Photo Oxidation Reaction Kinetics and Mechanistics of 4-Hydroxy-2-Butanone with Cl atoms and OH radicals in the Gas phase

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Table S1. Vibrational frequencies of reactants, transition states, and products at M062X/6-31G (d, p) level of theory for the reaction of 4H2BN with Cl atoms.

4H2BN	TS1	TS2	TS3	TS4	TS5	TS6	TS7
58.7	-1122.2	-1043.6	-961.6	-983.4	-1486.6	-1433.1	-143.4
103.9	39.7	35.9	51.9	10.3	50.9	39.6	38.1
169.1	53.4	55.8	68.9	71.2	62.9	68.5	60.8
251.6	92.1	93.1	85.3	74.1	84.7	122.5	70.9
341.0	183.8	183.1	114.8	107.2	132.7	150.2	123.1
456.7	248.6	246.0	143.1	189.4	156.3	225.1	214.8
502.2	339.4	333.1	252.5	226.2	229.4	258.9	268.0
557.1	368.9	379.6	301.7	332.6	361.8	348.2	353.3
641.8	423.6	425.9	396.9	388.2	387.9	427.3	439.5
786.3	462.6	481.2	463.9	475.1	416.3	486.4	500.4
864.7	505.3	494.7	513.1	511.5	515.8	529.0	554.1
986.4	545.3	505.2	549.6	553.0	531.9	680.5	580.0
991.3	626.4	624.7	614.7	638.5	656.7	699.5	629.3
1027.9	779.3	774.9	781.6	776.8	830.7	817.9	689.4
1134.6	812.2	817.7	826.4	839.4	916.2	931.2	771.9
1158.6	874.1	912.0	848.3	866.3	1022.4	1015.2	825.8
1227.2	950.7	943.9	957.1	964.8	1031.3	1045.4	889.6
1265.7	974.2	974.6	992.1	985.6	1112.7	1077.4	988.4
1303.5	1005.2	984.2	1044.9	989.9	1159.1	1176.9	1016.1
1435.8	1063.6	1069.4	1081.2	1052.2	1202.0	1211.1	1045.4
1447.3	1128.7	1127.5	1093.8	1127.0	1280.2	1285.0	1183.4
1460.9	1147.2	1156.5	1124.4	1166.7	1288.7	1295.8	1191.8
1480.7	1185.4	1191.7	1193.6	1203.4	1305.5	1337.1	1237.1
1495.3	1226.2	1216.9	1241.0	1234.3	1360.8	1381.6	1358.0
1515.9	1256.8	1259.1	1371.5	1344.3	1429.8	1440.5	1390.0
1529.3	1394.2	1391.6	1395.0	1387.1	1492.1	1517.4	1402.7
1561.1	1403.4	1402.9	1415.2	1422.5	1534.2	1545.6	1445.2
1868.4	1428.4	1422.2	1425.2	1427.5	1569.7	1570.0	1475.9
3099.7	1445.6	1441.5	1472.4	1471.8	1584.4	1583.4	1478.7
3105.7	1460.8	1461.3	1480.5	1477.0	1596.3	1586.0	1483.9
3118.6	1512.9	1511.9	1503.3	1481.1	1600.0	1598.9	1827.0
3143.1	1780.2	1788.2	1796.7	1800.8	1993.6	1977.3	2371.0
3177.5	3057.1	3057.0	3070.7	2978.3	3187.3	3171.4	2981.7
3179.0	3060.0	3065.3	3086.0	3067.4	3205.8	3188.8	3085.0
3231.1	3105.3	3105.1	3143.0	3127.5	3248.9	3251.2	3139.9
3965.5	3145.1	3145.9	3153.0	3138.4	3259.5	3258.3	3165.4
	3146.2	3148.9	3164.9	3149.8	3286.5	3297.1	3195.6
	3258.9	3262.0	3198.1	3202.2	3307.3	3311.6	3208.5
	3861.1	3883.5	3842.5	3835.2	4181.6	4062.5	3663.6

P1	P2	P3	P4	P5	P6	P7	P(HCl)
62.3	62.3	67.4	64.9	47.4	55.8	47.2	3030.1
164.3	164.3	79.0	76.8	72.7	131.8	102.0	
250.8	250.8	136.2	136.0	99.0	184.5	133.9	
346.4	346.4	240.4	240.6	227.0	257.9	256.8	
376.0	375.9	342.5	342.5	335.5	336.4	348.1	
452.6	452.5	466.3	466.4	345.5	436.2	464.0	
506.3	506.4	513.9	514.2	444.8	488.1	472.2	
556.3	556.3	561.0	561.3	471.4	558.6	550.0	
622.8	622.8	616.6	616.7	584.0	679.0	642.9	
745.9	745.9	702.1	702.2	682.9	701.9	796.0	
787.9	787.8	830.6	830.7	808.8	803.8	864.6	
889.6	889.6	943.4	943.1	848.2	869.7	953.5	
956.9	956.9	1002.4	1002.3	963.2	990.9	986.0	
1021.1	1021.0	1016.9	1016.7	1009.2	993.5	1064.0	
1057.7	1057.7	1037.2	1037.2	1065.0	1047.5	1095.4	
1128.1	1128.1	1159.9	1160.4	1177.0	1192.5	1159.8	
1193.7	1193.7	1206.8	1206.9	1192.5	1195.1	1208.6	
1222.1	1222.0	1243.1	1243.2	1237.6	1230.0	1226.7	
1265.6	1265.6	1345.3	1345.2	1312.8	1353.7	1367.3	
1394.4	1394.4	1394.1	1393.9	1321.3	1381.3	1380.4	
1404.1	1404.1	1446.1	1446.3	1396.2	1411.4	1387.2	
1426.3	1426.3	1462.1	1462.2	1431.4	1439.5	1411.8	
1450.5	1450.5	1481.9	1481.8	1470.3	1465.2	1455.9	
1484.2	1484.2	1484.1	1483.5	1479.8	1469.7	1472.1	
1506.6	1506.6	1486.7	1486.7	1482.6	1481.0	1484.0	
1675.2	1675.4	1680.0	1679.8	1859.4	1836.3	1858.6	
3055.0	3055.0	2976.2	2975.6	3055.9	2941.1	2992.3	
3057.0	3056.9	3073.0	3072.9	3066.3	3067.2	3037.6	
3103.4	3103.4	3120.2	3119.9	3104.9	3115.3	3062.8	
3130.9	3131.0	3145.2	3145.5	3139.8	3140.3	3066.4	
3197.3	3197.2	3194.1	3192.9	3183.5	3191.2	3126.4	
3317.8	3317.7	3213.1	3213.3	3193.2	3224.1	3137.6	
3831.8	3831.8	3805.1	3804.8	3914.7	3735.2	3191.6	

Table S2. Vibrational frequencies of reactants, transition states, and products at M062X/6-31+G(d, p) level of theory for the reaction of 4H2BN with OH radicals.

4H2BN	TS1	TS2	TS3	TS4	TS5	TS6	TS7
55.8	-1095.0	-1455.6	-717.1	-973.3	-1253.0	-748.8	-1481.1
107.8	27.9	28.3	47.9	53.2	53.1	26.3	53.3
181.5	40.5	67.3	69.2	61.5	77.6	101.3	83.8
251.1	88.1	133.5	78.1	85.6	112.0	126.7	122.7
335.2	139.3	186.4	106.8	118.1	179.2	141.6	149.4
441.4	182.9	255.8	118.4	181.2	190.8	196.3	196.4
484.0	244.4	272.8	179.4	232.0	248.3	243.2	264.4
540.3	316.2	319.1	255.4	292.9	342.8	314.8	326.8
622.3	350.7	398.9	338.8	331.2	425.5	339.3	343.9
769.9	440.5	433.0	453.8	437.4	458.1	442.7	409.5
838.0	478.8	483.7	487.0	482.0	495.8	485.3	475.1
950.7	510.4	512.3	536.1	484.1	608.1	561.5	493.3
965.6	604.7	603.7	618.8	609.8	626.3	602.6	610.5
995.8	752.7	701.8	668.7	743.0	752.2	711.1	760.5
1095.9	776.8	815.9	769.2	769.6	817.9	783.1	778.6
1137.9	851.9	835.5	816.0	849.9	871.0	842.5	839.8
1189.9	897.1	895.5	946.2	900.5	939.5	907.9	952.2
1223.2	959.7	956.8	962.0	970.5	967.0	972.5	965.2
1255.4	994.1	980.9	997.2	990.5	980.2	993.2	1031.7
1383.0	1057.9	1033.1	1083.5	1055.8	1013.5	1080.1	1090.1
1394.9	1120.6	1083.7	1124.8	1120.8	1117.1	1145.3	1103.7
1413.2	1165.4	1135.8	1149.1	1190.5	1122.3	1181.1	1191.5
1426.2	1190.6	1196.8	1188.3	1207.9	1174.9	1197.2	1223.3
1445.0	1232.1	1222.0	1231.5	1232.0	1207.7	1237.5	1261.9
1472.0	1256.5	1239.0	1262.4	1273.2	1238.7	1293.1	1356.2
1483.4	1290.5	1260.6	1368.4	1350.4	1367.9	1381.1	1375.4
1510.8	1381.8	1389.9	1392.5	1377.7	1382.0	1413.4	1383.6
1842.3	1396.0	1399.6	1405.0	1390.8	1413.1	1419.1	1402.6
3049.7	1410.7	1421.7	1415.6	1408.4	1424.7	1440.4	1444.7
3060.8	1425.7	1439.3	1432.3	1443.8	1471.2	1467.6	1472.3
3075.9	1446.3	1443.5	1471.6	1470.7	1481.1	1470.2	1484.2
3105.5	1460.9	1484.8	1478.6	1482.7	1499.6	1482.9	1507.5
3132.0	1509.4	1508.5	1509.5	1688.5	1547.9	1725.3	1773.6
3147.0	1822.4	1816.0	1834.5	1838.6	1824.6	1832.5	1862.0
3198.2	3052.7	3056.6	3065.0	3063.2	3056.4	3057.7	3067.0
3859.9	3061.1	3061.2	3075.4	3069.6	3074.6	3073.2	3071.6
	3106.4	3105.5	3105.2	3074.8	3123.4	3117.5	3075.1

	3126.5	3114.5	3136.4	3117.2	3143.1	3131.3	3126.6
	3133.8	3135.2	3146.7	3146.8	3146.9	3146.7	3137.0
	3219.1	3194.5	3199.1	3197.5	3199.0	3199.2	3149.9
	3778.3	3739.9	3789.3	3775.8	3691.4	3766.7	3196.2
	3864.5	3871.9	3854.4	3812.3	3837.4	3827.4	3832.3

P1	P2	P3	P4	P5	P6	P7	P (H2O)
53.3	53.3	28.8	28.8	51.6	51.6	45.0	1598.4
174.5	174.5	68.5	68.5	139.7	139.7	95.1	3882.8
251.2	251.2	137.3	137.3	186.7	186.7	142.7	4007.6
344.5	344.5	239.4	239.4	257.7	257.7	251.8	
358.8	358.8	344.3	344.3	336.4	336.4	347.7	
449.3	449.3	465.0	465.0	437.2	437.2	463.1	
501.4	501.4	511.0	511.0	487.6	487.6	474.4	
534.0	534.0	555.1	555.1	549.4	549.4	571.6	
621.7	621.7	612.9	612.9	663.8	663.8	671.8	
741.1	741.1	703.4	703.4	696.2	696.2	802.6	
789.0	789.0	831.7	831.7	802.5	802.5	868.1	
887.1	887.1	945.9	945.9	871.0	871.0	952.7	
957.1	957.1	1004.1	1004.1	992.2	992.2	984.9	
1022.1	1022.1	1017.0	1017.0	992.9	992.9	1063.5	
1058.9	1058.9	1037.6	1037.6	1047.1	1047.1	1101.1	
1129.3	1129.3	1158.1	1158.1	1192.7	1192.7	1160.2	
1194.2	1194.2	1209.9	1209.9	1194.1	1194.1	1206.4	
1221.0	1221.0	1244.6	1244.6	1231.0	1231.0	1229.8	
1266.2	1266.2	1345.2	1345.2	1352.6	1352.6	1369.4	
1393.8	1393.8	1393.1	1393.1	1381.2	1381.2	1379.9	
1402.8	1402.8	1448.2	1448.2	1410.4	1410.4	1385.7	
1427.4	1427.4	1462.3	1462.3	1439.6	1439.6	1408.3	
1450.7	1450.7	1481.9	1481.9	1465.7	1465.7	1454.9	
1483.7	1483.7	1484.4	1484.4	1470.1	1470.1	1471.7	
1510.2	1510.2	1489.8	1489.8	1482.7	1482.7	1482.5	
1670.3	1670.3	1675.8	1675.8	1838.5	1838.5	1862.9	
3050.8	3050.8	2967.5	2967.5	2941.9	2941.9	2979.1	
3062.2	3062.2	3076.3	3076.3	3073.6	3073.6	3033.1	
3108.1	3108.1	3122.6	3122.6	3121.5	3121.5	3064.9	
3133.0	3133.0	3147.9	3147.9	3144.9	3144.9	3071.7	
3194.9	3194.9	3196.2	3196.2	3199.2	3199.2	3124.4	
3314.6	3314.6	3214.1	3214.1	3228.8	3228.8	3142.1	
3847.7	3847.7	3816.3	3816.3	3744.3	3744.3	3197.1	

Table S3. Optimized geometries in Cartesian Coordinates of reactants, transition states and products at M062X/6-31G(d,p) level of theory for the reaction of 4H2BN with Cl atoms.

4-hydroxy 2-butanone

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.32312	-0.23965	-0.15629
2	6	-0.8842	0.144192	0.043566
3	1	-2.93692	0.647587	-0.23542
4	1	-2.43744	-0.85586	-1.0433
5	1	-2.65702	-0.83282	0.692001
6	6	0.141313	-0.95962	-0.0581
7	6	1.532729	-0.53056	0.372227
8	1	-0.19915	-1.81087	0.530318
9	1	0.160896	-1.29435	-1.09506
10	1	2.207526	-1.37685	0.309207
11	1	1.51038	-0.2032	1.411226
12	8	-0.56161	1.279381	0.274172
13	8	2.064699	0.469619	-0.45427
14	1	1.526667	1.248136	-0.33667

TS1

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.027423	1.443834	-0.37534
2	6	-0.31675	0.902316	-0.03661
3	1	1.828304	0.369856	-0.06339
4	1	1.286407	1.547359	-1.42848
5	1	1.40628	2.20927	0.299014
6	6	-0.92539	-0.12632	-0.96192
7	6	-2.34367	-0.50572	-0.54657
8	1	-0.90246	0.260544	-1.98874
9	1	-0.27562	-1.0124	-0.94292
10	1	-2.75131	-1.22228	-1.26354
11	1	-2.98314	0.38737	-0.55992
12	8	-0.87606	1.28503	0.977214
13	8	-2.37486	-1.13518	0.71386
14	1	-2.15157	-0.46975	1.377496
15	17	2.700046	-0.79726	0.150852

TS2

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.945352	1.256137	0.710838
2	6	-0.29452	0.706217	0.099355
3	1	1.280109	2.214509	0.319148
4	1	1.112118	1.074987	1.772271
5	1	1.889427	0.394571	0.19609
6	6	-0.8437	-0.58841	0.6531
7	6	-2.05474	-1.07898	-0.13347
8	1	-0.03561	-1.33284	0.648091
9	1	-1.11861	-0.42332	1.703116
10	1	-2.39552	-2.0318	0.278364
11	1	-1.77025	-1.24562	-1.18099
12	8	-0.8228	1.303391	-0.82329
13	8	-3.14171	-0.18468	-0.03701
14	1	-2.91359	0.602395	-0.54813
15	17	2.891393	-0.58661	-0.25203

TS3

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.090656	2.302519	0.451523
2	6	-0.60003	1.068007	-0.05781
3	1	-0.24142	3.171085	-0.11621
4	1	-0.13415	2.442924	1.513646
5	1	1.175425	2.18379	0.358698
6	6	-0.2511	-0.24781	0.570117
7	6	-0.92257	-1.4678	-0.02109
8	1	1.062721	-0.38429	0.208245
9	1	-0.13374	-0.23196	1.656755
10	1	-0.5326	-2.37825	0.437153
11	1	-0.74041	-1.50809	-1.10086
12	8	-1.42608	1.088758	-0.95346
13	8	-2.30404	-1.40543	0.272319
14	1	-2.67982	-0.70684	-0.28116
15	17	2.480182	-0.58732	-0.16962

TS4

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.68023	-2.30518	0.166759
2	6	-1.03124	-0.85045	0.01374
3	1	-0.81987	-2.61971	1.205695
4	1	-1.30705	-2.9052	-0.49192
5	1	0.376328	-2.45323	-0.08141
6	6	-0.26321	0.141089	0.835767
7	6	-0.63423	1.598352	0.723683
8	1	-0.01079	-0.20368	1.84219
9	1	0.946497	0.056356	0.26454
10	1	0.104639	2.207467	1.251713
11	1	-1.59773	1.726352	1.251693
12	8	-1.89854	-0.45609	-0.74664
13	8	-0.69836	2.071856	-0.59105
14	1	-1.35061	1.538961	-1.06683
15	17	2.358064	-0.10449	-0.23023

TS5

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.005831	-1.00022	0.461549
2	6	1.941653	-0.15976	-0.1989
3	1	3.968264	-0.79088	0.016169
4	1	3.039381	-0.76423	1.521688
5	1	2.774398	-2.05717	0.370698
6	6	0.496389	-0.51473	0.132728
7	6	-0.45049	0.618396	-0.15946
8	1	0.230455	-1.38283	-0.46567
9	1	0.405897	-0.80508	1.17374
10	1	-1.62232	0.085269	-0.13166
11	1	-0.41479	0.996452	-1.17188
12	8	2.204306	0.722931	-0.9572
13	8	-0.39526	1.571946	0.804554
14	1	-0.80667	2.375861	0.529342
15	17	-3.05925	-0.56933	-0.11981

TS6

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.29677	-1.40705	-0.19954
2	6	-1.46667	-0.19234	0.114611
3	1	-2.93152	-1.64751	0.641338
4	1	-2.898	-1.24074	-1.08833
5	1	-1.63318	-2.24267	-0.40425
6	6	-0.69672	0.440567	-1.03382
7	6	0.575525	1.154445	-0.61162
8	1	-0.45742	-0.30337	-1.78503
9	1	-1.36528	1.164443	-1.50124
10	1	1.152627	1.53569	-1.44155
11	1	1.343458	0.209674	-0.21146
12	8	-1.42091	0.279906	1.214527
13	8	0.47311	2.090668	0.351955
14	1	-0.10735	1.786705	1.040511
15	17	2.222757	-1.07062	0.152962

TS7

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.348104	-1.20753	-0.16674
2	6	1.108506	-0.37432	0.053642
3	1	2.081405	-2.26219	-0.23413
4	1	2.873186	-0.88704	-1.07139
5	1	3.032441	-1.05944	0.675872
6	6	1.250429	1.129643	-0.08353
7	6	0.002569	1.87958	0.369299
8	1	2.135803	1.453878	0.479193
9	1	1.454633	1.350187	-1.14004
10	1	0.174013	2.956774	0.29831
11	1	-0.20849	1.639842	1.420759
12	8	0.041093	-0.8848	0.335665
13	8	-1.11159	1.593841	-0.44715
14	1	-1.41537	0.346119	-0.24489
15	17	-1.75419	-1.04557	-0.01929

P(HCl)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	17	0	0	0.071136
2	1	0	0	-1.20932

P1

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.318308	0.257436	-0.20424
2	6	0.943064	-0.09245	0.049335
3	1	2.608978	1.27347	-0.44466
4	1	3.069631	-0.52108	-0.15559
5	6	-0.11056	1.000824	-0.01205
6	6	-1.49046	0.486867	0.383749
7	1	0.198861	1.829511	0.638112
8	1	-0.14222	1.394463	-1.03629
9	1	-2.2101	1.309323	0.359842
10	1	-1.45623	0.09539	1.409739
11	8	0.635876	-1.26105	0.305274
12	8	-1.96422	-0.49217	-0.51462
13	1	-1.40428	-1.27139	-0.3971

P2

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.31827	-0.25748	-0.20439
2	6	-0.94305	0.092502	0.049398
3	1	-3.06974	0.52091	-0.15579
4	1	-2.60892	-1.27349	-0.44498
5	6	0.110583	-1.00084	-0.01187
6	6	1.490512	-0.48685	0.383694
7	1	-0.19886	-1.82932	0.638554
8	1	0.142043	-1.39474	-1.03602
9	1	2.210183	-1.30926	0.359692
10	1	1.456455	-0.09534	1.409684
11	8	-0.63593	1.261062	0.3054
12	8	1.964168	0.492167	-0.51477
13	1	1.40426	1.271388	-0.39713

P3

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.319059	-0.27385	0.179864
2	6	0.873762	0.102751	-0.05604
3	1	2.937575	0.621757	0.126062
4	1	2.434464	-0.74049	1.163044
5	1	2.654189	-0.99702	-0.57023
6	6	-0.12542	-0.94141	-0.0256
7	6	-1.57679	-0.63978	-0.23292
8	1	0.196778	-1.97541	0.061696
9	1	-2.18437	-1.4661	0.146358
10	1	-1.76029	-0.58563	-1.32245
11	8	0.548527	1.274273	-0.28201
12	8	-2.02395	0.527472	0.411911
13	1	-1.41865	1.242612	0.164454

P4

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.31908	-0.274	-0.17959
2	6	-0.87378	0.102705	0.05621
3	1	-2.65228	-1.00309	0.56558
4	1	-2.93849	0.620547	-0.11862
5	1	-2.4354	-0.73348	-1.16605
6	6	0.125468	-0.9414	0.025883
7	6	1.57713	-0.64028	0.231732
8	1	-0.19684	-1.97547	-0.06013
9	1	2.183987	-1.46596	-0.15024
10	1	1.762132	-0.58897	1.32119
11	8	-0.54866	1.274423	0.281473
12	8	2.023764	0.52829	-0.41076
13	1	1.41759	1.242548	-0.16288

P5

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.21499	-0.4102	-0.37539
2	6	-0.90351	0.177618	0.094598
3	1	-2.08244	-0.81314	-1.38531
4	1	-2.51963	-1.24186	0.267699
5	1	-2.98563	0.360659	-0.39046
6	6	0.207696	-0.82947	0.422053
7	6	1.560716	-0.22656	0.502391
8	1	-0.06202	-1.2963	1.378861
9	1	0.19222	-1.62808	-0.33056
10	1	1.803079	0.460508	1.308276
11	8	-0.73849	1.369988	0.216552
12	8	2.097946	0.041667	-0.72592
13	1	2.879312	0.596603	-0.63548

P6

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.30089	0.23866	-0.06782
2	6	-0.8483	-0.1522	0.018819
3	1	-2.54937	0.961417	0.715466
4	1	-2.4783	0.729508	-1.03108
5	1	-2.93301	-0.64544	0.012452
6	6	0.162832	0.967414	0.209541
7	6	1.531501	0.648499	-0.30571
8	1	-0.21046	1.887532	-0.25104
9	1	0.169967	1.15587	1.30231
10	1	2.236135	1.455632	-0.47085
11	8	-0.49682	-1.31659	-0.03246
12	8	2.128401	-0.50441	0.088905
13	1	1.441554	-1.19083	0.142197

P7

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.14554	-0.47497	-0.3978
2	6	-0.87908	0.15899	0.121467
3	1	-2.93802	0.270009	-0.46657
4	1	-1.94848	-0.89425	-1.39067
5	1	-2.45391	-1.30363	0.247698
6	6	0.255688	-0.78392	0.50267
7	6	1.617693	-0.11	0.387538
8	1	0.07343	-1.10327	1.53832
9	1	0.225368	-1.68648	-0.11699
10	1	2.406882	-0.65868	0.925521
11	1	1.57448	0.89462	0.849084
12	8	-0.76196	1.357954	0.25072
13	8	2.007916	0.109684	-0.90943

Table S4. Optimized geometries in Cartesian Coordinates of reactants, transition states and products at M062X/6-31+G(d,p) level of theory for the reaction of 4H2BN with OH radicals.

4-hydroxy 2-butanone

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.33119	-0.23611	-0.16291
2	6	-0.88372	0.140443	0.043127
3	1	-2.93968	0.66259	-0.2632
4	1	-2.44265	-0.87407	-1.04462
5	1	-2.67657	-0.81353	0.701694
6	6	0.142781	-0.97212	-0.05358
7	6	1.533776	-0.52537	0.382501
8	1	-0.20541	-1.82693	0.541169
9	1	0.17063	-1.31005	-1.09837
10	1	2.222489	-1.37322	0.342411
11	1	1.496187	-0.16974	1.421587
12	8	-0.55268	1.286035	0.282989
13	8	2.06305	0.464895	-0.47122
14	1	1.522199	1.256459	-0.3497

TS1

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.728908	0.948631	-0.31138
2	6	0.282603	0.735006	0.026677
3	1	2.235332	-0.11732	-0.2068
4	1	1.914167	1.205311	-1.35651
5	1	2.224668	1.617919	0.390698
6	6	-0.57672	0.029418	-0.99976
7	6	-2.02127	-0.12911	-0.53944
8	1	-0.5235	0.586145	-1.94461
9	1	-0.12138	-0.95253	-1.18783
10	1	-2.59964	-0.63429	-1.31702
11	1	-2.46654	0.861769	-0.37661
12	8	-0.1576	1.072535	1.111481
13	8	-2.12352	-0.92469	0.621595
14	1	-1.74764	-0.4108	1.348085
15	8	2.567875	-1.42329	0.08768
16	1	2.309289	-1.45633	1.027933

TS2

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.517236	-1.05171	0.405935
2	6	0.293368	-0.25741	0.042221
3	1	1.618882	-1.14566	1.490564
4	1	1.586353	-2.02492	-0.08266
5	1	2.480566	-0.39402	0.060434
6	6	-0.99546	-1.01867	-0.18266
7	6	-2.16496	-0.09747	-0.51436
8	1	-0.82397	-1.74901	-0.98476
9	1	-1.21013	-1.59786	0.725272
10	1	-3.06435	-0.69556	-0.68148
11	1	-1.94786	0.453952	-1.4387
12	8	0.335739	0.957882	-0.04457
13	8	-2.45622	0.784151	0.547086
14	1	-1.73736	1.427799	0.587874
15	8	3.207902	0.629903	-0.24703
16	1	2.497406	1.301395	-0.22721

TS3

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.63234	1.500411	0.328588
2	6	0.273903	0.954757	-0.01915
3	1	1.692698	2.553215	0.053941
4	1	1.825668	1.374297	1.39853
5	1	2.395962	0.921869	-0.20198
6	6	-0.02464	-0.47314	0.388043
7	6	-1.31573	-1.02293	-0.197
8	1	0.892156	-1.08319	-0.00907
9	1	0.010281	-0.56941	1.479863
10	1	-1.43198	-2.07622	0.070133
11	1	-1.28422	-0.94817	-1.29131
12	8	-0.56305	1.607465	-0.61375
13	8	-2.43343	-0.34239	0.331917
14	1	-2.3968	0.560505	-0.01254
15	8	2.109263	-1.7573	-0.31032
16	1	1.998638	-2.54971	0.246777

TS4

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.397586	0.417219	0.0939
2	6	1.088447	-0.32072	-0.00152
3	1	3.112872	-0.00246	-0.61281
4	1	2.22877	1.476518	-0.12703
5	1	2.79442	0.353587	1.111978
6	6	-0.04017	0.154041	0.877183
7	6	-1.29036	-0.70154	0.795816
8	1	0.284068	0.382593	1.897758
9	1	-0.33561	1.215708	0.421565
10	1	-2.05907	-0.30605	1.463695
11	1	-1.06135	-1.7302	1.105359
12	8	0.916656	-1.24151	-0.78078
13	8	-1.8392	-0.68447	-0.51083
14	1	-1.21843	-1.16299	-1.07941
15	8	-0.96628	2.061477	-0.44951
16	1	-1.56813	1.395292	-0.84438

TS5

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.713447	-0.85317	0.157178
2	6	1.478164	-0.00264	-0.00011
3	1	3.570937	-0.22519	0.398119
4	1	2.564151	-1.6128	0.929932
5	1	2.902837	-1.38031	-0.78438
6	6	0.141713	-0.72617	-0.04341
7	6	-0.9822	0.168454	-0.52539
8	1	0.230491	-1.62121	-0.67052
9	1	-0.07994	-1.07666	0.973996
10	1	-1.9684	-0.46737	-0.49228
11	1	-0.86308	0.473854	-1.57378
12	8	1.542393	1.208803	-0.08901
13	8	-1.23151	1.253453	0.320886
14	1	-0.43612	1.807783	0.321819
15	8	-3.15686	-0.88007	0.107925
16	1	-3.25982	-0.07446	0.649031

TS6

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.501669	-0.04945	-0.21039
2	6	1.047825	-0.16839	0.16073
3	1	2.843815	-0.94085	-0.74373
4	1	2.61126	0.801957	-0.89182
5	1	3.10481	0.122368	0.680895
6	6	0.103739	-0.72188	-0.88856
7	6	-1.35689	-0.47052	-0.54946
8	1	0.353663	-0.27714	-1.85886
9	1	0.294143	-1.80164	-0.97102
10	1	-2.01982	-0.77135	-1.36463
11	1	-1.47758	0.67846	-0.46922
12	8	0.637788	0.180402	1.254891
13	8	-1.78935	-1.10519	0.61109
14	1	-1.21025	-0.81841	1.331914
15	8	-1.04583	2.108531	-0.29125
16	1	-0.69897	1.998045	0.614726

TS7

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.232902	0.3497	-0.48136
2	6	1.056647	-0.3414	0.159129
3	1	3.023197	0.499673	0.253987
4	1	2.605992	-0.22351	-1.33575
5	1	1.884837	1.319564	-0.85152
6	6	-0.00532	-0.89265	-0.78798
7	6	-1.35702	-1.06759	-0.10048
8	1	-0.10136	-0.25048	-1.66902
9	1	0.352641	-1.87219	-1.13277
10	1	-2.00828	-1.68374	-0.72739
11	1	-1.19649	-1.54946	0.87102
12	8	0.954572	-0.4796	1.357973
13	8	-2.04044	0.154194	0.085287
14	1	-1.39531	0.940114	0.464867
15	8	-0.60938	1.844693	0.048428
16	1	-1.16649	2.377415	-0.54279

P1

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.318164	0.25742	-0.20477
2	6	0.943016	-0.09242	0.049487
3	1	2.60861	1.273475	-0.44543
4	1	3.069638	-0.52096	-0.15612
5	6	-0.1106	1.000906	-0.01152
6	6	-1.49054	0.486672	0.383731
7	1	0.198751	1.829222	0.639151
8	1	-0.14209	1.395082	-1.03556
9	1	-2.21028	1.30903	0.359905
10	1	-1.45658	0.094756	1.40955
11	8	0.635865	-1.26098	0.305756
12	8	-1.96387	-0.4921	-0.51522
13	1	-1.40421	-1.27147	-0.39738

P2

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.31822	-0.2575	0.204487
2	6	0.943042	0.092526	-0.04943
3	1	3.069747	0.520851	0.155946
4	1	2.608744	-1.2735	0.445218
5	6	-0.11058	-1.00085	0.011775
6	6	-1.49048	-0.48678	-0.38374
7	1	0.198847	-1.82928	-0.63871
8	1	-0.14205	-1.39478	1.035902
9	1	-2.21018	-1.30918	-0.35997
10	1	-1.45634	-0.09505	-1.40964
11	8	0.635925	1.261058	-0.30549
12	8	-1.96413	0.492084	0.514922
13	1	-1.4044	1.271431	0.397276

P3

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.31905	-0.2739	-0.17992
2	6	-0.87378	0.102702	0.056068
3	1	-2.93748	0.621791	-0.12661
4	1	-2.43437	-0.74101	-1.16288
5	1	-2.65438	-0.99669	0.570466
6	6	0.125484	-0.9414	0.025709
7	6	1.576879	-0.63974	0.232881
8	1	-0.19656	-1.97543	-0.06167
9	1	2.184465	-1.46604	-0.14649
10	1	1.760484	-0.58561	1.32237
11	8	-0.54864	1.274268	0.282034
12	8	2.023897	0.52753	-0.41193
13	1	1.418508	1.242567	-0.16446

P4

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.319063	0.273807	-0.17995
2	6	0.873767	-0.10264	0.056068
3	1	2.937424	-0.62191	-0.12623
4	1	2.434495	0.740493	-1.1631
5	1	2.654392	0.996886	0.570153
6	6	-0.12548	0.941425	0.025626
7	6	-1.57682	0.639622	0.233068
8	1	0.196545	1.975463	-0.06185
9	1	-2.18453	1.466025	-0.14584
10	1	-1.76013	0.58504	1.322594
11	8	0.548545	-1.27418	0.282147
12	8	-2.02389	-0.52741	-0.41213
13	1	-1.41858	-1.24256	-0.16478

P5

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.30094	-0.23863	0.067643
2	6	-0.84829	0.152175	-0.01877
3	1	-2.93296	0.645546	-0.01246
4	1	-2.54943	-0.96114	-0.71586
5	1	-2.47848	-0.72966	1.030782
6	6	0.162819	-0.96745	-0.20937
7	6	1.531548	-0.64845	0.305713
8	1	-0.21042	-1.88746	0.251455
9	1	0.169866	-1.15614	-1.30209
10	1	2.23619	-1.45558	0.470846
11	8	-0.49681	1.316561	0.032641
12	8	2.128413	0.504409	-0.08911
13	1	1.441575	1.190833	-0.14225

P6

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.300919	-0.23865	-0.06776
2	6	0.848282	0.152177	0.018831
3	1	2.549458	-0.96129	0.715605
4	1	2.478387	-0.7295	-1.031
5	1	2.932967	0.645506	0.012447
6	6	-0.16285	-0.96745	0.209493
7	6	-1.53152	-0.64846	-0.30576
8	1	0.210456	-1.88749	-0.25123
9	1	-0.16996	-1.15604	1.302226
10	1	-2.23614	-1.45561	-0.47084
11	8	0.496832	1.316569	-0.03253
12	8	-2.12841	0.504411	0.088997
13	1	-1.44159	1.190856	0.142212

P7

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.14529	-0.47527	0.397847
2	6	-0.87906	0.159009	-0.12155
3	1	-2.93814	0.269363	0.466105
4	1	-2.45318	-1.30451	-0.24712
5	1	-1.9481	-0.8938	1.391018
6	6	0.255788	-0.78361	-0.5033
7	6	1.61768	-0.10964	-0.38751
8	1	0.225493	-1.6866	0.115744
9	1	0.073617	-1.10225	-1.53918
10	1	2.407055	-0.65786	-0.92567
11	1	1.574524	0.895313	-0.84836
12	8	-0.76211	1.358032	-0.25041
13	8	2.007614	0.109142	0.909721

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Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0	0	0.115559
2	1	0	0.768774	-0.46224
3	1	0	-0.76877	-0.46224