Supplementary information

Computational study on the mechanism and kinetics for the reaction between HO_2 and n-propyl peroxy radical

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SUMMARY:

42 pages, including 9 Figures and 7 Tables.

Figure Captions:

Fig. S1. Five different conformers (G_1G_2, G_1T_2, $G_1'G_2$, T_1G_2 and T_1T_2) of the n-$C_3H_7O_2$ radical optimized at the B3LYP/6-311g(d,p) level of theory.

Fig. S2. Schematic energy diagram of the HO_2 + G_1T_2 reaction computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/6-311G(d,p) level of theory on both the singlet and triplet potential energy surfaces. Energies are in units of kcal mol^{-1}.

Fig. S3. Schematic energy diagram of the HO_2 + $G_1'G_2$ reaction computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/6-311G(d,p) level of theory on both the singlet and triplet potential energy surfaces. Energies are in units of kcal mol^{-1}.

Fig. S4. Schematic energy diagram of the HO_2 + T_1G_2 reaction computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/6-311G(d,p) level of theory on both the singlet and triplet potential energy surfaces. Energies are in units of kcal mol^{-1}.

Fig. S5. Schematic energy diagram of the HO_2 + T_1T_2 reaction computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/6-311G(d,p) level of theory on both the singlet and triplet potential energy surfaces. Energies are in units of kcal mol^{-1}.

Fig. S6. Selected geometric structures of the reactants, intermediates and transition states of the HO_2 + G_1T_2 reaction computed at the B3LYP/6-311G(d,p) level of theory on the triplet potential energy surface. Bond distances are given in angstroms.

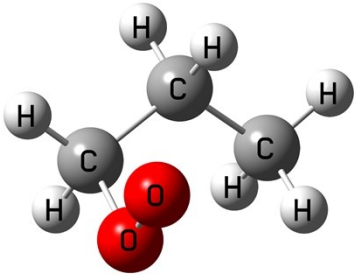
Fig. S7. Selected geometric structures of the reactants, intermediates and transition states of the HO_2 + $G_1'G_2$ reaction computed at the B3LYP/6-311G(d,p) level of theory on the triplet potential energy surface. Bond distances are given in angstroms.

Fig. S8. Selected geometric structures of the reactants, intermediates and transition

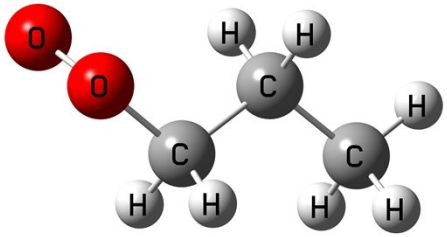
states of the HO_2 + T_1G_2 reaction computed at the B3LYP/6-311G(d,p) level of theory on the triplet potential energy surface. Bond distances are given in angstroms.

Fig. S9. Selected geometric structures of the reactants, intermediates and transition states of the HO_2 + T_1T_2 reaction computed at the B3LYP/6-311G(d,p) level of theory on the triplet potential energy surface. Bond distances are given in angstroms.

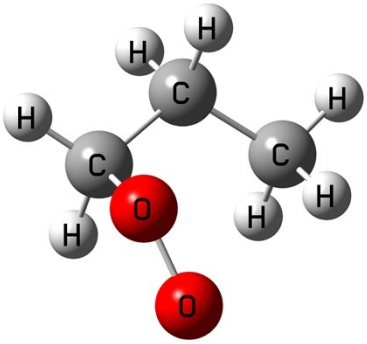
Fig. S1.



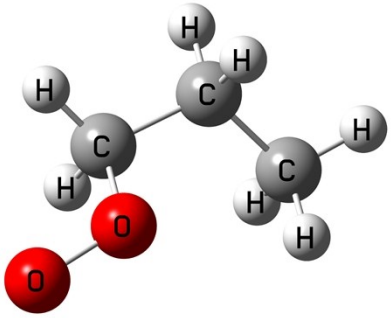
G_1G_2



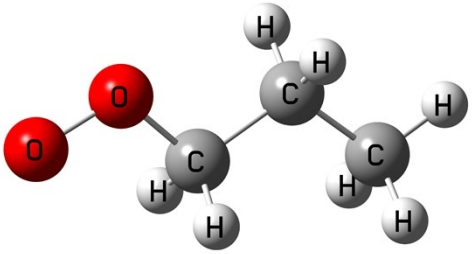
G_1T_2



$G_1'G_2$



T_1G_2



T_1T_2

Fig. S2.

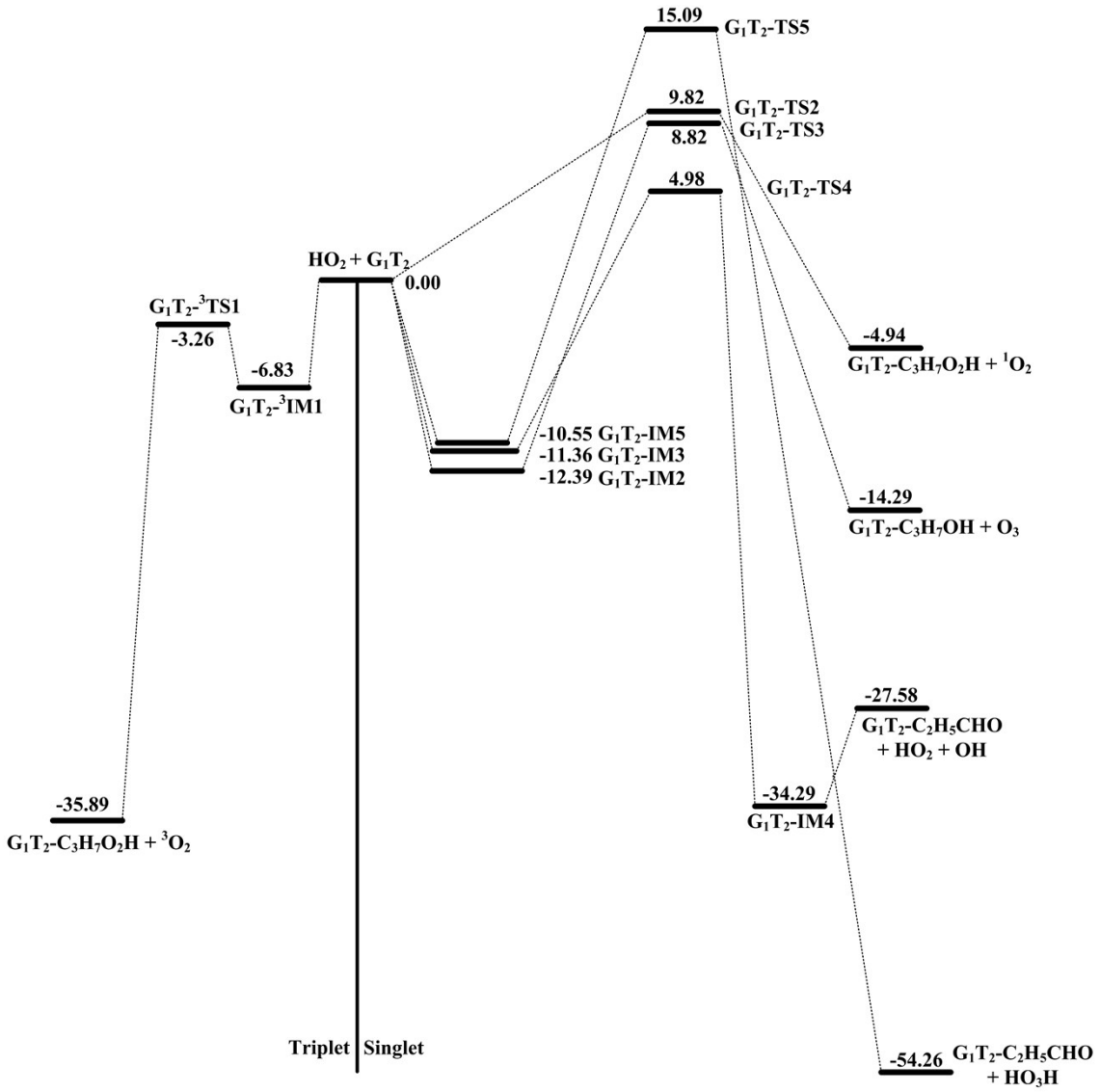

15.09
G1T2-TS5
9.82
G1T2-TS2
8.82
G1T2-TS3
4.98
G1T2-TS4
HO2 + G1T2
0.00
G1T2-3TS1
-3.26
-6.83
G1T2-3IM1
-4.94
G1T2-C3H7O2H + 1O2
-10.55 G1T2-IM5
-11.36 G1T2-IM3
-12.39 G1T2-IM2
-14.29
G1T2-C3H7OH + O3
-27.58
G1T2-C2H5CHO
+ HO2 + OH
-35.89
G1T2-C3H7O2H + 3O2
-34.29
G1T2-IM4
Triplet
Singlet
-54.26
G1T2-C2H5CHO
+ HO3H

Fig. S3.

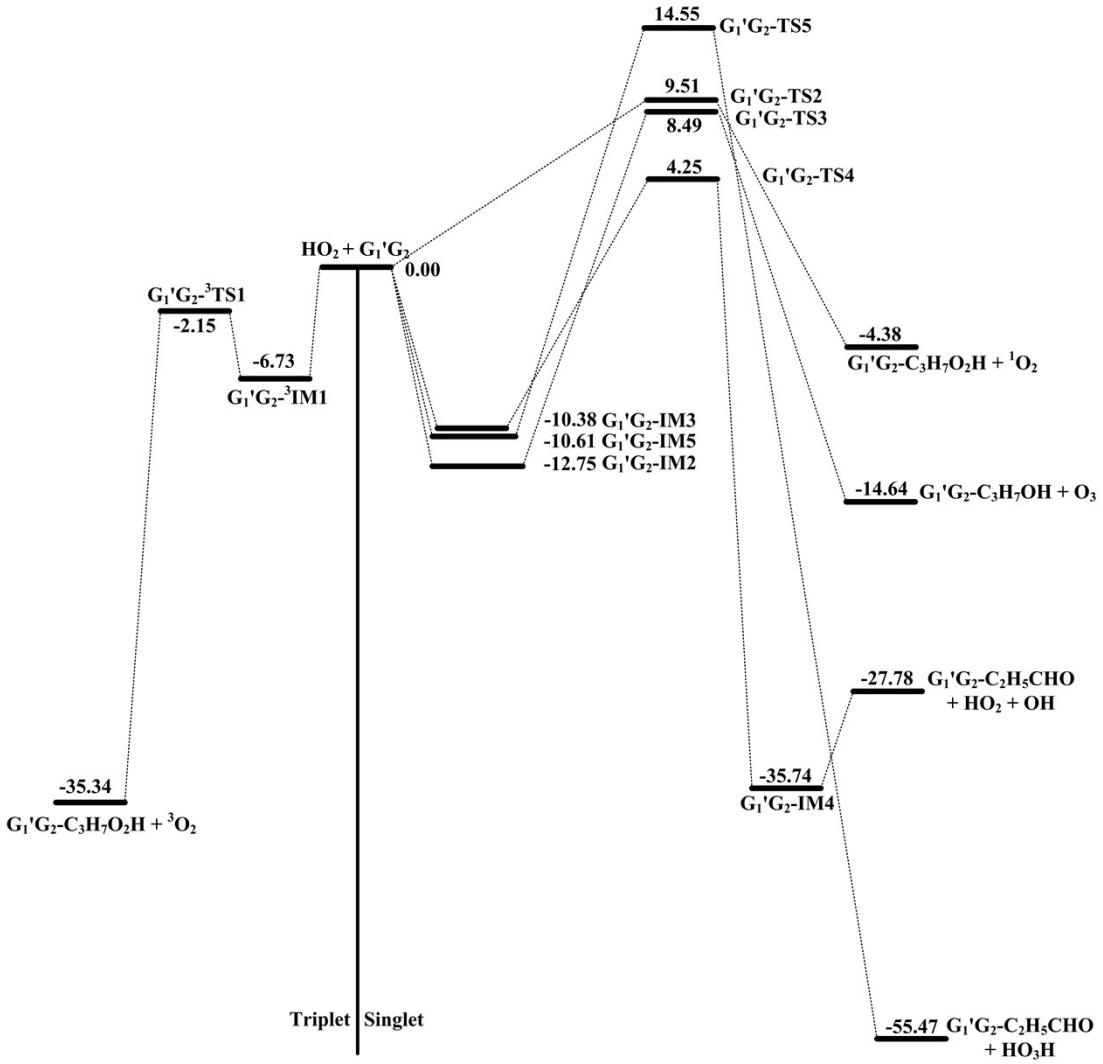

14.55
G1'G2-TS5
9.51
G1'G2-TS2
8.49
G1'G2-TS3
4.25
G1'G2-TS4
HO2 + G1'G2
0.00
G1'G2-3TS1
-2.15
-6.73
G1'G2-3IM1
-4.38
G1'G2-C3H7O2H + 1O2
-10.38 G1'G2-IM3
-10.61 G1'G2-IM5
-12.75 G1'G2-IM2
-14.64 G1'G2-C3H7OH + O3
-27.78 G1'G2-C2H5CHO
+ HO2 + OH
-35.74
G1'G2-IM4
-35.34
G1'G2-C3H7O2H + 3O2
Triplet
Singlet
-55.47 G1'G2-C2H5CHO
+ HO3H

Fig. S4.

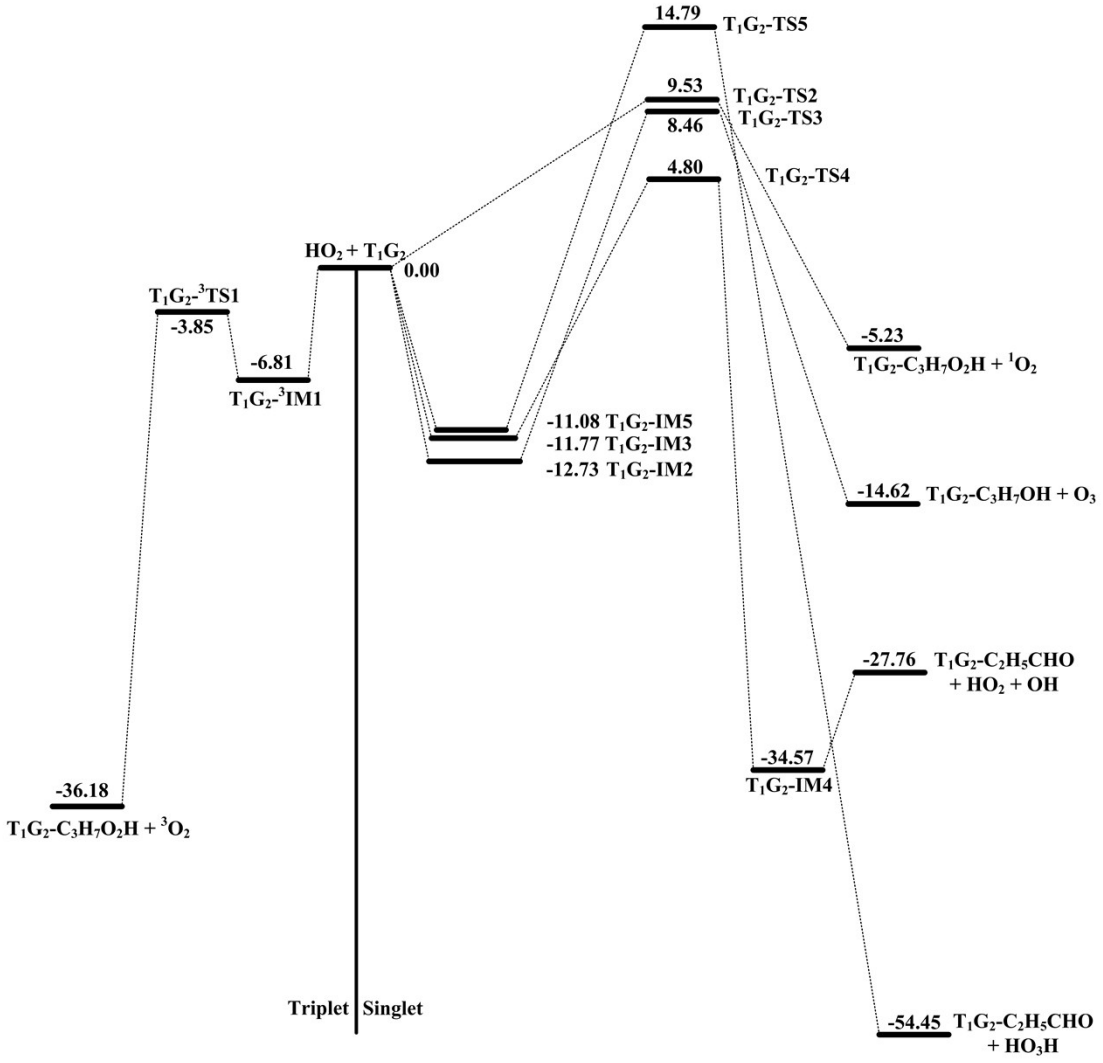

14.79 T1G2-TS5
9.53 T1G2-TS2
8.46 T1G2-TS3
4.80 T1G2-TS4
HO2 + T1G2
0.00
T1G2-3TS1
-3.85
-6.81
T1G2-3IM1
-5.23
T1G2-C3H7O2H + 1O2
-11.08 T1G2-IM5
-11.77 T1G2-IM3
-12.73 T1G2-IM2
-14.62 T1G2-C3H7OH + O3
-27.76 T1G2-C2H5CHO
+ HO2 + OH
-34.57
T1G2-IM4
-36.18
T1G2-C3H7O2H + 3O2
Triplet Singlet
-54.45 T1G2-C2H5CHO
+ HO3H

Fig. S5.

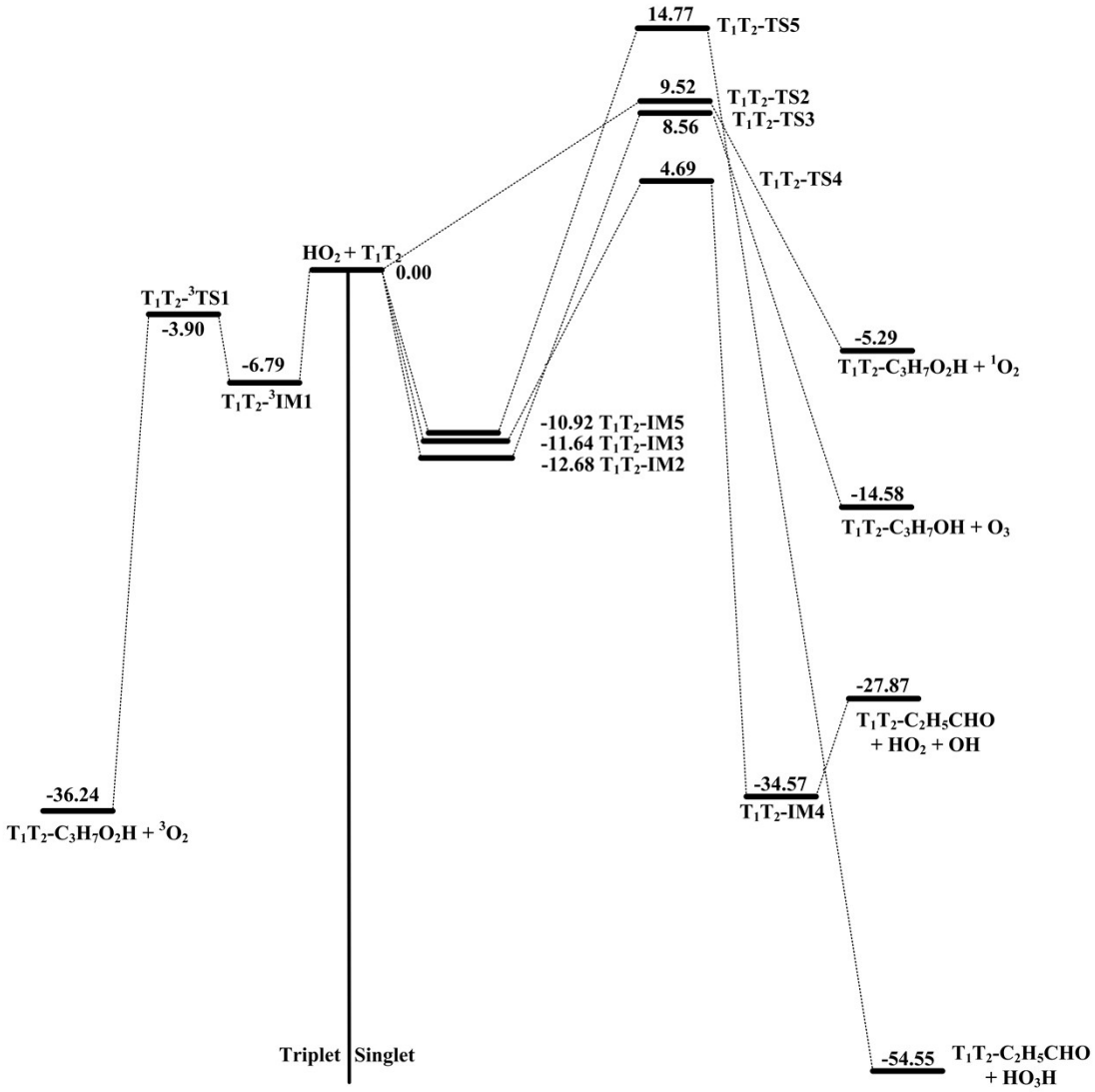

14.77
T1T2-TS5
9.52
T1T2-TS2
8.56
T1T2-TS3
4.69
T1T2-TS4
HO2 + T1T2
0.00
T1T2-3TS1
-3.90
-6.79
T1T2-3IM1
-10.92 T1T2-IM5
-11.64 T1T2-IM3
-12.68 T1T2-IM2
-5.29
T1T2-C3H7O2H + 1O2
-14.58
T1T2-C3H7OH + O3
-27.87
T1T2-C2H5CHO
+ HO2 + OH
-34.57
T1T2-IM4
-36.24
T1T2-C3H7O2H + 3O2
Triplet
Singlet
-54.55
T1T2-C2H5CHO
+ HO3H

Fig. S6.

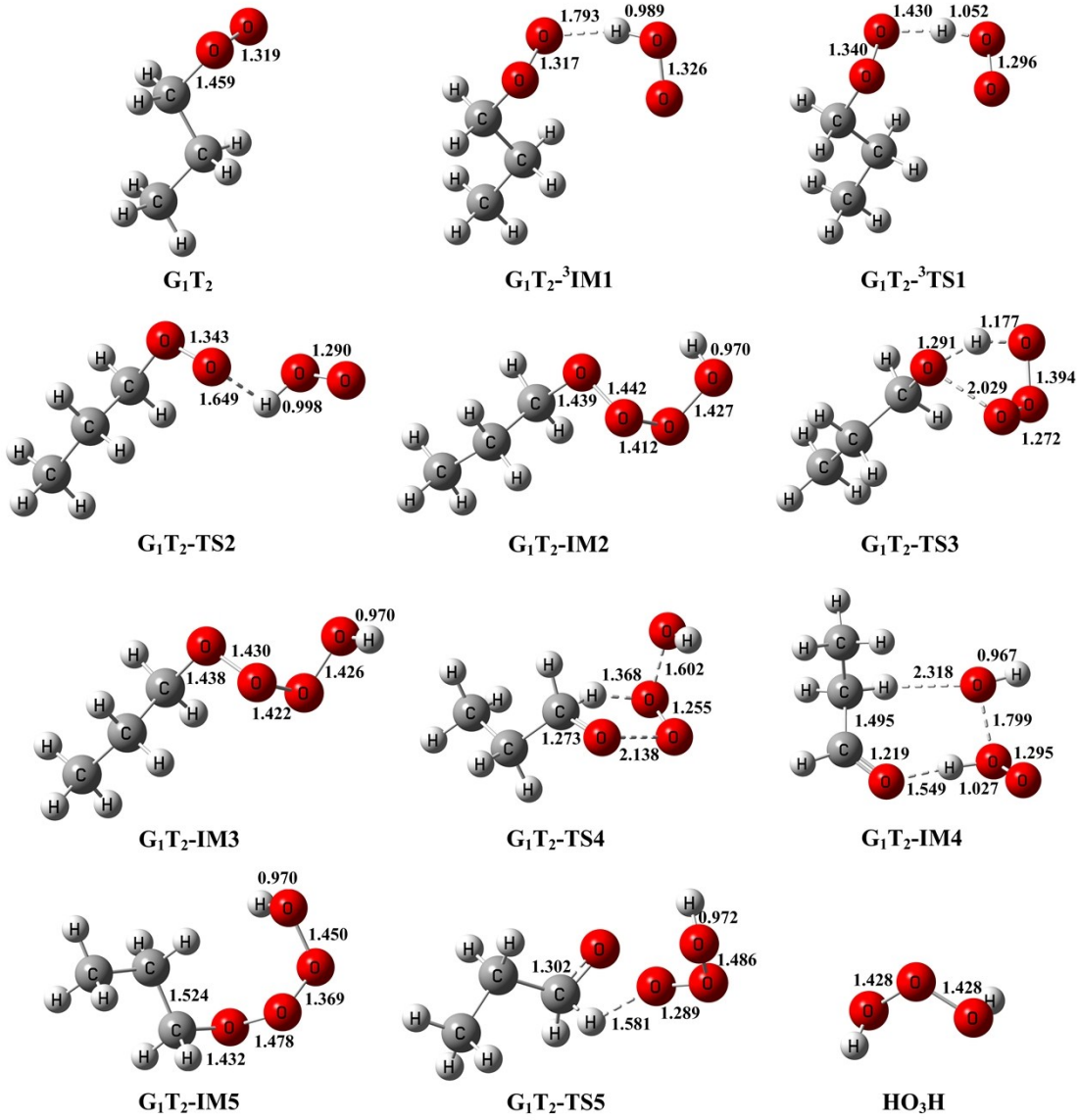
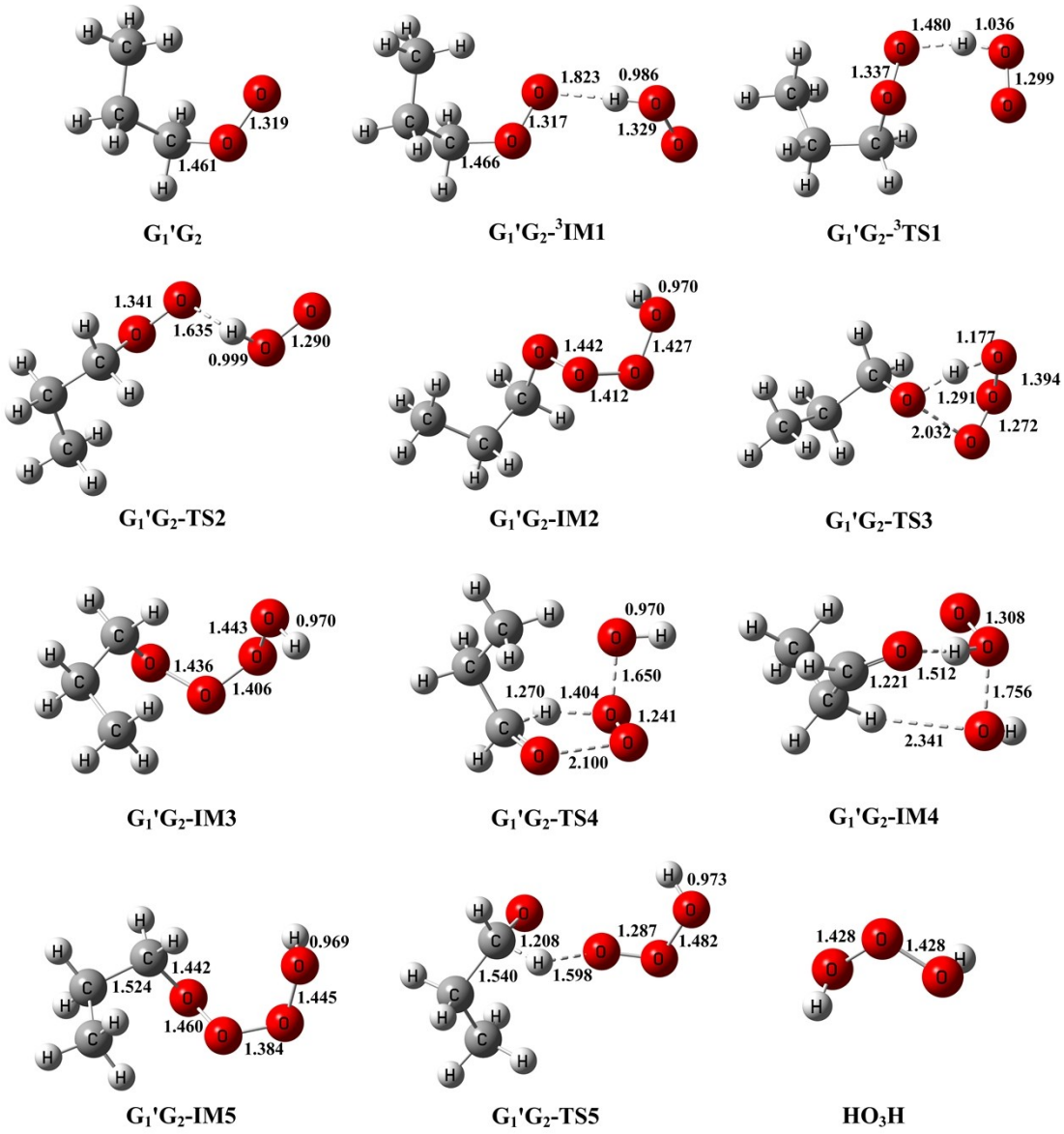

1.319
1.459
G1T2
1.793
0.989
1.317
1.326
G1T2-3IM1
1.430
1.052
1.340
1.296
G1T2-3TS1
1.343
1.290
1.649
0.998
G1T2-TS2
0.970
1.442
1.439
1.427
1.412
G1T2-IM2
1.177
1.291
1.394
2.029
1.272
G1T2-TS3
0.970
1.430
1.438
1.426
1.422
G1T2-IM3
1.602
1.368
1.255
1.273
2.138
G1T2-TS4
0.967
2.318
1.799
1.495
1.219
1.295
1.549
1.027
G1T2-IM4
0.970
1.450
1.524
1.369
1.478
1.432
G1T2-IM5
0.972
1.486
1.302
1.289
1.581
G1T2-TS5
1.428
1.428
HO3H

Fig. S7.



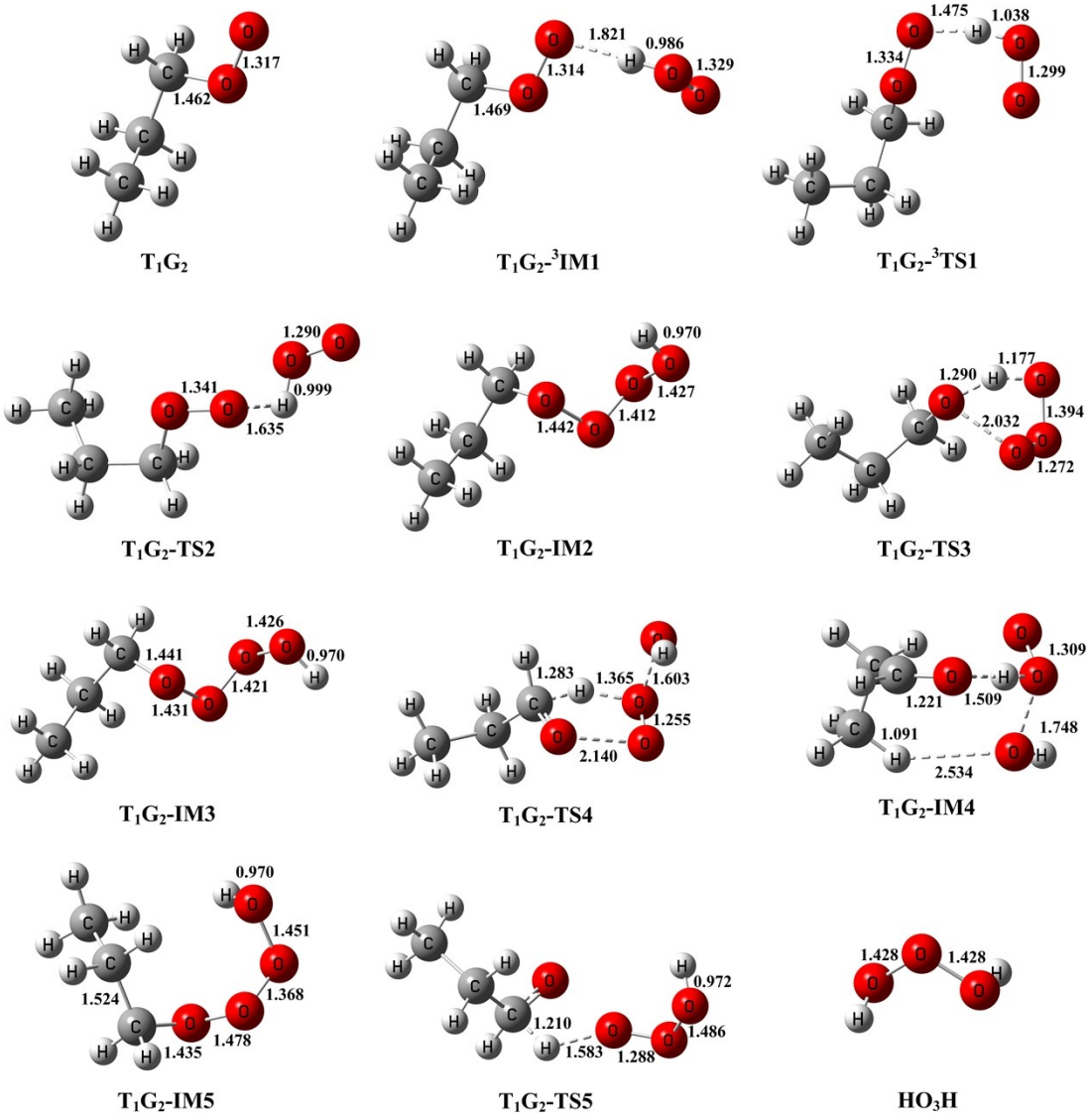
$G_1'G_2$ $G_1'G_2$-^{3}IM1 $G_1'G_2$-^{3}TS1

$G_1'G_2$-TS2 $G_1'G_2$-IM2 $G_1'G_2$-TS3

$G_1'G_2$-IM3 $G_1'G_2$-TS4 $G_1'G_2$-IM4

$G_1'G_2$-IM5 $G_1'G_2$-TS5 HO_3H

Fig. S8.



T_1G_2 T_1G_2-^{3}IM1 T_1G_2-^{3}TS1

T_1G_2-TS2 T_1G_2-IM2 T_1G_2-TS3

T_1G_2-IM3 T_1G_2-TS4 T_1G_2-IM4

T_1G_2-IM5 T_1G_2-TS5 HO_3H

Fig. S9.

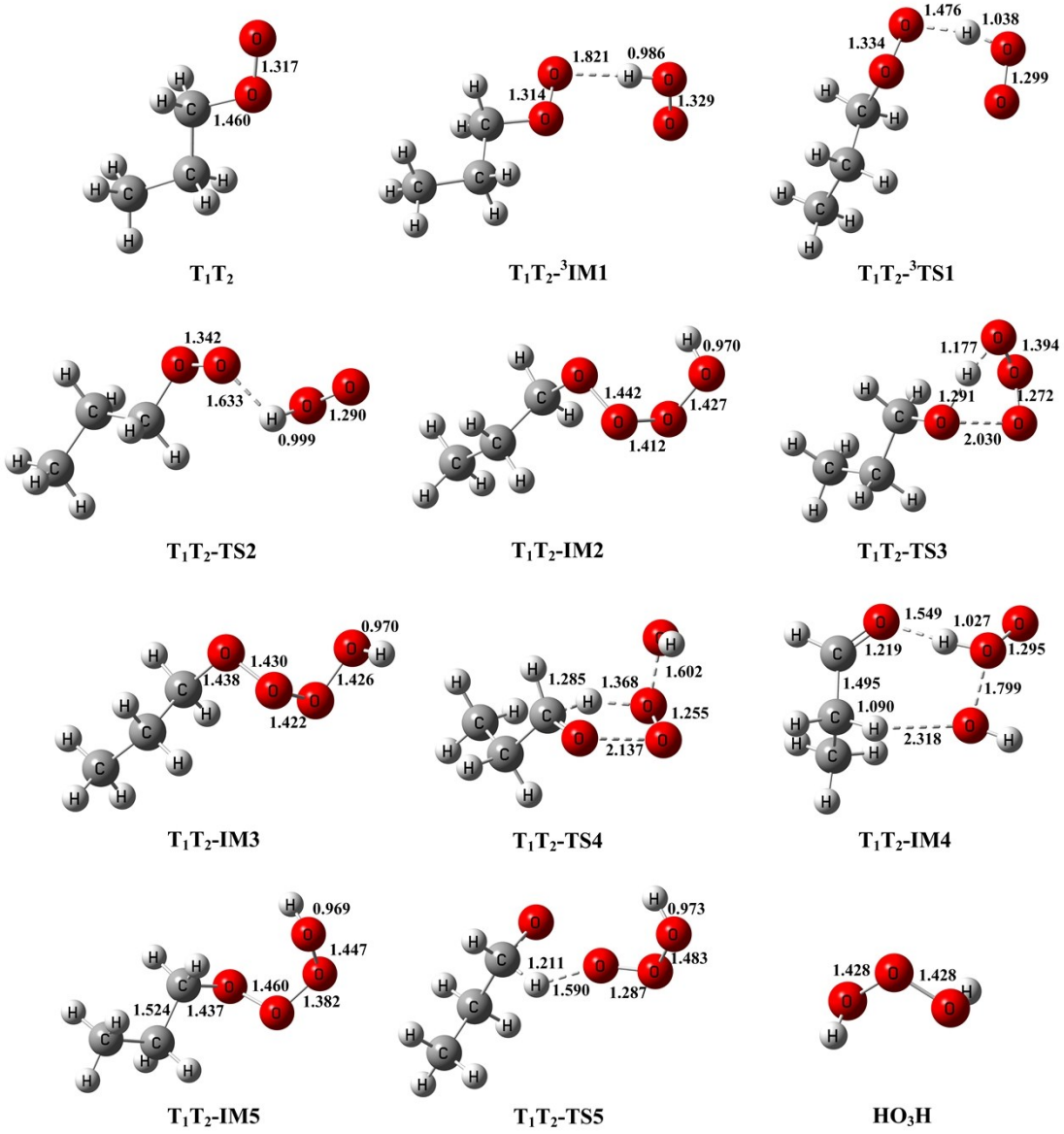

1.317
1.460
T1T2
1.821
0.986
1.314
1.329
T1T2-3IM1
1.476
1.038
1.334
1.299
T1T2-3TS1
1.342
1.633
1.290
0.999
T1T2-TS2
0.970
1.442
1.427
1.412
T1T2-IM2
1.177
1.394
1.291
1.272
2.030
T1T2-TS3
0.970
1.430
1.438
1.426
1.422
T1T2-IM3
1.285
1.368
1.602
1.255
2.137
T1T2-TS4
1.549
1.027
1.219
1.295
1.495
1.799
1.090
2.318
T1T2-IM4
0.969
1.447
1.460
1.524
1.437
1.382
T1T2-IM5
0.973
1.211
1.483
1.590
1.287
T1T2-TS5
1.428
1.428
HO3H

Table S1. Vibrational frequencies of all stationary points involved in the HO_2 + n-$C_3H_7O_2$ reaction at the B3LYP/6-311G(d,p) level of theory.

Species	Frequencies/cm^{-1}
G_1G_2	82, 145, 225, 293, 427, 549, 758, 854, 881, 940, 1046, 1106, 1148, 1188, 1286, 1299, 1374, 1387, 1421, 1479, 1483, 1503, 1509, 3031, 3032, 3059, 3072, 3096, 3108, 3120
HO_2	1163, 1428, 3613
G_1G_2-^{3}IM1	41, 49, 65, 86, 146, 158, 221, 243, 295, 432, 551, 630, 761, 851, 879, 938, 1042, 1109, 1157, 1190, 1196, 1290, 1296, 1374, 1386, 1429, 1478, 1481, 1504, 1515, 1530, 3030, 3032, 3064, 3073, 3096, 3111, 3129, 3368
G_1G_2-^{3}TS1	629i, 36, 67, 82, 110, 155, 224, 287, 334, 434, 539, 760, 775, 859, 878, 941, 963, 1044, 1111, 1168, 1237, 1288, 1304, 1373, 1382, 1424, 1476, 1482, 1503, 1514, 1638, 1648, 3030, 3031, 3059, 3070, 3094, 3118, 3122
G_1G_2-$C_3H_7O_2H$	85, 171, 174, 223, 284, 423, 535, 765, 856, 868, 923, 979, 1061, 1111, 1173, 1281, 1303, 1367, 1378, 1394, 1417, 1469, 1487, 1500, 1508, 3019, 3026, 3031, 3058, 3073, 3090, 3098, 3783
$^3O_2$	1641
G_1G_2-TS2	430i, 39, 67, 82, 106, 185, 199, 244, 300, 428, 497, 557, 764, 857, 886, 943, 1033, 1053, 1109, 1176, 1238, 1285, 1299, 1374, 1386, 1421, 1463, 1481, 1482, 1503, 1508, 3027, 3031, 3039, 3067, 3094, 3103, 3109, 3213
$^1O_2$	1627
G_1G_2-IM2	57, 71, 122, 149, 210, 238, 328, 381, 421, 563, 614, 624, 775, 857, 912, 920, 930, 994, 1045, 1150, 1189, 1263, 1317, 1338, 1406, 1411, 1420, 1498, 1503, 1510, 1526, 3022, 3028, 3038, 3058, 3077, 3097, 3100, 3725
G_1G_2-TS3	1451i, 59, 96, 133, 201, 238, 250, 327, 474, 523, 619, 756, 771, 889, 901, 910, 1025, 1034, 1100, 1143, 1184, 1271, 1315, 1328, 1373, 1383, 1415, 1481, 1496, 1500, 1510, 1853, 2901, 3027, 3032, 3041, 3071, 3095, 3098
G_1G_2-C_3H_7OH	135, 229, 265, 328, 458, 768, 889, 895, 1028, 1069, 1099, 1145, 1250, 1318, 1336, 1395, 1414, 1431, 1492, 1503, 1506, 1520, 2967, 3002, 3023, 3049, 3069, 3085, 3093, 3825
O_3	747, 1191, 1249
G_1G_2-IM3	57, 75, 107, 147, 227, 261, 329, 360, 434, 582, 595, 619, 760, 847, 888, 893, 918, 995, 1038, 1128, 1191, 1285, 1322, 1336, 1403, 1407, 1417, 1471, 1495, 1502, 1512, 3022, 3027, 3046, 3065, 3074, 3097, 3100, 3725
G_1G_2-TS4	764i, 77, 103, 130, 136, 209, 242, 334, 374, 420, 496, 551,

	618, 760, 782, 878, 961, 1034, 1107, 1119, 1181, 1230, 1280, 1296, 1317, 1353, 1418, 1456, 1472, 1503, 1509, 1625, 2849, 3022, 3026, 3079, 3099, 3101, 3759
G_1G_2-IM4	43, 84, 101, 132, 186, 198, 210, 245, 329, 346, 376, 526, 547, 819, 894, 936, 997, 1014, 1128, 1133, 1182, 1282, 1323, 1334, 1407, 1431, 1492, 1504, 1517, 1558, 1747, 2580, 2959, 3024, 3034, 3088, 3104, 3128, 3790
G_1G_2-C_2H_5CHO	78, 211, 327, 508, 760, 874, 920, 1010, 1132, 1156, 1273, 1326, 1413, 1425, 1468, 1502, 1507, 1819, 2838, 3010, 3031, 3082, 3101, 3105
OH	3705
G_1G_2-IM5	67, 82, 150, 184, 226, 265, 346, 402, 462, 519, 576, 642, 770, 809, 864, 896, 953, 973, 1059, 1110, 1175, 1289, 1311, 1363, 1382, 1397, 1417, 1469, 1487, 1499, 1510, 3024, 3027, 3035, 3068, 3076, 3091, 3098, 3738
G_1G_2-TS5	580i, 21, 39, 60, 88, 177, 221, 224, 243, 354, 483, 512, 726, 741, 780, 870, 913, 1001, 1044, 1109, 1143, 1160, 1255, 1294, 1329, 1379, 1398, 1405, 1479, 1497, 1506, 1755, 2876, 3026, 3030, 3070, 3093, 3103, 3688
HO_3H	378, 434, 537, 791, 935, 1391, 1395, 3722, 3728
G_1T_2	104, 110, 234, 264, 369, 559, 768, 871, 899, 937, 1040, 1123, 1152, 1202, 1282, 1323, 1327, 1398, 1420, 1481, 1498, 1503, 1513, 3027, 3039, 3058, 3071, 3092, 3100, 3119
G_1T_2-^{3}IM1	29, 41, 66, 94, 107, 161, 220, 233, 270, 379, 551, 618, 765, 869, 900, 928, 1039, 1120, 1158, 1187, 1206, 1283, 1324, 1329, 1396, 1419, 1478, 1497, 1503, 1512, 1526, 3028, 3049, 3065, 3075, 3096, 3103, 3129, 3343
G_1T_2-^{3}TS1	423i, 60, 65, 79, 102, 136, 233, 264, 331, 363, 558, 768, 801, 873, 896, 938, 990, 1038, 1122, 1189, 1239, 1280, 1322, 1329, 1395, 1419, 1478, 1499, 1503, 1514, 1622, 1884, 3027, 3048, 3058, 3076, 3096, 3102, 3121
G_1T_2-$C_3H_7O_2H$	98, 153, 206, 236, 275, 362, 538, 766, 858, 893, 915, 1020, 1045, 1127, 1191, 1280, 1320, 1330, 1367, 1409, 1419, 1472, 1499, 1504, 1513, 3014, 3023, 3030, 3056, 3072, 3091, 3094, 3782
G_1T_2-TS2	427i, 46, 69, 84, 110, 165, 202, 236, 281, 376, 495, 565, 765, 877, 896, 945, 1036, 1047, 1122, 1192, 1238, 1280, 1320, 1328, 1394, 1417, 1463, 1482, 1497, 1502, 1513, 3024, 3028, 3043, 3069, 3088, 3100, 3107, 3218
G_1T_2-IM2	57, 88, 89, 168, 229, 262, 296, 384, 493, 569, 603, 627, 763, 836, 889, 897, 925, 988, 1040, 1131, 1194, 1283, 1322, 1332, 1406, 1408, 1418, 1481, 1497, 1503, 1512, 3023, 3029, 3041, 3064, 3076, 3097, 3098, 3724
G_1T_2-TS3	1474i, 57, 79, 115, 207, 234, 287, 311, 414, 537, 647, 748,

	761, 872, 896, 913, 1027, 1058, 1123, 1133, 1151, 1259, 1310, 1323, 1357, 1413, 1420, 1451, 1494, 1502, 1510, 1854, 2888, 2925, 3024, 3035, 3064, 3088, 3098
G_1T_2-C_3H_7OH	127, 235, 274, 275, 457, 774, 889, 906, 1035, 1063, 1099, 1186, 1265, 1270, 1323, 1354, 1416, 1463, 1496, 1503, 1510, 1529, 2956, 2981, 3021, 3031, 3059, 3085, 3093, 3842
G_1T_2-IM3	53, 88, 91, 176, 229, 262, 296, 377, 466, 560, 613, 626, 765, 846, 889, 896, 914, 990, 1040, 1130, 1195, 1283, 1322, 1332, 1403, 1407, 1419, 1483, 1498, 1503, 1513, 3024, 3033, 3041, 3063, 3079, 3096, 3097, 3725
G_1T_2-TS4	797i, 67, 78, 117, 158, 197, 227, 314, 360, 422, 494, 552, 620, 741, 779, 877, 966, 1031, 1115, 1143, 1168, 1232, 1284, 1317, 1346, 1349, 1421, 1459, 1476, 1503, 1504, 1618, 2857, 3022, 3026, 3065, 3088, 3100, 3699
G_1T_2-IM4	17, 58, 108, 136, 154, 182, 196, 228, 330, 336, 363, 521, 536, 810, 893, 931, 946, 997, 1131, 1163, 1179, 1253, 1284, 1334, 1408, 1433, 1477, 1499, 1511, 1552, 1761, 2752, 2944, 3027, 3036, 3101, 3121, 3130, 3803
G_1T_2-C_2H_5CHO	78, 211, 327, 508, 760, 874, 920, 1010, 1132, 1156, 1273, 1326, 1413, 1425, 1468, 1502, 1507, 1819, 2838, 3010, 3031, 3082, 3101, 3105
G_1T_2-IM5	64, 98, 102, 174, 234, 264, 317, 371, 458, 530, 585, 647, 761, 814, 886, 896, 955, 1006, 1042, 1129, 1194, 1286, 1322, 1335, 1369, 1407, 1420, 1471, 1499, 1504, 1515, 3020, 3024, 3029, 3064, 3075, 3097, 3099, 3738
G_1T_2-TS5	458i, 56, 75, 103, 149, 166, 237, 307, 329, 483, 557, 648, 678, 734, 788, 867, 930, 1031, 1073, 1090, 1118, 1240, 1275, 1292, 1331, 1350, 1409, 1422, 1480, 1503, 1505, 1899, 2879, 3025, 3027, 3067, 3089, 3097, 3722
$G_1'G_2$	79, 120, 227, 312, 429, 519, 768, 837, 904, 928, 1051, 1100, 1150, 1190, 1288, 1299, 1376, 1385, 1424, 1473, 1478, 1502, 1506, 3022, 3034, 3052, 3063, 3095, 3109, 3122
$G_1'G_2$-^{3}IM1	18, 23, 50, 62, 92, 136, 215, 227, 310, 440, 518, 627, 767, 835, 898, 928, 1048, 1100, 1159, 1190, 1198, 1291, 1301, 1376, 1385, 1425, 1474, 1478, 1501, 1506, 1523, 3028, 3036, 3059, 3073, 3100, 3108, 3135, 3427
$G_1'G_2$-^{3}TS1	210i, 29, 54, 90, 119, 142, 228, 294, 325, 427, 518, 752, 769, 837, 903, 928, 1030, 1050, 1104, 1174, 1232, 1289, 1300, 1374, 1382, 1424, 1472, 1477, 1500, 1506, 1595, 2221, 3024, 3034, 3055, 3072, 3096, 3110, 3132
$G_1'G_2$-$C_3H_7O_2H$	81, 150, 186, 242, 324, 391, 514, 770, 832, 882, 927, 982, 1076, 1116, 1168, 1292, 1313, 1361, 1380, 1403, 1423, 1460, 1476, 1501, 1509, 3006, 3014, 3028, 3049, 3065, 3085, 3121, 3777

$G_1'G_2$-TS2	436i, 29, 67, 85, 120, 177, 190, 213, 306, 382, 485, 532, 756, 885, 914, 935, 1058, 1065, 1133, 1160, 1244, 1253, 1307, 1374, 1399, 1423, 1465, 1479, 1491, 1504, 1510, 3015, 3031, 3033, 3064, 3078, 3095, 3111, 3195
$G_1'G_2$-IM2	60, 71, 115, 183, 221, 251, 353, 406, 499, 570, 601, 624, 770, 837, 863, 898, 929, 963, 1056, 1113, 1181, 1286, 1306, 1381, 1394, 1410, 1419, 1478, 1485, 1502, 1510, 3025, 3028, 3037, 3064, 3082, 3093, 3108, 3724
$G_1'G_2$-TS3	1475i, 45, 106, 137, 181, 228, 309, 332, 460, 524, 640, 753, 791, 868, 893, 913, 981, 1081, 1110, 1124, 1144, 1257, 1300, 1349, 1377, 1402, 1419, 1449, 1479, 1501, 1510, 1852, 2903, 2925, 3024, 3028, 3056, 3091, 3109
$G_1'G_2$-C_3H_7OH	150, 226, 249, 327, 478, 777, 864, 930, 985, 1063, 1117, 1160, 1251, 1272, 1327, 1383, 1411, 1455, 1479, 1496, 1513, 1524, 2960, 2989, 3024, 3025, 3055, 3085, 3111, 3844
$G_1'G_2$-IM3	25, 91, 114, 163, 236, 307, 349, 390, 435, 531, 604, 612, 775, 820, 843, 910, 929, 954, 1067, 1111, 1170, 1294, 1310, 1373, 1380, 1399, 1421, 1474, 1477, 1501, 1507, 3014, 3028, 3049, 3055, 3087, 3108, 3110, 3734
$G_1'G_2$-TS4	712i, 88, 109, 137, 147, 203, 250, 310, 375, 419, 542, 590, 641, 762, 804, 842, 954, 1025, 1093, 1111, 1177, 1238, 1283, 1300, 1324, 1347, 1417, 1459, 1478, 1496, 1515, 1654, 2857, 3002, 3044, 3054, 3108, 3127, 3757
$G_1'G_2$-IM4	47, 68, 92, 123, 176, 209, 222, 241, 331, 341, 379, 526, 549, 817, 892, 933, 996, 1005, 1128, 1131, 1180, 1276, 1320, 1340, 1403, 1432, 1492, 1506, 1514, 1551, 1750, 2598, 2956, 3032, 3035, 3098, 3111, 3128, 3790
$G_1'G_2$-C_2H_5CHO	78, 211, 327, 508, 760, 874, 920, 1010, 1132, 1156, 1273, 1326, 1413, 1425, 1468, 1502, 1507, 1819, 2838, 3010, 3031, 3082, 3101, 3105
$G_1'G_2$-IM5	47, 80, 108, 156, 235, 294, 358, 396, 440, 511, 600, 644, 781, 828, 844, 913, 943, 961, 1067, 1112, 1170, 1292, 1307, 1376, 1379, 1396, 1423, 1464, 1477, 1501, 1508, 3015, 3031, 3035, 3053, 3088, 3094, 3108, 3740
$G_1'G_2$-TS5	-393, 53, 91, 118, 134, 154, 227, 286, 357, 546, 553, 615, 713, 759, 805, 832, 924, 1014, 1075, 1080, 1112, 1244, 1266, 1294, 1336, 1382, 1400, 1428, 1484, 1494, 1510, 1920, 2880, 3014, 3036, 3054, 3097, 3116, 3707
T_1G_2	61, 133, 198, 298, 381, 519, 750, 879, 905, 923, 1059, 1121, 1155, 1196, 1249, 1306, 1373, 1397, 1420, 1478, 1491, 1504, 1510, 3031, 3033, 3049, 3064, 3095, 3107, 3110
T_1G_2-^{3}IM1	16, 32, 40, 60, 110, 142, 201, 219, 300, 391, 525, 626, 751, 877, 898, 922, 1055, 1119, 1157, 1190, 1215, 1250, 1307, 1374, 1399, 1423, 1479, 1488, 1504, 1510, 1525, 3033, 3036,

	3056, 3068, 3098, 3110, 3117, 3426
T_1G_2-^{3}TS1	240i, 35, 58, 89, 117, 170, 195, 289, 327, 377, 513, 751, 757, 882, 901, 924, 1045, 1063, 1126, 1157, 1241, 1251, 1306, 1372, 1399, 1421, 1481, 1485, 1503, 1510, 1600, 2185, 3032, 3035, 3050, 3070, 3096, 3109, 3113
T_1G_2-$C_3H_7O_2H$	95, 127, 177, 198, 295, 363, 505, 761, 885, 919, 933, 983, 1066, 1143, 1176, 1254, 1307, 1363, 1375, 1399, 1419, 1480, 1497, 1510, 1525, 2995, 3025, 3030, 3041, 3060, 3090, 3113, 3772
T_1G_2-TS2	431i, 27, 69, 88, 122, 178, 192, 216, 305, 382, 486, 532, 755, 886, 912, 935, 1057, 1064, 1133, 1159, 1243, 1253, 1307, 1374, 1400, 1421, 1465, 1478, 1492, 1503, 1510, 3015, 3031, 3033, 3064, 3078, 3095, 3111, 3196
T_1G_2-IM2	60, 71, 115, 183, 221, 251, 353, 406, 499, 570, 601, 624, 770, 837, 863, 898, 929, 963, 1056, 1113, 1181, 1286, 1306, 1381, 1394, 1410, 1419, 1478, 1485, 1502, 1510, 3025, 3028, 3037, 3064, 3082, 3093, 3108, 3724
T_1G_2-TS3	1476i, 43, 103, 136, 181, 226, 310, 330, 458, 524, 640, 753, 790, 867, 891, 913, 980, 1081, 1109, 1124, 1144, 1256, 1299, 1348, 1377, 1401, 1417, 1449, 1479, 1500, 1510, 1852, 2903, 2925, 3023, 3027, 3056, 3090, 3108
T_1G_2-C_3H_7OH	150, 226, 249, 327, 478, 777, 864, 930, 985, 1063, 1117, 1160, 1251, 1272, 1327, 1383, 1411, 1455, 1479, 1496, 1513, 1524, 2960, 2989, 3024, 3025, 3055, 3085, 3111, 3844
T_1G_2-IM3	55, 67, 112, 186, 221, 253, 357, 385, 480, 557, 615, 623, 768, 846, 864, 896, 919, 964, 1055, 1112, 1181, 1286, 1305, 1379, 1393, 1403, 1418, 1480, 1484, 1502, 1509, 3025, 3028, 3042, 3064, 3087, 3093, 3106, 3725
T_1G_2-TS4	788i, 58, 82, 119, 164, 194, 239, 277, 364, 427, 497, 582, 620, 762, 794, 875, 970, 1022, 1111, 1128, 1168, 1232, 1290, 1309, 1344, 1365, 1405, 1457, 1478, 1497, 1506, 1623, 2864, 3029, 3031, 3073, 3095, 3108, 3699
T_1G_2-IM4	43, 84, 101, 132, 187, 198, 210, 245, 329, 346, 376, 526, 547, 819, 894, 936, 997, 1014, 1128, 1133, 1182, 1282, 1323, 1334, 1407, 1431, 1492, 1504, 1517, 1557, 1747, 2580, 2959, 3024, 3034, 3088, 3104, 3128, 3790
T_1G_2-C_2H_5CHO	78, 211, 327, 508, 760, 874, 920, 1010, 1132, 1156, 1273, 1326, 1413, 1425, 1468, 1502, 1507, 1819, 2838, 3010, 3031, 3082, 3101, 3105
T_1G_2-IM5	66, 82, 150, 184, 226, 265, 345, 402, 462, 519, 576, 642, 770, 809, 864, 896, 953, 973, 1059, 1110, 1175, 1289, 1311, 1362, 1382, 1397, 1417, 1469, 1487, 1499, 1510, 3024, 3027, 3036, 3068, 3076, 3091, 3098, 3738
T_1G_2-TS5	444i, 47, 87, 93, 148, 165, 237, 262, 376, 493, 559, 642, 697,

	762, 787, 871, 905, 1014, 1077, 1087, 1112, 1241, 1264, 1288, 1353, 1355, 1403, 1415, 1478, 1496, 1505, 1912, 2882, 3027, 3031, 3070, 3092, 3104, 3720
T_1T_2	62, 109, 200, 233, 397, 493, 764, 889, 922, 943, 1044, 1148, 1160, 1191, 1254, 1317, 1330, 1406, 1420, 1495, 1499, 1503, 1515, 3029, 3038, 3049, 3065, 3090, 3103, 3107
T_1T_2-^{3}IM1	15, 23, 43, 59, 97, 121, 184, 235, 238, 397, 501, 632, 764, 888, 922, 929, 1042, 1149, 1160, 1190, 1212, 1255, 1321, 1333, 1407, 1421, 1493, 1498, 1504, 1515, 1523, 3030, 3041, 3057, 3070, 3093, 3107, 3117, 3426
T_1T_2-^{3}TS1	239i, 32, 48, 85, 109, 162, 204, 238, 304, 404, 486, 755, 766, 890, 921, 938, 1035, 1057, 1150, 1163, 1240, 1257, 1320, 1332, 1407, 1421, 1490, 1499, 1504, 1515, 1600, 2187, 3029, 3040, 3049, 3071, 3092, 3104, 3113
T_1T_2-$C_3H_7O_2H$	106, 114, 182, 193, 233, 402, 454, 775, 910, 911, 927, 1024, 1049, 1152, 1189, 1257, 1313, 1333, 1366, 1412, 1419, 1498, 1502, 1511, 1531, 2992, 3026, 3033, 3038, 3067, 3092, 3097, 3773
T_1T_2-TS2	439i, 39, 56, 81, 106, 164, 196, 227, 237, 406, 471, 516, 769, 898, 921, 959, 1042, 1064, 1150, 1172, 1243, 1257, 1319, 1334, 1408, 1421, 1464, 1495, 1499, 1503, 1515, 3013, 3028, 3042, 3062, 3077, 3098, 3103, 3196
T_1T_2-IM2	57, 88, 89, 168, 229, 262, 296, 384, 493, 569, 603, 627, 763, 836, 889, 897, 925, 988, 1040, 1131, 1194, 1283, 1322, 1332, 1406, 1408, 1418, 1481, 1497, 1503, 1512, 3023, 3029, 3041, 3064, 3076, 3097, 3098, 3724
T_1T_2-TS3	-1477, 60, 79, 117, 207, 237, 289, 312, 414, 538, 647, 749, 761, 872, 897, 913, 1027, 1059, 1123, 1133, 1152, 1259, 1309, 1325, 1358, 1414, 1421, 1453, 1493, 1503, 1510, 1851, 2890, 2926, 3024, 3035, 3063, 3088, 3098
T_1T_2-C_3H_7OH	127, 235, 274, 275, 457, 774, 889, 906, 1035, 1063, 1099, 1186, 1265, 1270, 1323, 1354, 1416, 1463, 1496, 1503, 1510, 1529, 2956, 2981, 3021, 3031, 3059, 3085, 3093, 3842
T_1T_2-IM3	53, 88, 91, 176, 229, 262, 296, 377, 466, 560, 613, 626, 765, 846, 889, 896, 914, 990, 1040, 1130, 1195, 1283, 1322, 1332, 1403, 1407, 1419, 1483, 1498, 1503, 1513, 3024, 3033, 3041, 3063, 3079, 3096, 3097, 3725
T_1T_2-TS4	-798, 67, 78, 117, 158, 197, 227, 314, 360, 422, 494, 552, 620, 741, 779, 877, 966, 1031, 1115, 1143, 1168, 1232, 1284, 1317, 1346, 1349, 1421, 1459, 1476, 1503, 1504, 1618, 2857, 3022, 3026, 3065, 3088, 3100, 3699
T_1T_2-IM4	17, 58, 108, 136, 154, 182, 196, 228, 330, 336, 363, 521, 536, 810, 893, 931, 946, 997, 1131, 1163, 1179, 1253, 1284, 1334, 1408, 1433, 1477, 1499, 1511, 1553, 1761, 2752, 2944, 3027,

	3036, 3101, 3121, 3130, 3803
T_1T_2-C_2H_5CHO	78, 211, 327, 508, 760, 874, 920, 1010, 1132, 1156, 1273, 1326, 1413, 1425, 1468, 1502, 1507, 1819, 2838, 3010, 3031, 3082, 3101, 3105
T_1T_2-IM5	52, 89, 104, 154, 235, 275, 345, 353, 438, 533, 611, 650, 762, 829, 884, 897, 940, 998, 1041, 1130, 1194, 1285, 1321, 1338, 1374, 1408, 1419, 1474, 1497, 1504, 1512, 3023, 3028, 3039, 3062, 3077, 3096, 3098, 3742
T_1T_2-TS5	-422, 68, 74, 127, 134, 140, 221, 298, 342, 485, 552, 630, 677, 747, 786, 866, 929, 1029, 1074, 1089, 1116, 1245, 1270, 1291, 1330, 1381, 1409, 1421, 1481, 1501, 1504, 1897, 2865, 3023, 3028, 3068, 3089, 3097, 3707

Table S2. Coordinates of all stationary points involved in the HO_2 + n-$C_3H_7O_2$ reaction at the B3LYP/6-311G(d,p) level of theory.

$HO_2 + G_1G_2$

G_1G_2				HO_2			
12				3			
C	-3.573646	0.153506	1.746746	O	0.055292	-0.609759	0.000000
H	-3.181666	-0.864592	1.795791	H	-0.884676	-0.869854	0.000000
H	-3.334452	0.651050	2.691463	O	0.055292	0.718490	0.000000
H	-4.661328	0.090312	1.669294				
C	-2.985877	0.912028	0.554155				
H	-3.269623	0.430950	-0.386102				
H	-3.383681	1.932262	0.518283				
C	-1.468805	1.016882	0.583491				
H	-1.096534	1.420565	1.527587				
H	-1.080317	1.601320	-0.252032				
O	-0.837760	-0.301238	0.509474				
O	-0.976888	-0.834677	-0.688246				

G_1G_2-^{3}IM1				G_1G_2-^{3}TS1			
15				15			
O	2.817365	-0.075156	0.082881	O	0.468865	0.170456	1.924125
H	2.030932	-0.655218	0.235047	H	-0.174117	0.832559	1.393883
O	2.322001	1.135741	-0.13727	O	1.573818	0.805317	2.139933
C	-1.529593	1.671426	-0.09056	C	0.943157	3.996698	3.405928
H	-0.445405	1.679145	-0.221128	H	1.543035	3.209964	2.945842
H	-1.992992	1.847474	-1.066179	H	1.383077	4.963552	3.142617
H	-1.795359	2.507687	0.559702	H	1.014521	3.882685	4.490055
C	-2.001322	0.348546	0.519373	C	-0.514578	3.913005	2.948184
H	-1.545318	0.194964	1.501664	H	-0.970552	2.969850	3.264316
H	-3.086115	0.358215	0.67413	H	-1.105294	4.712476	3.409456
C	-1.691139	-0.868258	-0.339854	C	-0.698424	4.041158	1.441608
H	-2.096253	-0.784903	-1.34995	H	-0.143294	4.885667	1.027464
H	-2.013134	-1.802561	0.122588	H	-1.750201	4.109507	1.159387
O	-0.248821	-0.989706	-0.579411	O	-0.146650	2.900149	0.718488
O	0.393952	-1.352764	0.510097	O	-0.957228	1.835807	0.827718

G_1G_2-$C_3H_7O_2H$	$^3O_2$

13

H	-1.615481	-1.480275	0.232227
C	1.871116	-0.605394	-0.277213
H	1.258971	-1.365808	-0.768402
H	2.354841	-0.016483	-1.062778
H	2.655125	-1.11638	0.287201
C	1.017877	0.281818	0.633337
H	0.600460	-0.30514	1.45688
H	1.638688	1.059791	1.092411
C	-0.132108	0.970316	-0.096025
H	0.230194	1.541683	-0.957774
H	-0.674233	1.651582	0.568511
O	-1.060946	0.066957	-0.69448
O	-1.812788	-0.548133	0.393371

G_1G_2-TS2

15

O	-1.487323	0.436184	-0.265289
H	-0.833898	0.527715	0.483585
O	-2.567815	-0.116960	0.171033
C	3.794517	-0.919347	1.351897
H	3.288098	-1.809228	0.972547
H	4.620996	-0.687674	0.673095
H	4.222354	-1.165151	2.326426
C	2.822727	0.257119	1.466306
H	2.027838	0.027532	2.181825
H	3.341017	1.146095	1.843037
C	2.171426	0.637949	0.141926
H	2.909585	0.824158	-0.641686
H	1.527735	1.517273	0.243811
O	1.374673	-0.442775	-0.405693
O	0.276889	-0.679609	0.331976

G_1G_2-IM2

15

O	1.359107	-0.921638	-0.21037
O	2.876656	0.794908	-0.024271
O	2.032075	-0.089695	0.711771
H	2.247305	1.485646	-0.285311
O	0.235101	-0.180716	-0.716232
C	-0.879733	-0.382556	0.170683

2

O	0.000000	0.000000	0.602813
O	0.000000	0.000000	-0.602813

$^1O_2$

2

O	0.000000	0.000000	0.603294
O	0.000000	0.000000	-0.603294

G_1G_2-TS3

15

O	0.927772	1.754604	0.045428
O	2.804843	1.428502	-0.957615
O	1.808734	2.356309	-0.646755
H	2.007840	0.579835	-1.099739
O	0.776314	0.180762	-1.216635
C	0.319331	0.655001	-2.451260

C	-2.057807	0.367341	-0.435785
H	-0.628579	0.006028	1.163029
H	-1.084635	-1.455175	0.245546
C	-3.324634	0.214534	0.41228
H	-1.794190	1.425127	-0.532135
H	-2.231911	-0.010596	-1.447482
H	-4.157610	0.760692	-0.035634
H	-3.623010	-0.834208	0.497774
H	-3.177839	0.603703	1.42396

G_1G_2-C_3H_7OH

12

H	-2.022309	-0.699266	0.647923
O	-1.909002	-0.093928	-0.091441
C	-0.619754	0.499887	0.029632
C	0.514801	-0.520595	-0.040160
H	-0.540863	1.085888	0.958080
H	-0.543418	1.203243	-0.804038
C	1.902801	0.123756	0.013622
H	0.405761	-1.229051	0.791695
H	0.398050	-1.101292	-0.960746
H	2.691825	-0.630844	-0.028264
H	2.054054	0.807443	-0.827221
H	2.041834	0.697019	0.935537

G_1G_2-IM3

15

O	1.548042	-0.677407	0.428385
H	-1.198701	1.320115	0.930428
O	2.628487	-0.713014	-0.499792
H	3.382822	-0.491649	0.068495
O	1.172661	0.680568	0.631799
C	-1.040808	0.911431	-0.073185
H	-1.563880	1.552747	-0.790439
O	0.334987	1.109103	-0.442468
C	-1.525074	-0.529967	-0.179678
C	-3.029867	-0.635349	0.089570
H	-0.973015	-1.151734	0.529189
H	-1.287747	-0.905439	-1.179532
H	-3.282612	-0.277895	1.092591
H	-3.608073	-0.045549	-0.628541

C	1.048440	-0.038675	-3.614956
H	0.520924	1.740607	-2.528229
H	-0.765822	0.515813	-2.509726
C	0.556496	0.464292	-4.975437
H	2.123135	0.142607	-3.512842
H	0.892807	-1.117325	-3.526817
H	1.075982	-0.050534	-5.786922
H	-0.515344	0.287044	-5.102449
H	0.735580	1.536949	-5.092897

O_3

3

O	0.000000	1.079161	-0.215286
O	0.000000	0.000000	0.430573
O	0.000000	-1.079161	-0.215286

G_1G_2-TS4

15

O	0.725357	0.250404	0.513370
H	-0.390042	-0.557908	0.646228
O	1.472959	-0.912059	-0.391375
H	2.258161	-0.387117	-0.613173
O	0.281860	1.188824	-0.168009
C	-1.590332	-0.668356	0.216629
H	-2.063412	-0.715096	1.223449
O	-1.677584	0.444561	-0.398395
C	-1.560039	-1.987204	-0.565590
C	-1.153173	-3.187789	0.289209
H	-0.881962	-1.858076	-1.411606
H	-2.566868	-2.131837	-0.975455
H	-0.118541	-3.093739	0.629479
H	-1.794857	-3.289291	1.170348

H	-3.367717	-1.671279	0.014172

G_1G_2-IM4

15

O	1.851029	-0.263561	0.004374
H	1.001594	-0.788392	-0.276449
O	1.326645	1.025084	-1.05358
H	2.051300	1.616459	-0.804342
O	1.736863	0.000695	1.281365
C	-1.349401	-1.080296	-0.23909
H	-2.265349	-1.540794	-0.652651
O	-0.275645	-1.508363	-0.631735
C	-1.537229	0.040528	0.730032
C	-1.927691	1.333875	-0.022155
H	-0.611712	0.189656	1.291626
H	-2.342981	-0.243024	1.416726
H	-1.091773	1.661694	-0.641031
H	-2.810393	1.190888	-0.651877
H	-2.155893	2.118022	0.701892

OH

2

O	0.000000	0.000000	0.108355
H	0.000000	0.000000	-0.866843

G_1G_2-TS5

15

H	-1.231574	-4.115947	-0.281125

G_1G_2-C_2H_5CHO

10

C	0.787530	-0.231106	0.301330
H	0.705925	-1.069045	1.033247
O	1.814662	-0.040622	-0.297063
C	-0.471917	0.589679	0.149223
C	-1.693261	-0.283084	-0.177680
H	-0.296251	1.348655	-0.616061
H	-0.639877	1.104643	1.104672
H	-1.577022	-0.776339	-1.145912
H	-1.843350	-1.058426	0.579361
H	-2.600839	0.322552	-0.216036

G_1G_2-IM5

15

O	1.279048	-0.869191	0.261679
H	-0.816990	-1.888599	0.971985
O	1.463886	1.427210	0.281517
H	0.905486	1.678744	-0.470548
O	2.022510	0.179981	-0.206937
C	-2.045322	1.067958	-0.449245
H	-1.248999	1.240646	-1.179466
H	-2.891999	0.641818	-0.995998
H	-2.356941	2.037384	-0.053386
C	-1.577032	0.133123	0.669263
H	-0.803967	0.616022	1.272057
H	-2.411208	-0.088686	1.344595
C	-1.029346	-1.192267	0.154853
H	-1.733828	-1.680825	-0.527229
O	0.143136	-1.064174	-0.662664

HO_3H

5

-1.570273	-0.539028	-0.752859	
-0.097858	-0.801471	-0.181102	
-2.125665	1.445946	0.243961	
-2.478995	0.721855	0.791679	
-1.773298	0.702912	-0.990666	
3.138472	0.577235	-0.034083	
3.342669	0.413688	1.026742	
3.678634	-0.184798	-0.604149	
3.541719	1.553433	-0.314271	
1.629718	0.510050	-0.302795	
1.110717	1.290516	0.261126	
1.424413	0.679965	-1.365171	
1.049737	-0.848607	0.106555	
1.377563	-1.687449	-0.542653	
1.006418	-1.138938	1.387865	
H	-0.491165	-0.128082	0.948518
O	0.388732	1.065781	-0.210108
O	0.680958	0.207379	-1.313341
H	0.103045	0.569595	-2.003008
O	-0.817005	0.599910	0.396550

$HO_2 + G_1T_2$

G_1T_2

12

C	2.296861	-0.105364	0.155926
H	2.663635	0.877913	-0.153241
H	2.346038	-0.152007	1.247675
H	2.987220	-0.853913	-0.238530
C	0.874456	-0.360044	-0.350860
H	0.850361	-0.334386	-1.444712
H	0.531234	-1.351232	-0.042907
C	-0.110888	0.666700	0.186110
H	0.111746	1.677344	-0.162876
H	-0.164902	0.653893	1.276772
O	-1.458908	0.419274	-0.315238
O	-2.002080	-0.634945	0.261583

G_1T_2-^{3}IM1

15

O	-2.345560	-0.653950	-1.607024
H	-2.144353	-0.263403	-0.720509
O	-1.164923	-0.963215	-2.125722
C	2.983593	-0.434443	1.245425
H	3.633825	0.409425	0.996796
H	2.886798	-0.474442	2.334305
H	3.489964	-1.346833	0.924163
C	1.617698	-0.312953	0.563699
H	1.728250	-0.294795	-0.523892
H	0.989847	-1.174519	0.805723
C	0.884042	0.946525	1.001549
H	1.418853	1.858129	0.728619
H	0.650746	0.949228	2.067916
O	-0.384557	1.072010	0.284886
O	-1.297333	0.256820	0.771796

G_1T_2-^{3}TS1

15

O	-0.433317	0.379398	0.352488
H	-0.360431	0.912426	1.256389
O	0.530835	0.798166	-0.404922
C	4.242444	0.764679	2.786512

G_1T_2-$C_3H_7O_2H$

13

H	-2.141230	-1.154710	-0.466835
C	2.339354	-0.148864	0.15465
H	2.732776	0.828252	-0.142459
H	2.383288	-0.206041	1.2465

H	4.940727	1.558879	2.506329
H	4.170716	0.750827	3.878006
H	4.679859	-0.184903	2.471269
C	2.871215	0.965579	2.135239
H	2.954426	0.953244	1.045660
H	2.194941	0.154517	2.417690
C	2.237934	2.283231	2.561157
H	2.820448	3.147030	2.234533
H	2.076816	2.331679	3.640898
O	0.945649	2.502873	1.927134
O	0.021285	1.662483	2.412451
H	3.013726	-0.910806	-0.243091
C	0.910478	-0.355577	-0.356394
H	0.889952	-0.316846	-1.450982
H	0.548634	-1.344314	-0.060584
C	-0.053749	0.694372	0.18618
H	0.229086	1.699395	-0.145529
H	-0.072171	0.687579	1.282514
O	-1.384483	0.565917	-0.307441
O	-1.960587	-0.618679	0.316672

G_1T_2-TS2

15

O	-1.525197	0.415039	-0.318763
H	-0.878665	0.518718	0.434055
O	-2.609564	-0.131326	0.117744
C	3.665095	1.357599	2.004574
H	4.455553	1.658663	1.310620
H	3.059498	2.241997	2.224219
H	4.144438	1.046009	2.935028
C	2.813333	0.222920	1.429009
H	3.431789	-0.659079	1.237661
H	2.040334	-0.076080	2.142073
C	2.130487	0.628025	0.128103
H	2.851283	0.846178	-0.663183
H	1.479579	1.498071	0.266494
O	1.339535	-0.450833	-0.423382
O	0.237327	-0.688777	0.306910

G_1T_2-IM2

15

O	0.991155	-0.290957	0.757998
O	3.032106	0.019461	-0.251967
H	2.757606	0.815392	-0.734413
O	1.831260	-0.751491	-0.279024
C	-3.218664	-0.380758	-0.320862
H	-3.627291	0.497345	-0.830528
H	-3.021975	-1.144116	-1.079747
H	-3.994840	-0.767831	0.342863
C	-1.950226	-0.033644	0.464720
H	-2.169881	0.713932	1.233171
H	-1.572690	-0.920790	0.980216
C	-0.853335	0.509020	-0.441049
H	-1.157925	1.444645	-0.921211
H	-0.578725	-0.203592	-1.225839
O	0.332863	0.897650	0.275322

G_1T_2-TS3

15

O	-0.414638	-1.343627	-0.373135
O	-0.957512	0.700562	0.032297
H	0.071318	0.557764	-0.521330
O	-0.902068	-0.598702	0.535304
C	3.952055	-1.016824	1.615764
H	4.412684	-0.030904	1.731135
H	3.376345	-1.223220	2.523256
H	4.757707	-1.752186	1.561890
C	3.069792	-1.080320	0.366070
H	3.666441	-0.896819	-0.532432

G_1T_2-C_3H_7OH

12

H	2.568008	0.397459	0.000036
C	-1.900868	0.141052	-0.000233
H	-2.042243	0.771979	0.882902
H	-2.041923	0.771203	-0.883969
H	-2.695878	-0.608397	-0.000043
C	-0.521199	-0.521251	0.000293
H	-0.408807	-1.165256	0.878352
H	-0.408356	-1.165676	-0.877405
C	0.617766	0.486205	0.000249
H	0.541614	1.131705	0.888608

H	2.634407	-2.078745	0.256070
C	1.931162	-0.071470	0.402252
H	2.296976	0.964863	0.525617
H	1.290018	-0.241391	1.290395
O	1.151078	-0.110629	-0.756541

G_1T_2-IM3

15

O	1.783513	-0.790826	-0.030730
H	-0.553256	-0.521790	-1.116675
O	2.961888	-0.085662	-0.414383
H	3.517630	-0.190343	0.373810
O	0.999813	0.052998	0.803497
C	-3.192556	-0.515995	-0.185468
H	-3.624809	0.154145	-0.934970
H	-2.965863	-1.465306	-0.680162
H	-3.961353	-0.710577	0.565710
C	-1.941753	0.093000	0.455554
H	-2.192822	1.027296	0.967497
H	-1.538381	-0.586596	1.211297
C	-0.857100	0.379427	-0.574583
H	-1.186894	1.120612	-1.309199
O	0.311561	1.002736	-0.014674

G_1T_2-IM4

15

O	1.930404	-0.002121	-0.400614
H	1.081786	-0.556305	-0.235556
O	0.879486	1.444918	-0.207553
H	1.594543	2.066882	-0.399829
O	2.752899	-0.222276	0.574855
C	-2.361923	0.941990	0.594251
H	-3.074416	0.408047	1.229503
H	-1.518690	1.274472	1.200643
H	-2.863788	1.824646	0.194411
C	-1.851122	0.066377	-0.571279
H	-2.685347	-0.186104	-1.236227
H	-1.078569	0.605124	-1.119654
C	-1.292622	-1.214113	-0.039108
H	-2.029459	-1.952924	0.330168
O	-0.111797	-1.501691	0.049981
H	0.541033	1.132324	-0.887616
O	1.846545	-0.237672	-0.000341

G_1T_2-TS4

15

O	-1.322129	-0.513516	-0.631707
H	-0.130313	-0.395298	0.029060
O	-2.076130	-1.188349	0.610329
H	-2.481100	-0.372616	0.955828
O	-1.653609	0.686777	-0.789836
C	2.577980	-0.998249	-0.159801
H	2.750880	-1.339501	0.865322
H	1.944268	-1.740532	-0.654535
H	3.542548	-0.994987	-0.671681
C	1.940887	0.391943	-0.184350
H	2.620232	1.128079	0.261573
H	1.750231	0.727318	-1.207822
C	0.624594	0.475120	0.596779
H	0.611249	-0.042789	1.581812
O	-0.131727	1.492268	0.476799

G_1T_2-C_2H_5CHO

10

C	1.693382	-0.282972	-0.177727
H	1.843297	-1.058701	0.578949
H	1.577366	-0.775699	-1.146255
H	2.600956	0.322704	-0.215559
C	0.471932	0.589526	0.149361
H	0.639733	1.104318	1.104923
H	0.296233	1.348699	-0.615732
C	-0.787598	-0.231262	0.301250
H	-0.706161	-1.069307	1.033049
O	-1.814715	-0.040471	-0.297085

G_1T_2-IM5

15

O	1.250890	-0.699595	0.614882
H	-1.077204	-1.377152	0.913554
O	1.746282	1.437253	-0.081363
H	1.426400	1.392723	-0.995890
O	2.241453	0.085377	0.089002
C	-2.919474	0.586933	0.237966
H	-3.574181	-0.028036	-0.387200
H	-3.057188	0.270136	1.276116
H	-3.263792	1.620507	0.160468
C	-1.453767	0.464420	-0.189894
H	-1.335034	0.809292	-1.223363
H	-0.821577	1.098512	0.436098
C	-0.953265	-0.971721	-0.096855
H	-1.495987	-1.628852	-0.784863
O	0.406075	-1.152400	-0.510299

G_1T_2-TS5

15

O	1.143717	0.311244	-0.419256
H	-0.363311	0.064886	-0.828763
O	2.764466	-1.040802	0.463463
H	2.632423	-0.542004	1.286638
O	2.388851	-0.003528	-0.532746
C	-2.816496	-1.116150	-0.311540
H	-3.437047	-0.572878	-1.030969
H	-2.154565	-1.779328	-0.876404
H	-3.481369	-1.743060	0.286774
C	-2.021179	-0.158212	0.575959
H	-2.701022	0.461405	1.171624
H	-1.391007	-0.705129	1.282679
C	-1.118279	0.794840	-0.222755
H	-1.611827	1.301011	-1.078747
O	-0.266604	1.532113	0.430686

$HO_2 + G_1'G_2$

$G_1'G_2$

12

C	-3.549065	0.102489	1.642213
H	-3.227157	-0.932974	1.516289
H	-3.194881	0.442198	2.619454
H	-4.641690	0.117232	1.655632
C	-3.014210	0.992792	0.518157
H	-3.416696	0.669511	-0.447587
H	-3.351521	2.025951	0.663198
C	-1.494486	1.033057	0.418074
H	-1.015516	1.281990	1.366385
H	-1.163295	1.718475	-0.364901
O	-0.963006	-0.262763	0.002651
O	-0.638220	-1.023083	1.030919

$G_1'G_2$-^{3}IM1

15

O	2.743390	-1.126049	-0.656796
H	1.905613	-0.867072	-0.205068
O	3.587848	-0.128971	-0.415451
C	-2.751910	-0.867767	0.174389
H	-1.911722	-1.468680	-0.179615
H	-2.857579	-1.043330	1.248438
H	-3.655153	-1.236142	-0.317211
C	-2.547495	0.618062	-0.128778
H	-2.487161	0.785011	-1.208937
H	-3.407708	1.197754	0.225426
C	-1.315725	1.228763	0.526270
H	-1.262740	1.039344	1.598882
H	-1.235002	2.297695	0.322073
O	-0.092298	0.672808	-0.058477
O	0.392302	-0.323258	0.653034

$G_1'G_2$-^{3}TS1

15

O	2.764917	-0.538576	0.254473
H	1.827792	-0.914106	0.021213

$G_1'G_2$-$C_3H_7O_2H$

13

H	2.331899	-0.920779	0.382359
C	-1.620593	-0.879691	0.038943

O	2.673478	0.753462	0.154034
C	-2.715104	-0.741072	0.311194
H	-2.192899	-1.502647	-0.270904
H	-2.542870	-0.956758	1.369373
H	-3.785640	-0.842185	0.116707
C	-2.236751	0.665861	-0.052839
H	-2.457645	0.885672	-1.102402
H	-2.778097	1.413077	0.539390
C	-0.752328	0.913663	0.189781
H	-0.436760	0.646122	1.199074
H	-0.473858	1.945408	-0.030032
O	0.066177	0.137080	-0.734717
O	0.378562	-1.065129	-0.240195
H	-0.933757	-1.564736	-0.458673
H	-1.619301	-1.126423	1.105126
H	-2.628128	-1.062335	-0.344835
C	-1.214245	0.578976	-0.191003
H	-1.227161	0.808978	-1.261814
H	-1.951272	1.243360	0.278224
C	0.155128	0.973897	0.357295
H	0.257396	0.720092	1.419134
H	0.305465	2.053163	0.243479
O	1.263526	0.434152	-0.362595
O	1.429364	-0.957954	0.038293

$G_1'G_2$-TS2

15

O	-1.934759	-0.234822	0.505268
H	-1.106813	-0.325404	1.057150
O	-2.686864	-1.268788	0.676583
C	1.623551	2.887703	-1.354386
H	1.052650	2.306652	-2.081086
H	0.922242	3.527346	-0.809805
H	2.309074	3.536734	-1.903926
C	2.391073	1.970718	-0.398017
H	3.118258	1.366783	-0.949759
H	2.962989	2.565713	0.322159
C	1.497160	1.036698	0.400868
H	0.711046	1.585859	0.932242
H	2.058965	0.429783	1.116122
O	0.861265	0.131335	-0.535481
O	0.120093	-0.797818	0.085552

$G_1'G_2$-IM2

15

O	0.803247	-0.526623	-0.545784
O	2.940565	-0.238468	0.247632
H	2.656422	0.041390	1.132254
O	1.920243	0.336279	-0.568109
C	-2.849469	-0.659084	0.057854
H	-2.254647	-1.562020	0.210075
H	-3.312897	-0.398325	1.014651
H	-3.650074	-0.896669	-0.646519
C	-1.978450	0.485073	-0.466578
H	-1.575669	0.235220	-1.452375
H	-2.579654	1.392290	-0.597815
C	-0.818610	0.836116	0.456002
H	-1.165693	1.058534	1.470422
H	-0.247792	1.694667	0.090162
O	0.087093	-0.263403	0.678196

$G_1'G_2$-TS3

15

O	-0.954109	-0.559634	0.658819
O	-0.733376	1.457822	-0.062426
H	-0.178566	0.638050	-0.699202
O	-0.740068	0.628442	1.058190
C	2.647726	-2.453604	-1.211084
H	1.717824	-2.631112	-1.754954
H	3.324691	-1.902018	-1.871167
H	3.107120	-3.421133	-0.995518

$G_1'G_2$-C_3H_7OH

12

H	2.245046	-0.732931	0.196799
C	-1.543467	-0.515384	0.128923
H	-1.103325	-1.471191	-0.160306
H	-1.691027	-0.527539	1.213888
H	-2.527501	-0.434329	-0.340147
C	-0.633209	0.642150	-0.289390
H	-0.546459	0.673851	-1.380784
H	-1.068724	1.598652	0.021524

C	2.374230	-1.673791	0.077412
H	1.735400	-2.262740	0.744404
H	3.309204	-1.487127	0.617969
C	1.690739	-0.336436	-0.167871
H	2.306764	0.336264	-0.793504
H	1.556316	0.214770	0.782788
O	0.453591	-0.482245	-0.804916
C	0.769587	0.545839	0.293363
H	0.712742	0.512640	1.392213
H	1.348628	1.437658	0.013636
O	1.384144	-0.636556	-0.219275

$G_1'G_2$-IM3

15

O	-2.069726	-0.038898	-0.378387
H	0.224816	-0.179335	1.385888
O	-2.082932	0.678904	0.873133
H	-2.209823	1.589976	0.566304
O	-0.764347	-0.023704	-0.899255
C	2.023291	1.214006	-0.307137
H	1.437608	1.228119	-1.228174
H	1.550359	1.904006	0.398595
H	3.019427	1.601302	-0.536279
C	2.114635	-0.198795	0.276637
H	2.592847	-0.872308	-0.442327
H	2.757810	-0.186595	1.165516
C	0.786251	-0.815349	0.699462
H	0.951576	-1.782880	1.182891
O	-0.066706	-1.178984	-0.408763

$G_1'G_2$-IM4

15

O	-1.788988	-0.010367	-0.458352
H	-0.981628	-0.658303	-0.507187
O	-1.767279	-0.218772	1.284687
H	-2.464674	0.434980	1.436982
O	-1.362421	1.154936	-0.871450
C	2.041651	1.268005	-0.045618
H	2.985521	1.024527	-0.541674
H	1.313325	1.586378	-0.792300
H	2.224399	2.101668	0.634426
C	1.478212	0.068860	0.751798
H	2.178756	-0.206908	1.547516
H	0.509075	0.318125	1.187866
C	1.324173	-1.107583	-0.156164
H	2.240251	-1.680225	-0.391913

$G_1'G_2$-TS4

15

O	0.685737	0.418189	0.275914
H	-0.261821	-0.508985	0.737291
O	1.769651	-0.794409	-0.004691
H	2.459834	-0.234144	-0.393601
O	0.139372	0.841153	-0.754901
C	-0.624929	-2.965719	-1.019065
H	-1.281389	-2.649836	-1.831476
H	0.362563	-2.539985	-1.200581
H	-0.542638	-4.055137	-1.044729
C	-1.173121	-2.506781	0.330525
H	-2.153038	-2.966254	0.518784
H	-0.524159	-2.829559	1.150704
C	-1.397243	-0.986983	0.429448
H	-1.909789	-0.648576	1.356765
O	-1.623331	-0.292890	-0.618647

$G_1'G_2$-C_2H_5CHO

10

C	1.693439	-0.282870	-0.177745
H	1.843397	-1.058674	0.578836
H	1.577490	-0.775507	-1.146329
H	2.600962	0.322889	-0.215500
C	0.471899	0.589470	0.149454
H	0.639603	1.104044	1.105152
H	0.296208	1.348845	-0.615440
C	-0.787585	-0.231447	0.301086
H	-0.705975	-1.069888	1.032420
O	-1.814775	-0.040328	-0.296988

O	0.285032	-1.462788	-0.689111

$G_1'G_2$-IM5

15

O	0.696486	-0.703591	-0.434634
H	-0.319276	0.841400	1.136777
O	2.379711	0.148111	0.885269
H	2.428030	1.063195	0.568742
O	2.067618	-0.534550	-0.349640
C	-2.275225	-1.039824	0.356367
H	-1.678602	-1.633474	-0.339127
H	-1.920941	-1.258906	1.367786
H	-3.311906	-1.377847	0.282621
C	-2.171615	0.455007	0.043115
H	-2.542433	0.655151	-0.967587
H	-2.813196	1.022904	0.728412
C	-0.767228	1.036210	0.158864
H	-0.785627	2.118102	-0.010214
O	0.134729	0.572669	-0.865680

$G_1'G_2$-TS5

15

O	0.156717	-0.426208	0.076830
H	-1.193241	-0.455092	0.931498
O	2.180727	0.577061	0.423137
H	1.685195	1.268707	-0.048136
O	1.425649	-0.624357	-0.006061
C	-2.535608	-2.512850	-0.509099
H	-2.267906	-2.222122	-1.526064
H	-1.635749	-2.905868	-0.028378
H	-3.270724	-3.319377	-0.561864
C	-3.095038	-1.316620	0.258933
H	-4.031884	-0.979173	-0.201257
H	-3.333181	-1.587631	1.292810
C	-2.148460	-0.102322	0.280798
H	-2.496459	0.742069	0.911154
O	-1.569517	0.255419	-0.831053

$HO_2 + T_1G_2$

T_1G_2

12

C	-3.534495	0.110385	1.694852
H	-3.162539	-0.915530	1.662314
H	-3.237166	0.545121	2.653788
H	-4.625885	0.074414	1.668753
C	-2.986627	0.931031	0.523597
H	-3.332942	0.514617	-0.427739
H	-3.367271	1.956976	0.569177
C	-1.471148	1.013825	0.494111
H	-1.047638	1.349436	1.443671
H	-1.101893	1.650464	-0.312723
O	-0.954923	-0.331532	0.245525
O	0.359933	-0.368273	0.300274

T_1G_2-^{3}IM1

15

O	-2.964998	0.163213	-1.050792
H	-2.224755	0.470157	-0.475483
O	-3.224685	-1.074724	-0.643789
C	2.933176	-0.119136	-0.830064
H	2.128483	-0.136969	-1.568053
H	3.322919	0.901927	-0.780040
H	3.735031	-0.764869	-1.194160
C	2.438373	-0.590220	0.540551
H	2.090714	-1.626689	0.487344
H	3.259198	-0.576884	1.265560
C	1.327351	0.266647	1.117338
H	1.567054	1.332056	1.125208
H	1.021949	-0.049367	2.116544
O	0.150541	0.106054	0.253714
O	-0.830525	0.901809	0.613975

T_1G_2-^{3}TS1

15

T_1G_2-$C_3H_7O_2H$

13

O	-2.800189	-0.202381	-0.113152
H	-2.142612	0.600610	-0.131733
O	-2.067306	-1.274806	-0.126001
C	2.899827	-0.155650	-0.617816
H	2.401822	0.183294	-1.528559
H	3.439931	0.695594	-0.192500
H	3.636341	-0.911483	-0.899405
C	1.891223	-0.726900	0.383181
H	1.383980	-1.600108	-0.037750
H	2.407432	-1.071395	1.285773
C	0.837580	0.270293	0.828908
H	1.266596	1.206777	1.195458
H	0.160031	-0.140508	1.578757
O	0.025740	0.605494	-0.339141
O	-0.948908	1.460538	-0.026167
H	-1.515419	1.349805	-0.045665
C	3.027242	-0.209916	-0.601188
H	2.549877	0.160755	-1.509688
H	3.603297	0.612745	-0.166727
H	3.729899	-0.998928	-0.881053
C	1.983684	-0.732144	0.390543
H	1.442947	-1.581268	-0.040573
H	2.474983	-1.103643	1.296547
C	0.970713	0.321406	0.825757
H	1.472278	1.213761	1.217846
H	0.297107	-0.070223	1.598833
O	0.218264	0.674705	-0.333602
O	-0.651787	1.775921	0.039280

T_1G_2-TS2

15

O	-1.519972	0.478737	-0.040300
H	-0.832303	0.347844	0.672629
O	-2.596792	-0.159250	0.272097
C	3.082542	1.537351	-1.965270
H	2.419752	0.933376	-2.587888
H	2.602107	2.507345	-1.805234
H	4.005531	1.710563	-2.523238
C	3.374417	0.839383	-0.633711
H	3.893987	-0.108441	-0.805659
H	4.042601	1.454195	-0.021081
C	2.131575	0.563338	0.196087
H	1.539414	1.472763	0.351546
H	2.366717	0.115987	1.165656
O	1.317174	-0.385458	-0.536927
O	0.241979	-0.774164	0.163945

T_1G_2-IM2

15

O	0.803118	-0.526932	-0.545187
O	2.940615	-0.238485	0.247640
H	2.656664	0.042144	1.132079
O	1.920248	0.335758	-0.568411
C	-2.849214	-0.659374	0.058259
H	-2.254137	-1.562024	0.211172
H	-3.312772	-0.398061	1.014840
H	-3.649707	-0.897703	-0.645988
C	-1.978508	0.484649	-0.466977
H	-1.575644	0.234192	-1.452584
H	-2.579964	1.391603	-0.598878
C	-0.818774	0.836707	0.455355
H	-1.165947	1.059978	1.469557
H	-0.248073	1.695024	0.088777
O	0.087088	-0.262472	0.678608

T_1G_2-TS3

30

O	1.406041	1.082754	-0.430673
O	2.278262	-0.853320	-0.070208
H	1.194114	-0.873185	-0.528458
O	2.076990	0.431909	0.431367
C	-2.938162	-0.005735	-0.450992
H	-2.501494	0.091584	-1.446972

T_1G_2-C_3H_7OH

12

H	2.245020	-0.732964	0.196809
C	-1.543442	-0.515407	0.128913
H	-1.103285	-1.471189	-0.160374
H	-1.690977	-0.527624	1.213882
H	-2.527489	-0.434347	-0.340130
C	-0.633226	0.642174	-0.289359

H	-3.288825	-1.036292	-0.335542
H	-3.809624	0.650836	-0.395039
C	-1.908652	0.352142	0.623964
H	-1.609258	1.400927	0.522712
H	-2.345255	0.242743	1.623304
C	-0.651799	-0.502798	0.556835
H	-0.871157	-1.576898	0.703248
H	0.039879	-0.245918	1.382182
O	0.011619	-0.375775	-0.668521

T_1G_2-IM3

15

O	1.878609	0.290213	-0.590110
H	-0.214274	1.673350	0.015167
O	2.915352	-0.050426	0.327688
H	3.342137	-0.793802	-0.126573
O	0.799271	-0.618016	-0.415057
C	-2.867306	-0.623895	0.056459
H	-2.299200	-1.524455	0.298952
H	-3.356970	-0.281391	0.973516
H	-3.648574	-0.898462	-0.656374
C	-1.951438	0.459044	-0.519488
H	-1.521257	0.126682	-1.468804
H	-2.526587	1.365813	-0.740230
C	-0.815987	0.853350	0.416676
H	-1.190265	1.152821	1.400694
O	0.059690	-0.240715	0.750200

T_1G_2-IM4

15

O	1.850830	-0.264055	0.004255
H	1.001298	-0.788329	-0.277369
O	1.327717	1.025763	-1.052713
H	2.052105	1.616831	-0.801933
O	1.736118	-0.000908	1.281470
C	-1.926709	1.334393	-0.022063
H	-1.090290	1.661762	-0.640511
H	-2.809253	1.192225	-0.652187
H	-2.154621	2.118541	0.702084
C	-1.537530	0.040561	0.730004
H	-0.612120	0.188906	1.292002
H	-2.343800	-0.242591	1.416234
H	-0.546536	0.673975	-1.380754
H	-1.068741	1.598642	0.021663
C	0.769598	0.545856	0.293331
H	0.712796	0.512711	1.392184
H	1.348645	1.437649	0.013536
O	1.384123	-0.636574	-0.219266

T_1G_2-TS4

15

O	1.649587	-0.137751	0.686526
H	0.434243	-0.590109	0.259083
O	2.473861	-0.972501	-0.405717
H	2.577797	-0.248653	-1.049114
O	1.589505	1.083321	0.402459
C	-3.106451	-0.099656	-0.076889
H	-3.124811	0.922050	-0.462546
H	-3.292201	-0.781569	-0.911823
H	-3.925385	-0.213723	0.637535
C	-1.755534	-0.392404	0.593067
H	-1.592247	0.299681	1.424001
H	-1.746038	-1.410580	0.996030
C	-0.603307	-0.223845	-0.400797
H	-0.502650	-1.018019	-1.172826
O	-0.217573	0.943976	-0.734846

T_1G_2-C_2H_5CHO

10

C	-1.693315	-0.283027	-0.177720
H	-1.577295	-0.775741	-1.146255
H	-1.843078	-1.058778	0.578960
H	-2.600969	0.322534	-0.215494
C	-0.471929	0.589602	0.149314
H	-0.296239	1.348664	-0.615888
H	-0.639807	1.104470	1.104815
C	0.787579	-0.231192	0.301327
H	0.706096	-1.069129	1.033268
O	1.814661	-0.040540	-0.297116

C	-1.349912	-1.080079	-0.239383
H	-2.265916	-1.540810	-0.652562
O	-0.276227	-1.507773	-0.632650

T_1G_2-IM5

15

O	1.278669	-0.869119	0.261936
H	-0.817582	-1.888962	0.971647
O	1.463638	1.427193	0.281360
H	0.905630	1.678893	-0.470897
O	2.022143	0.179704	-0.206815
C	-2.044402	1.068420	-0.449157
H	-1.247908	1.240804	-1.179249
H	-2.891188	0.642770	-0.996104
H	-2.355616	2.037927	-0.053208
C	-1.576703	0.133196	0.669276
H	-0.803453	0.615627	1.272182
H	-2.411031	-0.088274	1.344503
C	-1.029565	-1.192352	0.154668
H	-1.734142	-1.680489	-0.527587
O	0.142963	-1.064513	-0.662731

T_1G_2-TS5

15

O	0.091798	-0.404613	-0.036584
H	-1.130540	-0.785143	0.894472
O	2.102727	0.611691	0.359581
H	1.689549	1.381517	-0.065662
O	1.350174	-0.486390	-0.300944
C	-3.924148	1.331212	1.395055
H	-3.832119	1.953599	0.501913
H	-4.727765	0.609028	1.222334
H	-4.222315	1.969540	2.230630
C	-2.594786	0.626224	1.692693
H	-1.806549	1.363946	1.867752
H	-2.681329	0.013879	2.596485
C	-2.158841	-0.266707	0.522262
H	-2.782731	-1.170388	0.362068
O	-1.754992	0.314769	-0.572747

$HO_2 + T_1T_2$

T_1T_2

15

C	-3.582573	0.079273	1.710117
H	-3.292002	-0.974939	1.730921
H	-3.340057	0.511575	2.685091
H	-4.666902	0.121651	1.589398
C	-2.880419	0.830691	0.574587
H	-3.155281	0.396993	-0.391482
H	-3.203469	1.875813	0.557189
C	-1.370628	0.785222	0.722005
H	-0.975466	-0.232663	0.679449
H	-1.024276	1.266811	1.639710
O	-0.792208	1.521381	-0.398076
O	0.523947	1.530129	-0.348184

T_1T_2-^{3}IM1

15

O	3.447345	0.110444	0.546489
H	2.598905	0.388779	0.127171
O	3.551238	-1.187507	0.281770
C	-3.660338	-0.279857	-0.147314
H	-3.986057	0.763561	-0.183933
H	-3.759652	-0.697976	-1.152992
H	-4.349301	-0.819422	0.505188
C	-2.223275	-0.401125	0.371291
H	-2.153312	0.000566	1.386401
H	-1.927410	-1.452920	0.422258
C	-1.248127	0.342090	-0.521642
H	-1.441307	1.416409	-0.562185
H	-1.209089	-0.059577	-1.536431
O	0.090384	0.172992	0.052233
O	1.007535	0.781469	-0.665667

T_1T_2-^{3}TS1

T_1T_2-$C_3H_7O_2H$

15

O	2.742195	-0.539923	-0.233946
H	2.256172	0.376019	-0.192199
O	1.871658	-1.432873	0.129799
C	-3.133880	-0.585527	-0.313337
H	-3.648582	0.315092	-0.660591
H	-2.886569	-1.189752	-1.190842
H	-3.838911	-1.156899	0.293713
C	-1.881433	-0.238738	0.498494
H	-2.155060	0.344318	1.383011
H	-1.392356	-1.150335	0.852272
C	-0.885494	0.554035	-0.327194
H	-1.286862	1.512399	-0.668279
H	-0.508313	-0.006946	-1.184232
O	0.255906	0.851152	0.531266
O	1.238407	1.443830	-0.149698

13

H	2.806179	-0.085277	0.755612
C	-2.450488	-0.291096	0.012296
H	-2.514561	-0.946908	-0.860868
H	-2.510156	-0.919194	0.906067
H	-3.328920	0.358202	0.004324
C	-1.161393	0.536134	-0.005009
H	-1.131581	1.172259	-0.894572
H	-1.128749	1.202247	0.862791
C	0.080736	-0.346208	0.003793
H	0.107562	-0.998635	-0.876811
H	0.115093	-0.974905	0.903566
O	1.204140	0.529591	-0.018180
O	2.392361	-0.304688	-0.090143

T_1T_2-TS2

15

O	-1.476353	0.482150	-0.170538
H	-0.797283	0.446414	0.561342
O	-2.562450	-0.098530	0.213796
C	4.361812	1.799107	-0.222786
H	3.879813	2.777366	-0.308398
H	4.629560	1.648523	0.827021
H	5.288761	1.835767	-0.798597
C	3.451702	0.678496	-0.735424
H	3.214452	0.837106	-1.791489
H	3.961621	-0.286529	-0.664607
C	2.154085	0.603439	0.051445
H	1.584068	1.536811	-0.025094
H	2.318766	0.368738	1.107227
O	1.357480	-0.461713	-0.519398
O	0.276082	-0.737558	0.225190

T_1T_2-IM2

15

O	0.991167	-0.290209	0.758463
O	3.031889	0.019055	-0.252372
H	2.757321	0.814608	-0.735407
O	1.830949	-0.751781	-0.278392
C	-3.218439	-0.381083	-0.320787
H	-3.627248	0.496782	-0.830719
H	-3.021576	-1.144621	-1.079447
H	-3.994542	-0.768125	0.343039
C	-1.950081	-0.033469	0.464702
H	-2.169851	0.714429	1.232806
H	-1.572469	-0.920341	0.980617
C	-0.853227	0.508906	-0.441280
H	-1.157923	1.444257	-0.921906
H	-0.578490	-0.204057	-1.225705
O	0.332903	0.898054	0.274916

T_1T_2-TS3

15

O	-1.521868	1.046643	0.443412
O	-2.279768	-0.770390	-0.429290
H	-1.409663	-0.916692	0.350344
O	-1.886505	0.545885	-0.667446

T_1T_2-C_3H_7OH

12

H	2.567994	0.397475	0.000075
C	-1.900858	0.141055	-0.000240
H	-2.042262	0.771923	0.882933
H	-2.041868	0.771270	-0.883938

C	3.076703	0.147270	-0.573846
H	3.397522	-0.883698	-0.751967
H	2.781248	0.574802	-1.536955
H	3.945550	0.705185	-0.218015
C	1.932765	0.210914	0.441887
H	2.254820	-0.195093	1.405502
H	1.638841	1.250135	0.621198
C	0.700146	-0.554355	-0.015646
H	0.924643	-1.616345	-0.227353
H	0.331365	-0.155916	-0.981985
O	-0.327111	-0.520307	0.931431
H	-2.695878	-0.608383	-0.000136
C	-0.521195	-0.521261	0.000304
H	-0.408815	-1.165248	0.878377
H	-0.408345	-1.165701	-0.877382
C	0.617760	0.486202	0.000253
H	0.541609	1.131690	0.888624
H	0.540995	1.132327	-0.887606
O	1.846541	-0.237667	-0.000356

T_1T_2-IM3

15

O	1.783514	-0.790825	-0.030749
H	-0.553261	-0.521767	-1.116690
O	2.961892	-0.085652	-0.414376
H	3.517628	-0.190351	0.373817
O	0.999809	0.052980	0.803493
C	-3.192555	-0.515994	-0.185473
H	-3.624813	0.154157	-0.934963
H	-2.965861	-1.465297	-0.680183
H	-3.961350	-0.710589	0.565704
C	-1.941752	0.092994	0.455556
H	-2.192822	1.027281	0.967514
H	-1.538376	-0.586613	1.211286
C	-0.857102	0.379440	-0.574579
H	-1.186896	1.120641	-1.309179
O	0.311562	1.002735	-0.014660

T_1T_2-TS4

15

O	-1.322268	-0.513385	-0.631921
H	-0.130279	-0.395278	0.028137
O	-2.075498	-1.188693	0.610382
H	-2.481081	-0.373220	0.955775
O	-1.653993	0.686943	-0.789477
C	2.577999	-0.998135	-0.160052
H	2.750554	-1.339971	0.864933
H	1.944305	-1.740048	-0.655360
H	3.542705	-0.994735	-0.671668
C	1.941097	0.392162	-0.184008
H	2.620311	1.127943	0.262698
H	1.750923	0.728209	-1.207350
C	0.624467	0.475025	0.596610
H	0.610731	-0.043237	1.581455
O	-0.131935	1.492138	0.476776

T_1T_2-IM4

15

O	1.930294	-0.001900	-0.400781
H	1.081775	-0.556304	-0.235858
O	0.878992	1.444902	-0.207178
H	1.593955	2.067087	-0.399083
O	2.752902	-0.222223	0.574533
C	-2.361678	0.942005	0.594026
H	-3.073970	0.408168	1.229590
H	-1.518272	1.274746	1.200027
H	-2.863719	1.824501	0.194061
C	-1.851031	0.066148	-0.571400

T_1T_2-C_2H_5CHO

10

C	1.693383	-0.282970	-0.177727
H	1.843297	-1.058702	0.578946
H	1.577368	-0.775694	-1.146257
H	2.600956	0.322706	-0.215556
C	0.471931	0.589526	0.149362
H	0.639731	1.104314	1.104927
H	0.296233	1.348701	-0.615727
C	-0.787597	-0.231265	0.301248
H	-0.706158	-1.069315	1.033040
O	-1.814716	-0.040469	-0.297084

H	-2.685339	-0.186564	-1.236159
H	-1.078600	0.604854	-1.119952
C	-1.292459	-1.214143	-0.038879
H	-2.029287	-1.952751	0.330831
O	-0.111630	-1.501753	0.050183

T_1T_2-IM5

15

O	-1.043459	-0.719832	-0.538600
H	0.428989	1.113070	0.304678
O	-2.303923	1.159515	-0.105927
H	-2.249554	1.219551	0.860094
O	-2.325591	-0.277546	-0.272069
C	3.107389	0.556516	-0.274521
H	2.831879	1.546716	-0.649895
H	3.528995	0.685898	0.727233
H	3.899706	0.168328	-0.918201
C	1.902838	-0.389298	-0.257527
H	1.513064	-0.518342	-1.271263
H	2.199947	-1.380315	0.099391
C	0.784160	0.132727	0.635534
H	1.116649	0.211601	1.676649
O	-0.331526	-0.767909	0.735396

T_1T_2-TS5

15

O	1.076783	-0.109128	-0.216038
H	-0.319099	-0.352463	0.505031
O	3.240252	-0.360496	0.476893
H	3.053185	0.560954	0.725660
O	2.226238	-0.554887	-0.587073
C	-2.990124	-1.027990	0.224192
H	-2.350675	-1.912906	0.297605
H	-3.339633	-0.785177	1.232566
H	-3.865714	-1.301035	-0.368948
C	-2.244898	0.148190	-0.407674
H	-1.884282	-0.102775	-1.408753
H	-2.915932	1.007381	-0.519364
C	-1.041322	0.616248	0.423644
H	-1.251206	0.767574	1.504482
O	-0.226845	1.486981	-0.099939

Table S3. T_1 diagnostic value for the species involved in the HO_2 + n-$C_3H_7O_2$ reaction.

Molecule	T_1	Molecule	T_1
G_1G_2	0.030	$G_1'G_2$-TS2	0.032
HO_2	0.039	$G_1'G_2$-IM2	0.018
G_1G_2-^{3}IM1	0.035	$G_1'G_2$-TS3	0.035
G_1G_2-^{3}TS1	0.047	$G_1'G_2$-C_3H_7OH	0.010
G_1G_2-$C_3H_7O_2H$	0.012	$G_1'G_2$-IM3	0.018
$^3O_2$	0.009	$G_1'G_2$-TS4	0.029
G_1G_2-TS2	0.032	$G_1'G_2$-IM4	0.027
$^1O_2$	0.016	$G_1'G_2$-C_2H_5CHO	0.014
G_1G_2-IM2	0.017	$G_1'G_2$-IM5	0.018
G_1G_2-TS3	0.035	$G_1'G_2$-TS5	0.026
G_1G_2-C_3H_7OH	0.010	T_1G_2	0.030
O_3	0.028	T_1G_2-^{3}IM1	0.034
G_1G_2-IM3	0.018	T_1G_2-^{3}TS1	0.032
G_1G_2-TS4	0.029	T_1G_2-$C_3H_7O_2H$	0.012
G_1G_2-IM4	0.028	T_1G_2-TS2	0.032
G_1G_2-C_2H_5CHO	0.014	T_1G_2-IM2	0.018
OH	0.012	T_1G_2-TS3	0.035
G_1G_2-IM5	0.018	T_1G_2-C_3H_7OH	0.010
G_1G_2-TS5	0.035	T_1G_2-IM3	0.018
HO_3H	0.018	T_1G_2-TS4	0.029
G_1T_2	0.030	T_1G_2-IM4	0.028
G_1T_2-^{3}IM1	0.035	T_1G_2-C_2H_5CHO	0.014
G_1T_2-^{3}TS1	0.045	T_1G_2-IM5	0.018
G_1T_2-$C_3H_7O_2H$	0.012	T_1G_2-TS5	0.025
G_1T_2-TS2	0.031	T_1T_2	0.030
G_1T_2-IM2	0.018	T_1T_2-^{3}IM1	0.034
G_1T_2-TS3	0.035	T_1T_2-^{3}TS1	0.042
G_1T_2-C_3H_7OH	0.010	T_1T_2-$C_3H_7O_2H$	0.012
G_1T_2-IM3	0.018	T_1T_2-TS2	0.032
G_1T_2-TS4	0.029	T_1T_2-IM2	0.018
G_1T_2-IM4	0.025	T_1T_2-TS3	0.035
G_1T_2-C_2H_5CHO	0.014	T_1T_2-C_3H_7OH	0.010
G_1T_2-IM5	0.018	T_1T_2-IM3	0.018
G_1T_2-TS5	0.025	T_1T_2-TS4	0.029
$G_1'G_2$	0.030	T_1T_2-IM4	0.025
$G_1'G_2$-^{3}IM1	0.034	T_1T_2-C_2H_5CHO	0.014
$G_1'G_2$-^{3}TS1	0.047	T_1T_2-IM5	0.018
$G_1'G_2$-$C_3H_7O_2H$	0.013	T_1T_2-TS5	0.026
G_1G_2	0.030	$G_1'G_2$-TS2	0.032
HO_2	0.039	$G_1'G_2$-IM2	0.018
G_1G_2-^{3}IM1	0.035	$G_1'G_2$-TS3	0.035

G_1G_2-^{3}TS1	0.047	$G_1'G_2$-C_3H_7OH	0.010

Table S4. Zero point energies (ZPE), relative energies (ΔE_{298K}), reaction enthalpies (ΔH_{298K}) and Gibbs free energies (ΔG_{298K}) of the stationary points involved in the HO_2 + G_1T_2 reaction. Energies are computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/6-311G(d,p) level of theory. Energy values are given in kcal mol^{-1}.

compound	ZPE	ΔE_{298K}	ΔH_{298K}	ΔG_{298K}
HO_2 + G_1T_2	71.60	0.00	0.00	0.00
G_1T_2-^{3}IM1	73.05	-6.19	-6.78	1.93
G_1T_2-^{3}TS1	71.22	-3.26	-3.85	6.92
G_1T_2-$C_3H_7O_2H$ + $^3O_2$	72.34	-35.87	-35.87	-34.31
G_1T_2-TS2	72.37	9.95	9.36	20.47
G_1T_2-$C_3H_7O_2H$ + $^1O_2$	72.31	-4.92	-4.92	-2.71
G_1T_2-IM2	74.11	-12.59	-13.18	-0.72
G_1T_2-TS3	70.89	8.31	7.71	20.73
G_1T_2-C_3H_7OH + O_3	72.49	-14.62	-14.62	-13.74
G_1T_2-IM3	74.09	-11.54	-12.14	0.29
G_1T_2-TS4	69.75	4.89	4.30	16.55
G_1T_2-IM4	72.40	-33.58	-34.18	-24.49
G_1T_2-C_2H_5CHO + HO_2 + OH	66.88	-26.79	-26.20	-36.56
G_1T_2-IM5	74.05	-10.77	-11.36	1.26
G_1T_2-TS5	70.09	15.00	14.40	26.31
G_1T_2-C_2H_5CHO + HO_3H	71.75	-54.37	-54.37	-54.26

Table S5. Zero point energies (ZPE), relative energies (ΔE_{298K}), reaction enthalpies (ΔH_{298K}) and Gibbs free energies (ΔG_{298K}) of the stationary points involved in the HO_2 + G_1'G_2 reaction. Energies are computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/6-311G(d,p) level of theory. Energy values are given in kcal mol^{-1}.

compound	ZPE	ΔE_{298K}	ΔH_{298K}	ΔG_{298K}
HO_2 + G_1'G_2	71.55	0.00	0.00	0.00
G_1'G_2-^{3}IM1	73.00	-5.96	-6.55	1.02
G_1'G_2-^{3}TS1	71.58	-2.14	-2.73	7.83
G_1'G_2-$C_3H_7O_2H$ + $^3O_2$	72.26	-35.30	-35.30	-33.79
G_1'G_2-TS2	72.28	9.70	9.10	19.99
G_1'G_2-$C_3H_7O_2H$ + $^1O_2$	72.24	-4.34	-4.34	-2.19
G_1'G_2-IM2	74.19	-12.99	-13.58	-0.91
G_1'G_2-TS3	70.98	7.94	7.35	20.57
G_1'G_2-C_3H_7OH + O_3	72.50	-14.98	-14.98	-14.02
G_1'G_2-IM3	73.99	-10.57	-11.16	1.07
G_1'G_2-TS4	70.11	4.05	3.45	16.34
G_1'G_2-IM4	72.51	-35.14	-35.73	-25.13
G_1'G_2-C_2H_5CHO + HO_2 + OH	66.88	-26.95	-26.36	-36.72
G_1'G_2-IM5	74.01	-10.80	-11.39	1.08
G_1'G_2-TS5	70.21	14.46	13.87	25.95
G_1'G_2-C_2H_5CHO + HO_3H	71.73	-55.61	-55.60	-55.21

Table S6. Zero point energies (ZPE), relative energies (ΔE_{298K}), reaction enthalpies (ΔH_{298K}) and Gibbs free energies (ΔG_{298K}) of the stationary points involved in the HO_2 + T_1G_2 reaction. Energies are computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/ 6-311G(d,p) level of theory. Energy values are given in kcal mol^{-1}.

compound	ZPE	ΔE_{298K}	ΔH_{298K}	ΔG_{298K}
HO_2 + T_1G_2	71.48	0.00	0.00	0.00
T_1G_2-^{3}IM1	72.98	-6.08	-6.67	1.08
T_1G_2-^{3}TS1	71.53	-3.88	-4.47	6.37
T_1G_2-$C_3H_7O_2H$ + $^3O_2$	72.23	-36.12	-36.12	-34.58
T_1G_2-TS2	72.29	9.64	9.04	20.19
T_1G_2-$C_3H_7O_2H$ + $^1O_2$	72.21	-5.17	-5.17	-2.98
T_1G_2-IM2	74.19	-13.04	-13.63	-0.72
T_1G_2-TS3	70.94	7.85	7.26	20.66
T_1G_2-C_3H_7OH + O_3	72.50	-15.04	-15.04	-13.82
T_1G_2-IM3	74.11	-12.04	-12.64	0.15
T_1G_2-TS4	69.85	4.66	4.07	16.56
T_1G_2-IM4	72.52	-35.17	-35.76	-24.75
T_1G_2-C_2H_5CHO + HO_2 + OH	66.88	-27.01	-26.41	-36.52
T_1G_2-IM5	74.07	-11.41	-12.00	1.15
T_1G_2-TS5	70.13	14.66	14.07	26.20
T_1G_2-C_2H_5CHO + HO_3H	71.73	-55.66	-55.66	-55.02

Table S7. Zero point energies (ZPE), relative energies (ΔE_{298K}), reaction enthalpies (ΔH_{298K}) and Gibbs free energies (ΔG_{298K}) of the stationary points involved in the $HO_2 + T_1T_2$ reaction. Energies are computed at the CCSD(T)/aug-cc-pVDZ//B3LYP/ 6-311G(d,p) level of theory. Energy values are given in kcal mol^{-1}.

compound	ZPE	ΔE_{298K}	ΔH_{298K}	ΔG_{298K}	ν
$HO_2 + T_1T_2$	71.45	0.00	0.00	0.00	
T_1T_2-^{3}IM1	72.92	-6.03	-6.62	0.81	
T_1T_2-^{3}TS1	71.50	-3.93	-4.52	6.09	-239.22
T_1T_2-$C_3H_7O_2H + {}^3O_2$	72.22	-36.21	-36.21	-34.56	
T_1T_2-TS2	72.27	9.63	9.04	-3.70	-438.54
T_1T_2-$C_3H_7O_2H + {}^1O_2$	72.20	-5.25	-5.25	-26.85	
T_1T_2-IM2	74.11	-12.99	-13.58	-0.71	
T_1T_2-TS3	70.92	7.92	7.33	20.82	-1476.56
T_1T_2-$C_3H_7OH + O_3$	72.49	-15.02	-15.02	-13.72	
T_1T_2-IM3	74.09	-11.95	-12.54	0.30	
T_1T_2-TS4	69.75	4.49	3.89	16.56	-797.68
T_1T_2-IM4	72.40	-33.99	-34.58	-24.47	
T_1T_2-$C_2H_5CHO + HO_2 + OH$	66.88	-27.19	-26.60	-36.54	
T_1T_2-IM5	74.07	-11.24	-11.83	1.02	
T_1T_2-TS5	70.03	14.58	13.99	26.37	-422.33
T_1T_2-$C_2H_5CHO + HO_3H$	71.75	-54.77	-54.77	-54.24	