

Theoretical mechanistic study on the radical-molecule reaction of Ketenyl with nitrogen dioxide

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Table S1. The harmonic vibrational frequencies (cm^{-1}) of reactants, some important

products, isomers, and transition states at the B3LYP/6-311G(d,p) level. Page S2

Figure S1. The B3LYP/6-311G(d,p) optimized geometries of unfavorable species for

$\text{CH}_2\text{OH} + \text{NO}_2$ reaction. Bond distances are in angstroms and angles are in degrees.

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Table S1. The harmonic vibrational frequencies (cm^{-1}) of reactants, some important products, isomers, and transition states at the B3LYP/6-311G(d,p) level.

Species	Frequencies	Expt ^a
CH_2OH	439, 588, 1061, 1207, 1367, 1488, 3112, 3256, 3840	420, —, 1056, 1183, 1357, 1465, —, 3650
NO_2	767, 1399, 1707	750, 1318, 1618
CH_2O	1202, 1270, 1539, 1827, 2869, 2919	1167, 1249, 1500, 1746, 2783, 2843
$\text{HONO-}trans$	591, 619, 834, 1298, 1793, 3776	
$\text{HONO-}cis$	638, 718, 893, 1338, 1720, 3585	
HNO_2	800, 1068, 1408, 1543, 1678, 3146	
HOCHO	633, 702, 1058, 1133, 1311, 1411, 1836, 3044, 3737	625, 638, 1033, 1105, 1229, 1387, 1770, 2943, 3570
HNO	1576, 1673, 2829	1511, 1569, 2854
1	112, 239, 376, 489, 577, 698, 887, 1064, 1163, 1234, 1355, 1409, 1426, 1506, 1661, 3018, 3156, 3774	
2^a	85, 191, 324, 412, 466, 634, 780, 1003, 1083, 1119, 1290, 1407, 1438, 1503, 1787, 3026, 3143, 3817	
2^b	153, 275, 345, 490, 539, 681, 855, 923, 1058, 1130, 1284, 1404, 1428, 1500, 1671, 3047, 3160, 3821	
TS1/2^a	211i, 201, 237, 279, 372, 442, 749, 785, 834, 1125, 1196, 1352, 1400, 1484, 1547, 3232, 3413, 3766	
TS1/P₁	943i, 153, 321, 359, 576, 646, 867, 880, 1085, 1214, 1214, 1315, 1457, 1629, 1681, 2008, 2964, 3017	
TS2^a/2^b	252i, 108, 245, 373, 508, 528, 790, 928, 1046, 1085, 1275, 1393, 1437, 1500, 1778, 2991, 3133, 3826	
TS2^a/P₂	883i, 149, 271, 308, 465, 528, 592, 725, 1072, 1184, 1261, 1280, 1367, 1454, 1586, 1926, 2960, 3768	
TS2^a/P₃	1107i, 130, 332, 444, 467, 638, 803, 831, 1092, 1227, 1247, 1306, 1422, 1610, 1680, 1899, 3009, 3083	
TS2^b/P₄	1254i, 204, 277, 341, 454, 585, 820, 874, 1209, 1231, 1277, 1363, 1391, 1449, 1634, 1795, 3040, 3134	

^aExperimental values from ref. 37.

Figure S1.

