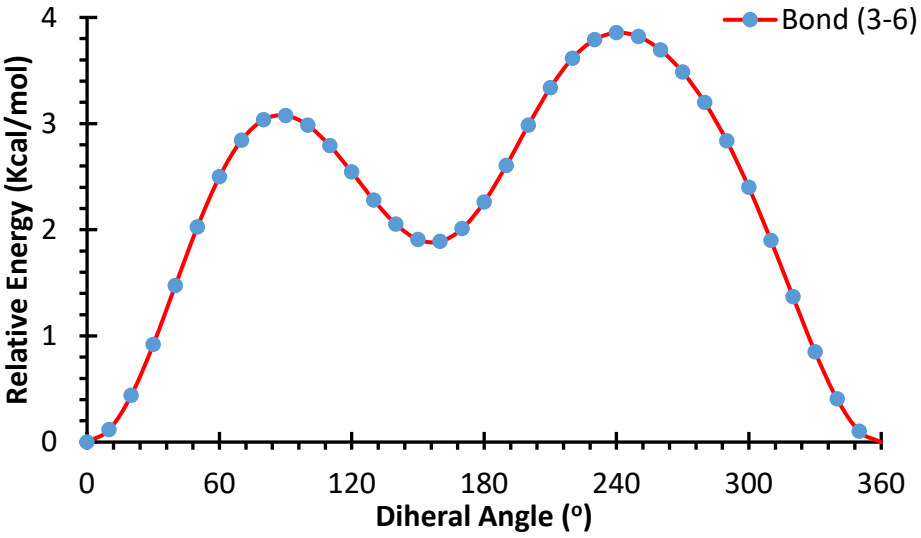
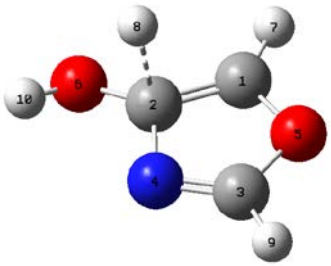
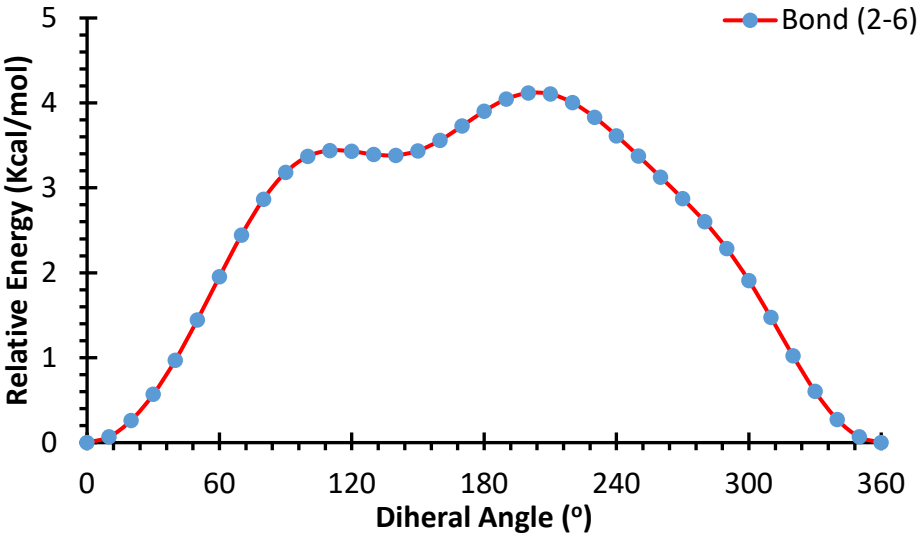
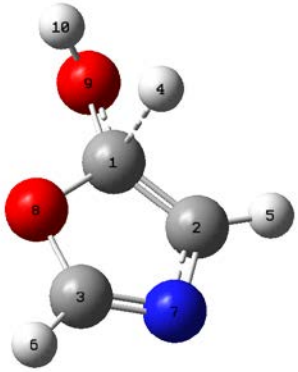
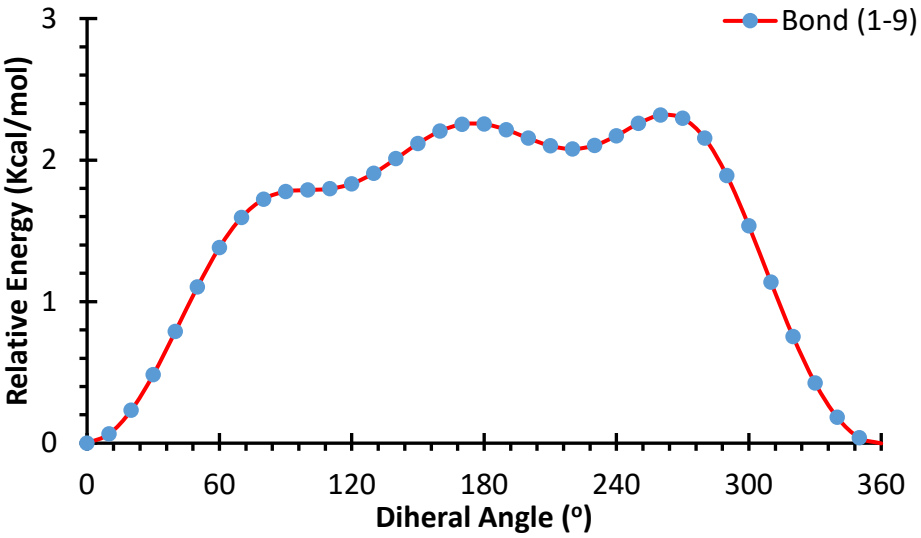


Figure S3: Plot of K_{eq} for the reaction of oxazole + OH → RC1 (K_{eq} = $[RC1]_{eq}/([OH]_{eq}\times[oxazole]_{eq})$ as a function of temperature (T = 299 – 468 K).

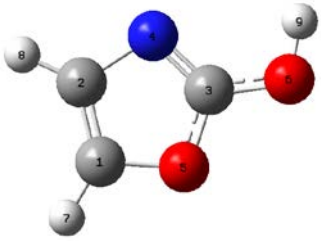
Species	Potential energy surfaces for the internal rotations
 I1	
 I2	
 I3	

Species	Potential energy surfaces for the internal rotations
 TS1	
 TS2[a]	
 TS3	

Species	Potential energy surfaces for the internal rotations
 TS4	
 TS5	
 TS6	

Species	Potential energy surfaces for the internal rotations
 TS7	
 TS8	
 TS9	

Species	Potential energy surfaces for the internal rotations



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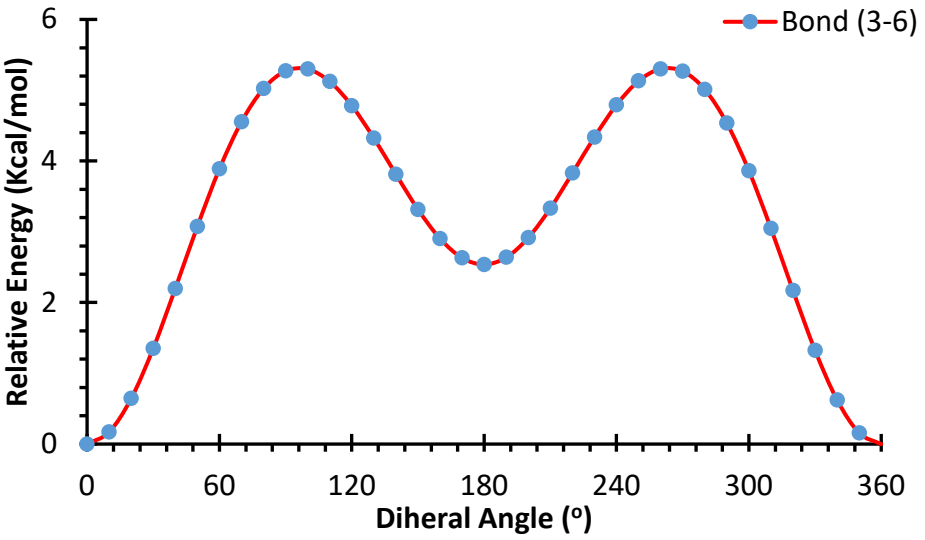

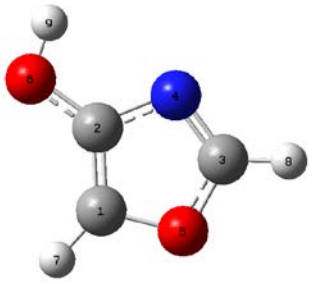

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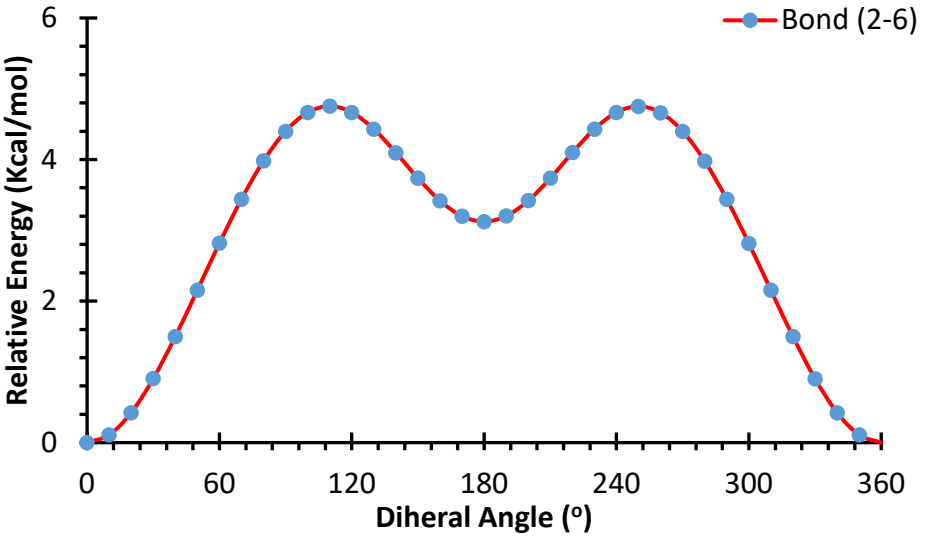

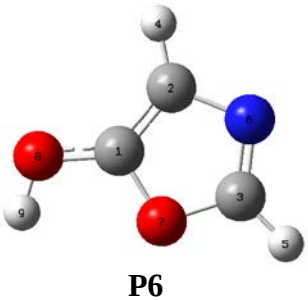

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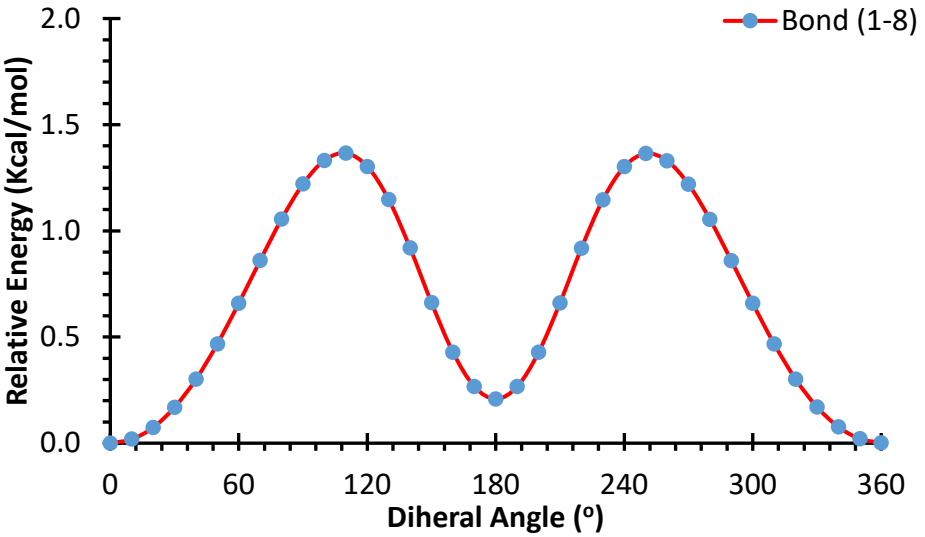

Figure S4: Hindrance potentials for the species involved in the oxazole + OH reaction, calculated at M06-2X/cc-pVDZ level of theory. ([a] assumed as **TS3**).

References:

1. K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure. IV. Constants of Diatomic Molecules*, Van Nostrand Reinhold Co, 1979.
2. T. Shimanouchi, *Tables of Molecular Vibrational Frequencies, Consolidated Volume 1, NSRDS NBS-39*.
3. A. Shiroudi, M. Abdel-Rahman, A. El-Nahas and M. Altarawneh, *New J. Chem.*, **2021**, 45, 2237-2248.