

Supporting Information for:

Thermal decomposition of 2,3,3,3- and *trans*-1,3,3,3-tetrafluoropropenes

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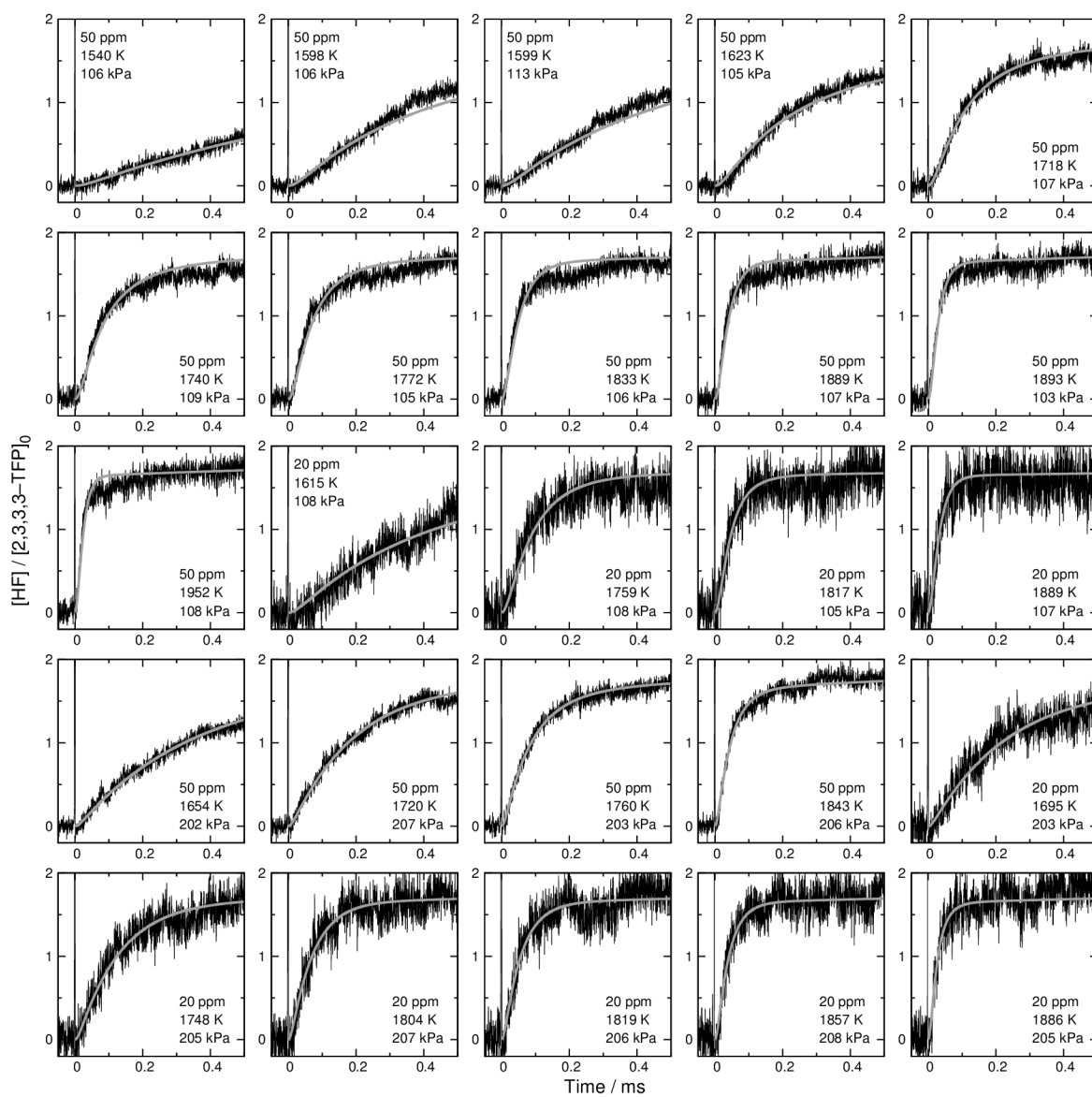


Figure S1. Experimental conditions and corresponding HF profiles for the decomposition of 2,3,3,3-TFP. The gray lines represent the fitted profiles.

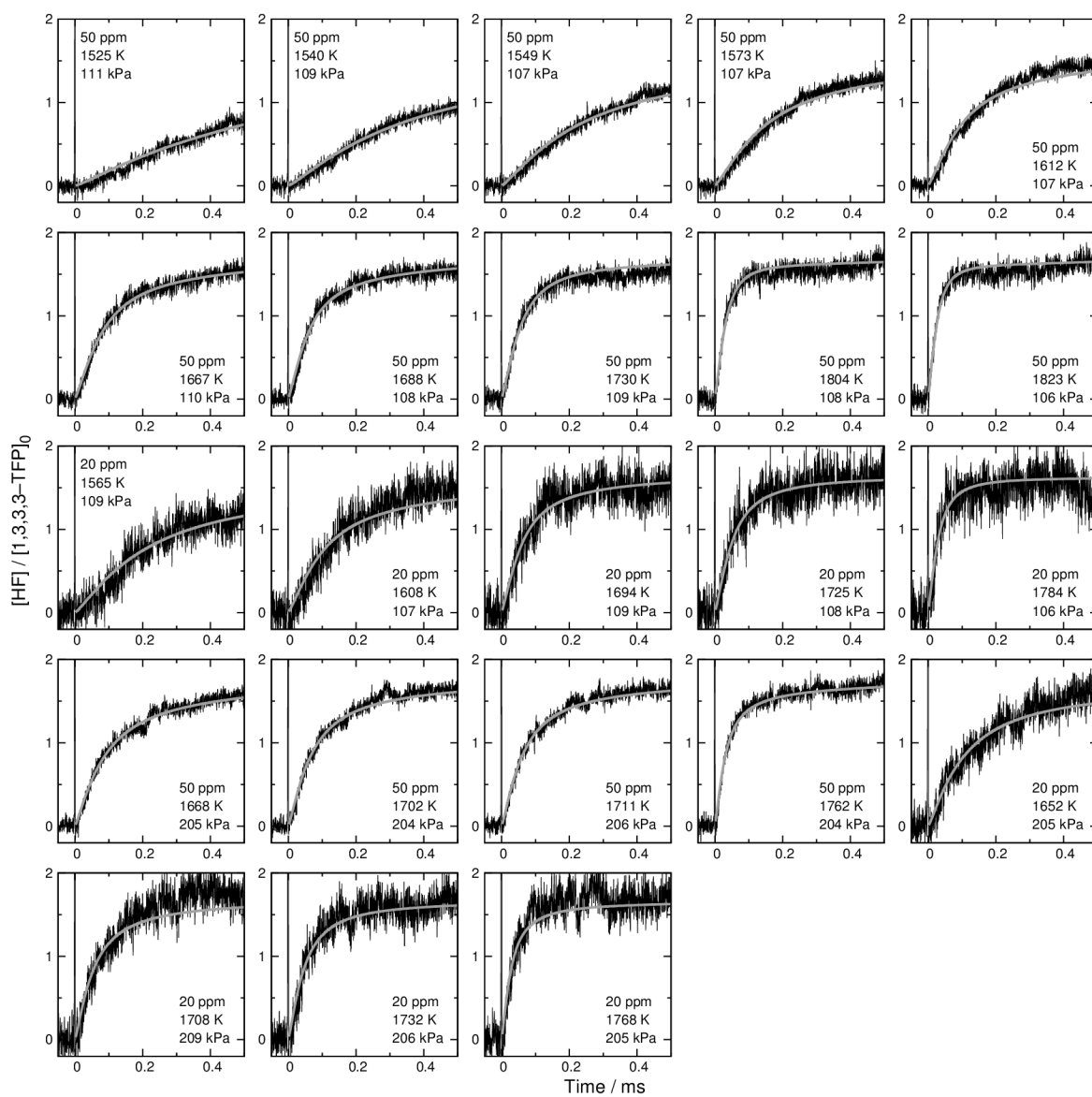


Figure S2. Experimental conditions and corresponding HF profiles for the decomposition of *trans*-1,3,3,3-TFP. The gray lines represent the fitted profiles.

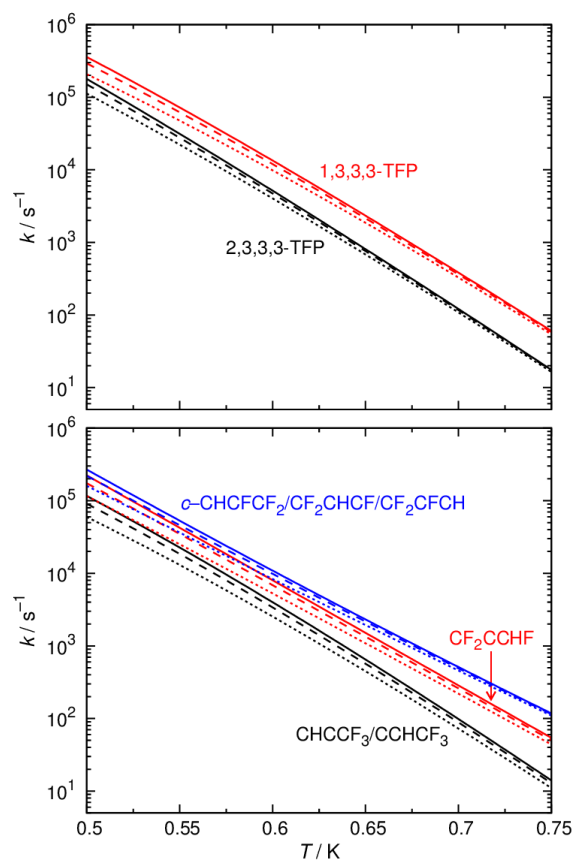


Figure S3. Effects of $\langle \Delta E_{\text{down}} \rangle$ on calculated rate constants for the thermal decomposition reactions at a pressure of 100 kPa. The solid, dashed, and dotted lines represent the results for $\langle \Delta E_{\text{down}} \rangle = 1600, 1200,$ and 800 cm^{-1} , respectively.

Table S1. The Optimized Geometries (in Cartesian Coordinates; Å) and Unscaled Harmonic Frequencies (cm⁻¹) for Stationary Points.

hydrogen fluoride (HF) H, 0.000000, 0.000000, -0.825136 F, 0.000000, 0.000000, 0.091682 Frequency: 4179	F, 0.755381, -2.376216, 0.000000 F, -1.220554, -1.525708, 0.000000 F, 0.067297, 1.939093, 1.093610 C, 0.598141, -0.054201, 0.000000 C, -0.230968, 1.177812, 0.000000 H, -1.306062, 0.992400, 0.000000 F, 0.067297, 1.939093, -1.093610 H, 1.674464, 0.046222, 0.000000 Frequencies: 54, 137, 180, 365, 481, 532, 555, 627, 654, 837, 964, 1069, 1085, 1162, 1248, 1341, 1374, 1451, 1828, 3129, 3245
2,3,3,3-tetrafluoropropene (CH₂CF₃) C, -0.108941, 0.577455, 0.000000 F, -0.835780, 0.892844, 1.079065 F, 0.984331, 1.346177, 0.000000 F, -0.835780, 0.892844, -1.079065 C, 0.256037, -0.886301, 0.000000 C, 1.476856, -1.378012, 0.000000 H, 2.327300, -0.712358, 0.000000 H, 1.636067, -2.447956, 0.000000 F, -0.835780, -1.656147, 0.000000 Frequencies: 62, 238, 238, 370, 422, 503, 578, 620, 687, 760, 799, 946, 965, 1167, 1180, 1213, 1384, 1426, 1782, 3195, 3299	1,3,3,3-tetrafluoropropylidene (CFCH₂CF₃) C, 0.827255, 0.017821, -0.000045 F, 1.067722, -0.732864, 1.081166 F, 1.066661, -0.731497, -1.082406 F, 1.723052, 1.021531, 0.000185 C, -0.580950, 0.567462, 0.000989 C, -1.627051, -0.511253, 0.000632 H, -0.720721, 1.206197, -0.880306 H, -0.720142, 1.203638, 0.884266 F, -2.776841, 0.125718, -0.000436 Frequencies: 21, 114, 172, 332, 376, 425, 521, 565, 691, 697, 882, 1008, 1066, 1124, 1222, 1289, 1297, 1357, 1418, 3041, 3097
1,1,2,3-tetrafluoropropene (CF₂CFCH₂F) C, 1.003493, -0.186770, 0.004671 F, 2.097691, 0.478666, -0.257586 F, 1.225724, -1.480900, 0.071778 F, -2.265608, -0.427646, -0.607438 C, -0.186923, 0.364236, 0.192832 C, -1.432632, -0.372131, 0.504813 H, -1.979446, 0.144029, 1.297632 H, -1.205952, -1.393687, 0.812416 F, -0.293166, 1.698507, 0.090585 Frequencies: 77, 140, 221, 264, 356, 472, 520, 595, 673, 800, 975, 1035, 1167, 1278, 1310, 1342, 1426, 1490, 1866, 3084, 3149	3,3,3-trifluoropropyne (CHCCF₃) C, 0.000000, 0.000000, 2.323480 C, 0.000000, 0.000000, 1.128805 H, 0.000000, 0.000000, 3.388183 C, 0.000000, 0.000000, -0.333581 F, 0.000000, 1.247802, -0.818534 F, 1.080629, -0.623901, -0.818534 F, -1.080629, -0.623901, -0.818534 Frequencies: 181, 181, 458, 458, 541, 620, 620, 752, 752, 817, 1176, 1176, 1261, 2281, 3481
trans-1,3,3,3-tetrafluoropropene (CHFCHCF₃(E)) C, -0.026668, -0.843604, 0.000000 F, 0.361459, -1.546862, 1.078306 F, -1.369942, -0.824018, 0.000000 F, 0.361459, -1.546862, -1.078306 C, 0.571286, 0.519828, 0.000000 C, -0.181044, 1.604465, 0.000000 H, -1.263700, 1.624323, 0.000000 H, 1.652345, 0.572827, 0.000000 F, 0.361459, 2.819821, 0.000000 Frequencies: 83, 198, 198, 391, 416, 426, 563, 586, 700, 877, 891, 973, 1111, 1157, 1210, 1270, 1345, 1360, 1776, 3232, 3238	trifluoroallene (CF₂CCHF) C, -0.191420, -0.932858, 0.000000 F, -0.203230, -1.691256, 1.076441 F, -0.203230, -1.691256, -1.076441 C, -0.168951, 0.360661, 0.000000 C, -0.203230, 1.657133, 0.000000 H, -1.103539, 2.261713, 0.000000 F, 0.904810, 2.407920, 0.000000 Frequencies: 114, 117, 300, 455, 595, 598, 642, 851, 912, 1105, 1258, 1313, 1532, 2151, 3207
cis-1,3,3,3-tetrafluoropropene (CHFCHCF₃(Z)) C, -0.102539, 0.728904, 0.000000 F, -0.413658, 1.471588, 1.079723 F, 1.220321, 0.557612, 0.000000 F, -0.413658, 1.471588, -1.079723 C, -0.882987, -0.543197, 0.000000 C, -0.413658, -1.779111, 0.000000 H, -1.957288, -0.414887, 0.000000 H, -1.054342, -2.652971, 0.000000 F, 0.874411, -2.097646, 0.000000 Frequencies: 11, 188, 260, 323, 475, 534, 554, 622, 772, 804, 864, 986, 1057, 1150, 1178, 1302, 1303, 1445, 1783, 3216, 3239	1H-trifluorovinylmethylene (CF₂CFCH) C, 0.000000, 0.606731, 0.000000 F, 0.942163, 1.472507, 0.000000 F, -1.159814, 1.170317, 0.000000 C, 0.173323, -0.753090, 0.000000 C, 1.445577, -1.270091, 0.000000 H, 1.401940, -2.368718, 0.000000 F, -1.017387, -1.435333, 0.000000 Frequencies: 115, 256, 375, 401, 525, 587, 713, 805, 805, 979, 1137, 1381, 1422, 1646, 3081
1,1,3,3-tetrafluoropropene (CF₂CHCF₂) C, 0.067297, -1.261108, 0.000000	2H-trifluorovinylmethylene (CF₂CHCF) C, -0.899365, -0.045615, -0.000062 F, -1.283870, 1.185293, -0.000091 F, -1.928100, -0.842311, 0.000223 C, 0.369813, -0.485710, 0.000015 C, 1.409473, 0.506738, -0.000104

F, 2.565959, -0.153328, -0.000053
H, 0.534571, -1.559358, 0.000189
Frequencies: 150, 197, 241, 426, 512, 638, 712,
860, 993, 1110, 1183, 1284, 1427, 1706, 3181

2H-trifluoromethylvinylidene (CCHCF3)

C, -0.022091, 0.276797, 0.000000
F, -0.480275, 0.924352, 1.078547
F, 1.309654, 0.369392, 0.000000
F, -0.480275, 0.924352, -1.078547
C, -0.480275, -1.147886, 0.000000
C, 0.237903, -2.231621, 0.000000
H, -1.555152, -1.346601, 0.000000
Frequencies: 99, 175, 345, 387, 534, 551, 608,
707, 836, 948, 1174, 1213, 1263, 1779, 3132

1,3,3-trifluoropropyne (CFCCHF2)

C, -0.250518, 1.543470, 0.000000
C, 0.088723, 0.401620, 0.000000
C, 0.553644, -0.981516, 0.000000
F, 0.088723, -1.639748, 1.096127
F, 0.088723, -1.639748, -1.096127
H, 1.643339, -1.055735, 0.000000
F, -0.621273, 2.754416, 0.000000
Frequencies: 113, 150, 408, 422, 474, 561, 604,
864, 1085, 1102, 1308, 1375, 1427, 2489, 3110

1H-trifluorocyclopropene (c-CHCF2)

C, 0.006465, 0.532270, 0.000000
F, -0.407728, 1.235000, 1.083214
F, -0.407728, -2.063878, 0.000000
F, -0.407728, 1.235000, -1.083214
C, 0.159479, -0.892088, 0.000000
C, 1.276890, -0.221664, 0.000000
H, 2.351666, -0.166201, 0.000000
Frequencies: 201, 284, 390, 505, 587, 624, 787,
834, 873, 1014, 1096, 1187, 1428, 1868, 3306

difluoropropadienylidene (CF2CC)

C, 0.000000, 0.000000, -0.279545
F, 0.000000, 1.059736, -1.022728
F, 0.000000, -1.059736, -1.022728
C, 0.000000, 0.000000, 1.039939
C, 0.000000, 0.000000, 2.307791
Frequencies: 133, 165, 550, 583, 723, 859,
1320, 1486, 2136

difluoromethylene (CF2)

C, 0.000000, 0.000000, 0.596771
F, 0.000000, 1.028696, -0.198924
F, 0.000000, -1.028696, -0.198924
Frequencies: 680, 1125, 1241

fluoroacetylene (CHCF)

C, 0.000000, 0.000000, -0.093056
F, 0.000000, 0.000000, 1.179049
C, 0.000000, 0.000000, -1.284461
H, 0.000000, 0.000000, -2.346342
Frequencies: 449, 449, 653, 653, 1095, 2350,
3503

1H-trifluorobutatrienylmethylene (CF2CCCFCH)

C, -0.000341, -2.068306, 0.000000
C, 1.236984, -2.670541, 0.000000
C, 0.076313, 1.840778, 0.000000
F, 1.186372, 2.514441, 0.000000
F, -0.950300, 2.638025, 0.000000

C, 0.000000, 0.530791, 0.000000
C, -0.013519, -0.717060, 0.000000
F, -1.229236, -2.677620, 0.000000
H, 1.141852, -3.767585, 0.000000
Frequencies: 33, 70, 107, 202, 332, 337, 486,
564, 613, 616, 657, 700, 704, 906, 1008, 1251,
1325, 1365, 1720, 2253, 3059

2H-trifluorobutatrienylmethylene (CF2CCCHCF)

C, 0.675077, 1.768210, 0.000000
C, 2.119729, 1.655954, 0.000000
F, 2.592876, 2.903736, 0.000000
H, 0.144474, 2.719564, 0.000000
C, -1.252303, -1.611274, 0.000000
F, -0.671817, -2.777155, 0.000000
F, -2.550289, -1.743183, 0.000000
C, -0.622737, -0.464488, 0.000000
C, 0.000000, 0.623242, 0.000000
Frequencies: 66, 73, 179, 181, 212, 383, 476,
552, 575, 607, 643, 804, 819, 1081, 1153, 1189,
1310, 1337, 1756, 2258, 3143

1H-trifluorovinylidenecyclopropene

C, -0.281497, -2.139163, 0.000000
C, -1.529045, -1.751051, 0.000000
C, 0.312902, 1.729805, 0.000000
F, 0.548275, 2.473796, 1.076238
F, 0.548275, 2.473796, -1.076238
C, -0.075528, 0.502154, 0.000000
C, -0.462775, -0.734739, 0.000000
F, 0.548275, -3.136250, 0.000000
H, -2.587773, -1.944098, 0.000000
Frequencies: 58, 91, 145, 304, 313, 444, 536,
572, 574, 615, 690, 781, 812, 965, 1050, 1198,
1248, 1606, 1858, 2163, 3308

trifluoropentatetraene (CF2CCCCHF)

C, 0.124787, 1.731630, 0.000000
C, 0.166051, 3.036233, 0.000000
F, -0.942540, 3.785877, 0.000000
H, 1.070021, 3.634256, 0.000000
C, 0.159589, -2.109417, 0.000000
F, 0.166051, -2.864756, 1.076781
F, 0.166051, -2.864756, -1.076781
C, 0.148797, -0.809586, 0.000000
C, 0.138097, 0.460882, 0.000000
Frequencies: 64, 70, 165, 179, 265, 400, 462,
496, 582, 589, 602, 734, 864, 1020, 1189, 1264,
1345, 1583, 2048, 2295, 3212

difluoropentatetraenylidene (CF2CCCC)

C, 0.000000, 0.000000, 2.531498
C, 0.000000, 0.000000, 3.805236
C, 0.000000, 0.000000, -1.330005
F, 0.000000, 1.066281, -2.074164
F, 0.000000, -1.066281, -2.074164
C, 0.000000, 0.000000, -0.019805
C, 0.000000, 0.000000, 1.235566
Frequencies: 57, 90, 192, 217, 462, 493, 560,
575, 671, 714, 1109, 1306, 1588, 2074, 2279

TS between 2,3,3,3- and

1,1,2,3-tetrafluoropropenes

C, 0.748501, 0.273895, 0.443702
C, 1.266257, -0.992706, 0.450390
C, -0.621898, 0.250503, 0.176099
F, 1.437913, 1.303968, -0.071818

H, 0.747511, -1.802744, 0.938106
H, 2.294017, -1.151481, 0.144766
F, -0.054695, -1.348178, -1.091248
F, -1.449081, -0.490071, 0.823099
F, -1.200658, 1.174734, -0.493813
Frequencies: 625i, 155, 173, 235, 261, 360,
465, 524, 607, 641, 797, 844, 959, 1030, 1215,
1391, 1418, 1552, 1604, 3194, 3310

**TS between 2,3,3,3-tetrafluoropropene and
3,3,3-trifluoropropyne + hydrogen fluoride**

C, -0.087499, 0.660163, 0.000000
F, -0.839762, 0.838329, 1.078609
F, 0.876631, 1.592655, 0.000000
F, -0.839762, 0.838329, -1.078609
C, 0.597852, -0.662891, 0.000000
C, 1.481143, -1.543719, 0.000000
H, 2.538597, -1.720088, 0.000000
H, 0.296320, -2.242998, 0.000000
F, -0.839762, -1.798007, 0.000000
Frequencies: 1855i, 69, 174, 183, 328, 449,
461, 528, 576, 616, 669, 757, 763, 835, 942,
1181, 1221, 1258, 1725, 1993, 3367

**TS between 1,1,2,3-tetrafluoropropene and
1H-trifluorovinylmethylene + hydrogen
fluoride**

C, 1.122351, -0.195933, -0.035606
F, 2.138449, 0.525002, -0.355268
F, 1.403830, -1.454706, -0.023228
F, -2.873373, -0.307293, -0.571320
C, -0.100782, 0.314738, 0.275485
C, -1.161397, -0.453530, 0.725135
H, -2.339569, -0.132973, 0.478572
H, -0.959876, -1.521341, 0.783013
F, -0.209083, 1.643960, 0.166297
Frequencies: 1050i, 69, 97, 161, 247, 362, 420,
538, 593, 605, 696, 817, 918, 1005, 1209, 1325,
1397, 1452, 1671, 1961, 3193

**TS between 1,1,2,3-tetrafluoropropene and
trifluoroallene + hydrogen fluoride**

C, 1.061595, -0.242792, 0.013832
F, 1.991314, 0.608762, -0.266624
F, 1.531643, -1.461365, 0.108702
F, -2.339286, -0.720484, -0.526233
C, -0.218045, -0.013280, 0.198970
C, -1.537079, -0.230946, 0.467352
H, -1.347349, 1.136784, 0.345764
H, -1.888212, -0.501154, 1.457505
F, -0.361810, 1.827141, 0.030355
Frequencies: 1971i, 82, 154, 185, 213, 350,
442, 515, 584, 639, 686, 787, 889, 1070, 1157,
1283, 1336, 1454, 1649, 1967, 3194

**TS between trans- and
cis-1,3,3,3-tetrafluoropropenes**

C, 0.792019, -0.001961, -0.019177
F, 0.721868, 1.338389, -0.112660
F, 0.929993, -0.295283, 1.285562
F, 1.913410, -0.387794, -0.643934
C, -0.412284, -0.665763, -0.609571
C, -1.699534, -0.640043, 0.058543
H, -1.978060, -1.249530, 0.909397
H, -0.276870, -1.109416, -1.592130
F, -2.434857, 0.478637, -0.072971

Frequencies: 895i, 15, 124, 242, 302, 387, 435,
512, 556, 648, 676, 846, 1065, 1128, 1149,
1203, 1258, 1336, 1392, 3169, 3213

**TS between trans-1,3,3,3- and
1,1,3,3-tetrafluoropropenes**

C, -0.269201, -0.908336, 0.261675
C, -1.278596, 0.031900, 0.375915
C, 0.933906, -0.238195, 0.128522
H, -0.426104, -1.801117, -0.325151
H, -1.254612, 0.931829, 0.974821
F, -2.476365, -0.281973, -0.029887
F, -0.183938, 1.156576, -0.907823
F, 1.358899, 0.672512, 0.940177
F, 1.897411, -0.707440, -0.585394
Frequencies: 537i, 133, 158, 260, 363, 414,
499, 520, 601, 644, 797, 953, 989, 1195, 1238,
1317, 1392, 1557, 1581, 3252, 3254

**TS between trans-1,3,3,3-tetrafluoropropene
and 1,3,3,3-tetrafluoropropylidene**

C, 0.845295, -0.013984, 0.003007
F, 1.037227, 1.297691, -0.066460
F, 1.309521, -0.449240, 1.180803
F, 1.585399, -0.589963, -0.959173
C, -0.601067, -0.432363, -0.137079
C, -1.625766, 0.472718, 0.089021
H, -0.747892, -1.509358, -0.253028
H, -1.024055, 0.473645, -1.060203
F, -2.814239, -0.160990, 0.020779
Frequencies: 1360i, 102, 182, 209, 381, 411,
429, 562, 582, 708, 897, 959, 1074, 1150, 1177,
1247, 1270, 1338, 1503, 2196, 3115

**TS between cis-1,3,3,3-tetrafluoropropene
and 1,3,3,3-tetrafluoropropylidene**

C, -0.712516, -0.003644, 0.002272
F, -0.830641, -0.662269, 1.158071
F, -1.866100, 0.643621, -0.220780
F, -0.552832, -0.894291, -0.976697
C, 0.440198, 0.987575, 0.066350
C, 1.803420, 0.720300, 0.125014
H, 0.153560, 2.018609, 0.254042
H, 1.293052, 1.276723, -0.938442
F, 2.068104, -0.589363, -0.013639
Frequencies: 1375i, 43, 161, 262, 318, 484,
525, 544, 609, 762, 812, 874, 1037, 1177, 1199,
1259, 1289, 1338, 1519, 2199, 3197

**TS between cis-1,3,3,3- and
1,1,3,3-tetrafluoropropenes**

C, 0.108742, -0.823242, -0.842456
C, 1.334801, -0.583415, -0.242543
C, -0.823639, 0.019489, -0.241827
H, -0.192351, -1.856977, -0.929334
F, 0.266226, -0.242208, 1.426466
F, -0.743451, 1.303884, -0.205686
F, -2.027939, -0.376874, -0.007974
H, 2.036044, -1.375105, -0.000798
F, 1.887040, 0.599097, -0.224908
Frequencies: 624i, 146, 181, 263, 317, 373,
429, 578, 655, 718, 819, 923, 1026, 1083, 1279,
1326, 1398, 1532, 1566, 3220, 3248

**TS between trans-1,3,3,3-tetrafluoropropene
and 3,3,3-trifluoropropyne + hydrogen
fluoride**

C, -0.012353, -0.884984, 0.000000

F, 0.604078, -1.372864, 1.082206
F, -1.264187, -1.370372, 0.000000
F, 0.604078, -1.372864, -1.082206
C, 0.029369, 0.591009, 0.000000
C, -0.730636, 1.586655, 0.000000
H, -1.561615, 2.264075, 0.000000
H, 0.910912, 1.661095, 0.000000
F, 0.604078, 2.818184, 0.000000
Frequencies: 1799i, 47, 135, 139, 362, 412, 454, 566, 606, 625, 678, 753, 856, 967, 1030, 1173, 1182, 1269, 1754, 1951, 3379

TS between trans-1,3,3,3-tetrafluoropropene and 2H-trifluoromethylvinylidene + hydrogen fluoride

C, -0.033839, -0.942788, 0.000000
F, 0.434736, -1.580141, 1.078861
F, -1.364707, -1.055494, 0.000000
F, 0.434736, -1.580141, -1.078861
C, 0.418186, 0.489757, 0.000000
C, -0.437527, 1.465495, 0.000000
H, -0.621887, 2.699802, 0.000000
H, 1.485455, 0.687544, 0.000000
F, 0.434736, 3.164428, 0.000000
Frequencies: 1234i, 92, 127, 133, 225, 392, 394, 556, 561, 602, 744, 772, 832, 876, 1096, 1181, 1234, 1280, 1714, 2240, 3202

TS between trans-1,3,3,3-tetrafluoropropene and trifluoroallene + hydrogen fluoride

C, -0.166326, -0.812519, 0.000000
F, -0.389059, -1.501541, 1.060555
F, -0.389059, -1.501541, -1.060555
F, 1.833917, -0.896785, 0.000000
C, 0.056888, 0.569189, 0.000000
C, -0.800550, 1.563827, 0.000000
H, -1.884457, 1.497963, 0.000000
H, 1.343721, 0.210054, 0.000000
F, -0.389059, 2.829757, 0.000000
Frequencies: 1745i, 81, 146, 210, 229, 243, 413, 514, 531, 662, 755, 930, 932, 1051, 1145, 1336, 1369, 1495, 1779, 1862, 3191

TS between cis-1,3,3,3-tetrafluoropropene and trifluoroallene + hydrogen fluoride

C, 0.614450, -0.095784, 0.000000
F, 1.217593, -0.486489, 1.059885
F, 1.217593, -0.486489, -1.059885
F, 1.217593, 1.837944, 0.000000
C, -0.657697, 0.497664, 0.000000
C, -1.860242, -0.029031, 0.000000
H, 0.019802, 1.639910, 0.000000
H, -2.786978, 0.530322, 0.000000
F, -2.076323, -1.354669, 0.000000
Frequencies: 1714i, 64, 121, 207, 230, 272, 446, 561, 589, 619, 835, 848, 909, 1058, 1109, 1337, 1386, 1476, 1785, 1866, 3238

TS between cis-1,3,3,3-tetrafluoropropene and 2H-trifluoromethylvinylidene + hydrogen fluoride

C, -0.509040, 0.538537, 0.000000
F, -0.987223, -0.075794, 1.079434
F, -0.987223, 1.793597, 0.000000
F, -0.987223, -0.075794, -1.079434
C, 1.001568, 0.586439, 0.000000
C, 1.836677, -0.404397, 0.000000
H, 2.063664, -1.629624, 0.000000

H, 1.467593, 1.570022, 0.000000
F, 1.016503, -2.115773, 0.000000
Frequencies: 1254i, 20, 107, 237, 257, 421, 438, 546, 557, 597, 695, 778, 802, 869, 1083, 1211, 1219, 1262, 1733, 2265, 3173

TS between 1,1,3,3-tetrafluoropropene and 2H-trifluorovinylmethylene + hydrogen fluoride

C, 1.206349, -0.132832, 0.035827
F, 2.365228, -0.525873, -0.383635
F, 1.273898, 1.017148, 0.595738
F, -1.465497, 1.660159, -0.494539
C, 0.091308, -0.875659, -0.110710
C, -1.135786, -0.346816, 0.337113
H, -1.362299, 0.801852, 0.487158
F, -2.148802, -1.132795, 0.120148
H, 0.167629, -1.837760, -0.599938
Frequencies: 942i, 86, 92, 172, 207, 292, 423, 509, 643, 689, 711, 861, 1003, 1203, 1219, 1306, 1404, 1511, 1702, 2287, 3231

TS between 1,1,3,3-tetrafluoropropene and trifluoroallene + hydrogen fluoride

C, -1.253667, -0.107106, 0.023480
F, -2.156966, -1.001891, -0.291992
F, -1.847243, 1.052996, 0.240846
F, 2.157250, -1.215361, 0.054773
C, 0.025762, -0.346245, 0.132906
C, 1.149560, 0.437517, 0.383942
H, 1.639766, 0.545920, 1.346297
F, 1.610051, 1.258926, -0.511289
H, 0.962464, -1.302940, -0.019301
Frequencies: 1762i, 65, 117, 147, 199, 409, 458, 531, 615, 635, 686, 881, 1011, 1029, 1189, 1264, 1308, 1486, 1752, 1914, 3211

TS between 1,1,3,3-tetrafluoropropene and 1,3,3-trifluoropropyne

C, 1.107339, 0.303459, 0.012613
F, 2.181477, -1.178540, 0.016352
F, 1.951319, 1.223302, -0.160534
F, -1.764662, 1.164192, -0.030866
C, 0.039452, -0.321373, 0.187470
C, -1.406523, -0.088792, 0.369186
H, -1.706576, -0.206003, 1.413005
F, -2.119138, -0.967857, -0.379597
H, 1.024005, -1.323625, 0.163181
Frequencies: 1771i, 34, 108, 155, 304, 405, 418, 467, 559, 662, 725, 875, 949, 1085, 1110, 1281, 1374, 1407, 1779, 2143, 3109

TS between 3,3,3-trifluoropropyne and 2H-trifluoromethylvinylidene

C, -0.325692, -0.002766, 0.000000
F, -0.793964, -0.637332, 1.076490
F, -0.793964, 1.243012, 0.000000
F, -0.793964, -0.637332, -1.076490
C, 1.155692, 0.046081, 0.000000
C, 2.397808, 0.170893, 0.000000
H, 2.070173, -1.000380, 0.000000
Frequencies: 942i, 114, 164, 212, 452, 483, 526, 608, 648, 811, 1191, 1205, 1236, 2060, 2527

TS between 3,3,3-trifluoropropyne and trifluoroallene

C, 0.288598, 0.388033, 0.000000

F, 0.147141, 1.106107, 1.062798
F, 0.147141, 1.106107, -1.062798
F, -1.267088, -0.547165, 0.000000
C, 1.076443, -0.793855, 0.000000
C, 0.147141, -1.654853, 0.000000
H, -0.317844, -2.621398, 0.000000
Frequencies: 597i, 223, 289, 338, 451, 586,
616, 717, 745, 918, 1064, 1338, 1436, 1777,
3380

**TS between 3,3,3-trifluoropropyne and
1H-trifluorovinylmethylene**

C, 0.530537, -0.157708, 0.000203
F, 1.246672, -0.199687, -1.053027
F, -0.827880, 1.510816, -0.002164
F, 1.246635, -0.195017, 1.053627
C, -0.859714, -0.187916, 0.000259
C, -1.723870, -1.068553, 0.001470
H, -2.670564, -1.559945, 0.002478
Frequencies: 489i, 22, 212, 276, 329, 476, 586,
591, 643, 783, 896, 1404, 1483, 2029, 3442

**TS between trifluoroallene and
2H-trifluorovinylmethylene**

C, -0.949670, 0.000628, -0.005122
F, -1.767386, -1.020828, -0.113217
F, -1.596493, 1.140252, -0.020121
C, 0.356480, -0.099393, 0.064723
C, 1.610837, 0.034540, 0.566606
H, 0.941823, -1.102892, 0.692040
F, 2.580801, 0.045935, -0.361027
Frequencies: 1336i, 146, 158, 325, 426, 558,
590, 601, 873, 958, 1059, 1309, 1364, 1968,
2235

**TS between 2H-trifluoromethylvinylidene and
2H-trifluorovinylmethylene**

C, 0.496403, 0.241019, -0.098657
F, 1.205561, 0.315367, 0.963370
F, -0.947363, -1.022444, 0.385123
F, 1.068563, -0.523192, -0.949008
C, -0.654158, 1.024148, -0.353402
C, -1.721703, 0.235427, -0.043822
H, -0.664101, 2.068850, -0.620083
Frequencies: 449i, 76, 240, 310, 534, 551, 607,
668, 805, 975, 1108, 1351, 1447, 1503, 3269

**TS between 1H-trifluorovinylmethylene and
1H-trifluorocyclopropene**

C, 0.578287, -0.018998, -0.021935
F, 1.061282, -1.134170, 0.438771
F, 1.531676, 0.766591, -0.382000
C, -0.970832, 1.416245, 0.384324
C, -0.786497, 0.199152, -0.127347
F, -1.596202, -0.877080, -0.316248
H, -1.896547, 1.623535, 0.925030
Frequencies: 216i, 260, 275, 408, 484, 596,
642, 808, 837, 871, 1075, 1346, 1549, 1630,
3153

**TS between 2H-trifluorovinylmethylene and
1H-trifluorocyclopropene**

C, -0.204760, -0.833144, 0.000000
F, -0.487348, -1.544258, 1.084054
F, 1.123950, 2.367232, 0.000000
F, -0.487348, -1.544258, -1.084054
C, 0.712771, 1.134313, 0.000000
C, -0.487348, 0.601233, 0.000000

H, -1.467272, 1.077142, 0.000000
Frequencies: 212i, 78, 232, 414, 470, 486, 583,
821, 947, 1101, 1173, 1217, 1404, 1775, 3134

**TS between trifluoroallene and
difluoropropadienylidene + hydrogen fluoride**

C, -0.342439, -0.998323, 0.000000
F, -0.351315, -1.729148, 1.065574
F, -0.351315, -1.729148, -1.065574
C, -0.336551, 0.319288, 0.000000
C, -0.351315, 1.567179, 0.000000
H, 0.082948, 2.646734, 0.000000
F, 1.380282, 2.572119, 0.000000
Frequencies: 1239i, 82, 89, 197, 271, 543, 590,
660, 704, 833, 856, 1348, 1512, 2098, 2580

**TS between 1H-trifluorovinylmethylene and
fluoroacetylene + difluoromethylene**

C, 0.647181, 0.597698, 0.000000
F, 0.414093, 1.361135, 1.042433
F, 0.414093, 1.361135, -1.042433
C, -0.482171, -1.068554, 0.000000
C, -1.612781, -0.628527, 0.000000
H, -2.493882, -0.032398, 0.000000
F, 0.414093, -1.985748, 0.000000
Frequencies: 429i, 60, 187, 197, 339, 487, 495,
572, 652, 663, 1062, 1114, 1176, 2185, 3475

**TS between 2H-trifluorovinylmethylene and
fluoroacetylene + difluoromethylene**

C, 0.239943, 1.191292, 0.000000
F, -0.569966, 1.104422, 1.047437
F, -0.569966, 1.104422, -1.047437
C, 1.358082, -0.370918, 0.000000
C, 0.569692, -1.315701, 0.000000
F, -0.569966, -1.871043, 0.000000
H, 2.382793, -0.068234, 0.000000
Frequencies: 444i, 21, 117, 258, 329, 470, 547,
650, 663, 908, 1066, 1083, 1144, 2127, 3401

**TS between 1H-trifluorobutatrienylmethylene
and difluoropropadienylidene +
fluoroacetylene**

C, 0.595411, -2.413414, 0.000000
C, 1.616879, -1.774482, 0.000000
C, -0.310730, 1.834389, 0.000000
F, -0.254170, 2.582872, 1.066773
F, -0.254170, 2.582872, -1.066773
C, -0.403310, 0.525634, 0.000000
C, -0.761491, -0.699220, 0.000000
H, 2.442022, -1.105126, 0.000000
F, -0.254170, -3.358225, 0.000000
Frequencies: 320i, 35, 72, 81, 178, 185, 291,
413, 462, 555, 589, 608, 631, 677, 856, 1085,
1290, 1486, 2093, 2255, 3492

**TS between 2H-trifluorobutatrienylmethylene
and difluoropropadienylidene +
fluoroacetylene**

C, -0.184537, -2.633385, 0.000000
C, 0.876679, -2.052084, 0.000000
F, 1.819394, -1.208816, 0.000000
H, -0.866749, -3.450735, 0.000000
C, -0.423460, 1.422507, 0.000000
F, -0.184537, 2.138159, 1.068749
F, -0.184537, 2.138159, -1.068749
C, -0.844150, 0.181686, 0.000000
C, -1.455554, -0.944857, 0.000000

Frequencies: 332i, 45, 54, 89, 162, 207, 349,
400, 433, 550, 591, 661, 664, 780, 862, 1100,
1277, 1473, 2074, 2246, 3460

**TS between 2H-trifluorobutatrienylmethylene
and 1H-trifluorovinylidenecyclopropene**

C, 0.071303, -2.425134, 0.000000
C, -1.093639, -1.822037, 0.000000
C, 0.201804, 1.948633, 0.000000
F, 0.433842, 2.663284, 1.079873
F, 0.433842, 2.663284, -1.079873
C, -0.219429, 0.688178, 0.000000
C, -0.556633, -0.504926, 0.000000
F, 0.433842, -3.679501, 0.000000
H, -2.134184, -2.131895, 0.000000
Frequencies: 450i, 57, 87, 104, 216, 303, 410,
443, 462, 496, 576, 739, 830, 1004, 1069, 1229,
1274, 1584, 1758, 2079, 3172

**TS between 2H-trifluorobutatrienylmethylene
and trifluoropentatetraene**

C, -1.739163, -0.094203, 0.126897
C, -3.029074, 0.061885, 0.539284
F, -3.926744, 0.115330, -0.458681
H, -2.367720, -1.128091, 0.587649
C, 2.115215, 0.015169, -0.026053
F, 2.828525, 1.115809, -0.006924
F, 2.887502, -1.041932, -0.119524
C, 0.812579, -0.024496, 0.039075
C, -0.448861, -0.054151, 0.100549
Frequencies: 1191i, 73, 80, 189, 205, 276, 381,
442, 523, 569, 582, 619, 750, 926, 968, 1148,
1289, 1477, 1897, 2195, 2274

**TS between trifluoropentatetraene and
difluoropentatetraenylidene + hydrogen
fluoride**

C, 0.648044, 1.581954, 0.000000
C, 0.977674, 2.789166, 0.000000
F, -0.428315, 4.250481, 0.000000
H, 0.854830, 3.937413, 0.000000
C, -0.252779, -2.171315, 0.000000
F, -0.428315, -2.885633, 1.069354
F, -0.428315, -2.885633, -1.069354
C, 0.063396, -0.897169, 0.000000
C, 0.348609, 0.322305, 0.000000
Frequencies: 1199i, 52, 57, 114, 140, 229, 272,
461, 481, 527, 586, 654, 656, 713, 806, 1122,
1327, 1592, 2059, 2261, 2613