Supporting Information

Kinetic Study and Rate Coefficients Calculations of the Reaction of

1-Hydroxyethyl Radical with Nitric Oxide

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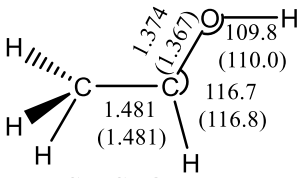
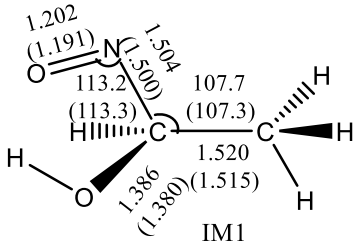
§1. Figures



CH_3CHOH



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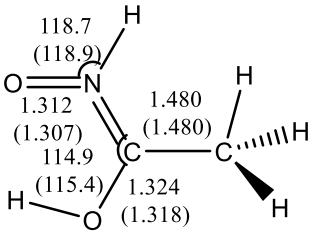

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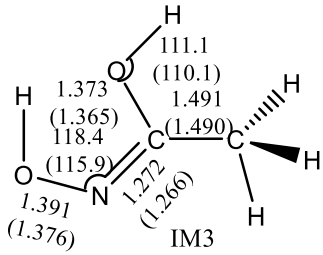

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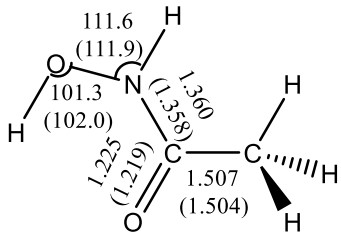

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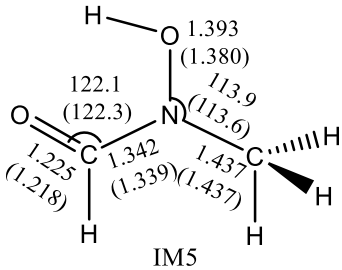

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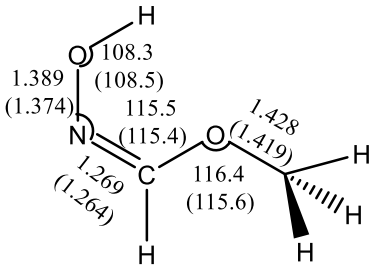

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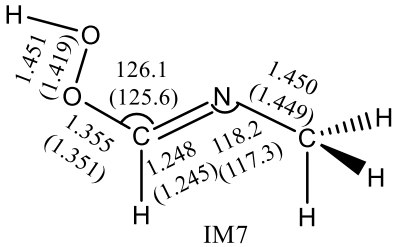

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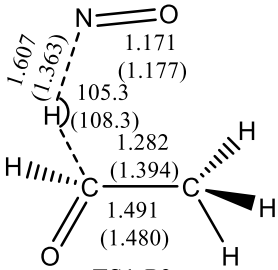

TS1-P3

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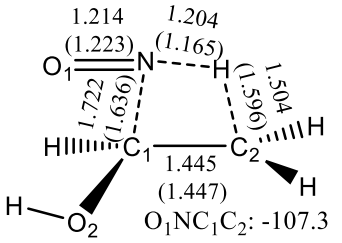

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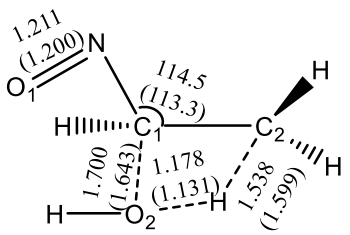

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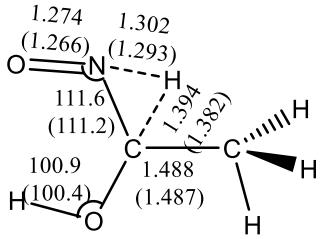

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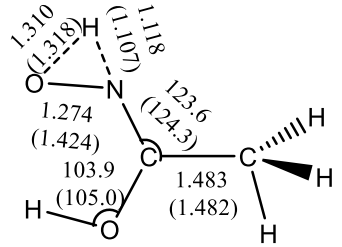

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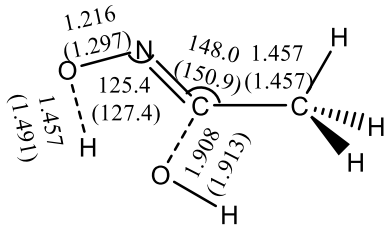

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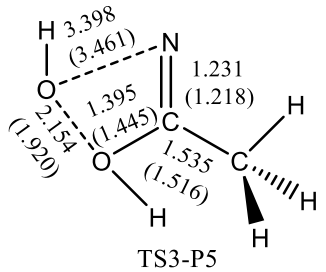

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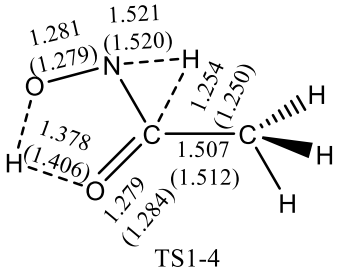

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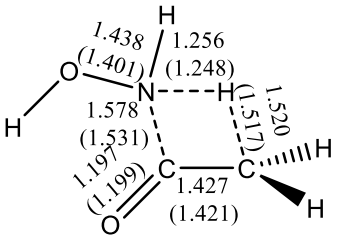

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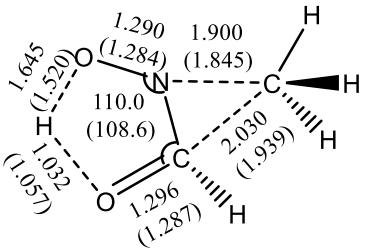

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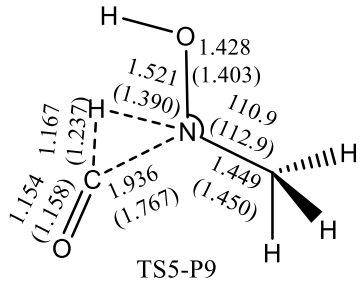

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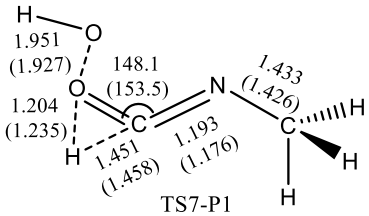

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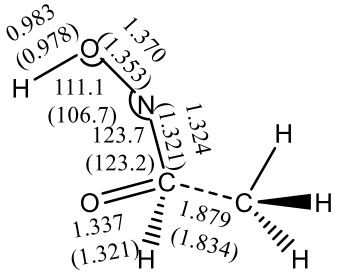

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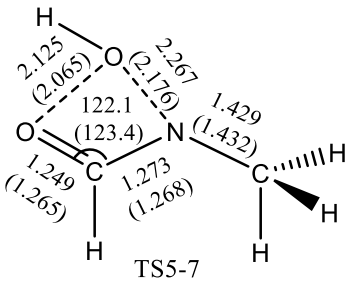

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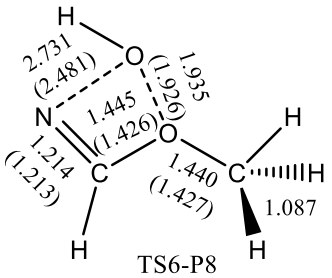

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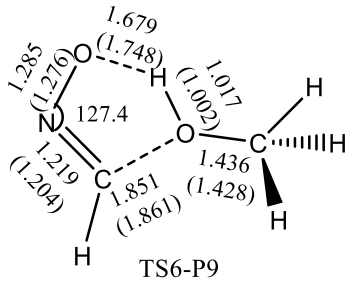

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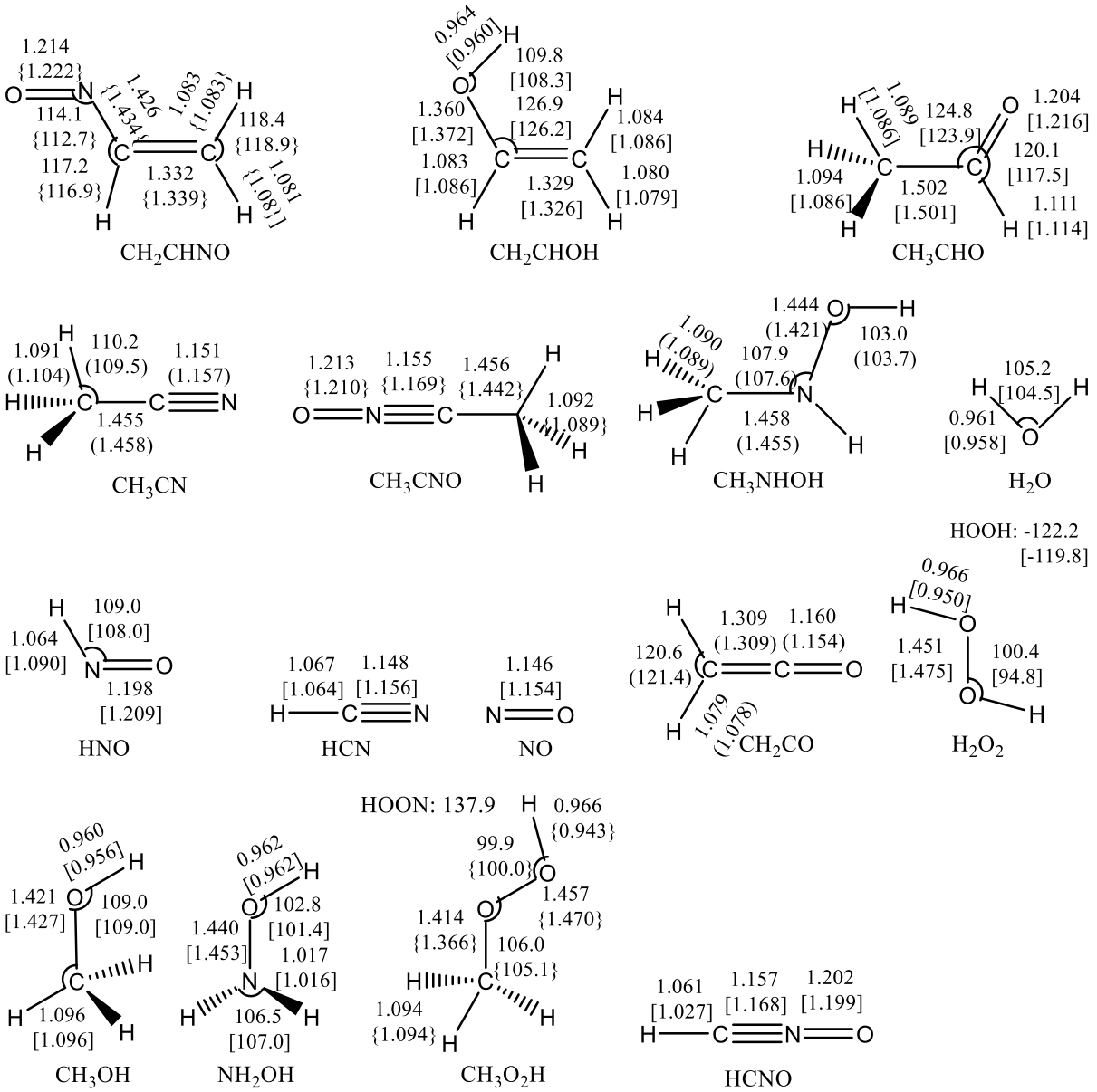

Figure S1. Optimized geometries of all species (bond lengths in angstroms (Å) and angles in degrees (°)) at the B3LYP/6-311++G(df, pd) and M06-2X/6-311++G(df,pd) level (the results in parentheses). The values in square brackets are the corresponding experimental data [17] and those in the braces are the corresponding calculated values from references [31-32].

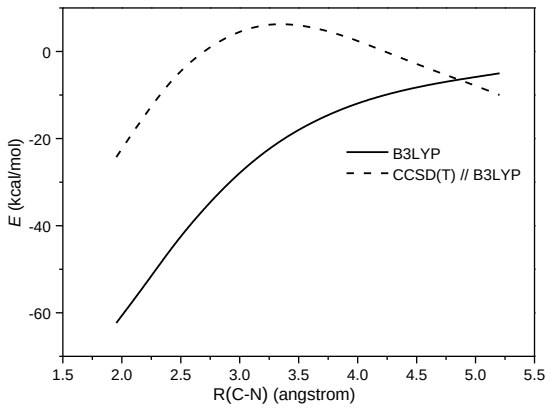

Figure S2. MEP for the reaction of CH_3CHOH + NO to form IM1* at the B3LYP/6-311++G(df,pd) and CCSD(T)/cc-pVTZ // B3LYP/6-311++G(df,pd) levels.

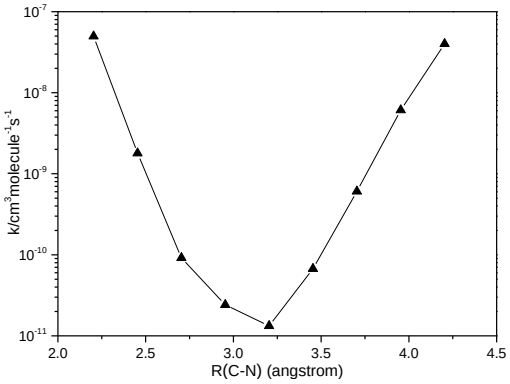

Figure S3. Variation of TST rate coefficients for CH_3CHOH + NO reaction to form IM1 at 298 K.

§2. Tables

Table S1. Theoretical and experimental harmonic vibrational frequencies (cm^{-1}), ZPE (kal/mol) and the T1 diagnostic values for the species of CH_3CHOH + NO system at the B3LYP/6-311++G(df,pd) level of theory.

Species	Methods	Frequencies	ZPE	T1 values
CH_3CHOH	B3LYP	178, 343, 399, 531, 906, 995, 1032, 1177, 1238, 1361, 1409, 1427, 1450, 2873, 2964, 3022, 3056, 3749	41.2	0.01377581
	Expt[a]	1242, 1507		
NO	B3LYP	1927	2.8	0.02430689
	Expt[a]	1904		
CH_2CHNO	B3LYP	175, 344, 599, 667, 869, 980, 996, 1114, 1256, 1384, 1540, 1635, 3064, 3079, 3168	30.6	0.01560050
CH_2CHOH	B3LYP	449, 480, 694, 817, 938, 973, 1093, 1290, 1320, 1414, 1653, 3065, 3109, 3162, 3709	35.4	0.01225111
	Expt[a]	388, 486, 699, 817, 948, 960, 1118, 1260, 1300, 1412, 1663, 3122, 3634		
HNO	B3LYP	1524, 1635, 2804	8.7	0.01518491
	Expt[a]	1501, 1565, 2684		
H2O	B3LYP	1581, 3741, 3839	13.4	0.00655052
	Expt[a]	1595, 3756, 3657		
CH_3CHO	B3LYP	148, 503, 765, 873, 1112, 1119, 1358, 1401, 1438, 1447, 1785, 2826, 2977, 3032, 3092	34.7	0.01421675
	Expt[a]	150, 509, 764, 867, 1102, 1114, 1352, 1395, 1431, 1433, 1743, 2716, 2923, 2964		
CH_3CNO	B3LYP	143, 144, 497, 497, 784, 1035, 1036, 1359, 1404, 1454, 1454, 2416, 2983, 3047, 3047	30.9	0.01860607
	Expt[a]	477, 780, 785, 1034, 1332, 1348, 1381, 1394, 1453, 2309, 2311, 2943, 3022		
H_2O_2	B3LYP	346, 933, 1262, 1421, 3721, 3722	16.6	0.01002754
	Expt[a]	371, 877, 1266, 1402, 3608		
CH_3CN	B3LYP	377, 377, 915, 1047, 1047, 1392, 1452, 1453, 2330, 3002, 3072, 3073	28.4	0.01238948
	Expt[a]	362, 920, 1041, 1385, 1448, 2267, 3009		
CH_2CO	B3LYP	437, 548, 602, 977, 1155, 1392, 2188, 3134, 3224	19.8	0.01658269
	Expt[a]	433, 528, 588, 977, 1118, 1388, 2152, 3166		
NH_2OH	B3LYP	429, 919, 1109, 1300, 1362, 1643, 3402, 3483, 3771	25.3	0.00869544
	Expt[a]	386, 895, 1115, 1295, 1353, 1605, 3294, 3359		
HCN	B3LYP	745, 745, 2169, 3390	10.2	0.01406920
	Expt[a]	712, 2089, 3312		
CH_3O_2H	B3LYP	133, 245, 433, 862, 1024, 1152, 1173, 1348,1428, 1437, 1489, 2962, 3028, 3066, 3729		0.01104520

CH_3OH	B3LYP	291, 1029, 1059 , 1152, 1340, 1460, 1473, 1484, 2941, 2989, 3064, 3792	32.0	0.00843718
	EXPT	200, 1033, 1060, 1165,1345, 1455, 1477, 1477, 2844, 2960, 3000		
HCNO	B3LYP	278, 539, 546, 1261, 2272, 3423	12.1	0.02079500
	Expt[a]	224, 537, 1254, 2196, 3336		
CO	B3LYP	2186	3.2	0.01826023
	Expt[a]	2170		
CH_3NHOH	B3LYP	258, 334, 431, 832, 951, 1036, 1132, 1199, 1328, 1421, 1451, 1464, 1494, 2949, 3027, 3060,3433, 3765	42.9	0.00950278
	Expt[a]	269, 1245	48.0	
IM1	B3LYP	133, 220, 321, 359, 399, 505, 672, 777, 892, 986, 1059, 1165, 1193, 1305, 1337, 1370, 1446, 1456, 1600, 2873, 2972, 3047,3054, 3566		0.01246500
IM2	B3LYP	163, 262, 272, 374, 556, 659, 664, 789, 942, 1000,1040, 1126, 1267, 1267, 1414, 1441,1450, 1492, 1665, 2987, 3043, 3072, 3266, 3428	49.0	0.02120243
IM3	B3LYP	126, 179, 284, 310, 395, 429, 594, 629, 875, 944, 1034, 1048, 1167, 1297, 1395, 1411, 1456, 1457, 1713, 2974, 3023, 3100, 3623, 3798	48.3	0.01346500
IM4	B3LYP	102, 232, 271, 376, 413, 442, 620, 640, 937, 991, 1039, 1081, 1251, 1377, 1388, 1447, 1467, 1529, 1696, 3001, 3075, 3078, 3516, 3587	48.7	0.01549852
IM5	B3LYP	50, 222, 247, 312, 455, 520, 811, 862, 895, 974, 1004, 1073, 1193, 1200, 1244, 1336, 1412, 1444, 1516, 2746, 3006, 3134, 3177, 3192	48.8	0.01603640
IM6	B3LYP	28, 141, 225, 384, 432, 562, 744, 836, 935, 1034, 1126, 1154, 1225, 1330, 1396, 1460, 1472, 1479, 1674, 2975, 3042, 3100, 3133, 3619	48.6	0.01391106
IM7	B3LYP	116, 170, 204, 218, 362, 369, 707, 863, 939, 1039, 1106, 1121, 1162, 1336, 1409, 1430, 1459, 1484, 1746, 2921, 2999, 3015, 3035,3721	47.6	0.01388659
TS1-P2	B3LYP	1206i, 197, 287, 319, 431, 480, 531, 676, 769, 906, 918, 1049, 1137, 1203,1302, 1321,1380,1420, 1466, 1879, 3052, 3059, 3165, 3395	44.5	0.01972024
TS1-P3	B3LYP	1896i, 37, 119, 162, 187, 350, 429, 501, 713, 884, 904, 1079, 1118, 1205, 1367, 1390, 1448, 1452, 1691, 2239, 2964, 2970, 3037, 3083	42.6	0.03147313
TS1-P4	B3LYP	1765i, 168, 206, 376, 414, 428, 600, 631, 721, 815, 823, 892, 1033, 1114, 1136, 1254, 1406, 1432, 1545, 1683, 3050, 3094, 3134, 3553	43.3	0.01833305
TS1-2	B3LYP	1310i, 216, 296, 324, 378, 622, 681, 895, 937, 979, 1024, 1135, 1212, 1212, 1386, 1417, 1447, 1450, 1487, 1838, 2994, 3000, 3066,3094	45.3	0.02138490

TS2-3	B3LYP	1719i, 147, 220, 264, 344, 391, 589, 630, 805, 861, 949, 1017, 1047, 1294, 1377, 1428, 1448, 1454, 1631, 2722, 2998, 3055, 3099, 3263	45.0	0.02153270
TS3-P1	B3LYP	676i, 130, 175, 267, 384, 449,576, 614, 669, 853, 992, 1043, 1132, 1281, 1383, 1430, 1462, 1572, 1856, 2019, 2989, 3052, 3068, 3778	44.6	0.02311870
TS3-P5	B3LYP	175i, 44, 125, 163, 170, 314, 388, 492, 541, 597, 774, 926, 1017, 1038, 1207, 1355, 1448, 1468, 1721, 2996, 3068, 3124, 3660, 3707	44.0	0.03572694
TS1-4	B3LYP	1164i, 181, 231, 371, 451, 634, 735, 892, 908, 1002, 1073, 1149, 1171, 1201, 1307, 1388, 1453, 1464, 1542, 1966, 2108, 3007, 3081, 3095	44.1	0.02341960
TS4-P6	B3LYP	1544i, 116, 199, 233, 464, 531, 621, 669, 730, 816, 909, 932, 1043, 1120, 1247, 1391, 1453, 1553, 1771, 1898, 3043, 3143, 3438, 3738	45.1	0.01601628
TS1-5	B3LYP	534i, 158, 247, 312, 455, 520, 811, 862, 895, 974, 1004,1073, 1193, 1200, 1244, 1336, 1412, 1444, 1516, 2746, 3006, 3134, 3177, 3192	46.3	0.02151690
TS5-P7	B3LYP	1478i, 86, 141, 230, 247, 263,301, 441,621, 869, 993, 1050, 1104, 1162, 1294, 1402, 1440, 1470, 1886, 2420, 2936, 2993, 3045, 3718	43.7	0.02276104
TS5-7	B3LYP	474i, 55, 117, 257, 291, 374, 403, 658, 845, 885, 967, 1067, 1121,1161,1366, 1409, 1432, 1478, 1632, 2934, 2934, 3012, 3036, 3741	45.3	0.03972494
TS7-P1	B3LYP	1309i, 64, 77, 103, 153, 219,368, 446, 493, 498, 743, 841, 1117, 1131, 1276, 1435, 1462, 1475, 1844, 2119, 2987, 3061, 3072, 3749	41.7	0.02890493
TS1-6	B3LYP	770i, 148, 214, 318, 462, 521, 675, 833, 858, 943, 982, 1004,1132, 1267, 1294, 1379, 1409, 1436, 1453, 3032, 3042, 3171, 3223, 3418	46.8	0.02448876
TS6-P8	B3LYP	475i, 78, 140, 186, 221, 335, 391, 577, 584, 793, 813, 972, 1075, 1132, 1178, 1414, 1454, 1463, 1767, 2993, 2993, 3078, 3107, 3567	44.0	0.09051890
TS6-P9	B3LYP	526i, 107, 133, 194, 311, 344, 550, 655, 942, 1009, 1047, 1148, 1158, 1214, 1444, 1466, 1475, 1491, 1687, 2782, 2990, 3063, 3089, 3314	45.9	0.02539379

[a] Ref.17.

Table S2. Reference enthalpies of formation ($\Delta_f H^0_{298}$).

Species	$\Delta_f H°(298\ K)$ (kcal/mol)
NO [a]	21.75 (± 0.02)
CH_3CHOH [b]	-15.2
CH_2CHNO [c]	39.5
H_2O [a]	-57.79 (± 0.08)
CH_2CHOH [a]	-30.59
HNO [a]	25.58 (± 0.06)
CH_3CHO [a]	-40.8 (± 0.35)
H_2O_2 [a]	-32.4 (± 0.04)
CH_3CN [a]	15.4
CH_2CO [a]	-11.5 (± 0.40)
NH_2OH [a]	-12.0 (± 2.45)
HCN [a]	31.5 (± 0.95)
CH_3O_2H [a]	-31.3
HCNO [d]	40.9
CH_3OH [a]	-48.0 (± 0.14)
CO [a]	-26.4 (± 0.04)

[a] Ref. 17.

[b] Ref. 34.

[c] Ref .35.

[d] Ref. 36.