

Table I Summary of scaled harmonic frequencies of the various species involved in the reaction of O (3P_2) with the methyl radical (B3LYP / 6-311G**)

CH ₃	495, 1375, 1376, 3043, 3218, 3219
CH ₂	1376, 2831, 2892
Methanal	1178, 1245, 1508, 1790, 2813, 2861
INT 1	704, 943, 1085, 1333, 1343, 1486, 2834, 2900, 2941
INT 2	430, 572, 1040, 1183, 1340, 1458, 3051, 3192, 3763
TS 1	1158i, 149, 555, 1076, 1218, 1468, 1626, 2876, 2950
TS 2	2001i, 704, 946, 1111, 1120, 1452, 2385, 2972, 3080

^ai represents imaginary frequency.

b represents zero-point energy (ZPE) corrections (scaling factor of 0.98)

Table II Summary of scaled harmonic frequencies of the various species involved in the reaction of O (3P_2) with the ethyl radical. (B3LYP / 6-311G**)

Species	Frequency (cm ⁻¹) ^{a,b}
Oxirane	802, 828, 872, 1019, 1117, 1120, 1145, 1148, 1275, 1475, 1510, 3014, 3022, 3093, 3108
C ₂ H ₅	107, 469, 797, 960, 1041, 1168, 1372, 1436, 1452, 1453, 2884, 2974, 3016, 3076, 3217
Ethene	817, 954, 955, 1045, 1213, 1352, 1443, 1657, 3059, 3073, 3128, 3156
Ethanal	155, 498, 761, 865, 1103, 1112, 1348, 1397, 1431, 1441, 1788, 2799, 2961, 3015, 3073
Methanal	1178, 1245, 1508, 1790, 2813, 2861
INT1	27, 267, 424, 850, 869, 1047, 1076, 1216, 1316, 1362, 1383, 1455, 1467, 2827, 2835, 2970, 3035, 3045

INT2	2150, 264, 404, 461, 841, 938, 1048, 1086, 1193, 1251, 1391, 1431, 1464, 2810, 2878, 3086, 3196, 3763
INT3	178, 358, 402, 571, 912, 1004, 1039, 1184, 1254, 1367, 1420, 1436, 1462, 2885, 2980, 3032, 3052, 3785
TS1	797 <i>i</i> , 174, 379, 445, 491, 794, 878, 1076, 1103, 1347, 1374, 1435, 1445, 1661, 2794, 2962, 3028, 3072
TS2	334 <i>i</i> , 135, 261, 489, 536, 588, 877, 1083, 1224, 1381, 1399, 1459, 1603, 2823, 2867, 3030, 3191, 3203
TS3	1947 <i>i</i> , 344, 705, 804, 904, 942, 1050, 1050, 1128, 1184, 1274, 1400, 1499, 1889, 2976, 3021, 3048, 3155
TS4	1285 <i>i</i> , 86, 491, 750, 758, 868, 873, 967, 1109, 1156, 1166, 1256, 1444, 1507, 2996, 3064, 3094, 3205
TS5	1918 <i>i</i> , 347, 405, 428, 688, 781, 932, 1066, 1145, 1233, 1279, 1369, 1415, 2100, 3024, 3073, 3194, 3746
TS6	1969 <i>i</i> , 180, 417, 589, 853, 882, 1039, 1088, 1149, 1330, 1375, 1411, 1453, 2351, 2934, 2988, 3008, 3049

^a*i* represents imaginary frequency.

^b represents zero-point energy (ZPE) corrections (scaling factor of 0.98)

Table III Summary of scaled harmonic frequencies of the species involved in the reaction of O (³P₂) with the propyl radical. (B3LYP / 6-311G**)

Species	Frequency (cm ⁻¹) ^{a,b}
<i>iso</i> -C ₃ H ₇	109, 117, 389, 865, 920, 926, 1008, 1123, 1153, 1341, 1380, 1385, 1441, 1449, 1450, 1462, 2872, 2877, 2953, 2954, 3019, 3020, 3099.
<i>n</i> -C ₃ H ₇	112, 243, 365, 473, 741, 863, 905, 1031, 1061, 1149, 1244, 1333, 1382, 1435, 1439, 1469, 1476, 2860, 2950, 2964, 3024, 3030, 3067, 3166
Cyclopropane	727, 728, 843, 865, 866, 1030, 1032, 1064, 1127, 1186, 1188, 1190, 1443, 1445, 1491, 3058, 3059,

	3069, 3131, 3132, 3154
Propene	209, 412, 581, 899, 920, 954, 998, 1037, 1148, 1307, 1378, 1422, 1462, 1465, 1673, 2965, 3014, 3038, 3059, 3070, 3142
Propanal	76, 206, 320, 498, 744, 857, 902, 989, 1109, 1133, 1247, 1296, 1385, 1396, 1439, 1472, 1477, 1783, 2781, 2950, 2970, 3020, 3039, 3042
Ethene	817, 954, 955, 1045, 1213, 1352, 1443, 1657, 3059, 3073, 3128, 3156
CH ₂ OH	430, 572, 1040, 1184, 1340, 1458, 3050, 3192, 3763
Acetone	51, 136, 369, 479, 525, 763, 864, 866, 1061, 1095, 1205, 1355, 1357, 1432, 1437, 1442, 1458, 1768, 2964, 2970, 3018, 3025, 3077, 3078
CH ₃	495, 1375, 1376, 3043, 3218, 3219
C ₂ H ₅	107, 469, 797, 960, 1041, 1168, 1372, 1436, 1452, 1453, 2884, 2974, 3016, 3076, 3217
Prop-2-ene-1-ol	116, 243, 324, 440, 640, 899, 934, 949, 1015, 1032, 1138, 1213, 1253, 1286, 1396, 14711442, 1478, 1681, 2897, 2935, 3062, 3079, 3146, 3760.
Oxetane	87, 757, 802, 830, 906, 927, 1009, 1024, 1130, 1141, 1175, 1215, 1246, 1246, 1294, 1358, 1465, 1488, 1518, 2950, 2960, 2991, 2992, 3011, 3062
Methyl-oxirane	206,359, 403, 757, 827, 888, 954, 1019, 1105, 1125, 1139, 1160, 1268, 1378, 1411, 1454, 1468, 1500, 2966, 3012, 3024, 3025, 3048, 3095
Cyclopropanol	319, 397, 402, 744, 800, 818, 909, 963, 1023, 1045, 1100, 1162, 1170, 1201, 1276, 1386, 1424, 1475, 3031, 3059, 3068, 3141, 3158, 3738
INT1	190, 233, 348, 391, 441, 786, 793, 893, 955, 1026, 1058, 1134, 1174, 1227, 1355, 1379, 1448, 1456, 1464, 1475, 2774, 2967, 2974, 3033, 3039, 3053, 3055
INT2	173, 241, 327, 351, 403, 465, 558, 819, 902, 939, 1004,

	1106, 1130, 1350, 1368, 1418, 1452, 1466, 2897, 2971, 3042, 3049, 3067, 3176, 3743
INT3	81, 120, 236, 268, 374, 558, 847, 906, 961, 997, 1101, 1118, 1189, 1246, 1351,1383, 1414, 1445, 1459, 1466, 2804, 2803, 2871, 2914,2993,3040,3104,3763
INT4	106, 138, 260, 270, 447, 487, 756, 865, 983, 1039, 1057, 1103, 1185, 1237,1278, 1320, 1427, 1435, 1445, 1496, 2876, 2907, 2939, 2987, 3071, 3171, 3766
INT5	35, 153, 224, 266, 463, 752, 866, 938, 1008, 1043, 1100, 1206, 1275, 1287, 1329, 1376, 1390, 1461, 1473, 1477, 2815, 2825, 2960, 2971, 2998, 3022, 3034,
INT6	82, 120, 237, 269, 374, 557, 847, 905, 961, 999, 1101, 1118, 1189, 1246, 1352, 1382, 1414, 1444, 1459, 1466, 2804, 2872, 2914, 2993, 3040, 3104, 3764
TS1	901 <i>i</i> , 143, 190, 360, 440, 496, 521, 540, 760, 864, 905, 1054, 1075, 1188, 1354, 1360, 1436, 1440, 1441, 1459, 1625, 2962, 2966, 3028
TS2	105 <i>i</i> , 205 ,330, 354, 453, 538, 630, 853, 866, 900, 1043, 1107, 1127, 1230, 1365, 1393, 1440, 1456, 1465, 2970, 2987, 3035, 3049,3071, 3178
TS3	418 <i>i</i> , 126, 177, 225, 324, 476, 568, 592, 830, 856, 927, 1042, 1092, 1338, 1365, 1385, 1402, 1441, 1447, 1548, 2810, 2962, 3026, 3027, 3062, 3184, 3196
TS4	1942 <i>i</i> , 240, 320, 349, 446, 681, 830, 867, 907, 957, 1049, 1062, 1118, 1164, 1256, 1356, 1387, 1402, 1454, 1467, 1887, 2965, 2972, 3031, 3039, 3040, 3149
TS5	213 <i>i</i> , 82, 96, 198, 371, 417, 763, 814, 908, 954, 1007, 1093, 1118, 1131, 1150, 1362, 1402, 1459, 1464, 1497, 2976, 3012, 3033, 3041, 3054, 3097
TS6	1915 <i>i</i> , 156, 216, 364, 641, 728, 860, 917, 947, 1037, 1092, 1111, 1127, 1164, 1273, 1331, 1384, 1455, 1461, 1496, 1882, 2940, 2960, 3005, 3006, 3037, 3061
TS7	1872 <i>i</i> , 142, 244, 269, 365, 545, 667, 715, 865, 937, 987, 1090, 1155, 1187, 1227, 1250, 1349, 1399, 1420, 1477, 2154, 2836, 2934, 3084, 3115, 3208, 3759

TS8	1079 <i>i</i> , 279, 372, 391, 489, 547, 614, 754, 827, 902, 980, 1047, 1061, 1111, 1134, 1175, 1200, 1262, 1389, 1407, 1466, 3046, 3053, 3084, 3128, 3193, 3742
TS9	1101 <i>i</i> , 129, 354, 455, 490, 533, 660, 742, 793, 848, 893, 958, 1161, 1173, 1190, 1266, 1359, 1404, 1434, 1453, 2892, 3027, 3041, 3063, 3140, 3170, 3684
TS10	1265 <i>i</i> , 246, 333, 386, 540, 630, 720, 747, 809, 859, 874, 1006, 1078, 1128, 1151, 1180, 1192, 1251, 1365, 1417, 1455, 3047, 3068, 3125, 3175, 3755
TS11	1339 <i>i</i> , 87, 425, 592, 663, 724, 727, 848, 926, 989, 1010, 1124, 1146, 1164, 1240, 1245, 1279, 1327, 1426, 1460, 1509, 2935, 2964, 3010, 3013, 3107
TS12	304 <i>i</i> , 68, 155, 178, 303., 529, 632, 810, 825, 977, 1043, 1099, 1190, 1220, 1373, 1447, 1449, 1449, 1463, 1593, 2812, 2856, 2922, 2994, 3034, 3069, 3160
TS13	1966 <i>i</i> , 98, 219, 266, 456, 588, 763, 876, 884, 1010, 1077, 1114, 1133, 1242, 1285, 1360, 1389, 1448, 1472, 1476, 2348, 2915, 2967, 2975, 2995, 3028, 3038,
TS14	1169 <i>i</i> , 48, 196, 236, 302, 485, 607, 665, 858, 889, 1020, 1091, 1107, 1245, 1303, 1365, 1393, 1421, 1474, 1475, 1614, 2875, 2916, 2971, 2985, 3030, 3043
TS15	213 <i>i</i> , 83, 96, 198, 371, 418, 764, 814, 908, 955, 1008, 1094, 1118, 1131, 1150, 1274, 1372, 402, 1459, 1464, 1497, 2976, 3013, 3033, 3041, 3053, 3096.38134
TS16	1118 <i>i</i> , 161, 308, 377, 511, 613, 651, 819, 910, 984, 1044, 1119, 1137, 1161, 1183, 1218, 1358, 1398, 1454, 1467, 1496, 2966, 2982, 3038, 3047, 3050, 3110,

^ai represents imaginary frequency.

b represents zero-point energy (ZPE) corrections (scaling factor of 0.98)

Table IV Summary of scaled harmonic frequencies of the various species involved in the reaction of O (3P_2) with the methyl radical (CBS-QB3).

Species	Frequency (cm ⁻¹) ^a
CH ₃	269, 1527, 1528, 3262, 3445, 3446
CH ₂	1558, 3112, 3180
Methanal	1326, 1377, 1666, 2023, 3130, 3203
INT1	817, 1104, 1208, 1570, 1581, 1652, 3161, 3233, 3252
INT2	424, 859, 1151, 1282, 1483, 1613, 3267, 3408, 4131
TS1	1763i, 493, 766, 993, 1315, 1438, 1669, 3224, 3335
TS2	2624i, 900, 1041, 1242, 1260, 1604, 2422, 3253, 3371

^ai represents imaginary frequency.

Table V Summary of scaled harmonic frequencies of the various species involved in the reaction of O (3P_2) with the ethyl radical (CBS-Q)

Species	Frequency (cm ⁻¹) ^a
Oxirane	878, 971, 985, 1152, 1279, 1280, 1289, 1293, 1423, 1636, 1691, 3274, 3288, 3362, 3379
C ₂ H ₅	174, 466, 861, 1075, 1107, 1299, 1537, 1596, 1620, 1625, 3148, 3218, 3254, 3297, 3397
Ethene	887, 1082, 1083, 1150, 1340, 1488, 1596, 1849, 3303, 3328, 3380, 3407
Ethanal	160, 543, 847, 956, 1223, 1256, 1519, 1555, 1598, 1607, 2029, 3124, 3190, 3251, 3309
Methanal	1326, 1377, 1666, 2023, 3130, 3203

INT1	128, 283, 453, 932, 959, 1160, 1200, 1372, 1517, 1557, 1584, 1619, 1633, 3170, 3193, 3205, 3263, 3274
INT2	176, 316, 420, 480, 942, 1050, 1152, 1217, 1357, 1391, 1552, 1612, 1654, 3100, 3161, 3310, 3422, 4124
INT3	199, 365, 436, 734, 988, 1127, 1150, 1286, 1409, 1517, 1580, 1609, 1628, 3161, 3234, 3261, 3278, 4130
TS1	1138i, 202, 492, 552, 607, 929, 994, 1185, 1216, 1485, 1537, 1599, 1612, 1648, 3184, 3198, 3264, 3304
TS2	56i, 142, 297, 569, 653, 782, 943, 1150, 1342, 1485, 1551, 1563, 1682, 3177, 3247, 3266, 3400, 3417
TS3	2908i, 394, 723,873, 1023, 1048, 1153, 1154, 1268, 1322, 1442, 1563, 1668, 1901, 3233, 3288, 3296, 3402
TS4 ^b	2486i, 293, 649, 775, 912, 916, 977, 1018, 1154, 1236, 1246, 1325, 1537, 1602, 3149, 3229, 3257, 3378
TS5	2485i, 369, 411, 463, 783, 873, 1037, 1179, 1283, 1372, 1413, 1509, 1573, 2188, 3281, 3315, 3437, 4116
TS6	2614i, 199, 451, 673, 963, 997, 1160, 1203, 1288, 1486, 1550, 1610, 1623, 2417, 3178, 3247, 3271, 3288

^a i represents imaginary frequency.

^b TS 4 was calculated at the second-order Møller-Plesset (MP2) level using the 6-31 G(d) basis set

Table VI Summary of scaled harmonic frequencies of the various species involved in the reaction of O (3P_2) with the propyl radical (CBS-Q).

Species	Frequency (cm ⁻¹) ^a
<i>iso</i> -C ₃ H ₇	133, 167, 373,482, 925, 1009,1025, 1135, 1204, 1279, 1477, 1552, 1553, 1612, 1621, 1624, 1630, 3134, 3140, 3206, 3210, 3250, 3251, 3314.
<i>n</i> -C ₃ H ₇	160, 270, 390, 490, 816, 940, 985, 1140, 1151, 1273, 1392, 1488, 1551, 1589, 1619, 1634, 1641, 3133, 3185, 3200, 3251, 3257, 3289, 3388
Cyclopropane	795, 796, 914, 955, 956, 1177, 1178, 1203, 1260, 1297, 1320, 1321, 1602, 1603, 1668, 3290, 3291, 3305, 3367, 3368, 3390
Propene	224, 440, 641, 978, 1046, 1050, 1110, 1167, 1270, 1439, 1539, 1579, 1627, 1630, 1871, 3191, 3251, 3266, 3304, 3325, 3388
Propanal	62, 235, 351, 542, 818, 937, 1000, 1082, 1243, 1258, 1368, 1458, 1549, 1555, 1607, 1635, 1639, 2026, 3107, 3188, 3193, 3253, 3274, 3277
Ethene	887, 1082, 1083, 1150, 1340, 1488, 1596, 1849, 3303, 3328, 3380, 3407
CH ₂ OH	887, 1082, 1083, 1150, 1340, 1488, 1596, 1849, 3303, 3328, 3380, 3407
Acetone	53, 147, 398, 530, 573, 842, 969, 973, 1182, 1231, 1342, 1530, 1541, 1598, 1601, 1605, 1624, 2018, 3189, 3197, 3250, 3258, 3311, 3312
CH ₃	269, 1527, 1528, 3262, 3445, 3446
C ₂ H ₅	174, 466, 861, 1075, 1107, 1299, 1537, 1596, 1620, 1625, 3148, 3218, 3254, 3297, 3397
Prop-2-ene-1-ol	122, 303, 357, 479, 705, 981, 1052, 1069, 1134, 1186, 1256, 1359, 1391, 1421, 1555, 1614, 1658, 1882, 3152, 3198, 3310, 3339, 3394, 4119
Oxetane	94, 819, 896, 903, 1003, 1025, 1140, 1168, 1266, 1272, 1314, 1340, 1387, 1438, 1523, 1628, 1658, 1689, 3205, 3213, 3244, 3252, 3254, 3297

Methyl-oxirane	220, 395, 438, 854, 947, 986, 1074, 1140, 1240, 1269, 1287, 1309, 1411, 1534, 1586, 1619, 1632, 1686, 3193, 3260, 3270,3276, 3298, 3364,
Cyclopropanol	355, 433, 441, 818, 881, 902, 1020, 1074, 1170, 1188, 1241, 1289, 1302, 1341, 1426, 1547, 1586, 1658, 3289, 3294, 3309, 3376, 3396, 4102
INT1	217, 265, 373, 381, 491, 872, 969, 999,1060, 1186, 1199, 1302, 1400, 1462, 1531, 1555, 1616, 1623, 1629, 1642, 3156, 3187, 3196, 3257, 3266, 3277, 3279
INT2	212, 266, 355, 375, 446, 506, 596, 896, 993, 1052, 1137, 1236, 1255, 1398, 1495, 1521, 1554, 1581, 1621, 1633, 3154, 3196, 3270, 3277, 3293, 3399, 4112
INT3	96, 157, 278, 314, 434, 624, 909, 1019, 1073, 1127, 1217, 1240,1340, 1387, 1494, 1554, 1598, 1617, 1630, 1653, 3096 ,3137, 3176, 3231, 3283, 3318, 4125
INT4	161, 296, 316, 474, 510, 824, 942, 1086, 1134, 1189, 1219, 1332, 1369, 1429, 1470, 1591, 1606, 1625, 1669, 3155, 3156, 3190, 3235, 3293, 3393, 4122
INT5	133, 241, 271, 292, 497, 822, 954, 1027, 1100, 1159, 1217, 1352, 1421, 1444, 1549, 1560, 1583, 1627, 1636, 1645, 3161, 3183, 3194, 3199, 3230, 3255, 3262
INT6	108, 250, 288, 360, 487, 723, 869, 953, 1111, 1177, 1192, 1278,1370, 1388, 1472, 1552, 1577, 1624, 1634, 1644, 3149, 3186, 3217, 3251, 3259, 3262, 4130
TS1	1215i, 181, 219, 305, 513, 547, 603, 674, 848, 993, 1043, 1172, 1182, 1337, 1540, 1541, 1583, 1607, 1612, 1624, 1657, 3188, 3193, 3260, 3266, 3306, 3308
TS2	1380i, 232, 353, 388, 479, 503, 519, 904, 963, 982, 1113, 1151, 1203, 1261, 1333, 1379, 1522, 1570, 1605, 1624, 1633, 3196, 3242, 3268, 3281, 3355, 3475
TS3	644i, 136, 203, 251, 354, 512, 682, 684, 896, 947, 1060, 1170, 1214, 1460, 1535, 1554, 1565, 1581, 1614, 1631, 3183, 3197, 3245, 3259, 3292, 3395, 3410

TS 4	2910i, 259, 348, 377, 487, 707, 914, 978, 995, 1037, 1156, 1185, 1230, 1287, 1418, 1507, 1558, 1573, 1621, 1630, 1903, 3191, 3233, 3263, 3273, 3289, 3395
TS5	225i, 21, 22, 66, 408, 458, 865, 938, 1013, 1078, 1131, 1235, 1251, 1290, 1305, 1419, 1531, 1582, 1628, 1629, 1682, 3200, 3264, 3272, 3282, 3305, 3360
TS6	2905i, 168, 223, 391, 663, 793, 943, 1013, 1077, 1140, 1183, 1219, 1261, 1302, 1432, 1489, 1554, 1623, 1628, 1667, 1901, 3174, 3220, 3242, 3271, 3272, 3315
TS7	2423i, 121, 294, 312, 393, 551, 797, 817, 948, 991, 1142, 1244, 1252, 1345, 1376, 1404, 1488, 1560, 1603, 1659, 2232, 3159, 3199, 3313, 3343, 3428, 4106,
TS 8	1496i, 272, 384, 424, 494, 563, 604, 814, 891, 990, 1098, 1109, 1132, 1221, 1276, 1317, 1332, 1410, 1547, 1561, 1631, 3281, 3317, 3338, 3362, 3452, 4111
TS9	930i, 82, 112, 318, 385, 473, 600, 689, 820, 856, 903, 1194, 1224, 1245, 1301, 1323, 1507, 1547, 1599, 1637, 3260, 3277, 3288, 3359, 3375, 3392, 4121
TS10	1420i, 213, 323, 350, 452, 521, 578, 718, 787, 858, 951, 1035, 1141, 1223, 1283, 1320, 1339, 1399, 1549, 1571, 1626, 3275, 3320, 3348, 3394, 3431, 4118
TS11	1644i, 6, 388, 451, 564, 735, 798, 927, 1058, 1075, 1102, 1145, 1185, 1262, 1313, 1375, 1424, 1486, 1585, 1628, 1674, 3191, 3231, 3241, 3292, 3329, 3440
TS12	544i, 77, 193, 209, 324, 600, 789, 908, 922, 991, 1109, 1214, 1322, 1342, 1486, 1540, 1606, 1626, 1626, 1680, 3169, 3174, 3235, 3256, 3264, 3290, 3380
TS13	612i, 112, 246, 294, 495, 675, 853, 957, 1010, 1104, 1199, 1234, 1271, 1383, 1433, 1531, 1554, 1620, 1634, 1641, 2415, 3169, 3188, 3230, 3256, 3265, 3269
TS14	1854i, 68, 239, 279, 397, 534, 703, 808, 917, 966, 1102, 1182, 1237, 1381, 1446, 1460, 1553, 1603, 1615, 1635, 1641, 3149, 3190, 3233, 3236, 3259, 3269

TS15	225i, 20, 21, 67, 408, 458, 864, 938, 1013, 1078, 1131, 1234, 1251, 1290, 1305, 1419, 1531, 1582, 1628, 1629, 1682, 3200, 3264, 3272, 3282, 3304, 3360
TS 16	1269i, 146, 295, 357, 442, 478, 557, 903, 1002, 1083, 1107, 1189, 1267, 1281, 1322, 1389, 1513, 1566, 1618, 1635, 1672, 3207, 3224, 3279, 3284, 3294, 3398

^ai represents imaginary frequency.

Table VII Summary of scaled harmonic frequencies of the various species involved in the reaction of O (³P₂) with the methyl radical. (CBS-QB3)

CH ₃	505, 1403, 1404, 3104, 3283, 3284
CH ₂	1404, 2889, 2951
Methanal	1202, 1270, 1539, 1827, 2870, 2919
INT1	718, 962, 1107, 1360, 1370, 1517, 2892, 2959, 3001
INT2	439, 584, 1061, 1208, 1367, 1488, 3112, 3257, 3840
TS1	1182i, 151, 566, 1098, 1243, 1498, 1659, 2935, 3010
TS2	2041i, 719, 965, 1135, 1144, 1482, 2437, 3032, 3142

^ai represents imaginary frequency.

Table VIII Summary of scaled harmonic frequencies of the various species involved in the reaction of O (³P₂) with the ethyl radical. (CBS-QB3)

Species	Frequency (cm ⁻¹) ^a
Oxirane	819, 845, 890, 1040, 1140, 1143, 1168, 1172, 1301, 1505, 1541, 3076, 3083, 3156, 3171

C ₂ H ₅	109, 479, 813, 980, 1062, 1192, 1400, 1465, 1482, 1483, 2943, 3035, 3078, 3139, 3238
Ethene	834, 973, 974, 1066, 1238, 1379, 1472, 1691, 3121, 3136, 3192, 3221
Ethanal	158, 508, 777, 882, 1125, 1135, 1375, 1426, 1460, 1471, 1824, 2856, 3022, 3077, 3136
Methanal	1202, 1270, 1539, 1827, 2870, 2919
INT1	27, 273, 433, 867, 887, 1069, 1098, 1241, 1343, 1390, 1411, 1485, 1496, 2885, 2893, 3031, 3098, 3107
INT2	153, 269, 412, 470, 858, 958, 1069, 1109, 1217, 1277, 1419, 1460, 1494, 2867, 2937, 3149, 3261, 3839
INT3	182, 356, 410, 583, 930, 1024, 1060, 1208, 1280, 1395, 1449, 1465, 1492, 2944, 3041, 3094, 3115, 3845
TS1	813i, 178, 387, 454, 501, 811, 896, 1098, 1125, 1375, 1402, 1464, 1474, 1695, 2851, 3023, 3090, 3135
TS2	341i, 138, 267, 499, 547, 600, 895, 1105, 1249, 1409, 1427, 1489, 1636, 2880, 2925, 3091, 3256, 3268
TS3	1986i, 351, 720, 821, 922, 961, 1071, 1072, 1151, 1208, 1300, 1429, 1530, 1928, 3037, 3083, 3110, 3219
TS4	1311i, 88, 501, 766, 774, 886, 891, 987, 1132, 1179, 1189, 1282, 1474, 1538, 3058, 3126, 3157, 3270
TS5	1957i, 354, 413, 436, 702, 797, 951, 1088, 1168, 1258, 1305, 1397, 1444, 2143, 3086, 3135, 3259, 3823
TS6	2009i, 184, 425, 601, 870, 900, 1060, 1110, 1172, 1357, 1403, 1470, 1483, 2398, 2994, 3049, 3069, 3111

^ai represents imaginary frequency.

Table IX Summary of harmonic frequencies of the various species involved in the reaction of O (3P_2) with the propyl radical. (CBS-QB3)

Species	Frequency (cm ⁻¹) ^a
<i>iso</i> -C ₃ H ₇	111, 119, 355, 397, 883, 939, 945, 1029, 1146, 1177, 1367, 1408, 1413, 1470, 1479, 1480, 1492, 2931, 2936, 3013, 3014, 3081, 3082, 3162
<i>n</i> -C ₃ H ₇	114, 248, 327, 483, 756, 881, 923, 1052, 1083, 1172, 1269, 1360, 1410, 1464, 1468, 1499, 1506, 2918, 3010, 3024, 3086, 3092, 3130, 3231,
Cyclopropane	742, 743, 861, 883, 884, 1051, 1053, 1086, 1150, 1210, 1211, 1214, 1472, 1474, 1521, 3120, 3121, 3129, 3195, 3196, 3218
Propene	209, 419, 593, 918, 938, 973, 1017, 1058, 1172, 1333, 1407, 1450, 1492, 1496, 1706, 3026, 3074, 3099, 3121, 3133, 3206
Propanal	92, 207, 293, 533, 657, 894, 895, 1032, 1119, 1147, 1279, 1328, 1417, 1426, 1450, 1503, 1504, 1817, 2837, 3029, 3031, 3056, 3091, 3103
Ethene	834, 973, 974, 1066, 1238, 1379, 1472, 1691, 3121, 3136, 3192, 3221
CH ₂ OH	439, 584, 1061, 1208, 1367, 1488, 3112, 3257, 3840
Acetone	37, 133, 377, 489, 535, 779, 881, 882, 1083, 1118, 1230, 1383, 1385, 1460, 1466, 1470, 1488, 1804, 3024, 3031, 3079, 3087, 3140, 3141
CH ₃	505, 1403, 1404, 3104, 3283, 3284
C ₂ H ₅	109, 479, 813, 980, 1062, 1192, 1400, 1465, 1482, 1483, 2943, 3035, 3078, 3139, 3238
Prop-2-ene-1-ol	118, 248, 331, 449, 653, 917, 953, 968, 1036, 1054, 1161, 1238, 1279, 1312, 1425, 1472, 1508, 1715, 2956, 2996, 3125, 3142, 3210, 3837

Oxetane	89, 773, 819, 847, 924, 946, 1030, 1045, 1153, 1164, 1199, 1240, 1271, 1320, 1386, 1495, 1519, 1549, 3010, 3020, 3052, 3053, 3072, 3124
Methyl-oxirane	211, 366, 411, 772, 844, 906, 973, 1040, 1128, 1148, 1162, 1184, 1294, 1406, 1440, 1484, 1498, 1532, 3027, 3073, 3086, 3087, 3110, 3158
Cyclopropanol	326, 405, 410, 759, 816, 835, 928, 983, 1044, 1066, 1122, 1186, 1194, 1226, 1302, 1414, 1453, 1505, 3093, 3121, 3131, 3205, 3222, 3814
INT1	194, 238, 355, 399, 450, 802, 889, 911, 975, 1047, 1080, 1157, 1198, 1252, 1383, 1407, 1479, 1486, 1494, 1505, 2831, 3028, 3035, 3096, 3102, 3115, 3117
INT2	177, 246, 324, 359, 412, 475, 569, 836, 920, 959, 1025, 1129, 1153, 1281, 1365, 1378, 1396, 1447, 1482, 1497, 2956, 3032, 3104, 3111, 3130, 3241, 3819
INT3	83, 122, 241, 274, 382, 569, 864, 924, 981, 1019, 1124, 1141, 1213, 1272, 1380, 1410, 1443, 1474, 1489, 1496, 2861, 2931, 2974, 3054, 3102, 3167, 3840
INT4	108, 141, 265, 276, 456, 497, 771, 883, 1003, 1060, 1079, 1126, 1209, 1262, 1304, 1347, 1456, 1464, 1475, 1527, 2935, 2966, 2999, 3048, 3134, 3236, 3843
INT5	36, 156, 229, 271, 472, 767, 884, 957, 1028, 1065, 1123, 1231, 1301, 1313, 1356, 1405, 1419, 1491, 1503, 1507, 2873, 2883, 3020, 3032, 3060, 3084, 3095
INT6	95, 228, 271, 372, 461, 584, 796, 896, 1044, 1083, 1095, 1195, 1253, 1271, 1349, 1414, 1452, 1484, 1499, 1509, 2924, 3021, 3026, 3085, 3097, 3099, 3845
TS1	918i, 146, 194, 367, 449, 506, 532, 551, 777, 882, 923, 1076, 1097, 1212, 1382, 1388, 1465, 1469, 1470, 1489, 1658, 3021, 3027, 3090, 3096, 3139, 3141
TS2	1072i, 209, 337, 361, 462, 549, 643, 870, 884, 918, 1064, 1130, 1150, 1158, 1197, 1255, 1393, 1422, 1469, 1486, 1495, 3032, 3047, 3097, 3111, 3134, 3243

TS3	427i, 129, 182, 230, 331, 486, 580, 604, 847, 875, 946, 1063, 1114, 1366, 1393, 1412, 1431, 1470, 1477, 1581, 2866, 3023, 3088, 3089, 3125, 3249, 3261
TS4	1983i, 245, 327, 356, 455, 695, 847, 885, 926, 977, 1071, 1084, 1141, 1188, 1282, 1384, 1415, 1432, 1484, 1497, 1927, 3026, 3034, 3093, 3101, 3103, 3213
TS5	217i, 84, 98, 202, 379, 426, 779, 831, 927, 974, 1028, 1116, 1141, 1154, 1173, 1300, 1400, 1431, 1489, 1494, 1528, 3037, 3074, 3095, 3104, 3116, 3160
TS6	1955i, 159, 221, 372, 654, 743, 878, 936, 966, 1058, 1114, 1134, 1149, 1188, 1299, 1357, 1412, 1485, 1491, 1527, 1922, 3000, 3021, 3066, 3067, 3099, 3123
TS7	1906i, 115, 250, 279, 371, 511, 725, 768, 889, 921, 988, 1143, 1158, 1246, 1260, 1288, 1371, 1430, 1456, 1509, 2204, 2956, 3007, 3146, 3167, 3261, 3806
TS8	1101i, 285, 380, 399, 499, 559, 627, 770, 844, 921, 1000, 1069, 1083, 1134, 1158, 1199, 1225, 1288, 1418, 1436, 1496, 3109, 3116, 3147, 3192, 3259, 3819
TS9	1124i, 131, 362, 465, 501, 543, 674, 757, 810, 866, 912, 978, 1185, 1197, 1215, 1291, 1387, 1433, 1464, 1482, 2953, 3089, 3104, 3126, 3204, 3235, 3760
TS10	1292i, 252, 340, 394, 553, 643, 735, 763, 826, 877, 892, 1027, 1100, 1151, 1174, 1204, 1217, 1277, 1393, 1446, 1485, 3109, 3131, 3138, 3189, 3240, 3832
TS11	1366i, 89, 434, 604, 677, 739, 747, 865, 945, 1009, 1031, 1147, 1169, 1189, 1265, 1271, 1305, 1354, 1455, 1490, 1540, 2995, 3025, 3072, 3075, 3123, 3170
TS12	310i, 71, 158, 182, 310, 540, 645, 827, 842, 997, 1065, 1121, 1214, 1245, 1401, 1476, 1478, 1479, 1493, 1625, 2870, 2915, 2982, 3055, 3096, 3131, 3224
TS13	2007i, 101, 223, 272, 465, 601, 778, 894, 902, 1031, 1099, 1138, 1157, 1268, 1312, 1388, 1417, 1477, 1502, 1506, 2396, 2974, 3028, 3036, 3056, 3090, 3100

TS14	1193i, 49, 200, 241, 308, 494, 620, 679, 876, 907, 1041, 1114, 1130, 1271, 1329, 1393, 1422, 1450, 1504, 1505, 1647, 2933, 2975, 3032, 3046, 3092, 3105
TS15	1273i, 150, 173, 304, 397, 508, 742, 826, 894, 971, 983, 1077, 1134, 1183, 1197, 1274, 1402, 1432, 1476, 1494, 1537, 3007, 3047, 3070, 3109, 3114, 3184
TS16	1139i, 164, 315, 385, 521, 626, 663, 837, 929, 1004, 1066, 1142, 1160, 1184, 1207, 1243, 1386, 1426, 1484, 1497, 1526, 3027, 3043, 3100, 3109, 3112, 3174

^ai represents imaginary frequency.