Supporting Information for

**Gas-Phase Study of the Elementary Reaction of the D1-Ethynyl Radical**

**(C2D; X2Σ+) with Propylene (C3H6; X1A’) Under Single Collision Conditions**

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**Table S1.** Optimized Cartesian coordinates (Å) and vibrational frequencies (cm−1) for all intermediates, transition states, reactants, and products involved in the C2H + propylene reaction at the ωB97X-D/6-311G(d,p) level.

**Reactants**

**Propene (C3H6)**

C -1.276382 -0.221005 0.000011

C -0.134665 0.454315 0.000065

C 1.230687 -0.162110 -0.000007

H -2.235678 0.284449 -0.000197

H -1.291429 -1.307503 0.000032

H -0.168945 1.542398 -0.000050

H 1.801146 0.152652 -0.879851

H 1.175233 -1.253094 0.000755

H 1.801836 0.153898 0.878900

**Frequencies**

182.1163 433.1263 584.8533

935.9604 946.6639 949.9836

1028.6410 1072.0141 1195.7134

1328.2163 1407.9847 1453.7621

1479.9109 1496.4393 1741.6224

3037.0035 3096.8485 3127.1754

3147.8492 3161.1146 3240.4151

**Ethynyl (C2H)**

C 0.000000 0.000000 0.728763

C 0.000000 0.000000 -0.472485

H 0.000000 0.000000 -1.537669

**Frequencies**

479.6131 479.6132 2105.5192

3467.3577

**Intermediate states**

**i1**

C 0.435423 0.067251 0.402465

C 1.178918 -1.163326 -0.136946

C -1.006460 -0.025483 0.117877

C -2.177429 -0.091750 -0.136275

C 0.976854 1.347526 -0.160654

H 0.544560 0.090481 1.494038

H 1.068302 -1.227461 -1.222314

H 0.780721 -2.080446 0.301116

H 2.242696 -1.090710 0.100655

H -3.215860 -0.152781 -0.356018

H 1.350879 1.368244 -1.178146

H 0.784862 2.287362 0.341861

**Frequencies**

52.2843 177.0370 226.4886

274.9168 355.8492 485.1906

534.7233 593.8586 688.3975

706.3797 805.2265 921.9487

961.0979 1061.8229 1143.5687

1186.6983 1317.1732 1332.6596

1412.9761 1457.3451 1499.4403

1506.2048 2237.0780 3039.6257

3054.2257 3135.3316 3143.2789

3155.7671 3271.0887 3484.6795

**i2**

C 0.580527 0.136687 0.499874

C 1.688996 -0.609415 -0.204384

C -0.825050 -0.058759 0.076467

C -1.846234 -0.830484 -0.020805

C -0.164209 1.255171 -0.206396

H 0.094430 1.463738 -1.240192

H 0.722560 0.279555 1.568454

H 1.812261 -1.608824 0.219666

H 2.638715 -0.075672 -0.107655

H 1.464176 -0.722547 -1.267981

H -2.850531 -0.808804 -0.414969

H -0.485789 2.113347 0.374138

**Frequencies**

180.8270 217.7740 320.1807

367.7494 449.3210 672.5861

739.5636 748.7619 856.5489

885.6046 931.5259 946.5295

1041.9071 1081.4755 1140.3249

1166.6831 1182.6140 1378.0281

1428.3132 1464.5717 1496.6867

1508.1727 1809.3341 3047.4418

3121.6670 3123.6991 3127.0002

3149.9132 3216.8646 3271.0181

**i3**

C 0.104673 0.626723 -0.032823

C -0.926799 -0.457292 -0.013950

C -2.368634 -0.100800 0.036229

C 2.604446 -0.280534 0.029200

C 1.480743 0.136163 0.002665

H -0.053398 1.309524 0.814885

H -0.020050 1.256222 -0.929576

H -0.615677 -1.476724 -0.204747

H -2.709389 0.360405 -0.904428

H -2.575112 0.630581 0.828002

H -2.994546 -0.977220 0.213227

H 3.601603 -0.648349 0.054706

**Frequencies**

61.5528 103.9672 156.9744

307.0908 337.5207 363.1863

514.1601 678.6571 693.3724

870.3411 891.2006 987.8227

992.5555 1114.3100 1150.8599

1202.5265 1289.1941 1392.9748

1417.5927 1452.9181 1475.6706

1490.4551 2254.9661 2970.7348

2980.5482 3015.1755 3043.2463

3130.3393 3217.7392 3484.2336

**i4**

C -1.226956 0.463469 -0.265802

C -1.601690 -0.930641 0.085679

C 1.224592 0.142746 0.019982

C 2.147923 -0.615179 -0.084061

C 0.087212 1.056033 0.150035

H 0.038896 1.385703 1.202081

H -1.990808 1.156663 -0.599803

H -0.809117 -1.636784 -0.183846

H -2.522985 -1.234662 -0.414739

H -1.763037 -1.046798 1.169686

H 2.969772 -1.283332 -0.176273

H 0.290792 1.960643 -0.432105

**Frequencies**

77.2630 145.1035 166.0933

328.1326 348.5903 398.9994

598.5643 691.5675 694.7446

857.9759 876.8576 952.0553

1000.5952 1101.7089 1159.5219

1228.1579 1339.3264 1378.6410

1427.5919 1452.2304 1480.7913

1491.8445 2250.0157 2960.6237

2977.2249 3070.5731 3074.7685

3132.1998 3198.2973 3484.5331

**i5**

C -0.850749 -0.343592 -0.042172

C -2.331890 -0.134598 0.016506

C 1.522085 0.450244 -0.029372

C 2.202317 -0.673077 0.046772

C 0.062885 0.631650 0.016703

H -0.507384 -1.371696 -0.141823

H -2.770821 -0.666663 0.868637

H -2.822802 -0.528300 -0.881030

H -2.587934 0.923613 0.108787

H 2.100270 1.376576 -0.133971

H 3.236942 -0.979235 0.030159

H -0.276152 1.661940 0.098620

**Frequencies**

44.5428 193.4510 203.7967

249.1474 382.6177 581.2466

613.6789 781.2283 849.6687

861.9355 900.9192 1001.3408

1048.9201 1066.3437 1126.9943

1269.2228 1326.8148 1343.6494

1413.6469 1478.6082 1490.2469

1637.4804 1707.4298 3008.0451

3011.0249 3048.5295 3090.2716

3127.1937 3136.5485 3245.5932

**i6**

C -1.303426 0.508757 0.000093

C -1.437781 -1.009821 -0.000026

C 1.219710 0.214243 -0.000001

C 2.203808 -0.504767 -0.000041

C 0.106633 1.019118 -0.000019

H -1.822469 0.929826 0.871868

H -1.822664 0.929990 -0.871481

H -0.961928 -1.445683 -0.881711

H -2.490424 -1.301297 0.000053

H -0.961759 -1.445835 0.881491

H 3.066328 -1.126207 -0.000038

H 0.259251 2.094024 -0.000221

**Frequencies**

57.9174 156.1498 257.9616

365.2581 384.6332 495.0886

565.5971 628.2811 663.1821

788.1300 859.3335 997.0678

1075.3162 1103.8947 1162.9934

1284.3523 1366.9661 1401.6846

1435.2845 1480.5151 1501.3198

1511.3022 2026.7060 3017.6102

3040.1461 3056.2531 3132.5336

3135.6487 3183.6786 3474.4880

**i7**

C 1.146570 0.582552 0.033202

C 1.540784 -0.859226 -0.043539

H 1.960483 1.300334 0.101531

H 1.684542 -1.280898 0.959258

H 2.485446 -0.979948 -0.581317

H 0.771026 -1.461959 -0.533686

C -1.360207 0.326936 -0.062985

C -1.564356 -0.966584 0.080962

C -0.101055 1.076043 0.026421

H -2.243075 0.945176 -0.268967

H -2.411149 -1.635836 0.045636

H -0.217680 2.154806 0.073173

**Frequencies**

86.9692 127.9951 221.1698

375.2709 417.3283 611.1505

671.9381 715.8242 850.1903

860.2409 904.4331 993.7330

1017.3344 1054.4650 1102.8729

1274.1613 1279.9476 1399.7284

1440.2382 1476.0818 1481.2348

1627.8176 1691.0090 3005.5056

3006.5915 3052.8281 3084.4790

3131.1913 3157.1139 3236.4052

**i8**

C -1.006349 0.045971 0.603440

C -2.144116 -0.348885 -0.345966

C 1.424551 0.120173 -0.089267

C 2.542631 -0.362965 -0.052130

C 0.158358 0.651018 -0.118553

H -0.671292 -0.825131 1.171320

H -1.388996 0.772580 1.332336

H -2.500359 0.516153 -0.912383

H -2.990282 -0.757447 0.211993

H -1.808279 -1.103791 -1.060837

H 3.518782 -0.782874 -0.020470

H -0.010028 1.548638 -0.707106

**Frequencies**

29.7020 182.6515 261.5818

337.0403 384.5115 483.4008

542.6707 620.8612 673.8804

784.2518 889.2375 1008.9730

1067.5716 1120.1009 1168.0270

1284.0152 1330.2978 1414.9843

1426.4876 1488.0011 1503.1664

1510.0957 2031.3926 3022.0314

3049.1228 3100.1501 3127.5664

3132.3573 3176.9394 3474.5984

**i9**

C -0.049913 0.638499 -0.063472

C -1.429892 0.163915 -0.013532

C -2.553063 -0.254545 0.027397

H 0.105664 1.199134 -0.990483

H 0.117795 1.340857 0.760203

H -3.550966 -0.619476 0.064779

C 0.974642 -0.506569 0.022260

C 2.379510 -0.023042 0.006207

H 0.800817 -1.211196 -0.797816

H 0.774297 -1.075815 0.944145

H 3.186165 -0.675276 -0.303985

H 2.638519 0.932221 0.449997

**Frequencies**

104.3449 157.6864 176.3147

350.7517 356.6233 498.0631

516.7562 685.6384 691.4793

743.9763 869.0743 977.2493

1001.9598 1093.5373 1113.0756

1193.2963 1294.1928 1315.4238

1388.5475 1463.1446 1473.4176

1484.7173 2251.0268 2981.4418

3055.0790 3072.1104 3100.1060

3156.9619 3265.4476 3483.8907

**i10**

C -0.027383 -0.962277 -0.272092

C 1.237182 -0.358308 0.367105

C -1.219180 -0.143920 -0.060600

C -2.185258 0.541846 0.126783

C 1.614103 0.967241 -0.188670

H -0.205541 -1.958879 0.143100

H 0.131712 -1.088737 -1.347688

H 2.627791 1.335207 -0.089330

H 2.062190 -1.069291 0.246616

H 1.066114 -0.280909 1.452985

H -3.047378 1.141911 0.291390

H 0.848327 1.653207 -0.532235

**Frequencies**

121.9389 164.0553 198.4734

353.4607 362.7020 497.2786

556.8645 684.3415 692.6719

769.2920 876.3469 945.8313

1000.4529 1080.1863 1122.0596

1195.6295 1287.2731 1362.3074

1379.1157 1466.6771 1472.4938

1483.8222 2251.1900 2978.9688

3054.7024 3069.6567 3098.9043

3157.5049 3266.3789 3486.8210

**i11**

C 1.026521 -0.035543 0.463444

C 2.030546 -0.498737 -0.273518

H 0.877515 -0.411542 1.472976

H 2.200369 -0.152675 -1.288666

H 2.723234 -1.238221 0.112688

C -1.352976 0.430107 -0.109597

C -1.985230 -0.714366 -0.060771

C 0.015133 0.987507 -0.006644

H -3.063887 -0.781788 -0.177315

H -1.457692 -1.660377 0.090671

H 0.316720 1.394911 -0.978336

H -0.000226 1.835882 0.690496

**Frequencies**

75.5130 155.7144 202.0040

404.4071 433.5156 474.8439

659.2508 886.8853 890.8017

910.9392 929.3940 949.1514

1016.1076 1030.9095 1116.0611

1237.4975 1302.1301 1323.1444

1409.7826 1445.7365 1461.7327

1698.4543 1736.6489 3000.0899

3038.4101 3040.6318 3124.7854

3139.2680 3143.2712 3209.2360

**i12**

C -1.111490 -0.048219 0.379400

C -0.048599 0.950234 -0.013156

C -2.140848 -0.395618 -0.347669

H -0.985285 -0.502962 1.369743

H -0.059468 1.775670 0.712019

H -0.307062 1.399688 -0.978547

H -2.996474 -1.049703 -0.269904

C 1.698679 -0.886840 -0.039884

C 1.354944 0.396513 -0.078546

H 2.737138 -1.191629 -0.100969

H 0.959427 -1.676223 0.043248

H 2.135609 1.148741 -0.176466

**Frequencies**

94.8587 149.5862 261.2462

397.3912 512.4101 573.0960

670.2748 780.0799 828.2312

907.6220 938.5341 953.0874

1031.0532 1045.8603 1109.2076

1207.1294 1275.4922 1326.1066

1348.6986 1444.8478 1467.7263

1678.2893 1706.4365 2996.7222

3011.8479 3040.4544 3122.0202

3137.3159 3216.2996 3239.1734

**i13**

C 1.333055 -0.307040 0.000129

C 1.530823 0.985185 -0.000008

C 0.041024 -1.089405 -0.000177

H 2.222998 -0.951380 0.000486

H 2.381982 1.649875 0.000002

H 0.063616 -1.768771 0.864873

H 0.063589 -1.767935 -0.865905

C -1.515654 0.935037 -0.000051

C -1.281653 -0.372530 0.000140

H -2.530866 1.317033 0.000193

H -0.712131 1.663640 -0.000372

H -2.134760 -1.049948 0.000526

**Frequencies**

67.3766 166.4240 226.4881

369.8941 516.8935 616.8735

630.2011 808.9787 821.0974

854.2551 943.9462 967.0059

1017.5074 1028.9874 1084.5895

1245.6107 1258.1739 1334.2598

1387.3866 1442.0943 1453.7389

1685.3034 1713.5386 2979.8521

2991.5512 2993.7626 3111.4752

3122.4734 3206.9262 3235.0516

**i14**

C -1.247024 0.391393 -0.000118

C -0.000038 -0.271576 -0.000085

C 2.460638 -0.227013 0.000079

C 1.246943 0.391212 0.000097

C -2.460578 -0.227030 0.000058

H -1.223363 1.479937 -0.000192

H -2.541681 -1.308868 0.000196

H -0.000216 -1.359604 -0.000161

H 3.384036 0.338074 -0.000014

H 2.542215 -1.308836 -0.000267

H 1.223518 1.479793 -0.000012

H -3.384157 0.337591 0.000271

**Frequencies**

157.1994 203.8249 255.7876

454.5763 492.6832 586.2926

627.0054 834.6782 854.7655

873.5676 921.8113 984.7204

1011.0370 1030.4246 1168.0496

1255.0541 1279.8851 1301.6895

1303.0369 1443.5366 1487.9647

1521.9903 1589.8185 3121.0417

3122.1092 3136.3543 3136.6552

3139.3291 3229.3588 3229.9683

**i15**

C 1.005914 -0.354273 -0.000157

C 0.047131 0.690515 -0.000119

C -2.074819 -0.623449 0.000073

C -1.361544 0.539533 0.000030

C 2.349610 -0.158664 0.000123

H 0.640397 -1.378079 -0.000450

H 0.433395 1.706226 -0.000118

H -3.157338 -0.608923 0.000101

H -1.601364 -1.598232 0.000157

H -1.930321 1.466511 0.000087

H 2.773650 0.840159 0.000401

H 3.043818 -0.989641 0.000121

**Frequencies**

141.4443 219.4607 236.5522

395.5770 577.3508 611.4989

623.1879 817.2661 847.8632

877.3821 919.7505 1000.0811

1011.8468 1038.5197 1096.2510

1195.0101 1270.3874 1312.2925

1379.8274 1444.8444 1479.5751

1545.7774 1591.4766 3128.2620

3134.3882 3139.9179 3148.3089

3152.7473 3227.4932 3232.3218

**i16**

C 0.924445 0.813963 0.100282

C 1.121523 -0.692477 -0.051689

C -1.259491 -0.401937 0.088694

C -0.058512 -1.279671 -0.056460

C -0.606656 1.005526 -0.118024

H 1.236459 1.136438 1.101396

H 1.515848 1.390020 -0.617806

H 2.093096 -1.167495 -0.102557

H -2.044673 -0.608500 -0.642720

H -1.706404 -0.511217 1.083562

H -1.034561 1.758524 0.546483

H -0.787627 1.329806 -1.145176

**Frequencies**

137.8487 372.4520 616.0320

749.2827 761.8559 808.4100

875.2964 889.0067 925.7360

969.8328 1011.5062 1049.2511

1134.5725 1190.1821 1212.2763

1230.9241 1291.4342 1301.7532

1332.2806 1481.3545 1489.4207

1505.0061 1673.9001 3007.3907

3020.8662 3045.6754 3056.6234

3067.9338 3099.5600 3193.5100

**i17**

C -1.284170 0.436808 0.102503

C -1.642337 -0.858283 -0.111563

H -2.087675 1.128344 0.349229

H -0.941946 -1.610939 -0.447292

H -2.674727 -1.166436 0.000497

C 0.000024 1.038614 0.000035

C 1.642236 -0.858304 0.111604

C 1.284268 0.436790 -0.102496

H 0.000051 2.124816 0.000013

H 2.674541 -1.166740 -0.000716

H 0.941847 -1.610968 0.447297

H 2.087780 1.128179 -0.349528

**Frequencies**

133.3319 243.5107 277.4382

376.8691 572.8968 590.7022

697.0076 806.5978 871.0013

877.1310 901.3722 989.1513

1004.7381 1009.0864 1122.1980

1179.3454 1269.0199 1314.8904

1416.2983 1448.8253 1471.7295

1556.7040 1599.7454 3117.7415

3122.3881 3149.4651 3151.3626

3158.6275 3235.6491 3246.0282

**i18**

C 0.666058 1.033790 -0.000266

C -0.666259 1.033670 0.000464

C 1.235890 -0.368801 -0.000036

C -1.235878 -0.368968 -0.000346

C 0.000105 -1.218883 0.000066

H 1.290483 1.919476 -0.000374

H -1.290603 1.919432 0.000635

H 1.881997 -0.550442 0.874899

H 1.882178 -0.550803 -0.874560

H -1.881734 -0.550894 -0.875242

H -1.882221 -0.551164 0.874252

H 0.000401 -2.300454 0.001099

**Frequencies**

205.8843 331.1613 390.0321

681.6008 742.8666 791.9530

896.0363 913.6082 924.0704

944.1522 961.7924 969.4016

1033.8085 1128.6138 1128.6583

1132.3383 1274.4514 1299.3070

1324.5548 1386.7380 1456.4985

1462.4737 1675.4155 2942.8478

2943.1634 2944.2467 2947.7481

3172.7613 3197.0995 3206.3454

**i19**

C 0.490839 1.145867 0.000023

C -0.971546 0.779126 -0.000127

C 1.273704 0.000770 -0.000020

C -0.970585 -0.780285 0.000131

C 0.492293 -1.145294 -0.000041

H 0.858065 2.163533 0.000594

H -1.491679 1.186472 -0.875740

H -1.492080 1.186978 0.875002

H 2.357468 0.001438 -0.000101

H -1.490527 -1.188659 -0.875080

H -1.490191 -1.188336 0.875703

H 0.860723 -2.162533 -0.000175

**Frequencies**

124.1706 449.7200 597.3540

641.9963 727.0993 804.5544

810.3011 905.6072 911.5470

948.8191 992.3520 1026.8690

1072.8327 1105.5569 1141.8848

1221.9749 1274.2185 1300.4541

1317.9040 1400.3031 1469.5809

1478.6199 1493.4128 2997.5239

3008.7137 3010.3043 3030.6200

3179.9963 3201.9144 3213.6407

**Transition states**

**i1 – i4**

C -1.053960 0.234157 -0.405692

C -1.406432 -1.102893 0.154786

C 1.384282 0.153452 -0.403495

C 2.336454 -0.368391 0.136757

C -0.679631 1.302803 0.325253

H -1.162549 0.357067 -1.479995

H -1.201063 -1.156623 1.224966

H -0.837029 -1.886717 -0.349428

H -2.468989 -1.306951 -0.013589

H 3.228400 -0.814223 0.511987

H -0.566734 1.234161 1.401803

H -0.476321 2.258517 -0.141396

**Frequencies**

-230.2626 44.5316 75.0690

171.2677 212.9421 270.2581

431.9510 617.5610 655.4169

682.0503 932.0187 959.4662

973.4057 1010.2083 1068.7275

1206.4643 1332.1459 1408.9985

1453.3384 1485.2350 1497.4575

1670.3154 2023.4371 3050.4629

3120.8220 3148.8531 3164.4163

3181.2579 3265.9176 3456.7649

**i1 – i2**

C -0.540531 -0.109148 0.476045

C -1.625705 0.707491 -0.202373

C 0.838126 0.193333 0.139451

C 1.963918 0.656157 -0.076966

C -0.073065 -1.361991 -0.192491

H -0.249978 -1.496885 -1.251330

H -0.700853 -0.217743 1.549555

H -1.675727 1.711876 0.223092

H -2.596079 0.221263 -0.073825

H -1.422499 0.800235 -1.271840

H 2.970909 0.657358 -0.430733

H 0.297769 -2.191151 0.393084

**Frequencies**

-715.2085 193.3926 226.5889

308.1422 368.9198 440.7574

493.5076 639.8831 706.1671

714.8351 838.0965 900.7783

930.3171 1083.5133 1165.7075

1170.9410 1228.4812 1364.8059

1417.5132 1451.5766 1496.4182

1501.4962 1964.5541 3049.1846

3100.5388 3131.2427 3136.7978

3167.3446 3288.1660 3416.6089

**i4 – i2**

C 0.710050 0.185232 0.527149

C 1.693236 -0.675860 -0.194981

C -1.023147 0.098466 -0.049150

C -1.945432 -0.726263 -0.056132

C -0.107864 1.213335 -0.188038

H 0.748261 0.247202 1.607742

H 1.812403 -1.646047 0.293278

H 2.682763 -0.200306 -0.234323

H 1.373398 -0.855779 -1.225259

H -2.401632 -1.666574 0.163483

H 0.195087 1.442548 -1.209803

H -0.371338 2.109498 0.371789

**Frequencies**

-711.9133 151.8863 168.5758

313.4035 367.4242 396.0944

511.2245 669.5866 718.8939

858.7633 919.5504 952.3033

1033.3051 1059.5540 1163.5471

1187.2179 1206.2619 1376.6112

1424.6575 1470.0399 1488.1939

1501.5807 1972.9726 3012.6328

3085.4848 3087.5893 3123.7747

3157.6930 3209.1574 3409.6758

**i4 – i3**

C 0.118997 0.789767 0.010648

C 2.467513 -0.467206 0.098824

C 1.416248 0.109207 0.067947

H -0.139963 1.144514 1.014239

H 0.232174 1.690204 -0.610802

H 3.400894 -0.975116 0.130964

C -0.972774 -0.089189 -0.523315

C -2.209310 -0.345870 0.259428

H -0.794747 -0.603278 -1.460346

H -2.702628 0.589614 0.556960

H -1.990434 -0.885791 1.193018

H -2.929332 -0.940409 -0.305221

**Frequencies**

-74.9989 101.2664 188.6175

324.4199 351.1258 387.2232

520.3430 690.6866 708.8621

856.9647 903.8081 968.9531

982.3896 1117.6125 1155.3746

1232.8035 1297.2686 1396.3077

1432.7001 1456.7154 1478.5519

1488.2920 2246.8691 2991.3156

3002.4047 3036.1848 3076.4140

3132.9112 3207.7067 3484.7609

**i1 – p1**

C 0.323554 0.459250 0.454563

C 1.226495 -1.523030 -0.148914

C -1.028475 0.106924 0.136352

C -2.161730 -0.188237 -0.117769

C 0.987384 1.428355 -0.233781

H 0.644802 0.216581 1.459488

H 0.963901 -1.530843 -1.196470

H 0.659388 -2.177710 0.498061

H 2.269658 -1.373046 0.090888

H -3.169645 -0.437546 -0.339527

H 0.603137 1.814248 -1.166893

H 1.945390 1.788743 0.111752

**Frequencies**

-537.9091 141.7631 150.2263

233.8153 243.5659 398.2040

544.2863 573.0534 577.1719

601.6090 675.1779 726.3108

837.9359 867.6707 905.7770

980.5340 1109.7311 1277.3224

1421.4244 1428.0737 1428.5578

1552.3892 2241.8578 3106.2021

3167.9653 3188.0073 3268.8136

3271.6299 3274.8814 3486.2214

**i1 – i8**

C 0.182794 0.326511 0.565741

C -1.147668 0.125437 0.163510

C -2.266756 -0.128039 -0.209333

C 1.213155 0.876785 -0.326264

H 0.365170 0.389659 1.629957

H -3.264854 -0.309007 -0.521686

H 0.939545 1.133618 -1.338355

H 2.059041 1.381708 0.115153

C 1.291883 -0.969064 -0.096474

H 0.987941 -1.268905 -1.092501

H 0.896037 -1.717598 0.608919

H 2.376669 -0.999257 0.015429

**Frequencies**

-1348.0386 124.2767 164.7858

215.1843 447.5530 542.6494

549.8578 561.2217 637.2207

673.1659 768.3627 813.3008

867.7284 990.8106 1038.2680

1109.3737 1213.5903 1337.6476

1395.2101 1430.8647 1469.5301

1497.6626 2160.4577 2894.0422

3046.6121 3157.5300 3193.2729

3195.4368 3277.3192 3481.4486

**i5 – i3**

C -0.070781 -0.471215 -0.071684

C 0.972171 0.432172 -0.007714

C 2.406628 0.018548 -0.005774

C -2.633851 0.236786 -0.119596

C -1.465636 -0.134338 0.014734

H -0.871838 -0.631751 1.124108

H 0.134619 -1.516676 -0.290359

H 0.739956 1.484137 0.122712

H 2.978021 0.565986 -0.762767

H 2.517680 -1.049924 -0.208212

H 2.885193 0.225635 0.959934

H -3.634817 0.430875 0.194787

**Frequencies**

-1859.1632 139.9078 159.2214

172.9508 360.5305 380.6251

494.7765 553.2996 630.4409

747.9513 787.5142 909.4547

1020.0927 1036.7801 1058.7067

1133.4569 1265.4053 1311.8950

1423.7004 1481.5887 1484.4944

1498.1040 1588.0710 2052.8143

3019.9116 3076.3583 3119.4043

3159.7434 3193.6657 3426.7581

**i4 – i6**

C -1.287030 0.499273 0.000145

C -1.566561 -0.966333 -0.014172

C 1.241531 0.172337 -0.023202

C 2.202016 -0.557943 0.000036

C 0.113177 1.021146 -0.023154

H -0.571801 0.991314 1.037707

H -2.051774 1.210248 -0.286814

H -1.427712 -1.382805 -1.021773

H -2.588814 -1.178518 0.304317

H -0.880504 -1.508697 0.642394

H 3.052334 -1.195422 0.012059

H 0.249466 2.053001 -0.325806

**Frequencies**

-1903.9331 141.5482 170.3721

228.9574 349.5593 401.2262

567.9529 596.7305 622.6735

703.0445 805.2899 862.2672

984.0051 1040.1524 1109.9744

1202.4985 1256.1771 1370.1537

1382.2963 1429.0850 1479.6171

1499.5028 2177.9552 2220.5722

3005.8569 3088.3827 3135.7029

3197.1372 3216.9779 3483.4782

**i8 – i3**

C 0.146249 0.536854 0.117294

C -0.973287 -0.448106 0.179278

C -2.360198 -0.026565 -0.181304

C 2.644491 -0.209093 -0.122759

C 1.494850 0.143042 -0.029702

H -0.118378 1.566545 -0.098975

H -0.692127 -1.494063 0.175125

H -2.495133 -0.001233 -1.271776

H -2.577470 0.980290 0.189734

H -3.107507 -0.705431 0.234003

H 3.658775 -0.512311 -0.217331

H -0.380792 0.189416 1.212378

**Frequencies**

-1912.5594 130.1267 158.8549

184.1308 349.0476 401.8859

519.7030 571.1697 662.5475

698.8488 769.9204 891.9372

1030.6656 1055.6540 1113.2631

1197.5537 1230.1668 1308.6612

1411.4711 1438.7858 1483.3918

1495.7469 2187.8396 2221.7212

3005.9444 3078.5395 3126.4108

3182.7464 3207.0630 3483.3676

**i7 – i5**

C -1.005400 0.351305 0.504811

C -1.908134 -0.541473 -0.285968

H -1.171723 0.447014 1.575936

H -2.115040 -0.130884 -1.281092

H -2.859792 -0.707399 0.224594

H -1.444769 -1.527501 -0.449147

C 1.431749 0.301856 -0.194073

C 1.734415 -0.951301 0.227704

C 0.196120 0.956143 -0.065528

H 2.241387 0.878343 -0.658898

H 2.523419 -1.630487 -0.073414

H 0.134013 1.971732 -0.459650

**Frequencies**

-746.2991 87.9199 127.7117

239.9593 264.5242 334.4937

416.4157 555.4742 657.1212

766.8098 873.5584 916.0154

979.9605 1051.9568 1087.7924

1170.8324 1196.1614 1321.9529

1384.2518 1396.6545 1448.6241

1472.5084 1483.5306 2957.5085

3011.6887 3026.0026 3082.7408

3086.9616 3118.8556 3192.9223

**i8 – i6**

C -1.180683 0.497452 0.354831

C -1.677767 -0.855860 -0.170479

H -1.085861 0.438501 1.446468

H -1.922364 1.272168 0.145429

H -1.827215 -0.823286 -1.252520

H -2.626559 -1.126768 0.299404

H -0.950897 -1.642440 0.045488

C 1.281362 0.159901 -0.064218

C 2.280090 -0.517449 0.095960

C 0.138275 0.909904 -0.232187

H 3.158338 -1.100937 0.231731

H 0.206892 1.819076 -0.819446

**Frequencies**

-50.7322 167.8761 254.0236

335.7985 376.6715 511.7778

555.1366 620.7428 675.4784

785.9946 881.2145 991.9979

1070.7983 1121.3823 1150.9653

1289.2963 1355.4230 1386.2630

1417.4168 1489.7429 1501.6013

1509.7410 2036.2540 3028.7772

3046.8278 3096.3501 3125.7003

3132.3927 3188.5227 3476.4472

**i3 – p3**

C -0.087374 0.452467 -0.148724

C 0.922253 -0.410910 0.107057

C 2.364501 -0.075517 -0.059999

C -2.625845 -0.227719 -0.012490

C -1.466330 0.079248 -0.061797

H 0.125112 1.393282 -0.649674

H -0.035872 1.577352 1.438825

H 0.677372 -1.387467 0.515071

H 2.874755 -0.086496 0.909658

H 2.500833 0.911541 -0.506603

H 2.867274 -0.815237 -0.690754

H -3.652708 -0.498391 0.039193

**Frequencies**

-862.4702 150.9339 167.6982

174.9903 314.4362 388.0097

427.1593 494.9497 547.0636

665.1093 711.7054 827.6708

916.8089 1007.9818 1047.5087

1060.1589 1140.7694 1310.8412

1313.0179 1420.6399 1481.3472

1490.3980 1648.2761 2245.2967

3038.5643 3100.4465 3129.6414

3170.2860 3189.2189 3487.0519

**i4 – p2**

C -1.213176 0.486500 0.145981

C -1.616123 -0.931083 -0.068876

C 1.210822 0.115977 0.047246

C 2.186445 -0.583367 0.019029

C 0.055433 0.960701 0.105650

H -2.009079 1.212528 0.285031

H -2.160166 -1.029613 -1.015569

H -2.294664 -1.264383 0.722110

H -0.753212 -1.597809 -0.097854

H 3.052432 -1.199499 -0.011810

H 0.239461 2.001257 0.351886

H 0.184816 1.585154 -1.727977

**Frequencies**

-864.5164 137.2677 162.5756

249.4072 299.5092 384.8594

416.8230 562.2459 661.5597

683.0046 703.0599 772.1900

907.5086 975.8409 1006.6747

1058.3335 1127.9923 1263.3439

1400.5555 1438.9236 1483.9274

1488.4462 1631.3346 2240.5266

3038.3741 3098.2182 3145.6556

3175.7536 3194.1978 3485.2313

**i6 – p2**

C 1.177922 0.485266 0.095049

C 1.542480 -0.966042 0.048606

C -1.247108 0.166442 0.023949

C -2.245161 -0.498357 -0.070079

C -0.080695 0.969500 0.138958

H 1.565120 0.933866 -1.919815

H 1.987421 1.190866 0.258011

H 1.827030 -1.305333 1.050589

H 2.396963 -1.136072 -0.609196

H 0.705970 -1.577903 -0.291874

H -3.128829 -1.084001 -0.152871

H -0.238307 2.037723 0.246264

**Frequencies**

-602.2680 101.2723 164.2499

200.0612 343.1166 355.7068

387.1659 509.1748 663.5490

666.9537 700.7308 781.3561

911.3865 976.6861 998.3205

1058.1260 1126.9191 1264.1491

1396.9781 1437.2396 1480.7999

1490.7029 1649.9260 2221.6879

3050.6210 3119.6347 3151.8873

3179.1616 3197.7294 3484.2281

**i5 – p3**

C -0.944115 -0.387109 -0.063246

C -2.402001 -0.059141 0.008763

C 1.430568 0.162487 0.007460

C 2.490843 -0.434876 0.042408

C 0.042129 0.509818 0.069583

H -0.681453 -1.427672 -0.236475

H -2.888753 -0.620137 0.814454

H -2.911905 -0.341093 -0.919266

H -2.569780 1.005842 0.182517

H 2.060709 1.897318 -0.486550

H 3.482206 -0.817783 0.024210

H -0.195566 1.556450 0.231300

**Frequencies**

-719.0065 41.6863 180.4338

198.9055 201.9972 398.5663

471.5628 512.4073 567.1619

627.8711 675.7954 816.4455

911.3163 990.6399 1037.1508

1066.0649 1128.7328 1314.2575

1330.8111 1413.8803 1478.2393

1488.4813 1688.1625 2103.8228

3013.7968 3056.3151 3099.5586

3146.1875 3158.7715 3464.3577

**i7 – p2**

C 1.213708 0.562787 0.028461

C 1.672324 -0.857612 -0.046604

C -1.205493 0.150839 0.000041

C -1.957710 -0.805932 0.051407

C -0.054131 1.002926 0.044975

H 1.994052 1.318435 0.074618

H 2.267506 -1.115391 0.836874

H 2.324003 -1.005317 -0.915004

H 0.837118 -1.554632 -0.115643

H -2.457223 1.501894 -0.493889

H -2.734434 -1.531744 0.049273

H -0.243207 2.068710 0.094088

**Frequencies**

-728.1593 22.9335 122.4887

188.9943 296.8966 410.6077

507.2691 524.8836 624.7440

653.3201 695.1906 746.7775

899.9434 968.3253 993.5846

1062.9889 1121.2010 1272.5740

1397.7895 1428.3015 1480.7644

1485.1735 1675.4422 2098.3421

3016.1894 3056.5604 3119.0148

3143.2158 3178.4430 3463.0839

**i8 – p1**

C -0.796511 0.906765 0.455765

C -2.260091 -0.918168 -0.133316

C 1.405237 0.018447 -0.098540

C 2.367550 -0.671897 0.117513

C 0.272897 0.827778 -0.370253

H -0.763743 0.468969 1.445597

H -1.599388 1.601636 0.244619

H -2.493103 -0.647104 -1.154888

H -3.027487 -0.772357 0.617564

H -1.538654 -1.709393 0.023290

H 3.219458 -1.276638 0.314767

H 0.268420 1.357339 -1.317966

**Frequencies**

-365.1698 79.7931 106.6010

216.1581 229.2923 386.4837

458.7615 488.2364 565.7888

641.2470 698.6775 733.5616

766.9352 897.2827 930.5398

980.5763 1116.3466 1293.6265

1417.0813 1419.0864 1428.6152

1587.4944 2207.8607 3102.4858

3172.7510 3186.9840 3271.9748

3272.5651 3282.2149 3484.4529

**i3 – i9**

C -0.089718 0.651872 -0.134251

C -1.451182 0.137239 0.006608

C -2.563503 -0.297495 0.110754

C 0.956754 -0.428136 -0.159667

C 2.373000 -0.081750 0.133297

H -0.030204 1.254168 -1.053597

H 0.116335 1.347197 0.688515

H -3.549169 -0.683660 0.208555

H 0.765484 -1.319891 -0.744575

H 1.568456 -0.697279 0.951427

H 3.164620 -0.716544 -0.241114

H 2.612373 0.925628 0.450343

**Frequencies**

-1917.4962 84.7542 161.6858

346.3319 347.0284 358.1815

519.4655 690.5439 699.2422

705.8327 734.6995 880.9623

930.4716 990.5415 1114.8316

1175.2094 1223.5894 1288.5040

1301.4880 1401.8458 1434.9528

1467.8089 2249.7812 2254.8603

2991.6497 3054.5242 3161.3307

3201.8020 3280.6792 3484.8423

**i10 – i4**

C 0.060922 1.041839 -0.174748

C -1.246153 0.417949 0.245066

C 1.214552 0.153451 -0.027012

C 2.149633 -0.587564 0.092632

C -1.589462 -0.974754 -0.144276

H 0.242182 1.953099 0.402693

H 0.002255 1.345552 -1.231623

H -2.071412 1.089016 0.452491

H -1.232356 -0.599357 1.050754

H 2.982893 -1.239375 0.198935

H -2.629425 -1.264472 -0.212566

H -0.831086 -1.589985 -0.610651

**Frequencies**

-1927.2184 110.7474 167.1374

337.7716 353.3847 365.0174

578.8928 686.6370 694.0266

698.7305 734.8841 872.7826

935.7533 949.1792 1080.1376

1173.8330 1255.6909 1272.2190

1348.4718 1369.6071 1435.7981

1465.0780 2247.5502 2250.8878

2985.5512 3086.8802 3164.9363

3198.0758 3285.8256 3484.8221

**i10 – i9**

C 0.074538 0.756655 -0.196517

C 1.372703 0.096494 -0.092011

C 2.431670 -0.458163 0.005118

H 0.173719 1.778514 0.180158

H -0.185940 0.850933 -1.255225

H 3.372905 -0.944959 0.090006

C -1.062979 0.018349 0.562213

C -2.173815 -0.433425 -0.315569

H -1.456141 0.664740 1.353686

H -0.627467 -0.844628 1.087957

H -3.152390 -0.640894 0.100122

H -1.977383 -0.743168 -1.336108

**Frequencies**

-121.4795 85.3605 202.1936

320.9953 383.2383 476.1153

533.3683 695.3035 725.2461

764.7964 894.3636 959.2661

974.5648 1090.2302 1118.5629

1218.0939 1258.2185 1341.3166

1378.0489 1466.3499 1474.6523

1485.7710 2251.3825 2992.6306

3062.5732 3071.1980 3103.3279

3153.9706 3261.9916 3486.5005

**i12 – i4**

C -1.352793 0.445651 -0.209928

C -1.467540 -0.908129 0.098135

C 0.984473 -0.113336 -0.020956

C 2.202954 -0.341645 -0.103376

C -0.035681 1.018346 0.202110

H -1.913770 0.897923 -1.018878

H -0.004567 -1.075380 -0.183019

H -2.209335 -1.520898 -0.407312

H -1.244704 -1.244679 1.112273

H 3.137386 -0.842834 -0.218598

H -0.000174 1.264101 1.270311

H 0.246688 1.916451 -0.350681

**Frequencies**

-2318.7568 107.4054 298.0507

342.2198 488.0320 496.2866

550.1756 676.4174 692.5587

740.2021 866.0974 893.2091

966.2420 981.4830 1068.1492

1168.3011 1210.7337 1238.5291

1287.7358 1417.7460 1469.5594

1487.0228 1533.2509 1920.5202

3044.3699 3096.3473 3114.4288

3191.6485 3214.2115 3432.0445

**i11 – i4**

C -1.142192 0.370209 -0.264336

C -1.222513 -0.948483 0.182286

C 1.252524 0.399357 -0.003365

C 1.466553 -0.830960 -0.127340

C 0.025198 1.228935 0.172021

H -1.622825 0.645768 -1.198191

H 0.107803 -1.272495 -0.133814

H -1.934168 -1.613440 -0.297598

H -1.073261 -1.145887 1.245152

H 2.227715 -1.585494 -0.193058

H -0.052911 1.505638 1.230914

H 0.070226 2.151565 -0.409003

**Frequencies**

-2151.7227 243.5174 348.1233

454.1456 473.2543 579.6057

650.1262 693.0854 802.6969

868.5227 905.0034 925.3801

945.6702 1041.3530 1099.8775

1201.9923 1240.5035 1254.4923

1289.9082 1408.2107 1434.5513

1470.8196 1538.1854 1899.2289

3039.3863 3099.3476 3117.8665

3183.4362 3209.5041 3343.5454

**i12 – i10**

C -0.047361 0.887737 -0.032750

C 1.024058 -0.120761 -0.431643

C -1.214406 -0.020505 0.047755

C -2.399253 -0.354422 0.123809

C 2.168704 -0.331446 0.288826

H -0.180870 1.706160 -0.745664

H 0.164700 1.319502 0.949319

H 1.003804 -0.412280 -1.480213

H -0.136059 -1.084147 -0.087830

H -3.267429 -0.971494 0.171159

H 2.929540 -1.019046 -0.059734

H 2.295863 0.097690 1.276975

**Frequencies**

-2164.7852 98.2960 200.8795

363.4914 408.9417 447.0347

492.2515 606.7895 658.5880

739.8006 814.7851 832.9982

917.6005 939.0958 1073.7020

1108.6503 1221.0986 1258.7009

1289.5835 1305.0336 1438.6660

1473.7158 1587.2237 2017.8455

3065.1454 3114.7887 3147.0424

3153.9381 3251.0186 3437.2899

**i9 – p4**

C 0.048878 0.728942 -0.049293

C 1.390535 0.154750 0.021100

C 2.491525 -0.317564 0.061430

C -1.044452 -0.288418 -0.299295

C -2.301384 -0.133300 0.141820

H -0.161751 1.281637 0.870981

H 0.030383 1.460635 -0.866041

H 3.464664 -0.743157 0.108267

H -0.370941 -1.650853 0.984863

H -0.823459 -1.047385 -1.044418

H -3.083968 -0.825364 -0.144562

H -2.565531 0.658025 0.836339

**Frequencies**

-782.7375 93.9926 172.9436

338.3710 363.4468 415.2081

426.8943 514.0214 613.8413

688.9684 720.7043 900.5893

919.2044 939.7612 1005.1624

1051.6249 1138.0766 1255.5393

1307.2193 1332.8923 1453.4611

1467.6848 1655.9317 2256.0514

3047.6138 3096.4602 3158.8319

3181.2781 3255.5801 3486.5372

**i12 – i11**

C 1.216017 -0.307256 -0.315619

C 2.236755 0.496726 -0.040982

C -1.285276 -0.193753 -0.152347

C -2.401058 0.458037 -0.156134

C 0.001008 -0.481070 0.560068

H 1.223167 -0.897193 -1.229319

H 2.257530 1.106988 0.856862

H 3.090336 0.574908 -0.704673

H -3.026983 1.168443 0.386701

H -2.177715 -0.445568 -1.047290

H 0.068191 0.171430 1.441723

H -0.039201 -1.515112 0.926083

**Frequencies**

-2104.4208 69.4566 123.0677

179.5453 290.2638 397.9880

419.3193 609.6745 636.0357

826.6905 892.7463 915.9859

948.9339 955.3099 1030.6987

1119.1497 1221.8712 1287.6507

1323.6738 1445.4776 1457.1408

1709.8645 1844.4594 2350.9335

2983.1789 3025.4946 3052.7533

3125.5190 3137.2847 3210.9770

**i3 – p4**

C -0.100834 0.748151 0.019137

C 0.972784 -0.237816 0.395437

C 2.090644 -0.430384 -0.310616

C -2.506310 -0.386859 -0.087171

C -1.426830 0.132465 -0.044222

H 0.133742 1.212529 -0.943312

H -0.126715 1.555112 0.762044

H 0.814385 -0.782233 1.322189

H 3.399708 1.024072 0.435870

H 2.243382 0.053344 -1.270344

H 2.823104 -1.170287 -0.010656

H -3.464329 -0.845883 -0.131188

**Frequencies**

-525.0145 74.5948 161.1767

234.3298 324.3423 346.4109

422.0076 503.5401 692.5659

695.2758 726.2101 912.0308

939.0268 990.6040 994.8629

1029.3956 1139.8341 1253.9397

1317.9994 1333.2281 1457.9100

1474.2420 1682.1020 2255.2514

3041.4900 3096.2691 3153.6790

3184.0945 3250.5367 3486.5653

**i3 – p5**

C 0.100835 0.748139 0.019156

C 2.506324 -0.386842 -0.087171

C 1.426836 0.132467 -0.044227

H 0.126711 1.555041 0.762127

H -0.133739 1.212595 -0.943255

H 3.464348 -0.845861 -0.131170

C -0.972775 -0.237863 0.395387

C -2.090675 -0.430339 -0.310627

H -0.814328 -0.782396 1.322061

H -2.243473 0.053517 -1.270280

H -2.823121 -1.170275 -0.010713

H -3.399673 1.024007 0.436120

**Frequencies**

-525.0629 74.5804 161.1737

234.3370 324.3507 346.4143

422.0044 503.5394 692.5617

695.2598 726.2125 912.0314

939.0263 990.5963 994.8619

1029.3692 1139.8355 1253.9362

1317.9935 1333.2254 1457.9071

1474.2474 1682.1003 2255.2492

3041.4827 3096.2736 3153.6957

3184.1017 3250.5496 3486.5608

**i10 – p6**

C -0.013874 -1.020601 -0.149434

C 1.306972 -0.291932 -0.009335

C -1.195384 -0.174087 -0.022504

C -2.164056 0.524589 0.079312

C 1.467776 1.035129 -0.112852

H -0.068384 -1.824354 0.590589

H -0.031441 -1.508528 -1.131430

H 2.180081 -0.938403 -0.033106

H 1.468738 -0.483241 1.948316

H -3.028876 1.135985 0.173828

H 2.456656 1.477054 -0.095365

H 0.614625 1.702896 -0.163954

**Frequencies**

-770.9930 119.4693 166.7775

340.5720 373.7158 394.5233

450.3408 579.6915 626.9950

689.3885 700.7436 876.5953

932.4916 958.1227 975.8944

1045.4702 1096.5138 1242.7093

1310.1461 1362.9881 1436.5038

1475.3286 1654.8529 2257.6209

3050.1749 3092.7474 3161.1091

3173.3816 3260.6996 3486.7150

**i12 – p6**

C -1.137246 0.138884 0.061810

C 0.031788 1.023073 -0.032492

C -2.135961 -0.503559 -0.183310

C 1.592165 -0.976230 -0.030902

C 1.377316 0.333270 -0.049709

H -0.892434 -0.301469 1.936658

H 0.010157 1.740678 0.795982

H -0.072954 1.621197 -0.947280

H -3.009485 -1.105888 -0.248960

H 2.599132 -1.376404 -0.049422

H 0.775328 -1.688173 0.005941

H 2.221876 1.017429 -0.085310

**Frequencies**

-674.3154 116.0700 153.4362

201.2634 389.1813 419.7650

475.5023 565.9675 614.9878

653.4663 683.6950 865.5704

947.9714 964.8534 965.6240

1029.4692 1094.0168 1237.2615

1325.9674 1353.5860 1444.0817

1462.5840 1712.7708 2133.1050

3008.4867 3035.3334 3133.0898

3145.3028 3224.5539 3464.1375

**i13 – p6**

C 1.151044 -0.135361 0.000004

C 1.879669 0.833540 0.000097

C -0.005793 -1.038201 0.000052

C -1.601660 0.943506 -0.000050

C -1.359663 -0.360906 0.000004

H 2.472515 -1.565020 -0.000550

H 2.633096 1.583535 -0.000160

H 0.061510 -1.703399 0.869827

H 0.061519 -1.703514 -0.869630

H -2.617816 1.320435 -0.000074

**Frequencies**

-641.9023 95.4826 166.0544

195.5698 351.5908 406.4738

468.5982 570.2041 617.3488

667.4709 674.7484 865.0490

946.2147 960.4500 964.1813

1027.5171 1090.6280 1245.1257

1324.6265 1352.2614 1441.2156

1461.8595 1713.1330 2137.2279

3014.1824 3030.4734 3130.4028

3143.6608 3223.5929 3465.5415

**i9 – p5**

C -0.048892 0.728848 -0.049224

C -1.390582 0.154724 0.021091

C -2.491630 -0.317467 0.061350

C 1.044481 -0.288501 -0.299114

C 2.301493 -0.133147 0.141637

H -0.030322 1.460462 -0.866022

H 0.161569 1.281607 0.871045

H -3.464859 -0.742886 0.107992

H 0.823353 -1.047903 -1.043750

H 0.371215 -1.651207 0.985236

H 3.084019 -0.825331 -0.144629

H 2.565800 0.658518 0.835691

**Frequencies**

-781.8517 93.7958 172.9211

338.3126 363.2911 415.0759

426.4806 514.0173 613.7746

688.9152 720.6609 900.5789

919.1921 939.7074 1005.1842

1051.6346 1138.0793 1255.5167

1307.2367 1332.8783 1453.4647

1467.6500 1655.9968 2256.0340

3047.7267 3096.5212 3158.8735

3181.3181 3255.6007 3486.4960

**i11 – p4**

C 1.196913 0.151774 -0.424330

C 2.246533 0.338583 0.366514

C -1.252168 -0.101501 -0.116298

C -2.330997 0.435964 -0.029039

C 0.044168 -0.775034 -0.104902

H 1.127498 0.678444 -1.372514

H 2.337328 -0.165402 1.323872

H 3.054195 1.004713 0.085941

H -2.913423 0.060258 1.919438

H -3.250290 0.956310 -0.147006

H 0.199928 -1.239859 0.875597

H 0.018068 -1.593180 -0.837004

**Frequencies**

-478.0087 41.3272 87.3294

177.8809 252.2285 390.9784

409.5842 486.0012 645.3983

660.3918 763.2465 895.0065

924.7482 954.9388 981.4982

1028.9433 1124.6331 1241.8229

1313.1821 1328.9423 1449.8453

1459.6135 1709.7480 2170.4386

3001.1478 3039.6286 3128.9094

3146.8465 3214.7246 3462.9564

**i4 – p6**

C -1.280804 0.424333 0.085713

C -1.507540 -0.887502 0.194558

C 1.206401 0.161509 -0.013596

C 2.136311 -0.592985 0.038275

C 0.069069 1.073842 -0.076158

H -2.118920 1.115853 0.070162

H -0.689422 -1.596529 0.263796

H -1.665732 -1.523525 -1.786259

H -2.511802 -1.266021 0.342897

H 2.965119 -1.257722 0.080878

H 0.187920 1.847592 0.691735

H 0.092214 1.605173 -1.035969

**Frequencies**

-529.4447 123.3922 165.5474

225.9914 331.9774 347.6882

388.4494 619.2805 641.3324

702.5690 704.4940 880.8639

964.2226 973.4739 993.1060

1031.2867 1098.3659 1240.3596

1322.9273 1362.3317 1435.0728

1471.0937 1679.1156 2256.2066

3037.4890 3066.7160 3160.4040

3180.8404 3256.0861 3484.4495

**i13 – i12**

C -1.279274 -0.279755 -0.239402

C -1.643621 0.862994 0.281311

H -1.955248 -0.745544 -0.966999

H -2.475127 1.546375 0.193372

C -0.027175 -1.075950 0.076418

C 1.516476 0.946592 -0.130602

C 1.293635 -0.343018 0.094481

H 0.052618 -1.902038 -0.640027

H -0.159773 -1.564599 1.051687

H 2.521812 1.350733 -0.091701

H 0.712844 1.637671 -0.356506

H 2.142628 -0.987776 0.316936

**Frequencies**

-111.8208 128.2582 223.1372

386.5574 533.8016 578.8678

655.5355 792.1702 836.3145

857.0331 944.7111 962.0470

1020.4479 1034.0929 1090.5951

1240.4556 1259.9804 1329.9726

1369.3455 1440.6318 1473.3350

1673.1192 1711.4109 2995.9901

3004.0111 3031.2607 3116.2311

3138.5439 3219.4603 3237.4768

**i14 – i11**

C 1.244896 -0.408971 -0.048780

C 2.453422 0.162794 -0.146695

C -1.282353 -0.261710 0.112274

C -2.519899 0.071588 -0.227925

C 0.019252 0.311032 0.269354

H 1.136075 -1.475965 -0.228310

H 2.595286 1.227268 0.009182

H 3.331786 -0.418986 -0.396516

H -2.705364 0.874854 -0.944406

H -3.388120 -0.470874 0.130061

H 0.101886 1.386248 0.450501

H -0.563455 -0.370940 1.230122

**Frequencies**

-1861.5061 134.9403 179.9150

257.5103 378.6433 468.3024

581.8199 686.4474 845.1498

867.6243 897.9569 910.9718

1000.0660 1012.8424 1077.8644

1117.9487 1185.3595 1267.8542

1315.1788 1431.7012 1460.7424

1652.9565 1669.4671 2095.8594

3051.6456 3057.8660 3134.5607

3141.8800 3174.0744 3224.2916

**i16 – i10**

C -0.368701 -1.195486 0.139437

C -1.215726 0.062733 -0.222089

C 1.023885 -0.745643 -0.030168

C 1.581078 0.352811 -0.096648

C -0.480375 1.311631 0.172362

H -0.631249 -2.050479 -0.486917

H -0.529121 -1.494015 1.180559

H -2.198074 0.002168 0.260231

H -1.382159 0.066495 -1.302254

H 2.383864 1.054130 -0.165811

H -0.498891 2.167265 -0.493175

H -0.385334 1.538163 1.230008

**Frequencies**

-584.1382 180.1101 331.7358

464.2893 510.5064 591.4287

678.0056 697.1304 800.5799

823.1210 878.8069 911.7923

1000.0391 1056.4549 1107.9323

1201.1535 1234.8076 1324.1634

1342.8054 1464.5693 1479.6200

1500.2683 1963.7546 3047.7970

3065.7076 3102.0802 3119.4048

3143.3002 3244.5452 3416.3076

**i13 – i18**

C -1.290607 0.068300 -0.000148

C -0.868071 -1.166239 -0.170515

C -0.253600 1.180725 0.152977

C 1.326502 -0.695719 0.224507

C 1.050738 0.549784 -0.260185

H -2.349719 0.325062 0.044756

H -1.349504 -2.128870 -0.276159

H -0.242822 1.539252 1.192102

H -0.504689 2.045205 -0.468443

H 2.095241 -1.311945 -0.230653

H 1.025731 -0.991621 1.223272

H 1.535997 0.901817 -1.164689

**Frequencies**

-518.3952 235.2388 315.8765

465.9473 603.2208 637.9660

695.1974 815.9137 871.6497

894.0825 907.1708 927.6301

945.9227 984.1812 1087.4920

1193.5268 1212.3706 1270.6601

1311.2295 1421.4046 1479.4873

1561.9783 1644.2632 2988.8245

3057.5818 3093.1520 3125.2523

3159.0753 3204.3096 3217.7943

**i17 – i7**

C 1.150176 0.570553 -0.026656

C 1.298534 -0.898904 0.026205

C -1.295398 0.360266 0.024687

C -1.273656 -0.968180 -0.044491

C -0.062009 1.153456 0.025368

H 2.037320 1.186776 -0.158314

H 1.438685 -1.308471 1.030702

H 2.013222 -1.331520 -0.676145

H 0.081629 -1.303061 -0.194877

H -2.240589 0.904876 0.031475

H -2.084671 -1.685691 -0.061465

H -0.151473 2.233943 -0.002057

**Frequencies**

-1581.2797 172.5470 352.3467

427.5580 520.5550 562.1910

614.9997 704.1404 763.2665

919.4956 932.0295 957.4266

968.7686 1033.2694 1045.4491

1112.1690 1212.7823 1274.0459

1328.0545 1412.1068 1443.9725

1530.9774 1586.1968 1670.4772

3044.6852 3086.8612 3109.2559

3122.2868 3174.4393 3194.6932

**i14 – i15**

C 1.121039 -0.310577 0.233124

C 0.048767 0.519301 -0.069556

C -2.278054 -0.338251 -0.330591

C -1.337231 0.277237 0.382286

C 2.427196 -0.091610 -0.156662

H 0.907471 -1.203990 0.816958

H 0.240063 1.424628 -0.643776

H -3.280227 -0.477691 0.060002

H -2.077648 -0.723611 -1.325039

H -1.597123 0.647211 1.376390

H 2.699650 0.779581 -0.742458

H 3.217504 -0.782728 0.106318

**Frequencies**

-215.5315 152.7076 242.3701

403.1961 485.9003 541.6318

664.3832 736.3868 802.1330

908.8416 958.5548 994.8227

1013.1578 1024.6439 1116.8707

1201.7816 1275.0303 1310.9043

1318.2832 1441.1722 1485.3075

1516.4523 1688.6661 3076.2654

3115.0551 3128.8164 3130.1695

3138.0784 3212.4288 3234.1540

**i15 – i17**

C -1.108108 0.148733 0.460526

C -1.983087 -0.461918 -0.335500

H -1.252715 0.084189 1.540928

H -1.886691 -0.431055 -1.415888

H -2.825072 -1.012948 0.069249

C 0.054765 0.937196 0.001442

C 1.726847 -0.879583 0.053348

C 1.341961 0.430494 -0.149671

H -0.105966 1.996635 -0.181277

H 2.755998 -1.186129 -0.083249

H 1.011415 -1.638404 0.346316

H 2.108760 1.138187 -0.456944

**Frequencies**

-168.8161 209.4259 242.2804

438.2514 502.2537 522.7862

678.4002 723.0430 810.1290

913.8033 958.2159 993.6987

1013.2995 1030.8765 1078.6176

1165.0680 1232.8215 1314.8892

1405.4693 1439.7497 1461.3403

1520.6434 1688.8658 3078.9838

3125.7685 3129.2176 3142.5224

3149.4894 3212.7053 3240.0962

**i17 – i19**

C -1.167622 0.481019 0.169240

C -1.183028 -0.837252 -0.229641

C 0.064421 1.202773 -0.084161

C 1.060133 -1.007791 0.197523

C 1.179266 0.438662 -0.086275

H -1.895098 0.870746 0.875350

H -0.777404 -1.121089 -1.192265

H -1.894266 -1.541685 0.193136

H 0.102930 2.283397 -0.174876

H 1.504767 -1.722064 -0.489823

H 1.080877 -1.316618 1.241709

H 2.159169 0.882847 -0.253347

**Frequencies**

-664.8297 211.4786 406.5081

451.7594 511.2242 642.6582

715.5318 736.0026 771.6530

862.3547 938.2213 963.8755

985.2993 1008.9120 1041.0700

1066.9963 1162.3060 1241.3689

1371.3908 1421.8352 1444.0492

1531.5551 1591.7899 3086.7849

3115.9201 3123.3195 3147.3168

3171.0700 3173.0264 3204.0590

**i19 – i18**

C 0.441477 1.146362 -0.004430

C -0.886014 0.889392 -0.019736

C 1.262304 -0.128955 -0.013311

C -1.138293 -0.538598 -0.020134

C 0.202511 -1.209030 -0.004442

H 0.888385 2.130920 0.045933

H -1.669877 1.635373 0.001899

H 1.955355 -0.187370 0.841336

H 1.911154 -0.198870 -0.905991

H -2.045711 -1.025311 -0.352008

H -0.678718 -1.067679 1.026481

H 0.347506 -2.242083 -0.285326

**Frequencies**

-1913.1968 271.2348 489.8277

557.9211 682.7480 729.0915

800.3762 826.8239 905.6700

923.7509 930.6590 946.3861

1006.3674 1054.8270 1121.8295

1132.0939 1239.0837 1268.2900

1291.6132 1318.5104 1389.2401

1465.2804 1566.9432 2162.2918

2884.2925 2936.8821 3186.7835

3194.3595 3210.1078 3217.1003

**i19 – i16**

C 1.212542 0.275436 -0.101696

C 0.602816 -1.104640 0.058299

C -1.192572 0.263512 -0.057997

C -0.789793 -1.093123 -0.140405

C -0.009311 1.219058 0.107525

H 2.011834 0.439876 0.627846

H 1.666660 0.430938 -1.090295

H 1.181349 -1.970147 0.359060

H -2.166821 0.608408 -0.396559

H -1.575998 -0.590252 0.841934

H 0.008668 1.694843 1.093136

H -0.067788 2.024866 -0.629468

**Frequencies**

-1516.1606 143.5922 464.5835

555.8428 607.4803 710.2109

787.2740 824.4365 891.3462

909.4491 971.3288 1008.3211

1066.0199 1125.2844 1176.2052

1221.3591 1240.1472 1261.6980

1305.8774 1325.3017 1385.0737

1463.7448 1482.5262 2025.7793

2985.5999 3034.2023 3049.6289

3074.5505 3140.0833 3182.1346

**i10 – p8**

C 0.351380 1.100772 -0.269619

C -1.481960 0.215985 0.517474

C 1.370774 0.151185 -0.083330

C 2.197014 -0.709152 0.104209

C -1.841348 -0.837910 -0.269415

H 0.360463 1.969364 0.381459

H 0.025850 1.286726 -1.286583

H -2.014656 1.157708 0.430794

H -0.992830 0.036028 1.468463

H 2.946283 -1.447684 0.256027

H -2.477334 -0.702798 -1.137164

H -1.422939 -1.824627 -0.108904

**Frequencies**

-628.4135 75.1420 127.2291

257.6510 354.8707 384.6389

471.9757 595.5308 635.4415

692.4277 779.4467 832.2936

856.7216 985.4235 1027.4327

1057.8173 1071.0137 1248.9297

1290.1937 1457.7301 1467.5501

1573.4791 2155.1124 3141.0378

3144.2314 3159.4417 3228.4142

3235.1854 3258.2662 3481.7977

**i11 – p10**

C 1.559101 0.020745 0.564551

C 2.349405 -0.477747 -0.354772

H 1.601972 0.009783 1.646482

H 2.134859 -0.388540 -1.417836

H 3.268894 -1.010564 -0.101070

C -1.418040 0.210915 -0.076135

C -2.302612 -0.737205 0.023132

C -0.421905 1.081313 -0.130734

H -3.345078 -0.580921 -0.241979

H -2.028857 -1.729786 0.376097

H 0.067337 1.295613 -1.074773

H -0.294819 1.816287 0.656829

**Frequencies**

-327.9283 22.9875 107.8199

169.6419 250.3638 339.2289

367.4767 379.4073 794.5197

850.1649 872.0135 872.8810

881.0343 934.8126 999.3580

1031.5405 1060.3622 1091.2476

1397.7565 1420.2789 1466.4312

1640.5715 1970.8349 3050.8367

3091.1607 3122.8526 3134.2764

3159.8259 3197.6003 3199.2879

**i18 – p7**

C 0.936518 0.823015 0.029571

C -0.357120 1.165408 -0.087956

C 1.058869 -0.677608 0.054114

C -1.181745 -0.054768 -0.141811

C -0.361747 -1.139357 -0.100231

H 1.778498 1.497116 0.108247

H -0.755321 2.170919 -0.120346

H 1.506022 -1.035708 0.992942

H 1.704159 -1.057373 -0.749677

H -2.241007 -0.069603 -0.359233

H -1.897564 -0.029093 1.752107

H -0.663434 -2.176402 -0.146159

**Frequencies**

-554.6787 263.1678 295.1440

377.0117 547.6056 691.7145

709.0503 811.0909 817.7765

919.7062 925.1422 955.3196

966.1770 970.5989 1006.5221

1106.3207 1124.5800 1128.7552

1271.0188 1313.1121 1393.2486

1414.6786 1516.4608 1620.5193

3001.3791 3024.8371 3195.7479

3204.1742 3219.1359 3226.2726

**i19 – p7**

C -0.404699 1.140896 -0.107060

C -1.157814 0.018479 -0.144619

C 0.999725 0.773475 0.041140

C -0.251133 -1.178523 -0.089469

C 1.108447 -0.565776 0.061649

H -0.775708 2.155720 -0.165819

H -2.221139 -0.036776 -0.330408

H -1.783971 0.028188 1.928027

H 1.813958 1.481812 0.121433

H -0.322855 -1.760574 -1.017829

H -0.498232 -1.862741 0.728921

H 2.020792 -1.136934 0.165832

**Frequencies**

-510.9544 227.5863 295.3875

372.6181 527.7159 697.0797

771.0298 818.3538 821.0934

916.7738 937.7575 969.1519

975.5928 983.5410 1030.0797

1110.1445 1132.4776 1135.5312

1278.0666 1327.1608 1406.0964

1423.3075 1546.1322 1648.7277

3048.7226 3097.1466 3220.7962

3231.2664 3248.9549 3255.6982

**i1 – p9**

C 0.416225 0.114368 0.058280

C 1.157571 -1.194457 -0.089941

C -1.018785 0.029488 0.010474

C -2.209319 -0.081527 -0.059138

C 1.025100 1.310647 -0.106457

H 0.460396 0.069966 1.943573

H 1.004781 -1.584311 -1.097668

H 0.790079 -1.937548 0.614237

H 2.223971 -1.050581 0.072223

H -3.265618 -0.172553 -0.119008

H 2.102647 1.373742 -0.169202

H 0.458993 2.230167 -0.123456

**Frequencies**

-990.6462 188.2601 242.2548

281.6569 387.3344 438.5722

498.6596 561.9958 584.0203

677.3083 686.9491 715.1876

781.3488 911.1495 965.9395

1048.3650 1076.2847 1294.2218

1419.3474 1434.7844 1496.7368

1508.3428 1608.2952 2243.0734

3061.4031 3133.8342 3158.1089

3171.2249 3270.7050 3484.1733

**Products**

**p1 including the methylradical (CH3)**

C 0.735469 0.110223 0.000086

C -1.659547 -0.371443 -0.000057

C -0.635848 0.488624 -0.000043

C 1.906556 -0.171716 -0.000032

H -2.682927 -0.016566 0.000061

H -1.500620 -1.443220 0.000192

H -0.832585 1.557992 0.000100

H 2.936361 -0.432338 -0.000074

**Frequencies**

224.2867 316.4180 557.7143

647.7405 680.3845 703.4961

892.2675 954.7839 1009.9860

1111.4766 1320.9319 1443.5005

1668.4638 2205.6653 3136.5876

3147.5830 3236.4066 3476.2183

**p2 including H**

C -1.202292 0.542763 -0.000079

C -1.645730 -0.885237 -0.000019

C 1.219844 0.145766 0.000002

C 2.221543 -0.524619 0.000053

C 0.066812 0.978728 0.000028

H -1.987388 1.294487 -0.000082

H -2.268509 -1.096578 -0.876600

H -0.798957 -1.572565 -0.002829

H -2.263492 -1.097953 0.879832

H 3.100856 -1.120378 -0.000332

H 0.256429 2.048577 0.000096

**Frequencies**

136.6859 157.8647 274.8248

374.7152 502.7787 630.2292

661.7995 679.5908 749.8505

901.1060 973.5395 987.8983

1063.3332 1120.7954 1265.7218

1398.6581 1430.3399 1482.6620

1483.8772 1683.1863 2199.3013

3015.0403 3055.6654 3113.9473

3136.8641 3156.1774 3476.3682

**p3 including H**

C 0.925056 -0.394350 0.000012

C 2.371246 -0.011169 -0.000008

C -1.466238 0.109466 0.000001

C -2.639574 -0.165085 0.000016

C -0.093017 0.477133 -0.000018

H 0.697974 -1.457539 0.000054

H 2.884328 -0.419494 -0.878030

H 2.884334 -0.419427 0.878041

H 2.502368 1.073139 -0.000050

H -3.671109 -0.417575 0.000030

H 0.117264 1.544925 -0.000060

**Frequencies**

167.0357 170.9676 199.8552

390.5346 450.1885 544.8979

626.0470 681.2255 816.2460

912.4616 986.8754 1046.6087

1065.7194 1128.4006 1314.4868

1328.7208 1414.4391 1477.7085

1489.6826 1695.6858 2203.1267

3012.8784 3054.9688 3097.4517

3125.2985 3147.4522 3477.9955

**p4 including H**

C -1.338270 0.111976 -0.043656

C -0.039083 0.772602 0.091737

C 2.193061 -0.313669 -0.301312

C 1.081494 -0.191272 0.414143

C -2.399348 -0.441833 -0.144895

H -0.113034 1.524078 0.889181

H 0.194377 1.317986 -0.828708

H 2.973102 -1.011742 -0.020010

H 2.364542 0.278153 -1.195387

H 0.931740 -0.805140 1.298553

H -3.337848 -0.930163 -0.239728

**Frequencies**

89.3954 187.7194 337.6049

408.6864 475.0917 644.9942

664.4057 680.2830 898.3696

925.9499 953.1208 982.0640

1030.8713 1127.9109 1245.4688

1314.0050 1330.0467 1450.5476

1464.4171 1709.5795 2223.6181

3001.9565 3049.7914 3127.8671

3146.0430 3213.3811 3477.6481

**p5 including H**

C 1.338364 0.111812 -0.043717

C 2.399674 -0.441361 -0.145081

C -1.081490 -0.191863 0.413768

C -2.193393 -0.313113 -0.301327

C 0.039087 0.772259 0.092273

H 3.338310 -0.929368 -0.240259

H -0.931447 -0.806970 1.297257

H -2.365269 0.279877 -1.194540

H -2.973410 -1.011459 -0.020609

H 0.112779 1.523095 0.890368

H -0.194414 1.318421 -0.827713

**Frequencies**

89.1871 187.4077 337.4265

408.6538 475.0295 644.9127

664.5444 680.3927 898.3509

925.9920 953.1322 982.0512

1030.8683 1127.9541 1245.4893

1314.0216 1330.0750 1450.5950

1464.4220 1709.6609 2223.9987

3001.8282 3049.6767 3127.9373

3146.1104 3213.3494 3477.6527

**p6 including H**

C -1.163693 0.167288 0.000096

C -2.133665 -0.541117 -0.000019

C 0.012695 1.031130 0.000113

C 1.538108 -0.994979 -0.000148

C 1.348571 0.318440 -0.000019

H -2.995522 -1.162115 -0.000082

H -0.032561 1.697068 0.872207

H -0.032649 1.697226 -0.871856

H 2.537300 -1.414736 -0.000236

H 0.705184 -1.689370 -0.000169

H 2.206159 0.987355 -0.000002

**Frequencies**

147.5206 162.0456 332.3985

378.7846 568.0392 614.7230

663.9413 681.5658 866.6468

947.0140 965.1155 966.7503

1030.0920 1093.1564 1237.7560

1325.0798 1353.6219 1441.0304

1463.1201 1712.5303 2226.1384

3000.4644 3016.9398 3131.0362

3143.4622 3223.0748 3476.4354

**p7 including H**

C 0.736623 0.987585 0.000000

C 1.178765 -0.283674 0.000003

C -0.732076 0.990950 -0.000042

C -0.002784 -1.215526 0.000012

C -1.180063 -0.278271 -0.000012

H 1.351623 1.878553 0.000008

H 2.208871 -0.612750 0.000074

H -1.342974 1.884740 0.000182

H -0.004416 -1.877171 0.877009

H -0.004230 -1.877090 -0.877061

H -2.211661 -0.602668 0.000024

**Frequencies**

348.6040 524.0849 681.4372

712.6337 816.8658 818.7255

917.4930 924.4380 954.1554

955.7283 970.8450 1012.4461

1111.9798 1125.8854 1129.9476

1266.1830 1314.9867 1397.1448

1414.9789 1552.2415 1638.8444

3010.5306 3032.0452 3186.7348

3196.8341 3215.4703 3222.0692

**p8 including the propargyl radical (C3H3)**

C 0.663422 0.000006 0.000021

C -0.663514 -0.000020 -0.000122

H 1.234985 -0.922431 0.000012

H 1.234746 0.922528 0.000061

H -1.234596 0.922630 0.000243

H -1.234582 -0.922640 0.000292

**Frequencies**

834.9037 973.0542 973.9308

1066.6751 1238.6866 1379.6577

1472.3233 1691.9537 3120.9179

3136.0676 3192.0523 3220.5232

**p9 including H**

C -1.004075 0.039682 -0.000023

C -2.202667 -0.079851 -0.000040

C 0.424308 0.121973 0.000002

C 1.167364 -1.194836 0.000087

C 1.046741 1.308301 -0.000048

H -3.261115 -0.169603 -0.000056

H 0.901453 -1.788033 0.879923

H 2.246492 -1.032930 0.000101

H 0.901489 -1.788125 -0.879698

H 2.129017 1.368606 -0.000029

H 0.492638 2.238473 -0.000109

**Frequencies**

176.0542 186.9003 268.6311

396.9905 546.3948 571.1248

650.0507 677.8309 743.9201

775.5743 931.9078 964.8473

1031.9442 1071.4830 1284.5910

1410.5281 1435.3005 1478.0144

1495.8336 1675.6068 2201.3420

3028.1446 3080.9802 3112.9291

3143.5745 3233.6641 3476.5419

**p10 including the vinyl radical (C2H3)**

C 1.302452 0.000002 -0.000016

C -0.000002 -0.000073 0.000117

C -1.302448 0.000028 -0.000019

H 1.866971 0.663127 0.648052

H 1.866901 -0.663016 -0.648258

H -1.867110 -0.648184 0.662825

H -1.866772 0.648328 -0.663111

**Frequencies**

371.7987 371.8106 866.2426

866.2584 885.0895 1017.1692

1017.1764 1109.3233 1422.4951

1479.5973 2052.4143 3117.2859

3121.3263 3192.2676 3192.2929

**Radicals**

**Methyl**

C -0.000035 -0.000090 0.000016

H -0.998670 -0.412387 -0.000033

H 0.856880 -0.658119 -0.000033

H 0.142001 1.071048 -0.000033

**Frequencies**

505.2897 1402.6327 1403.3797

3104.1952 3282.8105 3283.7762

**Vinyl**

C 0.586665 0.029432 -0.000348

C -0.706546 -0.142672 -0.000013

H 1.282549 -0.806960 0.001029

H 1.038849 1.025354 0.000631

H -1.602110 0.461046 0.000505

**Frequencies**

710.0974 818.1174 921.1459

1045.3942 1390.9565 1649.7997

3038.3302 3135.2321 3236.1642

**Propargyl**

C -1.337790 -0.000036 -0.000137

C 1.251310 0.000077 -0.000077

C -0.115777 0.000017 0.000412

H -2.399972 0.000257 -0.000456

H 1.806292 -0.930175 -0.000367

H 1.807221 0.929569 -0.000368

**Frequencies**

351.7867 402.9866 468.4694

637.7994 681.7457 1031.4004

1089.4462 1455.3690 2011.5641

3139.3202 3229.8787 3468.0096

**Table S2.** Rate constants *k* (s−1) for all unimolecular reactions in the C2H + propylene system calculated using RRKM theory at *E*c = 41.1 kJ mol−1.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Reaction** | ***k*** | **Reaction** | ***k*** | **Reaction** | ***k*** |
| **i14 – i15** | 4.19E+12 | **i5 – i7** | 4.63E+06 | **i11 – i4** | 1.19E+07 |
| **i15 – i14** | 2.79E+12 | **i6 – p2** | 3.56E+08 | **i4 – i11** | 1.71E+07 |
| **i15 – i17** | 1.96E+12 | **i4 – i6** | 2.97E+08 | **i12 – i4** | 1.88E+06 |
| **i17 – i15** | 4.48E+12 | **i6 – i4** | 4.10E+07 | **i4 – i12** | 6.78E+05 |
| **i17 – i19** | 7.76E+09 | **i1 – i4** | 3.09E+05 | **i1 – i8** | 2.60E+03 |
| **i19 – i17** | 6.48E+09 | **i4 – i1** | 2.63E+05 | **i8 – i1** | 1.76E+02 |
| **i19 – p7** | 2.20E+10 | **i8 – p1** | 2.04E+09 | **i4 – i2** | 1.15E+10 |
| **i15 – p2** | 1.39E+07 | **i4 – p6** | 3.41E+08 | **i2 – i4** | 6.20E+12 |
| **i19 – i18** | 1.89E+09 | **i4 – p2** | 6.17E+08 | **i12 – i10** | 1.28E+06 |
| **i18 – i19** | 1.53E+10 | **i1 – i2** | 1.26E+10 | **i10 – i12** | 1.06E+06 |
| **i15 – p3** | 1.19E+07 | **i2 – i1** | 5.81E+12 | **i4 – i3** | 5.39E+12 |
| **i13 – i18** | 4.45E+10 | **i10 – p8** | 3.31E+10 | **i3 – i4** | 1.95E+12 |
| **i18 – i13** | 9.21E+08 | **i10 – p6** | 2.24E+08 | **i5 – i3** | 1.06E+06 |
| **i18 – p7** | 1.40E+11 | **i10 – i4** | 6.65E+07 | **i3 – i5** | 8.85E+05 |
| **i13 – i21** | 2.23E+12 | **i4 – i10** | 2.91E+07 | **i3 – p4** | 1.45E+08 |
| **i12 – i13** | 2.17E+12 | **i10 – i8** | 1.04E+08 | **i3 – p3** | 2.85E+08 |
| **i19 – i16** | 1.57E+05 | **i8 – i10** | 7.26E+06 | **i8 – i3** | 1.74E+07 |
| **i16 – i19** | 8.74E+07 | **i7 – i4** | 5.26E+07 | **i3 – i8** | 7.94E+07 |
| **i13 – p6** | 5.92E+08 | **i4 – i7** | 5.05E+07 | **i3 – p5** | 1.45E+08 |
| **i12 – p6** | 3.78E+08 | **i16 – i10** | 1.47E+10 | **i10 – i9** | 6.06E+12 |
| **i17 – i7** | 2.90E+09 | **i10 – i16** | 4.15E+09 | **i9 – i10** | 3.97E+12 |
| **i7 – i17** | 6.91E+11 | **i1 – p1** | 1.60E+09 | **i3 – i9** | 1.45E+07 |
| **i7 – p2** | 5.07E+09 | **i1 – p9** | 5.79E+07 | **i9 – i3** | 6.00E+07 |
| **i5 – p3** | 1.13E+09 | **i8 – i6** | 9.26E+11 | **i9 – p4** | 1.23E+08 |
| **i7 – i5** | 1.11E+07 | **i6 – i8** | 1.61E+12 | **i9 – p5** | 1.23E+08 |

**Table S3.** Rate constants *k* (s−1) for all unimolecular reactions in the C2H + propylene system calculated using RRKM theory at *E*c = 0 kJ mol−1.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Reaction** | ***k*** | **Reaction** | ***k*** | **Reaction** | ***k*** |
| **i14 – i15** | 3.53E+12 | **i5 – i7** | 1.55E+05 | **i11 – i4** | 1.98E+06 |
| **i15 – i14** | 2.42E+12 | **i6 – p2** | 5.06E+07 | **i4 – i11** | 3.00E+06 |
| **i15 – i17** | 1.70E+12 | **i4 – i6** | 5.56E+07 | **i12 – i4** | 9.06E+04 |
| **i17 – i15** | 4.09E+12 | **i6 – i4** | 5.93E+06 | **i4 – i12** | 3.14E+04 |
| **i17 – i19** | 3.93E+09 | **i1 – i4** | 1.55E+03 | **i1 – i8** | 4.78E+00 |
| **i19 – i17** | 2.65E+09 | **i4 – i1** | 1.23E+03 | **i8 – i1** | 2.32E-01 |
| **i19 – p7** | 8.68E+09 | **i8 – p1** | 4.37E+08 | **i4 – i2** | 5.63E+09 |
| **i15 – p2** | 1.35E+06 | **i4 – p6** | 3.95E+07 | **i2 – i4** | 4.47E+12 |
| **i19 – i18** | 7.15E+08 | **i4 – p2** | 9.54E+07 | **i12 – i10** | 3.52E+04 |
| **i18 – i19** | 6.87E+09 | **i1 – i2** | 6.77E+09 | **i10 – i12** | 2.92E+04 |
| **i15 – p3** | 9.69E+05 | **i2 – i1** | 4.25E+12 | **i4 – i3** | 5.27E+12 |
| **i13 – i18** | 3.09E+10 | **i10 – p8** | 1.07E+10 | **i3 – i4** | 1.90E+12 |
| **i18 – i13** | 3.06E+08 | **i10 – p6** | 2.31E+07 | **i5 – i3** | 4.18E+04 |
| **i18 – p7** | 6.27E+10 | **i10 – i4** | 6.68E+06 | **i3 – i5** | 3.66E+04 |
| **i13 – i21** | 2.20E+12 | **i4 – i10** | 2.78E+06 | **i3 – p4** | 1.54E+07 |
| **i12 – i13** | 2.02E+12 | **i10 – i8** | 1.62E+07 | **i3 – p3** | 4.28E+07 |
| **i19 – i16** | 1.37E+04 | **i8 – i10** | 8.29E+05 | **i8 – i3** | 2.50E+06 |
| **i16 – i19** | 1.19E+07 | **i7 – i4** | 5.00E+06 | **i3 – i8** | 1.46E+07 |
| **i13 – p6** | 6.12E+07 | **i4 – i7** | 5.05E+06 | **i3 – p5** | 1.54E+07 |
| **i12 – p6** | 3.55E+07 | **i16 – i10** | 4.92E+09 | **i10 – i9** | 5.46E+12 |
| **i17 – i7** | 1.26E+09 | **i10 – i16** | 2.10E+09 | **i9 – i10** | 3.59E+12 |
| **i7 – i17** | 5.18E+11 | **i1 – p1** | 3.45E+08 | **i3 – i9** | 1.37E+06 |
| **i7 – p2** | 6.94E+08 | **i1 – p9** | 7.79E+06 | **i9 – i3** | 5.99E+06 |
| **i5 – p3** | 1.49E+08 | **i8 – i6** | 9.21E+11 | **i9 – p4** | 1.11E+07 |
| **i7 – i5** | 3.72E+05 | **i6 – i8** | 1.60E+12 | **i9 – p5** | 1.11E+07 |