Supplementary Information for

Comment on "Atmospheric oxidation reactions of imidazole initiated by hydroxyl radicals: kinetics and mechanism of reactions and atmospheric implications" by Zahra Safaei, Abolfazl Shiroudi, Ehsan Zahedi and Mika Sillanpää, Phys. Chem. Chem. Phys., 2019, 21, 8445

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Contents

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 M06-2X/aug-cc-pVTZ level of theory for the title reaction.

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	/
Imidazole (C_s)	6	0.991895000	-0.521600000	-0.000178000	-226.212273	0.072087	570.1515 655.6537 690.2652
	6	-1.127693000	-0.299045000	-0.000065000			768.9928 862.3679 909.8507
	6	-0.624370000	0.968315000	0.000090000			910.1665 949.0447 1087.7462
	7	0.739049000	0.813005000	0.000276000			1105.7237 1153.7695 1186.5050
	1	1.422618000	1.548851000	-0.000180000			1291.5984 1390.1990 1451.8367
	1	1.993403000	-0.918125000	-0.000052000			1525.8087 1585.7463 3272.6666
	1	-2.160789000	-0.600026000	0.000694000			3279.1160 3306.9022 3688.5662
	1	-1.092079000	1.935582000	-0.001241000			(539; 621; 663; 674; 758; 831; 898; 923; 988; 1013; 1062; 1098;
	7	-0.110784000	-1.220476000	-0.000033000			1188; 1265; 1328; 1404; 1448; 3110; 3123; 3143; 3517)[3]
RC (C_1)	6	-0.341720000	-1.026595000	0.000393000	-301.959810	0.083475	27.7239 49.7737 163.3562
	6	-0.430063000	1.111320000	0.000336000			564.4323 582.2844 649.9751
	6	-1.723257000	0.684212000	-0.000434000			665.7123 704.3271 770.7221
	7	-1.651890000	-0.686462000	-0.000389000			868.1818 912.1842 923.9577
	1	-2.428755000	-1.323644000	-0.000852000			951.4751 1091.1359 1112.3555
	1	-0.004356000	-2.049134000	0.000604000			1157.6952 1193.1697 1294.1036
	1	-0.062268000	2.122107000	0.000556000			1392.4034 1458.4002 1535.0027
	1	-2.659382000	1.210961000	-0.001001000			1594.0495 3282.2318 3284.9411
	7	0.421819000	0.034885000	0.000856000			3313.7299 3414.8382 3682.9096
	8	3.302539000	-0.005683000	-0.000567000			
	1	2.315185000	0.032594000	0.000190000			
Addition channels							

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
TS1	6	0.449183000	0.068890000	0.778685000	-301.951405	0.083283	-442.7900	143.8862	155.9370
(C_1)	6	-1.183757000	-0.818475000	-0.281396000			261.7786	581.4107	617.5111
	6	-1.318494000	0.544442000	-0.436791000			650.6518	716.4407	788.6317
	7	-0.302689000	1.092908000	0.276252000			866.8406	907.2479	914.3586
	1	-0.044201000	2.063977000	0.293289000			943.9409	1086.4518	1112.3499
	1	1.214036000	0.225880000	1.517267000			1139.8109	1220.7718	1264.3800
	1	-1.812168000	-1.590234000	-0.691540000			1353.0264	1421.7157	1510.8125
	1	-2.027656000	1.138371000	-0.984206000			1539.6449	3273.5671	3294.7634
	7	-0.111707000	-1.104055000	0.491391000			3304.1177	3682.7795	3804.0832
	8	1.994986000	0.047131000	-0.634695000					
	1	1.929281000	-0.906160000	-0.793740000					
TS2	6	1.202696000	-0.713535000	-0.291502000	-301.947967	0.083421	-424.7340	156.5320	161.4007
(C_1)	6	-0.532433000	-0.058146000	0.778008000			227.8314	553.3099	595.6916
	6	0.146043000	1.093167000	0.379666000			661.7717	767.5356	821.2313
	7	1.219101000	0.656329000	-0.324491000			875.5081	900.2722	936.2628
	1	1.877414000	1.230318000	-0.821687000			941.5155	1071.2117	1097.7393
	1	1.961736000	-1.302112000	-0.779966000			1136.3143	1158.5841	1291.0282
	1	-1.292094000	-0.130475000	1.533777000			1381.7081	1438.7126	1491.9378
	1	-0.105613000	2.132665000	0.477976000			1582.5447	3270.5304	3292.2473
	7	0.199493000	-1.173198000	0.388918000			3312.2982	3680.6377	3813.1188
	8	-1.935110000	0.074615000	-0.641397000					
	1	-1.788556000	-0.838148000	-0.926946000					
TS3	6	-1.340225000	-0.415590000	-0.447051000	-301.953424	0.083182	-293.6567	127.9530	130.4954
(C_1)	6	-0.107973000	1.062062000	0.456445000			205.7824	572.1014	610.7690
	6	0.441996000	-0.161775000	0.813182000			666.7836	696.6670	841.3414
	7	-0.404490000	-1.088884000	0.264312000			867.7178	901.2285	908.9851
	1	-0.259788000	-2.083255000	0.265911000			948.1575	1084.9843	1102.9637
	1	-2.103953000	-0.917214000	-1.017488000			1149.8118	1202.3980	1288.5681
	1	0.254651000	2.039859000	0.723251000			1357.1944	1426.9058	1507.6938
	1	1.197278000	-0.421442000	1.529219000			1552.9041	3273.9711	3279.2812
	7	-1.193358000	0.884874000	-0.343925000			3320.3477	3684.7559	3802.8287
	8	2.052236000	-0.086903000	-0.586840000					
	1	1.716072000	0.597169000	-1.184332000					
IM1	6	0.728704000	-0.017358000	0.446380000	-301.995581	0.085842	129.1930	222.6640	310.7978

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
(C_1)	6	-1.274870000	-0.770904000	-0.138685000			438.9893	556.4630	605.4417
	6	-1.371637000	0.628230000	-0.205535000			703.4831	811.1898	872.6772
	7	-0.178920000	1.114911000	0.203558000			918.7739	958.5380	1011.2295
	1	0.153850000	2.050946000	0.051656000			1080.3666	1092.7747	1156.7321
	1	1.118417000	0.031238000	1.465272000			1242.9464	1301.3748	1306.0026
	1	-2.070038000	-1.461887000	-0.376480000			1408.2341	1440.9812	1474.9430
	1	-2.193556000	1.254019000	-0.505959000			1521.2047	3075.9441	3235.4717
	7	-0.089995000	-1.188131000	0.244731000			3285.9659	3675.3258	3842.6288
	8	1.844352000	0.013810000	-0.400934000					
	1	1.625727000	-0.512058000	-1.178007000					
IM2	6	-1.443910000	-1.303623000	-0.735797000	-301.978996	0.085185	140.3318	261.2880	329.4712
(C_1)	1	-1.523539000	-2.112049000	-0.008989000			362.4059	446.8638	519.8841
	1	-2.022153000	-1.542452000	-1.628902000			614.3735	798.6812	880.8039
	6	-0.014917000	-0.903727000	-1.047932000			908.2420	942.5778	1017.0983
	1	0.008512000	-0.222671000	-1.903088000			1073.0264	1111.2017	1135.2959
	1	0.537283000	-1.797015000	-1.366088000			1253.5175	1277.3243	1312.1700
	6	0.777307000	-0.279778000	0.116596000			1394.5793	1421.1071	1447.6038
	6	0.260408000	2.043588000	-0.417337000			1661.4651	3036.7871	3224.9656
	1	-0.308457000	1.818734000	-1.324822000			3293.0285	3685.4617	3842.1325
	1	-0.203140000	2.899817000	0.071793000					
	1	1.288922000	2.305407000	-0.681515000					
	1	-2.056067000	-0.405891000	-0.241099000					
	8	0.213015000	0.981912000	0.515737000					
	6	0.682343000	-1.133841000	1.374916000					
	1	1.336314000	-0.726382000	2.147928000					
	1	-0.339401000	-1.137045000	1.758656000					
	1	0.983382000	-2.162836000	1.163689000					
	6	2.240208000	-0.105874000	-0.292087000					
	1	2.720734000	-1.083939000	-0.361480000					
	1	2.340655000	0.382516000	-1.264060000					
	1	2.768944000	0.486476000	0.458199000					
	8	-2.568481000	0.584379000	0.525240000					
	1	-1.696899000	0.866528000	0.861809000					
IM3	6	-1.362634000	-0.576320000	-0.202586000	-301.990918	0.085373	111.8891	303.8544	340.0462

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
(C_1)	6	-0.190484000	1.151722000	0.214111000			429.2277	540.0630	599.0506
	6	0.753659000	0.006714000	0.457437000			635.7587	806.1415	822.6098
	7	-0.179012000	-1.083857000	0.233736000			893.6490	935.4359	1042.1312
	1	0.092148000	-2.049937000	0.207283000			1046.5429	1122.7825	1185.8826
	1	-2.185094000	-1.205525000	-0.501296000			1233.9762	1251.6076	1302.0933
	1	0.065830000	2.191635000	0.331263000			1323.5370	1419.1947	1471.1579
	1	1.183442000	-0.032947000	1.460258000			1532.9465	3072.9383	3257.1357
	7	-1.393497000	0.743090000	-0.208128000			3266.1203	3693.7479	3834.8887
	8	1.881627000	-0.030252000	-0.400976000					
	1	1.594975000	0.231470000	-1.282729000					
TS-IM1a	6	0.644447000	-0.038719000	0.082155000	-301.939203	0.078751	-1054.2256	278.2412	311.2573
(C_1)	6	-1.360404000	-0.750048000	-0.045324000			413.3013	504.1168	566.4830
	6	-1.447726000	0.614169000	-0.042261000			594.9989	646.5838	728.7360
	7	-0.151322000	1.067918000	-0.034980000			762.1572	809.7743	905.8808
	1	0.165140000	2.016973000	0.059659000			928.9285	1008.3741	1100.7872
	1	0.650687000	-0.078846000	1.790991000			1142.9257	1154.9237	1229.3117
	1	-2.170163000	-1.458358000	-0.065215000			1329.7931	1399.9548	1520.0361
	1	-2.289811000	1.281206000	-0.044058000			1528.0083	1579.3892	3278.5094
	7	-0.057081000	-1.156852000	-0.028922000			3307.1288	3682.8852	3855.0298
	8	1.967193000	0.088184000	-0.144741000					
	1	2.347525000	-0.796319000	-0.103552000					
TS-IM1b	6	0.658891000	-0.117227000	0.412257000	-301.900400	0.076950	-747.2610	180.2814	240.5513
(C_1)	6	-1.350352000	-0.714850000	-0.189929000			306.6913	440.3886	458.9173
	6	-1.298539000	0.759682000	-0.039423000			599.3855	630.6665	805.4009
	7	-0.111889000	1.133209000	0.248880000			864.7160	875.2766	958.4460
	1	0.792162000	1.999317000	-1.126554000			968.8570	995.9030	1020.0356
	1	0.827831000	-0.226607000	1.487568000			1196.5693	1247.3376	1295.1087
	1	-2.224416000	-1.299393000	-0.448620000			1311.7941	1347.9901	1414.3051
	1	-2.117106000	1.453847000	-0.177412000			1588.7443	1699.4018	3078.5475
	7	-0.208354000	-1.231679000	0.017455000			3203.5004	3217.6156	3830.9152
	8	1.891012000	-0.108542000	-0.195077000					
	1	1.775133000	0.064835000	-1.136142000					
TS-IM2a	6	1.273859000	-0.792610000	-0.036631000	-301.932920	0.078760	-1096.1964	219.1447	300.9284
(C_1)	6	-0.683541000	0.044032000	0.082530000			417.3443	544.0547	567.5351

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	6	0.182242000	1.126516000	-0.041006000			614.5620	642.9880	695.3685
	7	1.429670000	0.557323000	-0.033842000			751.0892	828.1037	879.8580
	1	2.304807000	1.050417000	-0.037892000			938.6511	998.2925	1088.7654
	1	2.115664000	-1.464531000	-0.059666000			1134.5010	1174.5285	1279.0542
	1	-0.713196000	0.073614000	1.736414000			1333.8404	1400.1362	1474.5905
	1	0.008804000	2.184541000	-0.003203000			1550.2022	1600.6899	3270.2745
	7	0.020822000	-1.142970000	-0.027851000			3320.9095	3689.1086	3857.2995
	8	-2.015034000	0.093916000	-0.163220000					
	1	-2.384617000	-0.763471000	0.072597000					
TS-IM2b (C_1)	6	-1.189888000	-0.803674000	0.061413000	-301.895552	0.076558	-847.7798	169.2166	213.9651
	6	0.765488000	0.013552000	-0.392433000			309.5219	376.9409	385.0023
	6	-0.253378000	1.108484000	-0.208510000			582.0475	626.0554	786.7280
	7	-1.415781000	0.619301000	0.013880000			866.6145	901.5601	955.0518
	1	-2.288275000	0.771179000	1.560338000			997.0154	1010.2279	1052.8091
	1	-2.031348000	-1.451227000	0.267724000			1188.3671	1211.2097	1283.1247
	1	1.060518000	-0.016158000	-1.451518000			1309.9285	1327.3016	1424.3916
	1	-0.061274000	2.169263000	-0.289277000			1594.6890	1705.8855	3001.4816
	7	-0.004532000	-1.200243000	-0.134961000			3228.6795	3233.2796	3863.7923
	8	1.870179000	0.167431000	0.445154000					
	1	2.367811000	-0.656082000	0.436254000					
TS-IM3a (C_1)	6	-1.427182000	-0.604596000	-0.010842000	-301.931486	0.078349	-775.5985	206.5242	296.8942
	6	-0.203025000	1.140451000	-0.053090000			387.1452	480.2467	572.0693
	6	0.666493000	0.063654000	0.036160000			594.1709	674.8900	676.4637
	7	-0.146270000	-1.048482000	-0.021074000			741.6812	851.0213	877.0916
	1	0.176206000	-1.999236000	0.034470000			925.8094	1029.1367	1110.5387
	1	-2.271336000	-1.273331000	0.001386000			1166.4001	1225.6018	1271.0578
	1	0.060338000	2.183777000	-0.069789000			1318.4385	1394.6486	1424.7131
	1	0.825622000	0.223464000	1.803013000			1513.8843	1603.0290	3273.0678
	7	-1.490913000	0.704984000	-0.032796000			3282.5212	3676.8264	3817.5175
	8	1.995285000	-0.050575000	-0.226944000					
	1	2.489460000	0.077366000	0.590193000					
TS-IM3b (C_1)	6	-1.297384000	-0.707917000	-0.031624000	-301.896932	0.076854	-772.7133	164.8947	247.4538
	6	-0.300350000	1.174464000	-0.016182000			313.2266	391.3494	534.0513
	6	0.676993000	0.101385000	0.409130000			587.3501	609.6689	767.4236

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	7	-0.119538000	-1.121963000	0.251656000			867.5587	898.1283	964.4561
	1	0.708081000	-1.924638000	-1.138402000			982.9616	1022.6721	1069.6307
	1	-2.144714000	-1.365021000	-0.165337000			1181.9993	1248.1515	1270.6196
	1	-0.073313000	2.231221000	-0.078467000			1330.9526	1335.1610	1407.9179
	1	0.834040000	0.224973000	1.488217000			1556.7794	1683.7977	3038.5705
	7	-1.465779000	0.696146000	-0.218109000			3216.4082	3237.0682	3806.7097
	8	1.930749000	0.088922000	-0.181273000					
	1	1.851579000	-0.304786000	-1.058598000					
P-IM1a (C_1)	6	-0.648687000	-0.043463000	-0.000212000	-301.4516126	0.07668	305.4508	388.5728	432.6472
	6	1.352168000	-0.745770000	-0.000283000			519.2337	647.0505	722.4406
	6	1.441972000	0.607749000	-0.000044000			723.3575	763.7087	896.8881
	7	0.130282000	1.058986000	0.000081000			931.5230	1023.4509	1085.9816
	1	-0.195703000	2.008811000	0.001306000			1147.5405	1163.1489	1230.7696
	1	2.153855000	-1.462647000	-0.000034000			1324.4494	1394.0675	1568.9186
	1	2.278159000	1.281428000	-0.000115000			1585.2269	1656.3296	3284.2272
	7	0.028247000	-1.149225000	0.000407000			3312.2275	3692.1458	3859.1644
	8	-1.983256000	0.086957000	-0.000294000					
	1	-2.352690000	-0.802667000	0.001012000					
P-IM1b (C_1)	6	0.681923000	0.000072000	0.396468000	-301.40619	0.075444	207.1895	210.2857	434.5146
	6	-1.296670000	-0.746904000	-0.133417000			605.8986	627.4426	809.3027
	6	-1.296794000	0.746755000	-0.133436000			874.9898	875.7376	950.5563
	7	-0.139406000	1.190638000	0.131897000			975.9096	1004.0613	1020.6148
	1	0.902664000	0.000229000	1.467102000			1186.4797	1250.5318	1299.9104
	1	-2.144124000	-1.388865000	-0.340510000			1303.2427	1345.4085	1412.0476
	1	-2.144375000	1.388525000	-0.340612000			1650.2052	1726.9111	3086.0481
	7	-0.139222000	-1.190555000	0.132073000			3196.7006	3208.4093	3853.4995
	8	1.886328000	0.000114000	-0.273806000					
	1	1.714846000	-0.000925000	-1.221012000					
P-IM2a (C_1)	6	1.256738000	-0.793683000	-0.000007000	-301.44691	0.076638	326.2778	337.9995	425.7654
	6	-0.687842000	0.057986000	0.000006000			546.9002	661.9456	695.9976
	6	0.165722000	1.122835000	-0.000064000			706.2619	762.9977	854.6757
	7	1.420688000	0.544610000	0.000028000			951.0476	1016.5282	1086.5264
	1	2.297134000	1.034491000	0.000029000			1154.2919	1183.2539	1282.0905
	1	2.084373000	-1.482053000	-0.000050000			1344.9452	1416.5528	1496.9795

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	1	0.004165000	2.183175000	0.000098000			1548.8267	1682.3561	3279.4832
	7	-0.014233000	-1.122148000	0.000009000			3322.4835	3694.3488	3861.6900
	8	-2.036541000	0.099544000	0.000012000					
	1	-2.346238000	-0.812023000	-0.000043000					
P-IM2b	6	1.280540000	-0.710668000	-0.121806000	-301.403099	0.075270	188.9474	216.3889	378.2622
(C_1)	6	-0.696387000	0.000233000	0.402211000			585.6328	612.0483	781.6698
	6	0.249831000	1.142014000	0.087740000			867.0722	903.5962	973.2147
	7	1.420431000	0.722424000	-0.181530000			1003.1187	1010.8345	1062.8536
	1	2.146766000	-1.325582000	-0.325104000			1167.3758	1253.4305	1268.5265
	1	-0.920361000	0.028109000	1.474483000			1324.6196	1334.1572	1404.5617
	1	-0.009292000	2.192900000	0.126511000			1629.8956	1718.8485	3053.7355
	7	0.134103000	-1.175122000	0.158665000			3211.4538	3229.1990	3860.4828
	8	-1.917018000	-0.002558000	-0.268964000					
	1	-1.766602000	-0.295547000	-1.172992000					
P-IM3a	6	1.425217000	-0.576113000	0.000232000	-301.438901	0.076136	192.9605	311.8828	405.9579
(C_1)	6	0.145961000	1.141172000	-0.000399000			537.0737	681.3832	687.0977
	6	-0.673200000	0.052132000	-0.000318000			696.4866	812.7147	833.2987
	7	0.137307000	-1.043121000	0.000272000			932.6502	1044.9155	1098.6332
	1	-0.175980000	-1.998286000	0.001143000			1141.6777	1172.5698	1287.7118
	1	2.274131000	-1.238252000	0.000221000			1302.0943	1411.6721	1516.5953
	1	-0.126655000	2.182195000	-0.000985000			1560.5852	1663.3663	3274.5823
	7	1.460365000	0.722338000	0.000110000			3278.5877	3680.7827	3894.5210
	8	-2.011386000	-0.139614000	-0.001446000					
	1	-2.451988000	0.713593000	0.011421000					
Abstraction channels									
TS4	6	-0.382513000	-0.122792000	-0.133936000	-301.933082	0.077070	-1690.9155	56.2313	109.0769
(C_1)	6	1.648187000	-0.686905000	0.051358000			173.8397	376.3936	553.8201
	6	1.638530000	0.676214000	0.072601000			645.5926	649.9671	759.7761
	7	0.312996000	1.033507000	-0.034420000			777.8738	880.2111	898.9137
	1	-0.071679000	1.961352000	-0.062107000			957.0491	1019.3392	1089.8823
	1	-1.623457000	-0.086286000	-0.255431000			1128.0263	1167.9615	1243.4591
	1	2.493020000	-1.349774000	0.113306000			1330.7739	1381.1741	1442.3933
	1	2.425047000	1.404797000	0.146432000			1523.8662	1587.9035	3281.6905
	7	0.359914000	-1.170976000	-0.065353000			3305.8139	3685.2190	3803.6917

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	8	-2.809919000	0.048949000	0.007106000					
	1	-2.879172000	-0.558502000	0.759228000					
TS5	6	1.426638000	-0.863941000	0.000067000	-301.933432	0.077255	-1646.3744	92.3011	94.1754
(C_s)	6	-0.419802000	0.160174000	-0.000249000			208.5779	412.1469	578.9108
	6	0.520603000	1.145992000	-0.000056000			606.8630	680.6669	753.7894
	7	1.713965000	0.461562000	0.000079000			810.3985	818.5724	859.0613
	1	2.632798000	0.869576000	0.000369000			922.4611	957.0728	1080.9508
	1	2.189508000	-1.623775000	0.000151000			1134.5876	1216.4121	1243.1062
	1	-1.657159000	0.304400000	-0.000478000			1357.4743	1446.4200	1471.5047
	1	0.459955000	2.217534000	0.000230000			1530.1095	1561.9296	3280.1552
	7	0.131825000	-1.070664000	-0.000118000			3317.8269	3674.9241	3800.4773
	8	-2.860561000	0.090168000	0.000084000					
	1	-2.825784000	-0.878712000	0.000760000					
TS6	6	1.563584000	-0.712586000	0.062853000	-301.930900	0.077390	-1589.7045	83.3313	111.3952
(C_1)	6	0.544763000	1.173974000	-0.036131000			210.3269	372.7757	558.3746
	6	-0.404421000	0.201713000	-0.139898000			620.5745	686.7543	718.3906
	7	0.241705000	-0.998499000	-0.050464000			857.3479	872.0428	878.3481
	1	-0.190022000	-1.904638000	-0.108701000			962.1520	1055.5942	1101.7819
	1	2.320140000	-1.476422000	0.126552000			1144.6847	1214.3634	1267.0049
	1	0.421942000	2.241608000	-0.052210000			1308.6102	1385.7404	1440.4486
	1	-1.667061000	0.213659000	-0.276697000			1486.3221	1570.9117	3274.2525
	7	1.776901000	0.578402000	0.072262000			3295.9275	3677.7942	3815.1624
	8	-2.800388000	-0.041092000	-0.010572000					
	1	-2.835694000	0.216611000	0.922106000					
TS7	6	-0.197366000	-1.001610000	-0.197098000	-301.935223	0.077606	-2261.3279	90.7369	105.9675
(C_1)	6	-1.706282000	0.409657000	0.242154000			185.2426	347.8740	612.8233
	6	-0.575621000	1.144803000	-0.093822000			636.4363	654.1329	808.2431
	7	0.361371000	0.246946000	-0.431621000			881.7345	911.4315	923.7563
	1	1.482080000	0.329808000	-0.380510000			960.4439	1026.1820	1121.2708
	1	0.382939000	-1.899532000	-0.331440000			1148.0625	1213.7311	1275.6655
	1	-2.691217000	0.781695000	0.471282000			1337.8832	1402.8617	1452.2645
	1	-0.424846000	2.206227000	-0.176864000			1560.8935	1734.8663	3266.3079
	7	-1.444921000	-0.932932000	0.173310000			3279.3411	3298.1830	3828.8470
	8	2.632473000	-0.025444000	0.177584000					

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	1	2.651720000	0.270158000	1.097629000					
PC4	6	-0.582340000	-1.093682000	-0.001225000	-301.959329	0.082766	42.3597	56.7622	78.0465
(C_1)	6	-1.923953000	0.526638000	0.001574000			149.5608	181.9364	244.9384
	6	-0.676209000	1.072759000	-0.000849000			586.1046	641.5161	764.1581
	7	0.200350000	0.002099000	-0.002664000			799.7167	870.9451	890.3774
	1	1.212291000	0.031449000	-0.004554000			939.7271	1093.3462	1108.6792
	1	3.664156000	-0.239486000	-0.763128000			1146.1781	1228.0821	1356.8006
	1	-2.875565000	1.028271000	0.003528000			1444.1585	1533.9258	1592.0564
	1	-0.332895000	2.091395000	-0.001482000			1622.1431	3279.8676	3304.5774
	7	-1.836441000	-0.859349000	0.001293000			3547.3845	3863.4074	3963.1058
	8	3.152806000	0.036576000	0.000989000					
	1	3.657211000	-0.237775000	0.770327000					
PC5	6	0.686858000	-1.032677000	-0.000076000	-301.959072	0.083048	43.6646	58.1810	137.3328
(C_s)	6	1.937721000	0.651303000	0.000067000			142.5221	145.8278	228.7655
	6	0.676960000	1.166872000	0.000003000			624.5531	665.4271	760.1268
	7	-0.127722000	0.046712000	-0.000012000			812.8989	857.9278	879.1136
	1	-1.140523000	0.030725000	-0.000027000			947.3876	1075.1154	1163.3380
	1	0.311848000	-2.042111000	-0.000134000			1209.3236	1263.8730	1356.1930
	1	-3.668870000	-0.047727000	-0.767292000			1442.7958	1504.2178	1541.5048
	1	0.286354000	2.166051000	0.000011000			1621.2896	3275.9446	3317.8384
	7	1.957717000	-0.681217000	0.000033000			3548.7846	3864.8424	3965.0024
	8	-3.092394000	-0.041329000	0.000003000					
	1	-3.668854000	-0.047761000	0.767309000					
PC6	6	-0.629964000	1.037681000	-0.001591000	-301.953756	0.082836	44.9081	56.5485	98.0804
(C_1)	6	-1.904829000	-0.694209000	0.002938000			138.9606	152.8567	233.5057
	6	-0.616808000	-1.123982000	-0.003595000			554.4090	679.3421	793.6191
	7	0.201540000	-0.040486000	-0.006515000			845.0572	853.3894	882.9284
	1	1.214672000	-0.037114000	-0.011120000			943.0478	1097.2204	1142.6404
	1	-0.260973000	2.049622000	-0.002400000			1188.2680	1261.6681	1353.5955
	1	-2.816945000	-1.261325000	0.006815000			1446.6211	1470.6095	1559.4244
	1	3.684348000	-0.215693000	0.775404000			1622.2287	3272.2166	3303.9497
	7	-1.889632000	0.684175000	0.004138000			3537.1977	3864.1841	3964.2768
	8	3.150199000	-0.018926000	0.002540000					
	1	3.703554000	-0.206838000	-0.758892000					

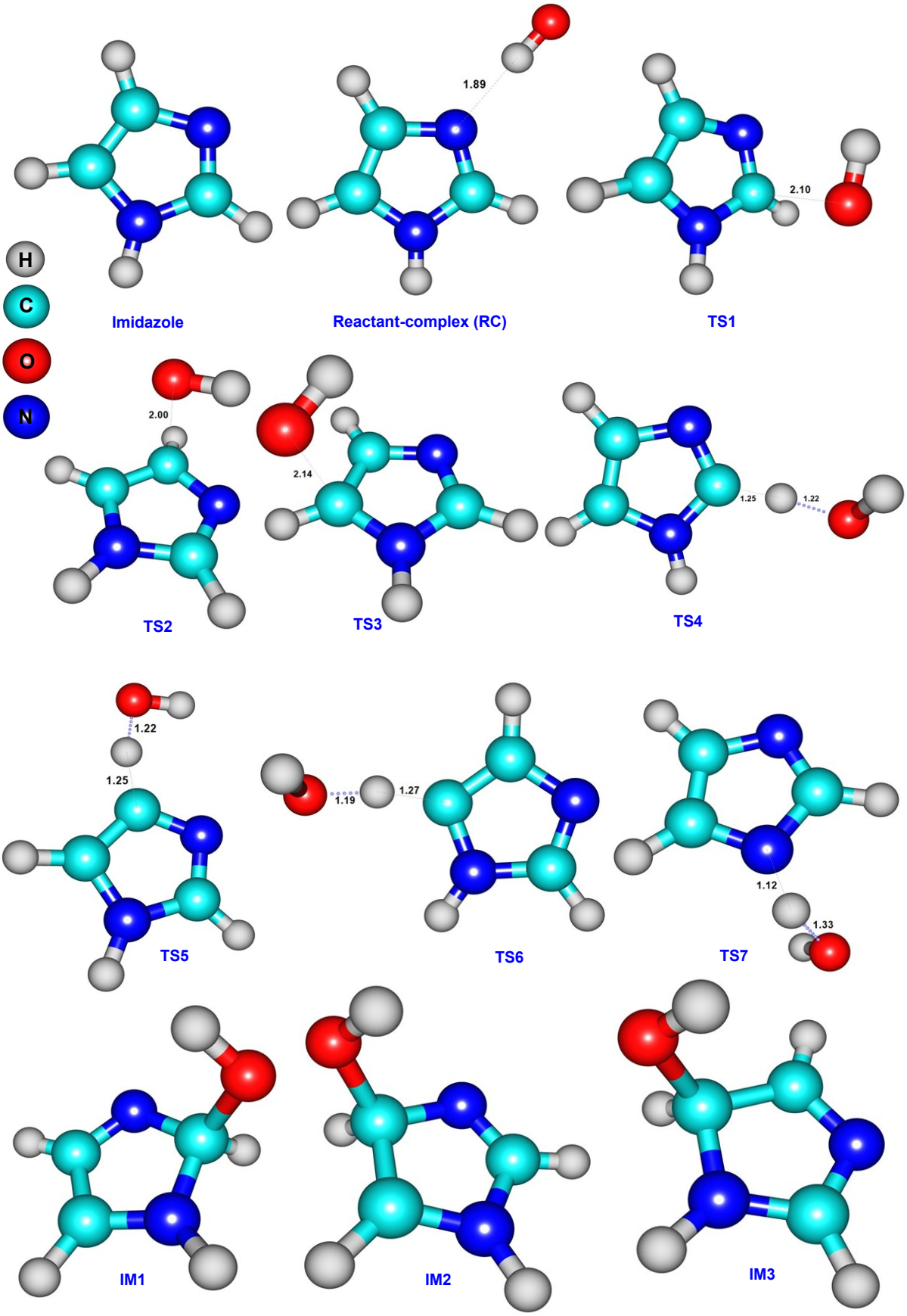
Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
PC7	6	-0.027081000	-0.730713000	0.003925000	-301.987121	0.081879	46.3109	68.6134	87.9763
(C_1)	6	-1.981401000	0.030699000	-0.002303000			163.9926	390.6920	489.0203
	6	-1.011444000	1.128472000	-0.000524000			549.6262	571.9272	785.5072
	7	0.195680000	0.619325000	0.003147000			802.1307	923.1850	926.2919
	1	2.217128000	0.516518000	-0.002027000			928.8760	1012.6109	1034.4694
	1	0.791686000	-1.434095000	0.006725000			1190.9561	1201.3379	1306.2714
	1	-3.058730000	0.099827000	-0.005376000			1333.3736	1483.1882	1564.5091
	1	-1.205707000	2.190248000	-0.002082000			1632.0989	3238.5971	3251.2559
	7	-1.336018000	-1.109268000	0.000490000			3262.3749	3747.2810	3948.0648
	8	2.950349000	-0.114551000	-0.009406000					
	1	3.754753000	0.402752000	0.045963000					
P4	6	-0.081162000	-1.154515000	-0.000004000	-225.519193	0.059146	504.4893	628.3427	640.5182
(Cs)	6	0.843656000	0.738359000	0.000029000			762.5651	863.2769	891.3957
	6	-0.494556000	0.983255000	-0.000033000			941.8152	1077.3892	1103.5223
	7	-1.095792000	-0.265330000	0.000022000			1140.8324	1209.3039	1355.5777
	1	-2.078562000	-0.468871000	0.000021000			1418.5640	1537.0357	1598.7132
	1	1.653363000	1.446256000	0.000043000			3282.4013	3307.5479	3698.9384
	1	-1.065058000	1.894079000	-0.000035000					
	7	1.079025000	-0.630964000	-0.000019000					
P5	6	-0.821106000	0.691955000	-0.000176000	-225.519074	0.059427	579.2094	626.7556	686.1431
(C_s)	6	0.090039000	-1.199738000	0.000105000			755.4364	849.7343	873.5978
	6	1.135751000	-0.329742000	0.000222000			949.5478	1069.6258	1127.6826
	7	0.517136000	0.905244000	0.000032000			1205.9998	1262.1517	1361.5550
	1	0.973649000	1.801180000	0.000105000			1432.4571	1498.4453	1535.4125
	1	-1.538086000	1.495287000	-0.000354000			3278.5293	3320.5552	3672.5255
	1	2.201679000	-0.450284000	0.000412000					
	7	-1.097900000	-0.593963000	-0.000186000					
P6	6	-0.696953000	0.810621000	-0.000140000	-225.513504	0.059251	499.2536	593.1680	684.6197
(C_s)	6	1.178666000	-0.247502000	0.000143000			838.1425	855.4684	875.9973
	6	0.186435000	-1.171750000	0.000121000			944.4563	1085.3405	1122.2526
	7	-1.006154000	-0.517856000	-0.000061000			1179.0030	1258.2986	1355.3255
	1	-1.921229000	-0.932194000	-0.000239000			1422.4844	1470.6671	1559.8973
	1	-1.450040000	1.580526000	-0.000273000			3275.3040	3304.2602	3684.0864
	1	2.243602000	-0.386001000	0.000283000					

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies [a] (cm^{-1})		
	7	0.594551000	1.002064000	-0.000013000					
P7	6	-0.002570000	-1.091399000	0.000025000	-225.547068	0.057567	531.7446	570.9612	772.0446
(C_s)	6	0.735522000	0.868602000	0.000027000			797.4632	910.3987	923.3898
	6	-0.731416000	0.872030000	-0.000019000			925.3158	1007.5195	1028.8139
	7	-1.158602000	-0.366453000	0.000003000			1190.9896	1199.6502	1299.6417
	1	-0.005138000	-2.170191000	-0.000008000			1331.0873	1478.0055	1560.9905
	1	1.401818000	1.718161000	0.000035000			3234.7830	3247.3260	3258.8921
	1	-1.393915000	1.724527000	-0.000020000					
	7	1.156891000	-0.371816000	-0.000032000					

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

Table S2: Calculated overall rate constants, k_{tot}, of the imidazole + OH → products over the range of temperature 297 – 440 K at different pressures, including the HIR treatments, Eckart quantum tunneling effects. Units are in cm^3/molecule/s.

T (K)	0.75 torr	7.5 torr	100 torr	750 torr	760 torr	7500 torr	75000 torr	750000 torr
297	1.80E-11	3.04E-11	3.44E-11	3.79E-11	3.80E-11	6.06E-11	1.67E-10	3.42E-10
316	1.51E-11	2.75E-11	3.16E-11	3.43E-11	3.45E-11	5.06E-11	1.32E-10	3.20E-10
331	1.27E-11	2.46E-11	2.88E-11	3.17E-11	3.16E-11	4.54E-11	1.06E-10	2.96E-10
344	1.14E-11	2.25E-11	2.69E-11	2.93E-11	2.91E-11	4.06E-11	8.63E-11	2.69E-10
352	1.03E-11	2.13E-11	2.56E-11	2.77E-11	2.76E-11	3.81E-11	7.60E-11	2.50E-10
362	9.29E-12	1.94E-11	2.44E-11	2.58E-11	2.57E-11	3.47E-11	6.47E-11	2.26E-10
386	6.97E-12	1.60E-11	2.10E-11	2.26E-11	2.26E-11	2.83E-11	4.65E-11	1.66E-10
402	5.95E-12	1.41E-11	1.89E-11	1.99E-11	1.98E-11	2.46E-11	3.81E-11	1.30E-10
425	4.42E-12	1.13E-11	1.56E-11	1.68E-11	1.69E-11	2.01E-11	2.95E-11	8.48E-11
440	3.69E-12	9.46E-12	1.36E-11	1.47E-11	1.46E-11	1.80E-11	2.49E-11	6.30E-11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C
O
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Imidazole
Reactant-complex (RC)
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1.22
TS2
TS3
TS4
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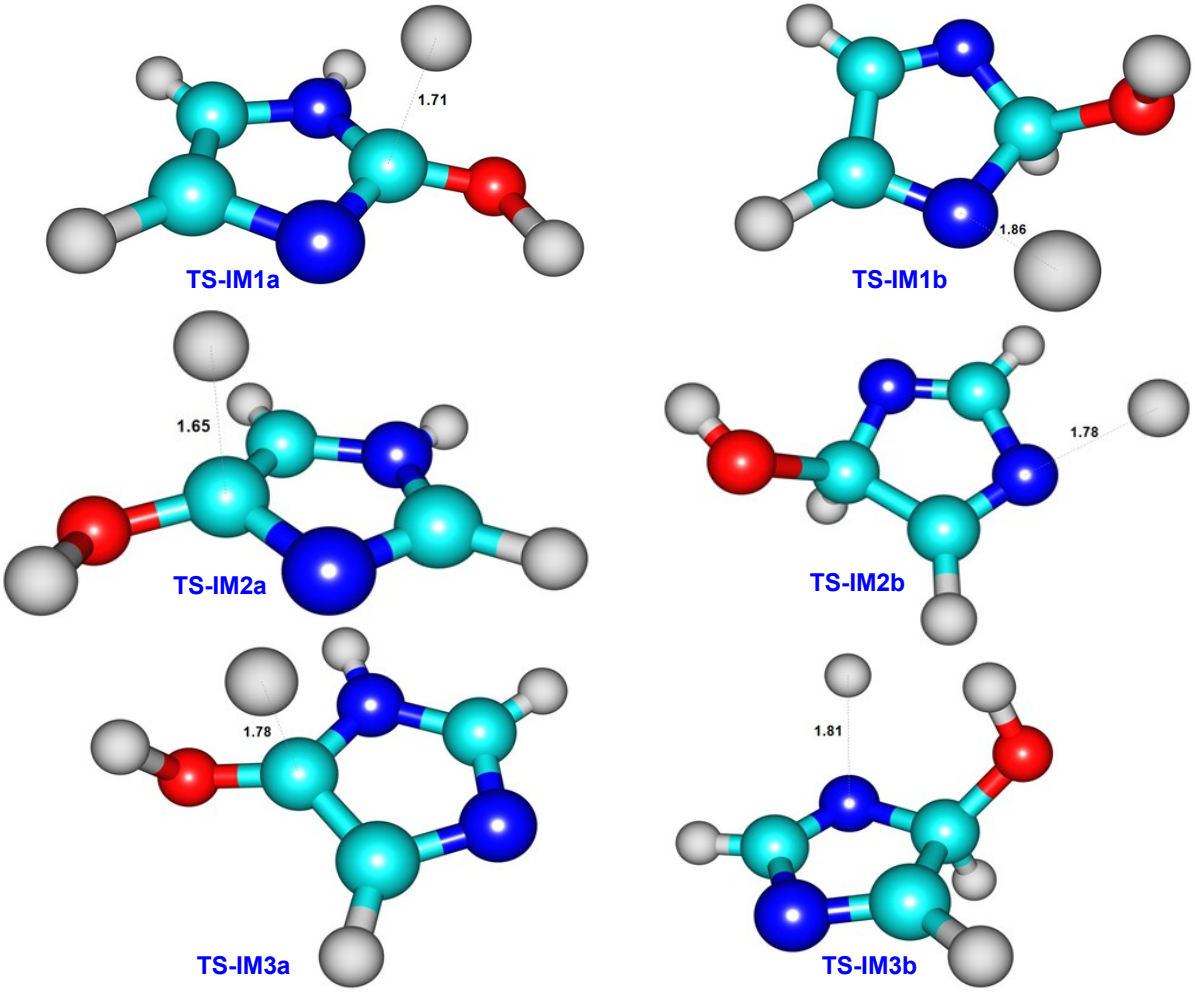
1.25
1.19
1.27
1.12
1.33
TS5
TS6
TS7
IM1
IM2
IM3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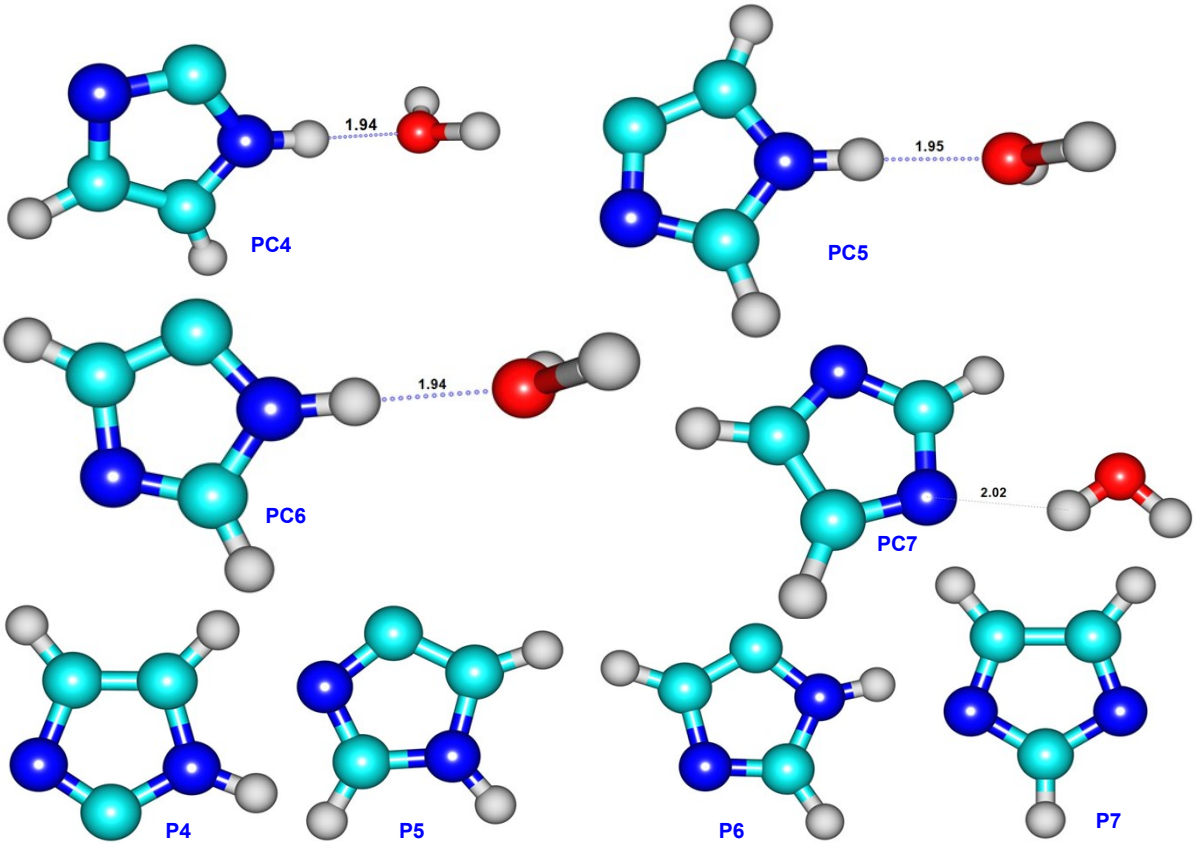
TS-IM3b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PC4
1.95
PC5
1.94
PC6
2.02
PC7
P4
P5
P6
P7

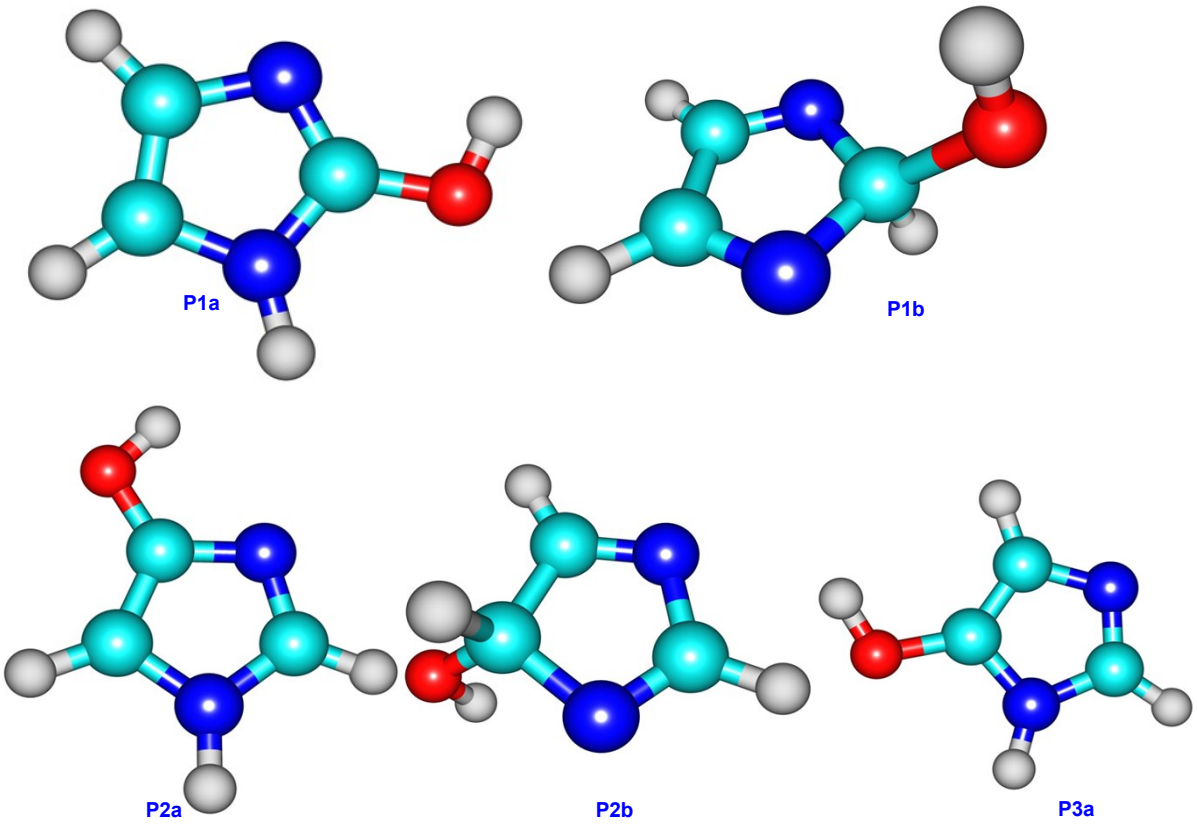


Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the imidazole + OH reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths are in Å.

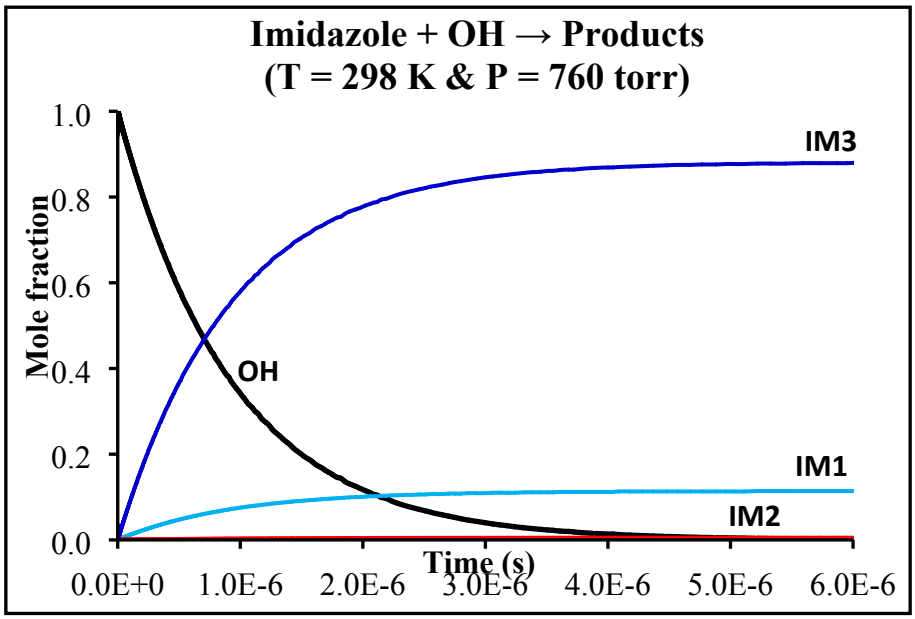
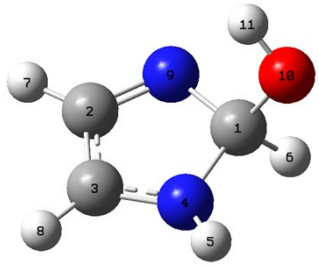
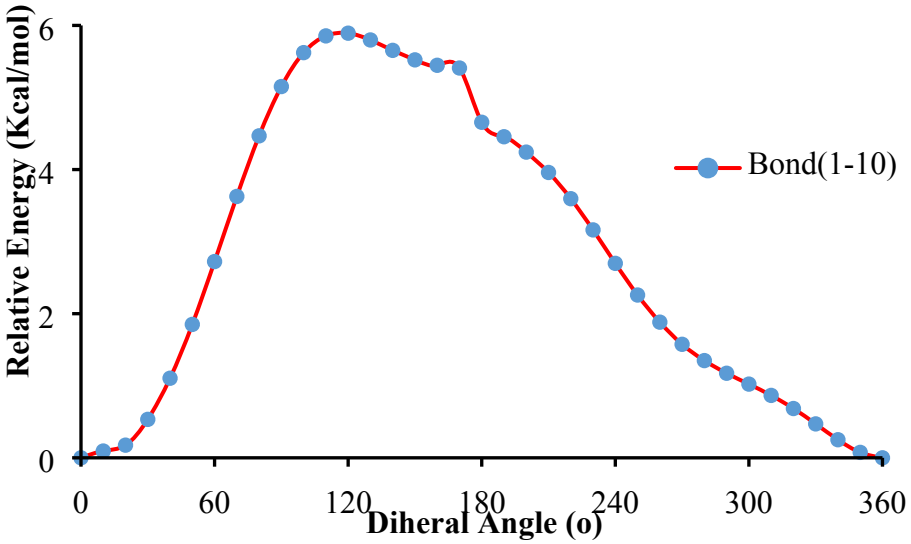
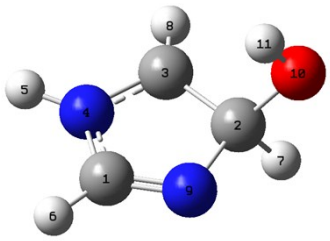
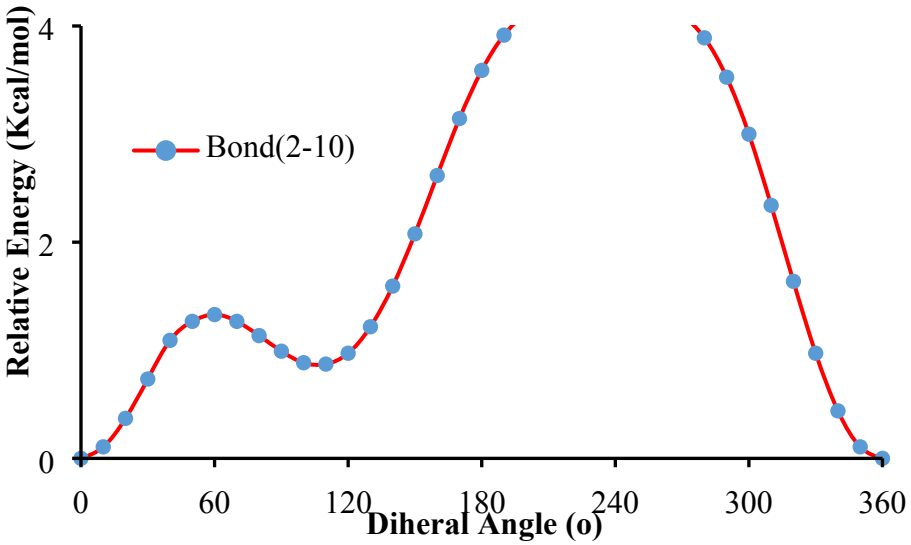
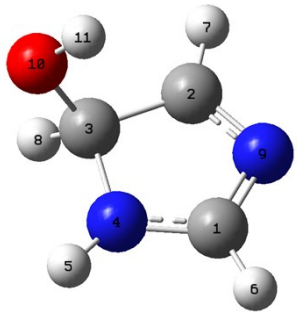
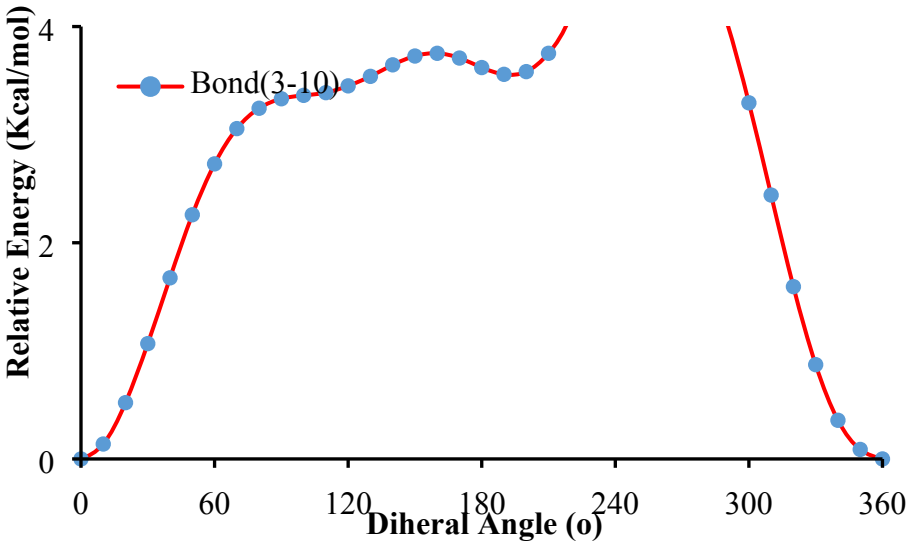
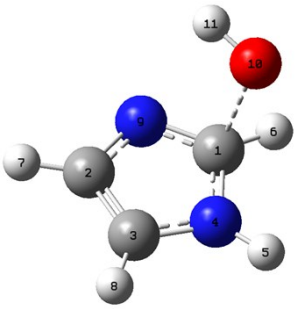
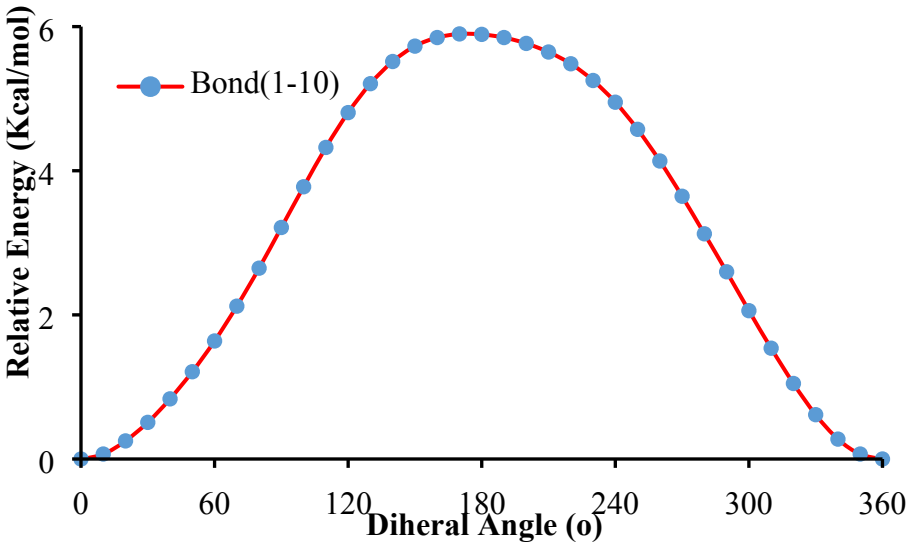
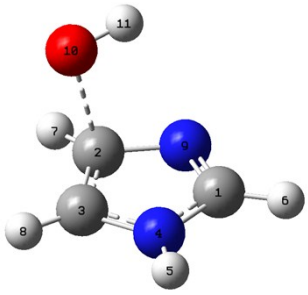
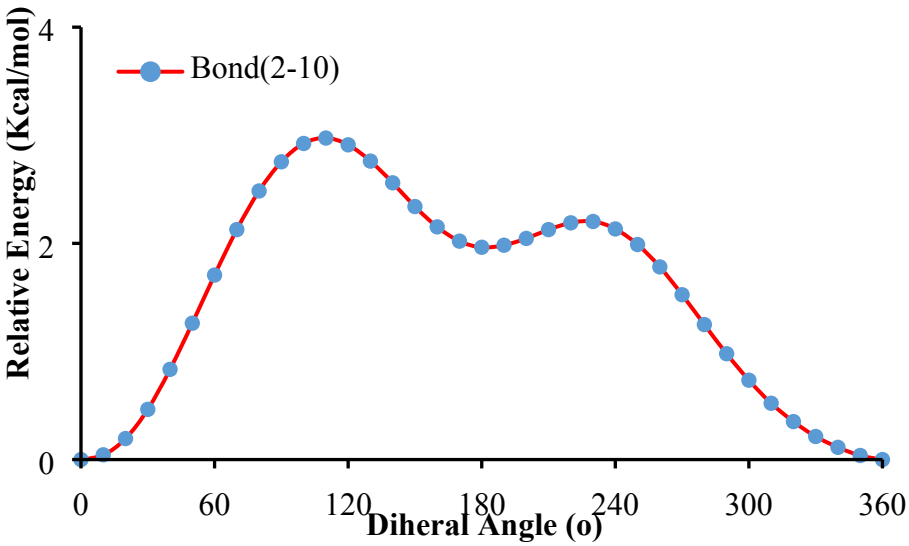
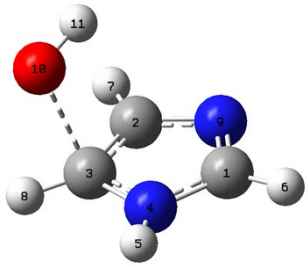
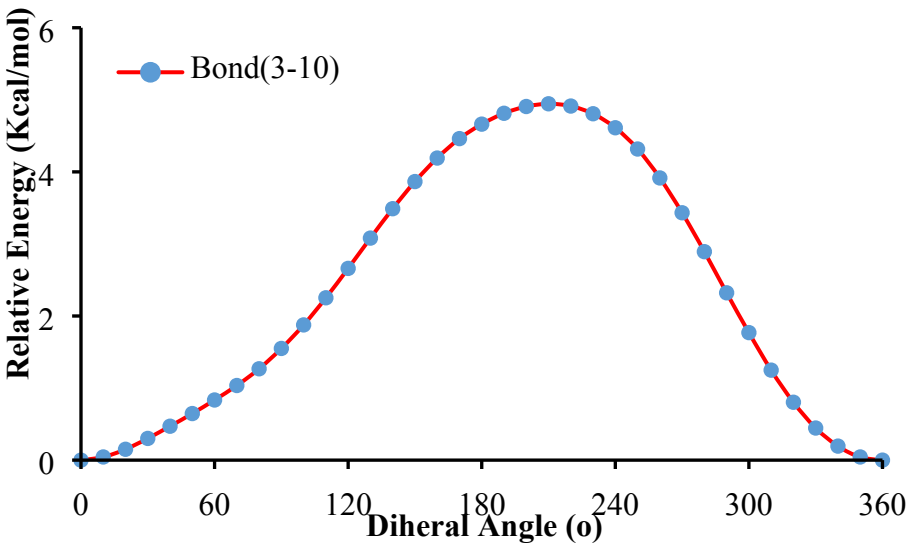
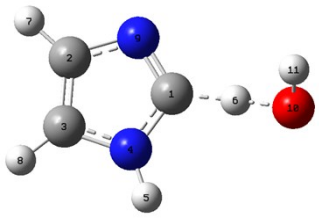
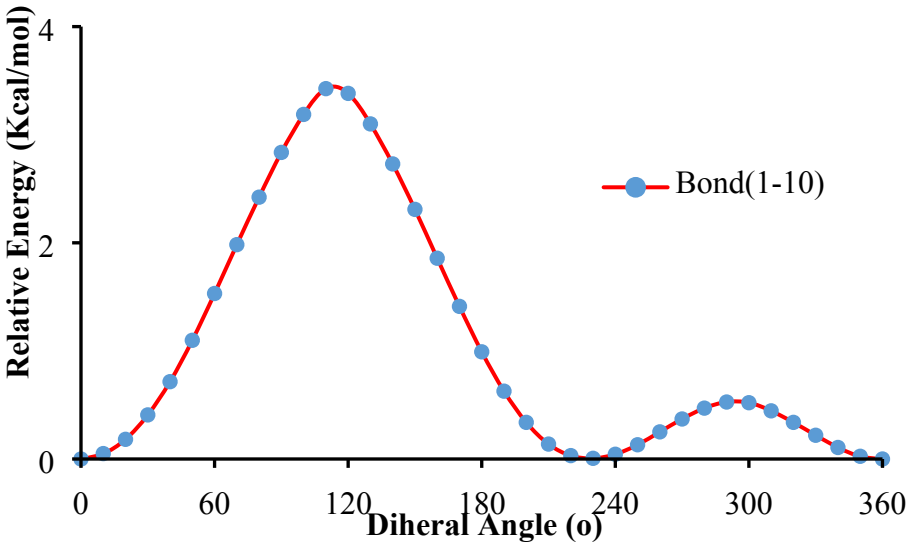
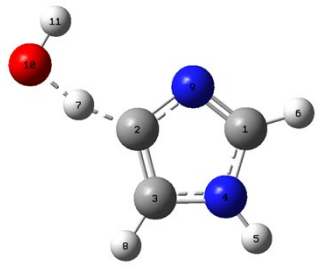
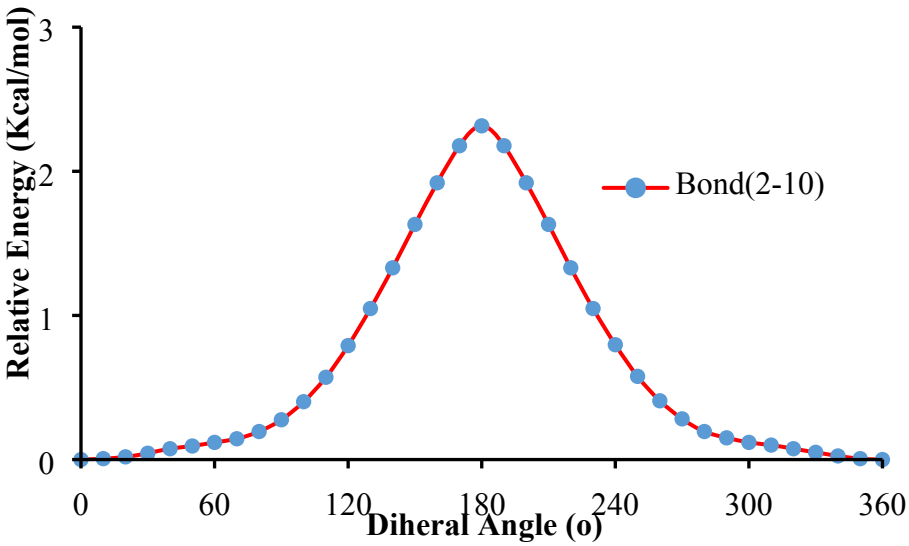
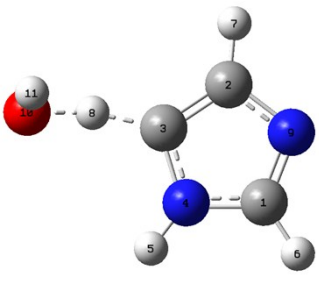
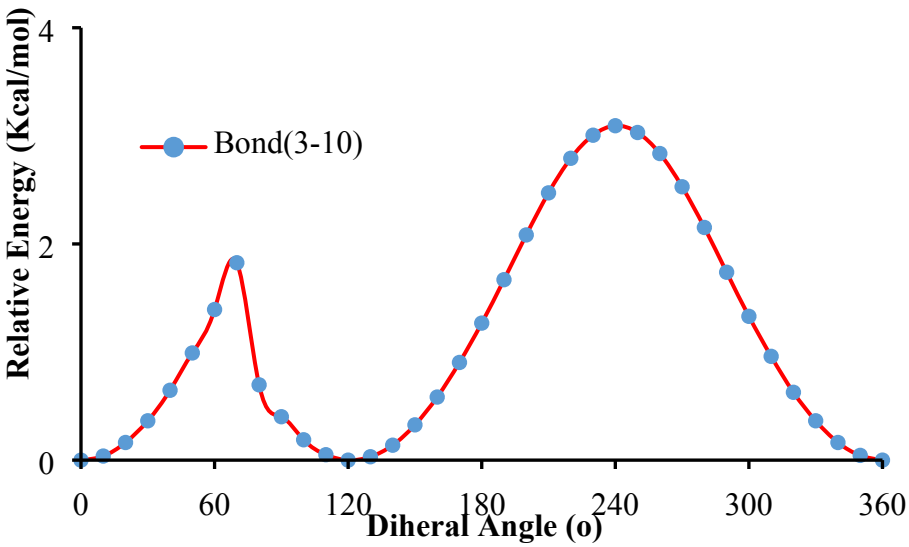
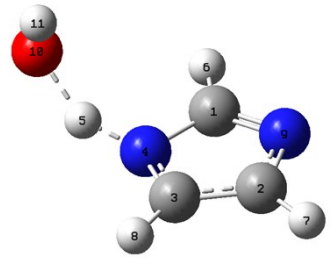
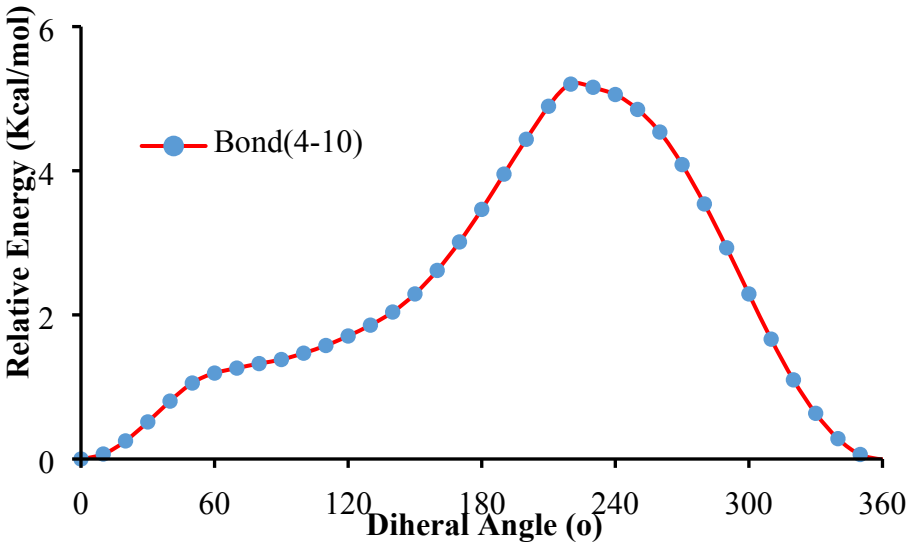
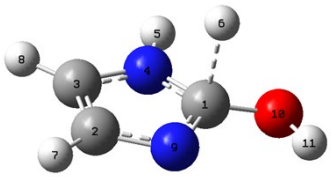
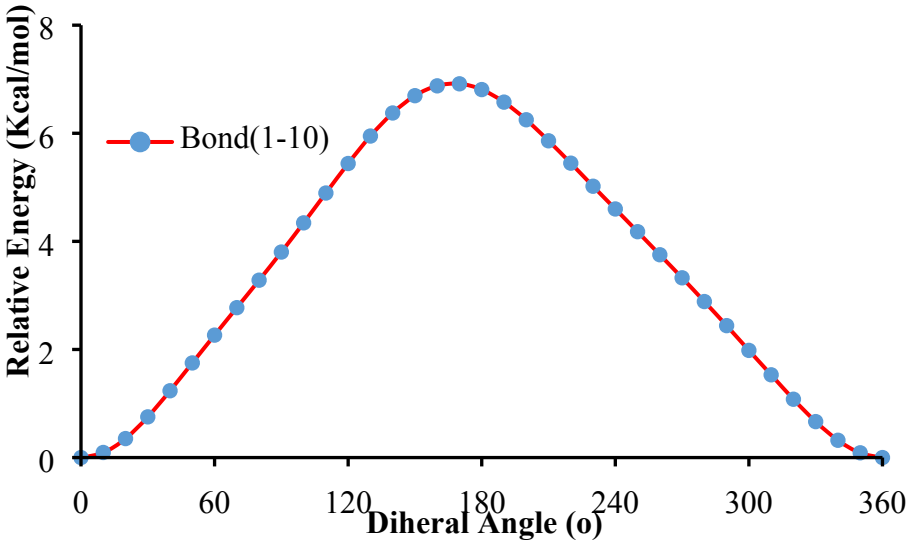
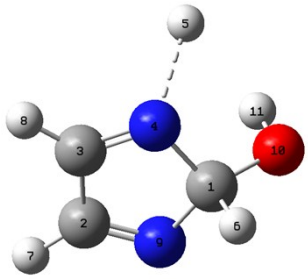
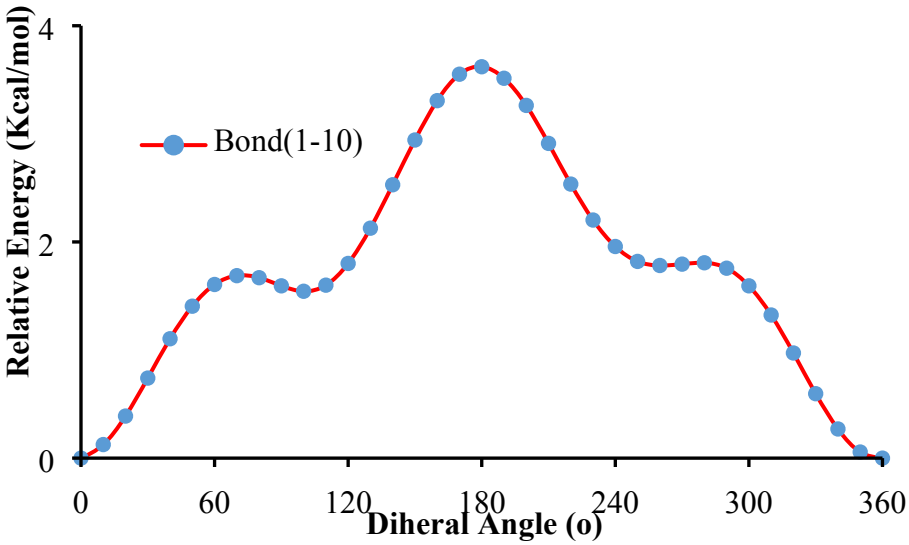


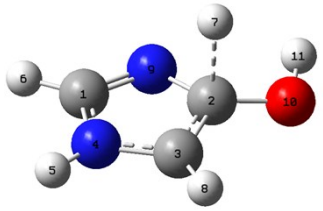
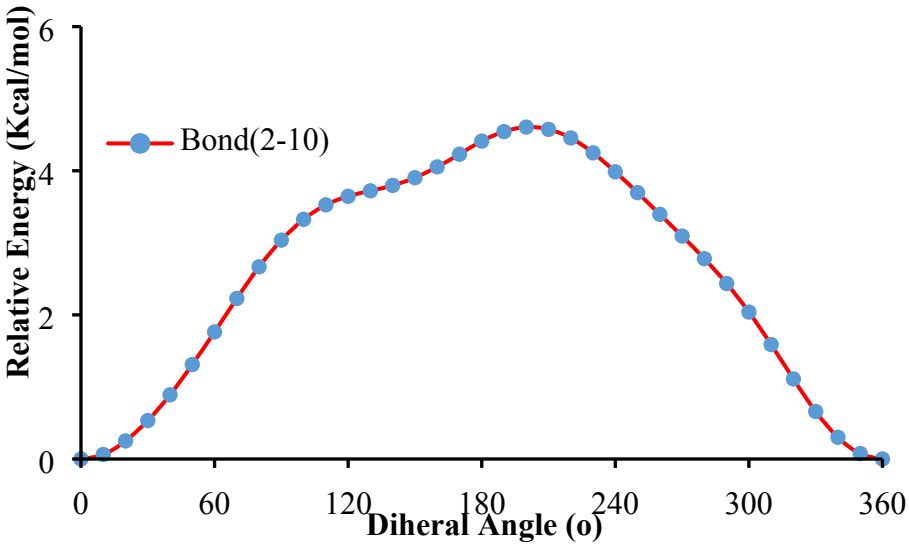
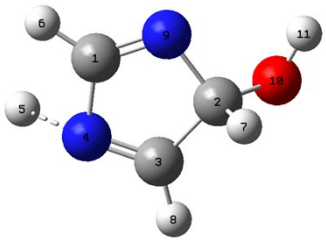
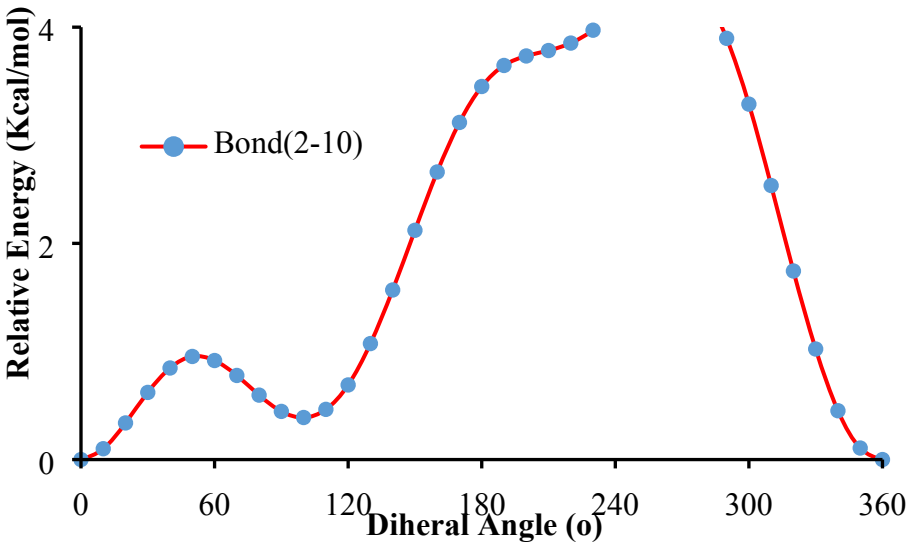
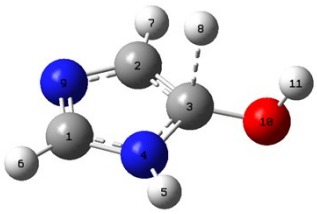
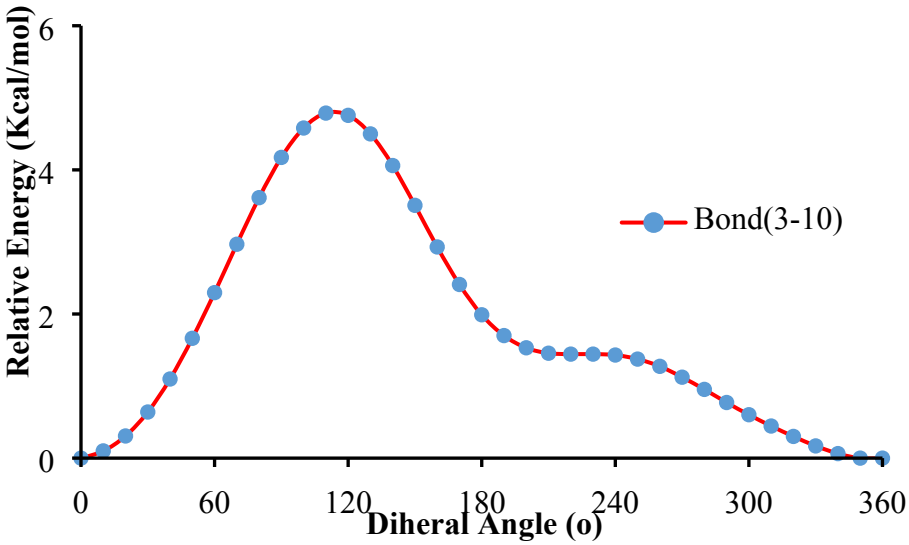
Figure S2: Time-resolved species profiles for the imidazole + OH reaction, simulated at the atmospheric condition using the stochastic (with 10^6 numbers of trials) approach with [imidazole]/[[Ar] = 10^{-3} and $[imidazole]_0 >> [OH]_0$ (Ar is the bath gas). The calculations were carried out using the simplified PES in Figure 1 (main text).

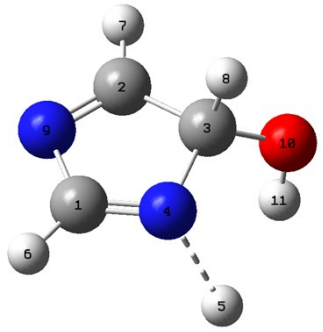
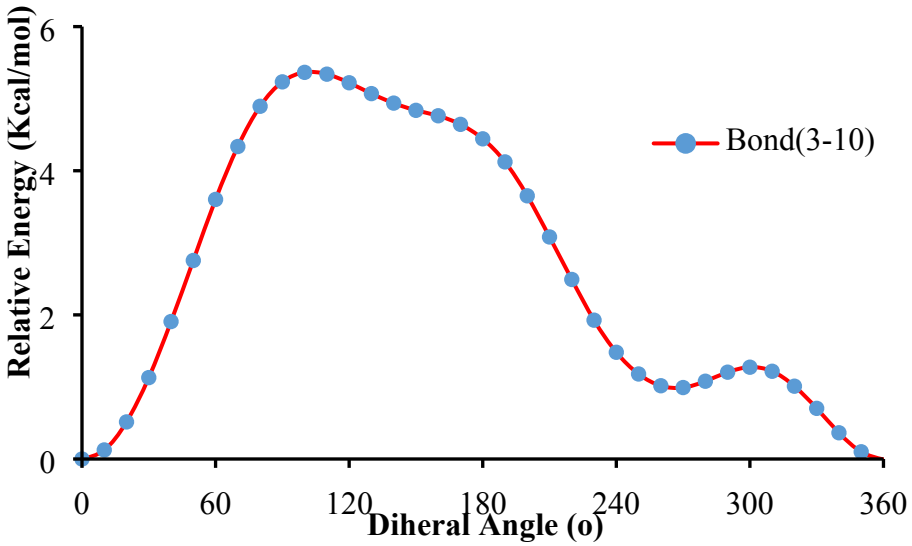
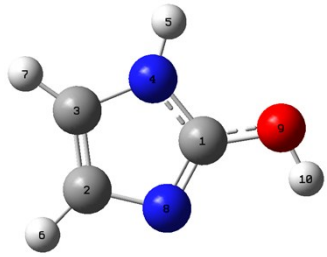
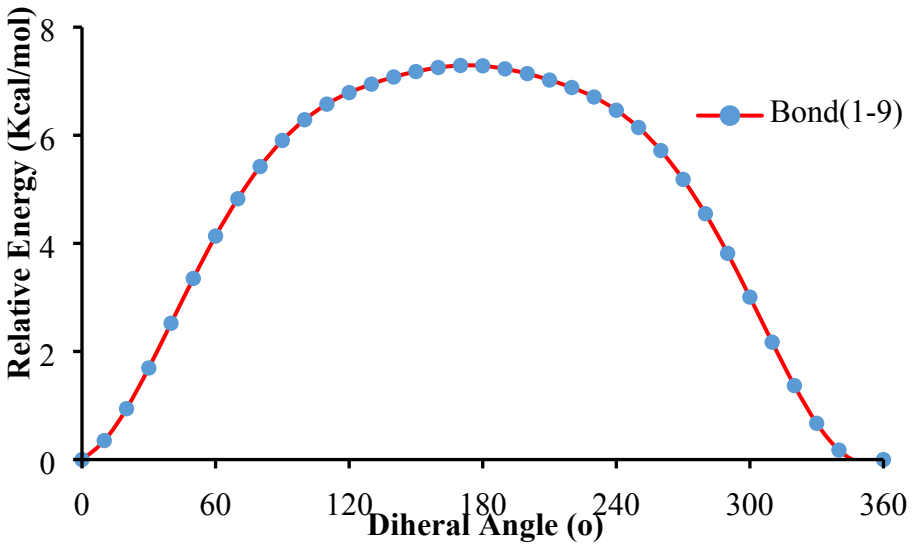
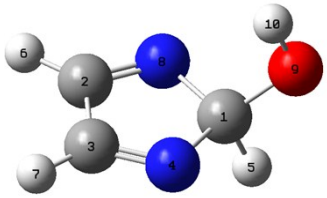
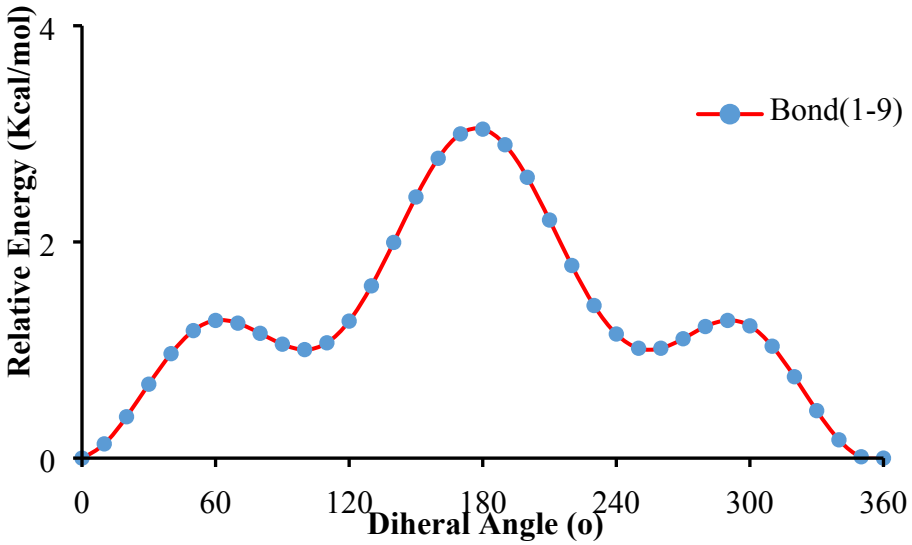
Species	Potential energy surfaces for the internal rotations
 IM1	
 IM2	
 IM3	

Species	Potential energy surfaces for the internal rotations
 TS1	
 TS2	
 TS3	

Species	Potential energy surfaces for the internal rotations
 TS4	
 TS5	
 TS6	

Species	Potential energy surfaces for the internal rotations
 TS7	
 TS-IM1a	
 TS-IM1b	

Species	Potential energy surfaces for the internal rotations
 TS-IM2a	
 TS-IM2b	
 TS-IM3a	

Species	Potential energy surfaces for the internal rotations
 TS-IM3b	
 P-IM1a	
 P-IM1b	

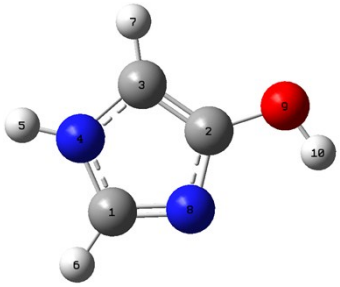
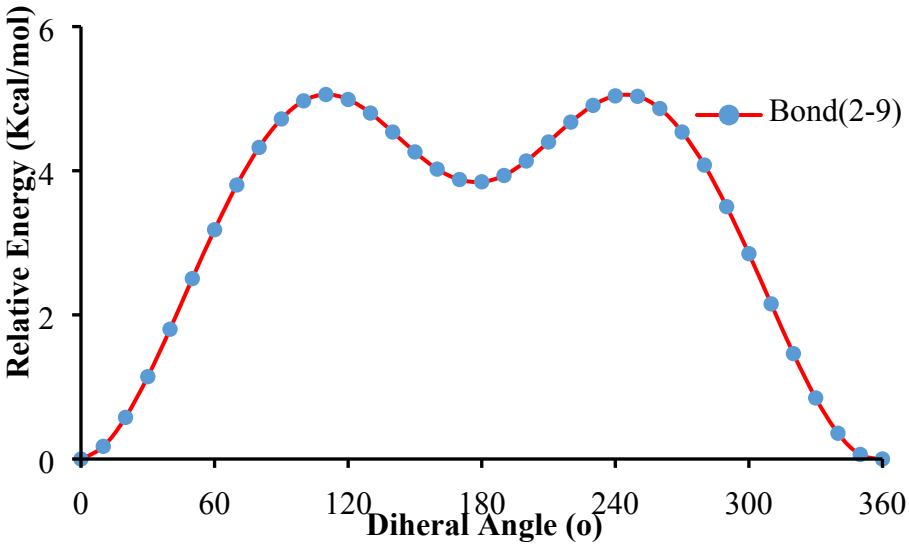
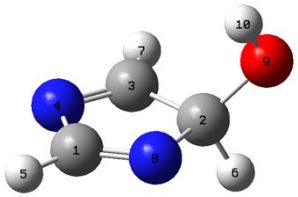
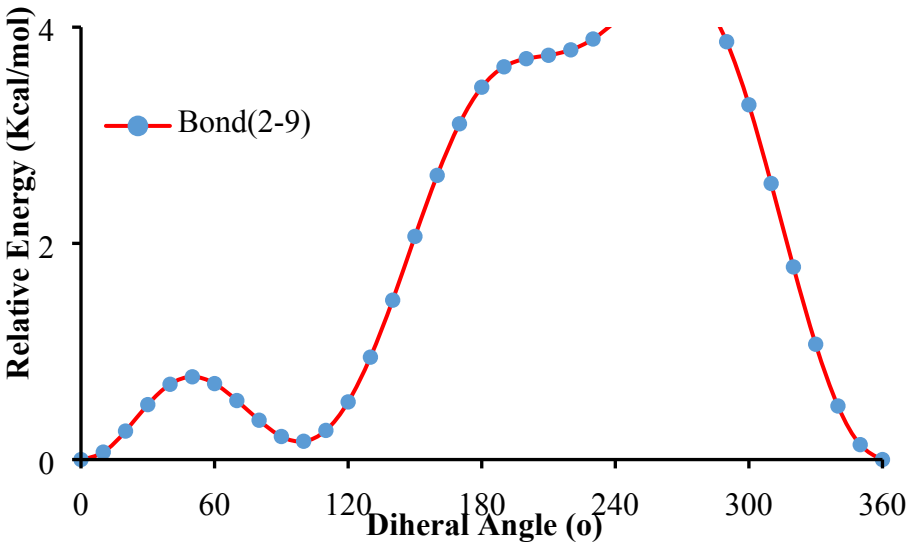
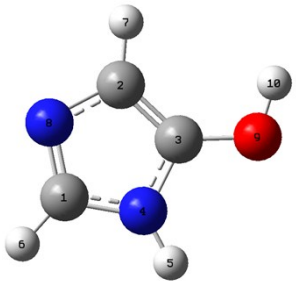
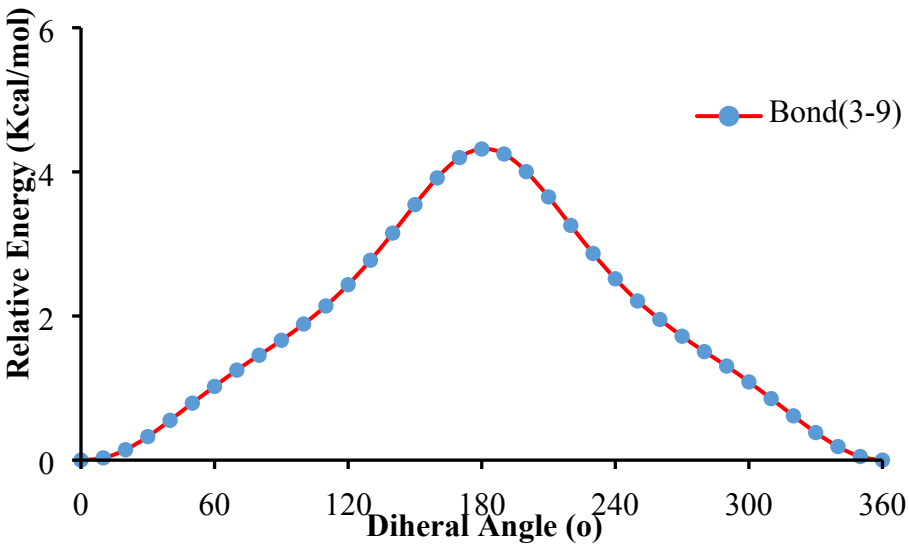
Species	Potential energy surfaces for the internal rotations
 P-IM2a	
 P-IM2b	
 P-IM3a	

Figure S3: Hindrance potentials for the species involved in the imidazole + OH reaction, calculated at M06-2X/cc-pVDZ level of theory.

References:

[1] K.P. Huber, 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] F. Billes, H. Endrédi, G. Jalsovszky, Journal of Molecular Structure: THEOCHEM 465 (1999) 157.