

**Table S1.** Calculated frequencies (in  $\text{cm}^{-1}$ ) for the reactants, products, transition states, and complexes for the title reactions at the B3LYP/6-311G(d,p) level.

species	B3LYP/6-311G(d,p)
R1	65, 71, 122, 149, 270, 278, 322, 362, 469, 533, 568, 648, 777, 838, 874, 1021, 1040, 1050, 1077, 1147, 1185, 1245, 1251, 1268, 1317, 1333, 1339, 1418, 1467, 1483, 1509, 1530, 2958, 2985, 3047, 3057, 3083, 3105, 3843
R2	36, 70, 102, 128, 210, 222, 235, 288, 309, 323, 333, 372, 380, 423, 508, 529, 538, 596, 650, 733, 777, 908, 942, 1097, 1121, 1134, 1156, 1183, 1219, 1225, 1267, 1288, 1345, 1402, 1436, 1497, 3022, 3129, 3819
HCl	2929
P1	67, 68, 122, 135, 257, 272, 331, 362, 478, 533, 572, 647, 768, 837, 914, 1020, 1055, 1056, 1072, 1155, 1217, 1265, 1284, 1294, 1341, 1354, 1400, 1421, 1481, 1504, 2881, 2889, 3045, 3055, 3081, 3103
P2	58, 70, 117, 126, 276, 327, 356, 370, 466, 532, 563, 593, 649, 787, 837, 985, 1031, 1057, 1110, 1144, 1201, 1229, 1252, 1268, 1328, 1330, 1407, 1458, 1481, 1494, 2956, 3048, 3057, 3101, 3103, 3843
P3	47, 55, 79, 210, 257, 276, 325, 362, 430, 511, 529, 567, 664, 812, 869, 923, 1020, 1055, 1132, 1134, 1143, 1219, 1248, 1264, 1307, 1348, 1370, 1462, 1464, 1493, 2903, 2945, 3031, 3089, 3191, 3841
P4	38, 50, 98, 168, 260, 270, 322, 326, 461, 470, 567, 588, 654, 793, 855, 1002, 1028, 1069, 1084, 1122, 1151, 1211, 1244, 1260, 1305, 1331, 1437, 1463, 1472, 1528, 2959, 2969, 3006, 3075, 3191, 3843
P5	29, 72, 93, 131, 213, 221, 233, 287, 301, 326, 333, 375, 396, 508, 530, 534, 597, 647, 711, 756, 896, 1017, 1059, 1119, 1159, 1166, 1211, 1221, 1255, 1275, 1324, 1345, 1510, 1520, 2976, 3048
P6	41, 62, 85, 141, 206, 225, 234, 287, 298, 322, 336, 365, 378, 460, 517, 531, 546, 584, 599, 655, 733, 783, 928, 1004, 1113, 1151, 1167, 1202, 1219, 1229, 1275, 1336, 1363, 1474, 3260, 3767
TS1	1113i, 21, 33, 78, 116, 128, 173, 276, 324, 361, 436, 467, 533, 566, 648, 754, 829, 838, 907, 976, 1000, 1037, 1050, 1127, 1151, 1166, 1207, 1255, 1264, 1315, 1340, 1360, 1411, 1425, 1482, 1506, 2900, 3026, 3050, 3062, 3091, 3114
TS2	277i, 26, 46, 83, 130, 135, 178, 285, 327, 362, 441, 467, 533, 565, 643, 660, 778, 841, 902, 948, 978, 1027, 1060, 1099, 1156, 1180, 1206, 1242, 1261, 1272, 1334, 1345, 1420, 1460, 1480, 1492, 3007, 3048, 3060, 3079, 3112, 3813
TS3	463i, 26, 59, 85, 118, 143, 156, 282, 322, 353, 395, 471, 528, 556, 624, 646, 757, 839, 852, 898, 917, 1048, 1065, 1086, 1110, 1164, 1184, 1236, 1266, 1282, 1303, 1400, 1409, 1425, 1455, 1476, 2973, 3002, 3008, 3073, 3127, 3793
TS4	690i, 45, 66, 74, 81, 115, 173, 270, 281, 321, 340, 449, 509, 540, 569, 660, 751, 824, 845, 874, 964, 1022, 1070, 1092, 1115, 1160, 1182, 1221, 1259, 1270, 1302, 1324, 1416, 1456, 1471, 1531, 2969, 2972, 3027, 3076, 3131, 3846
TS5	1194i, 18, 31, 33, 71, 119, 142, 212, 215, 228, 284, 305, 324, 332, 375, 391, 428, 506, 529, 538, 596, 649, 733, 775, 829, 894, 908, 1010, 1119, 1126, 1157, 1170, 1182, 1217, 1224, 1257, 1289, 1340, 1369, 1404, 2964, 3061

TS6	847i, 23, 49, 62, 75, 130, 161, 210, 227, 240, 281, 291, 325, 336, 369, 379, 422, 502, 530, 541, 587, 604, 657, 736, 789, 910, 919, 1031, 1103, 1125, 1161, 1172, 1184, 1201, 1222, 1229, 1283, 1328, 1339, 1439, 3163, 3750
ER1	25, 40, 80, 117, 126, 159, 258, 282, 323, 362, 452, 485, 533, 569, 648, 773, 837, 869, 1002, 1024, 1039, 1061, 1147, 1177, 1232, 1246, 1267, 1318, 1329, 1343, 1414, 1447, 1484, 1498, 1516, 2999, 3049, 3051, 3062, 3088, 3112, 3800
ER2	29, 46, 82, 128, 135, 158, 280, 314, 340, 362, 435, 482, 532, 573, 649, 754, 835, 846, 981, 1019, 1028, 1058, 1115, 1149, 1159, 1197, 1236, 1261, 1271, 1331, 1343, 1351, 1420, 1453, 1480, 1493, 3018, 3028, 3059, 3088, 3112, 3810
ER5	24, 35, 49, 75, 99, 118, 171, 217, 227, 235, 288, 329, 333, 348, 380, 397, 504, 519, 532, 543, 596, 651, 732, 778, 908, 941, 1070, 1122, 1130, 1162, 1183, 1218, 1226, 1254, 1286, 1342, 1380, 1424, 1496, 3068, 3156, 3774
EP1	6, 26, 66, 76, 89, 130, 162, 274, 341, 361, 375, 481, 532, 547, 576, 593, 648, 780, 838, 946, 1016, 1054, 1061, 1067, 1160, 1217, 1264, 1280, 1297, 1340, 1348, 1399, 1424, 1481, 1504, 2635, 2877, 2896, 3047, 3058, 3085, 3107
EP2	26, 36, 70, 87, 122, 125, 192, 279, 328, 360, 436, 473, 532, 569, 640, 650, 701, 768, 835, 840, 998, 1029, 1061, 1128, 1153, 1211, 1234, 1257, 1269, 1332, 1341, 1417, 1461, 1480, 1491, 1982, 2987, 3057, 3065, 3080, 3108, 3822
EP3	14, 55, 64, 72, 80, 96, 194, 266, 287, 295, 329, 356, 434, 475, 524, 530, 566, 643, 820, 867, 922, 1034, 1062, 1103, 1129, 1164, 1195, 1256, 1270, 1306, 1383, 1411, 1432, 1459, 1482, 2870, 2944, 2970, 2979, 3075, 3173, 3792
EP4	9, 17, 24, 40, 84, 98, 175, 262, 266, 275, 301, 330, 340, 469, 492, 567, 600, 653, 793, 856, 996, 1031, 1068, 1077, 1103, 1140, 1208, 1248, 1275, 1303, 1328, 1436, 1462, 1470, 1529, 2884, 2953, 2971, 3011, 3084, 3184, 3843
EP5	14, 23, 28, 72, 82, 95, 141, 213, 217, 227, 284, 308, 313, 332, 351, 373, 385, 390, 503, 529, 540, 595, 649, 723, 737, 790, 908, 1046, 1083, 1121, 1154, 1185, 1218, 1219, 1257, 1291, 1342, 1350, 1387, 2809, 2949, 2977
EP6	22, 33, 44, 56, 65, 84, 142, 151, 207, 211, 228, 242, 287, 292, 325, 337, 367, 379, 451, 513, 529, 545, 585, 599, 654, 731, 779, 927, 1017, 1108, 1142, 1168, 1204, 1220, 1233, 1266, 1332, 1366, 1474, 2908, 3256, 3758

**Table S2.** Calculated frequencies (in  $\text{cm}^{-1}$ ) for the species of the subsequent reactions of  $\text{CF}_3(\text{CX}_2)_2\text{C}\cdot\text{HOH}$  ( $\text{X}=\text{H}, \text{F}$ ) at the B3LYP/6-311G(d,p) level.

species	B3LYP/6-311G(d,p)
$\text{CF}_3(\text{CH}_2)_2\text{C}\cdot\text{HOH}$	58, 70, 117, 126, 276, 327, 356, 370, 466, 532, 563, 593, 649, 787, 837, 985, 1031, 1057, 1110, 1144, 1201, 1229, 1252, 1268, 1328, 1330, 1407, 1458, 1481, 1494, 2956, 3048, 3057, 3101, 3103, 3843
$\text{CF}_3(\text{CF}_2)_2\text{C}\cdot\text{HOH}$	41,62, 85, 141, 206, 225, 234, 287, 298, 322, 336, 365, 378, 460, 517, 531, 546, 584, 599, 655, 733, 783, 928, 1004, 1113, 1151, 1167, 1202, 1219, 1229, 1275, 1336, 1363, 1474, 3260, 3767
$\text{O}_2$	1626
$\text{HO}_2\cdot$	1163, 1428, 3605
$\text{NO}$	1988
$\text{NO}_2$	766, 1399, 1706
$\text{CF}_3\text{CH}_2\text{CH}_2\text{CHO}$	54, 66, 105, 160, 288, 355, 370, 507, 533, 566, 645, 774, 829, 864, 1007, 1033, 1073, 1158, 1161, 1243, 1265, 1297, 1338, 1408, 1421, 1471, 1487, 1825, 2851, 3026, 3056, 3098, 3117
$\text{CF}_3\text{CF}_2\text{CF}_2\text{CHO}$	20, 57, 71, 142, 209, 222, 237, 262, 287, 329, 351, 371, 415, 500, 528, 572, 598, 653, 724, 774, 866, 1009, 1128, 1135, 1165, 1196, 1213, 1232, 1287, 1344, 1391, 1853, 2965
$\text{CF}_3(\text{CH}_2)_2\text{C}(\text{OO}\cdot)\text{HOH}$	35, 65, 79, 119, 134, 206, 304, 322, 361, 425, 460, 509, 533, 578, 608, 661, 728, 821, 843, 996, 1035, 1061, 1142, 1150, 1162, 1201, 1241, 1267, 1282, 1335, 1345, 1362, 1422, 1480, 1484, 1496, 3019, 3059, 3068, 3102, 3121, 3781
$\text{CF}_3(\text{CF}_2)_2\text{C}(\text{OO}\cdot)\text{HOH}$	26, 50, 66, 73, 115, 163, 209, 236, 243, 290, 302, 316, 328,, 345, 371, 386, 399, 501, 532, 570, 593, 625, 671, 735, 801, 897, 928, 1122, 1135, 1153, 1175, 1187, 1199, 1223, 1234, 1255, 1304, 1329, 1360, 1481, 3076, 3800
$\text{CF}_3(\text{CH}_2)_2\text{C}(\text{OONO})\text{HOH}$	23, 40, 51, 70, 124, 134, 212, 218, 268, 326, 357, 370, 392, 431, 452, 529, 533, 580, 608, 658, 763, 835, 841, 874, 940, 1015, 1033, 1063, 1118, 1153, 1160, 1238, 1266, 1281, 1335, 1341, 1390, 1418, 1464, 1481, 1495, 1813, 3006, 3060, 3070, 3106, 3125, 3819
$\text{CF}_3(\text{CF}_2)_2\text{C}(\text{OONO})\text{HOH}$	30, 38, 52, 64, 73, 121, 166, 198, 220, 235, 245, 262, 280, 292, 316, 328, 346, 373, 388, 408, 436, 504, 531, 576, 594, 623, 669, 735, 796, 837, 925, 942, 1013, 1119, 1135, 1138, 1175, 1182, 1221, 1228, 1252, 1302, 1333, 1383, 1460, 1854, 3063, 3832
$\text{CF}_3(\text{CH}_2)_2\text{C}(\text{O}\cdot)\text{HOH}$	40, 68, 122, 141, 226, 231, 320, 359, 398, 465, 533, 550, 581, 647, 786, 830, 896, 922, 998, 1048, 1065, 1132, 1160, 1178, 1217, 1245, 1265, 1308, 1329, 1340, 1416, 1485, 1500, 2720, 3060, 3075, 3108, 3129, 3812
$\text{CF}_3(\text{CF}_2)_2\text{C}(\text{O}\cdot)\text{HOH}$	42, 64, 75, 122, 182, 191, 214, 239, 259, 289, 297, 329, 348, 373, 406, 500, 529, 552, 574, 601, 641, 715, 744, 856, 978, 1040,

	1105, 1121, 1169, 1178, 1201, 1210, 1237, 1261, 1289, 1325, 1385, 2935, 3802
TS-H-O2	863 <i>i</i> , 30, 56, 107, 117, 143, 192, 320, 354, 368, 494, 497 533, 577, 629, 653, 720, 771, 841, 903, 1012, 1041, 1058, 1086, 1159, 1170, 1248, 1264, 1296, 1305, 1339, 1376, 1420, 1468, 1487, 1609, 1865, 3002, 3027, 3061, 3093, 3115
TS-F-O2	837 <i>i</i> , 18, 54, 66, 101, 121, 180, 213, 237, 263, 276, 290, 320, 336, 374, 377, 493, 526, 538, 572, 597, 664, 676, 724, 746, 816, 916, 1009, 1040, 1118, 1135, 1165, 1195, 1220, 1232, 1289, 1308, 1341, 1373, 1626, 1880, 3079

**Table S3.** Calculated frequencies (in  $\text{cm}^{-1}$ ) for the species of the subsequent reactions of  $\text{CF}_3(\text{CX}_2)_2\text{C}(\text{O}\bullet)\text{HOH}$  ( $\text{X}=\text{H}, \text{F}$ ) at the B3LYP/6-311G(d,p) level.

species	B3LYP/6-311G(d,p)
$\text{CF}_3(\text{CH}_2)_2\text{C}(\text{O}\bullet)\text{HOH}$	40, 68, 122, 141, 226, 231, 320, 359, 398, 465, 533, 550, 581, 647, 786, 830, 896, 922, 998, 1048, 1065, 1132, 1160, 1178, 1217, 1245, 1265, 1308, 1329, 1340, 1416, 1485, 1500, 2720, 3060, 3075, 3108, 3129, 3812
$\text{CF}_3(\text{CF}_2)_2\text{C}(\text{O}\bullet)\text{HOH}$	42, 64, 75, 122, 182, 191, 214, 239, 259, 289, 297, 329, 348, 373, 406, 500, 529, 552, 574, 601, 641, 715, 744, 856, 978, 1040, 1105, 1121, 1169, 1178, 1201, 1210, 1237, 1261, 1289, 1325, 1385, 2935, 3802
$\text{O}_2$	1626
$\text{HO}_2\bullet$	1163, 1428, 3605
$\text{CF}_3(\text{CH}_2)_2\text{C}(\text{O})\text{OH}$	23, 64, 104, 122, 221, 330, 357, 471, 523, 533, 569, 602, 666, 670, 796, 837, 897, 992, 1073, 1129, 1141, 1175, 1238, 1264, 1303, 1332, 1377, 1438, 1469, 1481, 1829, 3054, 3080, 3086, 3125, 3758
$\text{CF}_3(\text{CF}_2)_2\text{C}(\text{O})\text{OH}$	20, 45, 63, 120, 179, 210, 228, 255, 286, 328, 342, 370, 374, 449, 515, 544, 555, 588, 605, 659, 674, 752, 771, 925, 1122, 1144, 1164, 1175, 1201, 1214, 1234, 1270, 1330, 1397, 1865, 3749
$\text{CF}_3\text{CH}_2\text{CH}_2\bullet$	44, 108, 216, 351, 402, 514, 530, 542, 655, 792, 817, 1021, 1076, 1140, 1188, 1249, 1321, 1347, 1462, 1475, 3043, 3090, 3153, 3261
$\text{CF}_3\text{CF}_2\text{CF}_2\bullet$	26, 75, 136, 200, 222, 272, 338, 364, 369, 499, 513, 542, 596, 635, 672, 762, 1011, 1147, 1179, 1206, 1213, 1279, 1300, 1360
$\text{HC}(\text{O})\text{OH}$	632, 701, 1058, 1132, 1310, 1411, 1836, 3043, 3736
$\text{CF}_3\text{CH}_2\text{CH}_2\text{CHO}$	54, 66, 105, 160, 288, 355, 370, 507, 533, 566, 645, 774, 829, 864, 1007, 1033, 1073, 1158, 1161, 1243, 1265, 1297, 1338, 1408, 1421, 1471, 1487, 1825, 2851, 3026, 3056, 3098, 3117
$\text{CF}_3\text{CF}_2\text{CF}_2\text{CHO}$	20, 57, 71, 142, 209, 222, 237, 262, 287, 329, 351, 371, 415, 500, 528, 572, 598, 653, 724, 774, 866, 1009, 1128, 1135, 1165, 1196, 1213, 1232, 1287, 1344, 1391, 1853, 2965
$\bullet\text{OH}$	3704
$\text{TS1O}_2$	480i, 28, 42, 67, 111, 123, 130, 160, 218, 291, 347, 360, 391, 452, 519, 533, 559, 621, 649, 744, 798, 841, 924, 1013, 1038, 1076, 1120, 1134, 1158, 1196, 1240, 1266, 1307, 1331, 1340, 1415, 1484, 1497, 1539, 1747, 3060, 3070, 3109, 3128, 3790
$\text{TS2O}_2$	685i, 31, 53, 55, 73, 116, 134, 166, 195, 216, 238, 255, 271, 289, 307, 334, 357, 365, 382, 445, 507, 532, 571, 596, 625, 679, 697, 738, 802, 891, 1060, 1118, 1127, 1153, 1180, 1183, 1212, 1230, 1284, 1289, 1326, 1346, 1547, 1703, 3793
$\text{TS1C-H}$	1040i, 40, 68, 122, 138, 224, 323, 359, 447, 512, 532, 543, 561, 572, 626, 677, 683, 800, 837, 906, 994, 1068, 1116, 1135, 1164, 1238, 1263, 1297, 1328, 1360, 1425, 1477, 1488, 1653, 3046, 3070, 3107, 3125, 3765
$\text{TS2C-H}$	963i, 36, 68, 76, 123, 191, 213, 235, 265, 288, 308, 328, 360, 372, 416,

	492, 515, 533, 558, 563, 596, 605, 668, 686, 745, 800, 902, 1110, 1132, 1147, 1165, 1183, 1220, 1228, 1293, 1326, 1359, 1707, 3761
TS1C-C	455i, 30, 53, 105, 124, 215, 247, 343, 360, 418, 530, 535, 552, 600, 645, 719, 824, 827, 943, 1026, 1049, 1074, 1098, 1160, 1204, 1256, 1276, 1319, 1341, 1369, 1475, 1480, 1536, 2956, 3063, 3116, 3120, 3211, 3767
TS2C-C	453i, 40, 57, 70, 109, 177, 199, 219, 236, 241, 286, 310, 342, 372, 383, 468, 505, 530, 578, 595, 605, 672, 689, 769, 947, 1053, 1102, 1150, 1190, 1205, 1209, 1247, 1274, 1296, 1302, 1332, 1492, 2978, 3767
TS1C-O	337i, 35, 56, 98, 112, 212, 227, 280, 361, 370, 423, 516, 537, 555, 650, 766, 800, 836, 932, 977, 1033, 1055, 1149, 1161, 1240, 1265, 1298, 1334, 1392, 1407, 1479, 1493, 1593, 2948, 3055, 3070, 3102, 3131, 3729
TS2C-O	319i, 23, 56, 66, 104, 180, 193, 207, 227, 237, 259, 286, 330, 356, 363, 391, 431, 504, 530, 585, 599, 671, 708, 747, 782, 888, 994, 1123, 1148, 1166, 1198, 1211, 1233, 1276, 1339, 1376, 1635, 3011, 3718

**Table S4.** The B3LYP/6-311G(d,p) electronic energies, CCSD(T)/6-311++G(d,p) energies, ZPE, thermal correction to the enthalpy (TZPE<sub>H</sub>), and Gibbs free energy (TZPE<sub>G</sub>) (in a.u.).

Speices	TZPE <sub>H</sub>	TZPE <sub>G</sub>	B3LYP	CCSD(T)//B3LYP
R1+Cl	0.126139	0.064163	-991.720618	-989.993451
TS1	0.117795	0.067132	-991.717987	-989.973214
TS2	0.119277	0.06937	-991.736772	-989.997821
TS3	0.118124	0.068277	-991.721982	-989.987124
TS4	0.117859	0.067536	-991.714054	-989.979299
P1+HCl	0.118334	0.052473	-991.716071	-989.980218
P2+HCl	0.119913	0.05396	-991.729098	-989.99565
P3+HCl	0.119123	0.052517	-991.718781	-989.986558
P4+HCl	0.119412	0.052369	-991.717092	-989.983726
R2+Cl	0.096693	0.028166	-1388.767691	-1386.307587
TS5	0.087975	0.029907	-1388.756005	-1386.279946
TS6	0.089559	0.032994	-1388.770992	-1386.298815
P5+HCl	0.091357	0.019262	-1388.751383	-1386.284598
P6+HCl	0.090564	0.018055	-1388.776839	-1386.307557

**Table S5.** The Cartesian coordinates of reactants, products, transition states for the title reactions at the B3LYP/6-311G(d,p) level..

R1	C	-1.432667	0.008808	0.000056
	C	-0.106184	0.728356	0.000008
	C	1.094524	-0.220752	-0.000046
	H	-0.097075	1.375052	-0.881943
	H	-0.097005	1.375039	0.881967
	C	2.417697	0.530297	-0.000116
	H	1.059897	-0.868225	0.879633
	H	1.059807	-0.868241	-0.879709
	H	2.479115	1.176540	-0.888693
	H	2.479163	1.176618	0.888402
	F	-2.464756	0.882641	0.000092
	F	-1.582956	-0.782010	1.087025
	F	-1.583037	-0.782014	-1.086897
	O	3.456485	-0.441593	-0.000101
H	4.300735	0.018151	-0.000240	
TS1	C	-0.916846	-0.666758	1.886763
	C	-0.125601	0.368260	1.120470
	C	1.171810	-0.194553	0.534120
	H	-0.781008	0.750897	0.333437
	H	0.076554	1.190056	1.813030
	C	1.937199	0.873065	-0.258997
	H	1.816085	-0.577643	1.328005
	H	0.948755	-1.024143	-0.141244
	H	1.335280	1.306606	-1.067243
	H	2.217666	1.697003	0.426703
	F	-2.050278	-0.135494	2.390602
	F	-0.212729	-1.169705	2.925486
	F	-1.272917	-1.709304	1.105688
	O	3.162764	0.415363	-0.723242
	H	3.150287	0.131715	-1.967904
	Cl	2.794435	-0.618364	-3.154004
TS2	C	-1.435420	-0.117612	-0.208299
	C	-0.107239	0.598998	-0.158851
	C	1.078165	-0.371514	-0.155069
	H	-0.072353	1.260803	-1.028545
	H	-0.105339	1.225236	0.735551
	C	2.402770	0.327769	-0.245929
	H	1.064020	-0.987356	0.748058
	H	0.995833	-1.059610	-1.006879
	H	2.516847	1.102546	-1.010861
	H	2.451942	1.233592	0.927599
	F	-2.461794	0.756445	-0.197063



	F	-1.601351	-0.949839	0.843239
	F	-1.561448	-0.868452	-1.328701
	O	3.456242	-0.525860	-0.113253
	H	4.282991	-0.063956	-0.295730
	Cl	2.542566	2.156158	2.050447
TS3	C	-1.490317	0.586874	-0.276431
	C	-0.029040	0.945783	-0.108283
	C	0.900907	-0.233850	-0.162902
	H	0.217017	1.647915	-0.916840
	H	0.077753	1.498741	0.829762
	C	2.382891	0.033982	-0.165777
	H	0.763360	-0.934690	1.161807
	H	0.591390	-1.074463	-0.782942
	H	2.631421	0.557183	-1.100886
	H	2.649120	0.714179	0.656472
	F	-2.258671	1.694662	-0.265835
	F	-1.929583	-0.223873	0.704686
	F	-1.710907	-0.047546	-1.449670
	O	3.160327	-1.142525	-0.159837
	H	3.062925	-1.563120	0.702909
	Cl	0.915605	-1.561557	2.441468
TS4	C	-1.358277	-0.387139	-0.115676
	C	-0.121733	0.466820	-0.148447
	C	1.202761	-0.224910	-0.214712
	H	-0.257900	1.358132	-0.759644
	H	-0.155467	1.145934	1.167344
	C	2.401242	0.717414	-0.199533
	H	1.297261	-0.958797	0.590067
	H	1.236400	-0.798522	-1.154904
	H	2.289568	1.471593	-0.992650
	H	2.452667	1.240302	0.763228
	F	-2.463063	0.347045	0.097674
	F	-1.296596	-1.336512	0.835057
	F	-1.517707	-1.020653	-1.305553
	O	3.549359	-0.091406	-0.415524
	H	4.331828	0.455745	-0.303284
	Cl	-0.120281	1.851936	2.416344
PI	C	1.380168	0.015569	0.000006
	C	0.036603	0.703711	-0.000263
	C	-1.142649	-0.272634	-0.000224
	H	0.012241	1.351082	0.881321
	H	0.012410	1.350821	-0.882038
	C	-2.491813	0.452246	-0.000016
	H	-1.092385	-0.919516	-0.879733

	H	-1.092208	-0.919742	0.879107
	H	-2.585473	1.136216	0.868373
	H	-2.585366	1.137396	-0.867417
	F	2.390562	0.912849	-0.000416
	F	1.546115	-0.771797	-1.086801
	F	1.546142	-0.770795	1.087543
	O	-3.588556	-0.357741	0.000053
P2	C	-1.394787	0.015957	-0.015253
	C	-0.058391	0.701403	-0.154836
	C	1.129751	-0.229713	0.110657
	H	-0.007562	1.111535	-1.166156
	H	-0.059362	1.543369	0.543079
	C	2.428775	0.485050	-0.027207
	H	1.026655	-0.672216	1.114140
	H	1.111299	-1.066770	-0.594624
	H	2.569304	1.466939	0.423090
	F	-2.412372	0.868822	-0.271065
	F	-1.591425	-0.472038	1.231916
	F	-1.524865	-1.024785	-0.869479
	O	3.520442	-0.344295	-0.067535
	H	4.321992	0.187320	-0.081757
P3	C	1.300349	0.026094	0.004617
	C	0.223195	-0.839956	-0.633153
	C	-1.104124	-0.753245	0.040996
	H	0.161662	-0.519953	-1.679520
	H	0.605084	-1.863943	-0.619498
	C	-2.028044	0.388077	-0.175481
	H	-1.354469	-1.451841	0.830037
	H	-1.741354	1.234207	0.475976
	H	-1.938245	0.752373	-1.212485
	F	2.479187	-0.099911	-0.642650
	F	1.515551	-0.297758	1.296284
	F	0.969509	1.340009	-0.025962
	O	-3.356451	-0.037907	0.116903
	H	-3.907541	0.745537	0.199338
P4	C	1.429762	0.031446	0.010788
	C	0.095643	0.574969	-0.324628
	C	-1.124680	-0.267220	-0.244702
	H	0.084567	1.548560	-0.799542
	C	-2.381912	0.533021	0.088912
	H	-1.300747	-0.769813	-1.209463
	H	-0.996792	-1.063187	0.493764
	H	-2.278841	0.982810	1.085718
	H	-2.503211	1.348364	-0.639556

	F	2.370912	0.998147	0.037861
	F	1.846659	-0.901719	-0.890613
	F	1.445363	-0.585197	1.219031
	O	-3.476490	-0.372443	0.036393
	H	-4.272340	0.098439	0.299206
R2	C	-1.641049	-0.235391	0.008566
	C	-0.322368	0.585147	-0.023755
	C	1.001197	-0.215415	0.030408
	C	2.237351	0.670975	0.181256
	H	2.174565	1.471381	-0.566122
	H	2.227872	1.116539	1.175183
	F	-2.675157	0.590992	-0.189598
	F	-1.798004	-0.834957	1.190632
	F	-1.644917	-1.161863	-0.954987
	F	-0.345900	1.435418	1.036789
	F	-0.324901	1.325745	-1.160291
	F	0.922167	-1.117384	1.043529
	F	1.111986	-0.926547	-1.137452
	O	3.414846	-0.089602	0.069287
	H	3.420547	-0.505638	-0.799803
TS5	C	1.447182	-0.919487	1.104494
	C	0.360243	0.071400	0.604130
	C	-1.061330	-0.503583	0.377640
	C	-2.013499	0.549751	-0.212014
	H	-2.051687	1.440565	0.423789
	H	-1.615971	0.851897	-1.195545
	F	2.582192	-0.244743	1.316624
	F	1.676380	-1.865928	0.191736
	F	1.068958	-1.494898	2.247858
	F	0.790049	0.594303	-0.575325
	F	0.266842	1.079372	1.505581
	F	-0.975028	-1.563737	-0.464374
	F	-1.546544	-0.944348	1.563525
	O	-3.262902	0.015883	-0.457243
	H	-4.190109	0.487472	0.287928
Cl	-4.905686	0.692994	1.517013	
TS6	C	-1.65481900	-0.13311400	-0.04450500
	C	-0.35404900	0.71057700	-0.18861600
	C	0.97202300	-0.09312600	-0.13632700
	C	2.21540100	0.73450200	0.16176800
	H	2.22009100	1.82192100	-0.68753500
	H	2.20444600	1.23391500	1.12675600
	F	-2.70686700	0.63785000	-0.32989500
	F	-1.78915800	-0.59423800	1.20039500

	F	-1.63285300	-1.16549500	-0.89534900
	F	-0.33308300	1.61474800	0.82470500
	F	-0.41655700	1.36966600	-1.36026800
	F	0.85482400	-1.06003300	0.82260600
	F	1.15410600	-0.73449900	-1.32744600
	O	3.37720700	0.06991500	-0.04231600
	H	3.30525400	-0.47692300	-0.83909400
	Cl	2.44411600	3.03089700	-1.56083800
P5	C	-1.603220	-0.224307	-0.000018
	C	-0.272194	0.580606	0.000008
	C	1.039050	-0.254506	0.000020
	C	2.284249	0.673018	-0.000079
	H	2.203422	1.288043	-0.906814
	H	2.203445	1.288199	0.906554
	F	-2.625554	0.638917	0.000037
	F	-1.692617	-0.992735	1.087727
	F	-1.692639	-0.992621	-1.087840
	F	-0.274229	1.373468	1.099710
	F	-0.274205	1.373487	-1.099681
	F	1.041259	-1.048734	1.096963
	F	1.041193	-1.048875	-1.096824
	O	3.399620	-0.118907	-0.000020
P6	C	-1.612925	-0.195936	-0.025973
	C	-0.269136	0.586119	-0.025966
	C	1.024076	-0.256360	0.112453
	C	2.227342	0.567785	0.344573
	H	2.265630	1.304120	1.130420
	F	-2.605309	0.641409	-0.352064
	F	-1.871674	-0.706717	1.179242
	F	-1.580647	-1.187276	-0.923700
	F	-0.312793	1.469111	1.006048
	F	-0.201169	1.282421	-1.183486
	F	0.805678	-1.190468	1.112639
	F	1.199181	-0.985223	-1.041205
	O	3.418658	0.137927	-0.116740
	H	3.269554	-0.526497	-0.804289