**Electronic Supporting Information**

The Hidden Path to the Resonance-Stabilized Fulvenallenyl Radical (C7H5) via the Bimolecular Reaction of Tricarbon (C3, X1Σg+) with 1,3-Butadiene (C4H6; X1Ag)

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Table of Contents

[**Figure S1**. Time-of-flight (TOF) spectra at different *m/z*’s for the reaction of the tricarbon (C3; X1g+): (a, d) with the 1,3-butadiene (C4H6, X1Ag); (b) with 1,3-butadiene-1,1,4,4-d4 (CD2CHCHCD2; X1Ag); (c) overlapped TOFs of H-loss channel for 1,3-dutadiene reaction with tricarbon with the sum of the H- and D-loss signals in the 1,3-butadiene-1,1,4,4-d4 reaction with tricarbon. 3](#_Toc209706918)

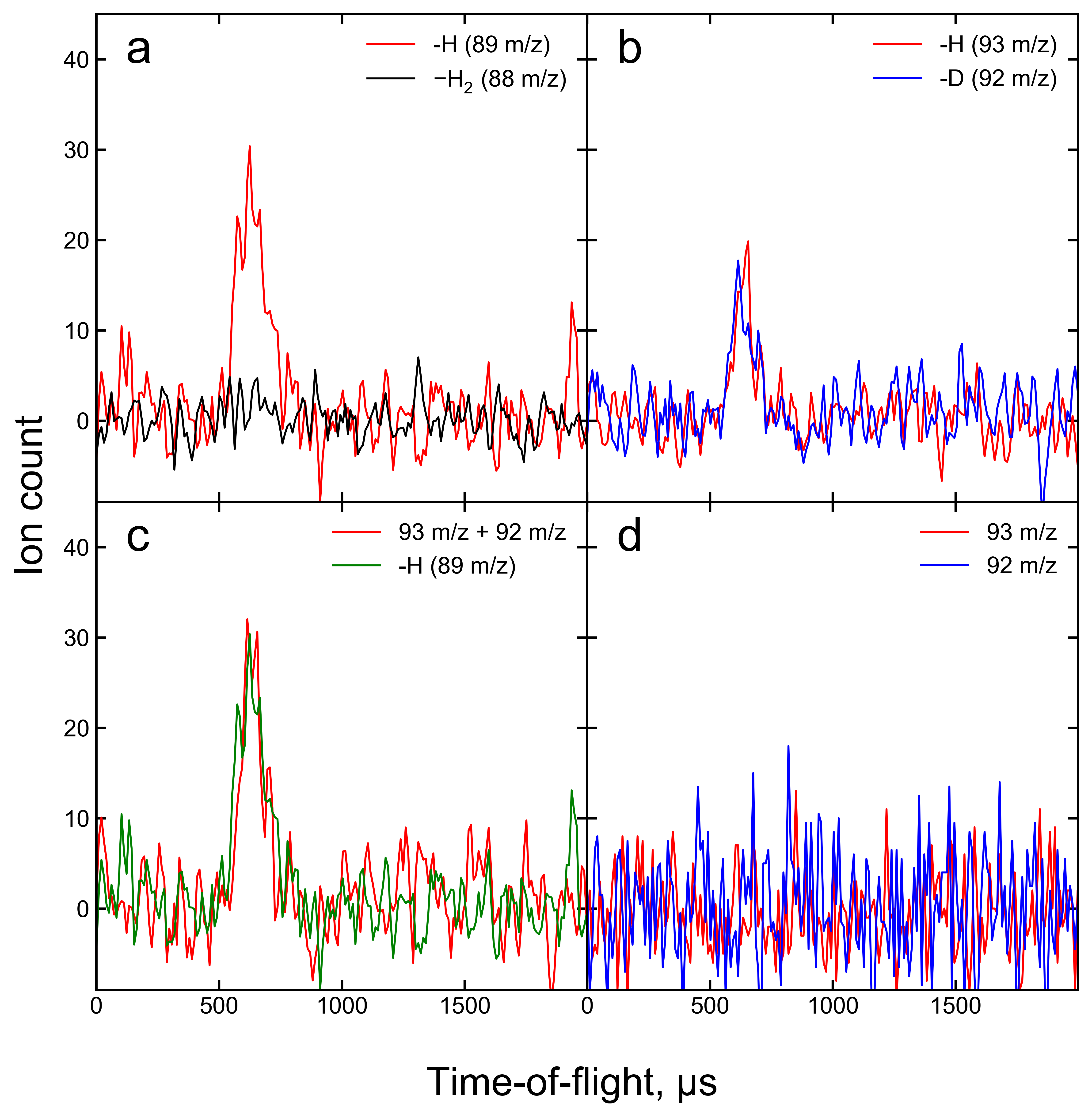
[**Figure S2.** Potential energy surface for the bimolecular reaction of the tricarbon (C3; X1g+) with the 1,3-butadiene-1,1,4,4-d4 (CD2CHCHCD2; X1Ag) leading to C7HD4/C7H2D3 isomers plus the atomic hydrogen/deuterium calculated at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory, with exception of structures with high T1 diagnostics, for which CASPT2(8,8)/cc-pVTZ were employed (see the COMPUTATIONAL section for more detail). Italics numbers calculated energies for deuterated intermediates and products. Grey atoms - carbon, white – hydrogen, blue – deuterium 4](#_Toc209706919)

[**Figure S3.** Possible C7H5 products. Energy (kJ mol–1) relative to the reactants. For unfavorable products **p5**-**p10**, relative energies were computed only at the ωB97X-D/6-311G(d,p) *+* ZPE(ωB97X-D/6-311G(d,p)) level of theory. 5](#_Toc209706920)

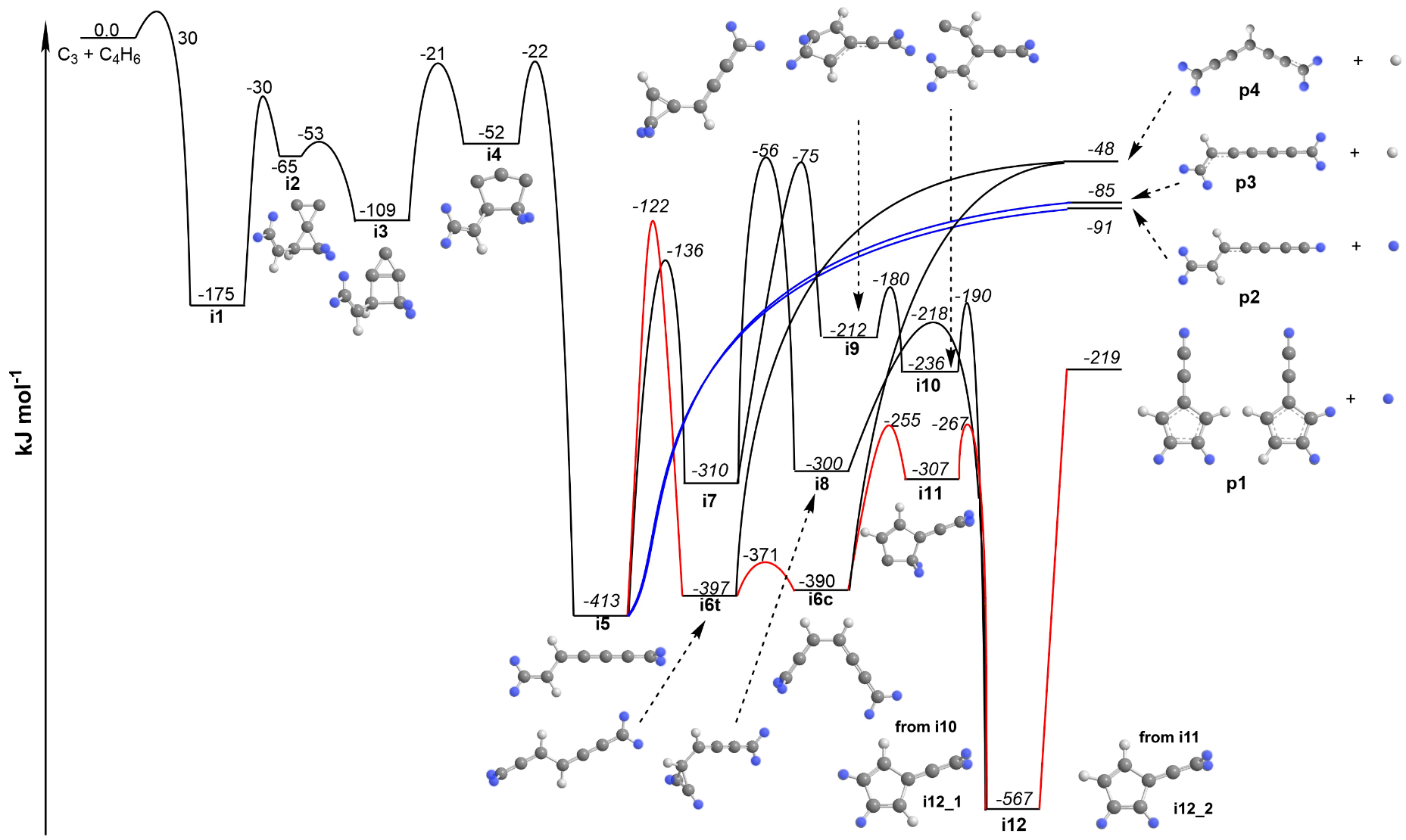
[**Table S1.** RRKM calculated statistical product branching ratios (%) for the reaction of tricarbon (C3; X1) with the 1,3-butadiene (C4H6, X1Ag) with ***i5*** as initial intermediates at different collision energies (*EC,* kJ mol–1). 6](#_Toc209706921)

[**Table S2.** RRKM calculated statistical product branching ratios (%) for the reaction of tricarbon (C3; X1) with 1,3-butadiene-1,1,4,4-d4 (CD2CHCHCD2; X1Ag) with ***i5*** as initial intermediates at different collision energies (*EC,* kJ mol–1). 6](#_Toc209706922)

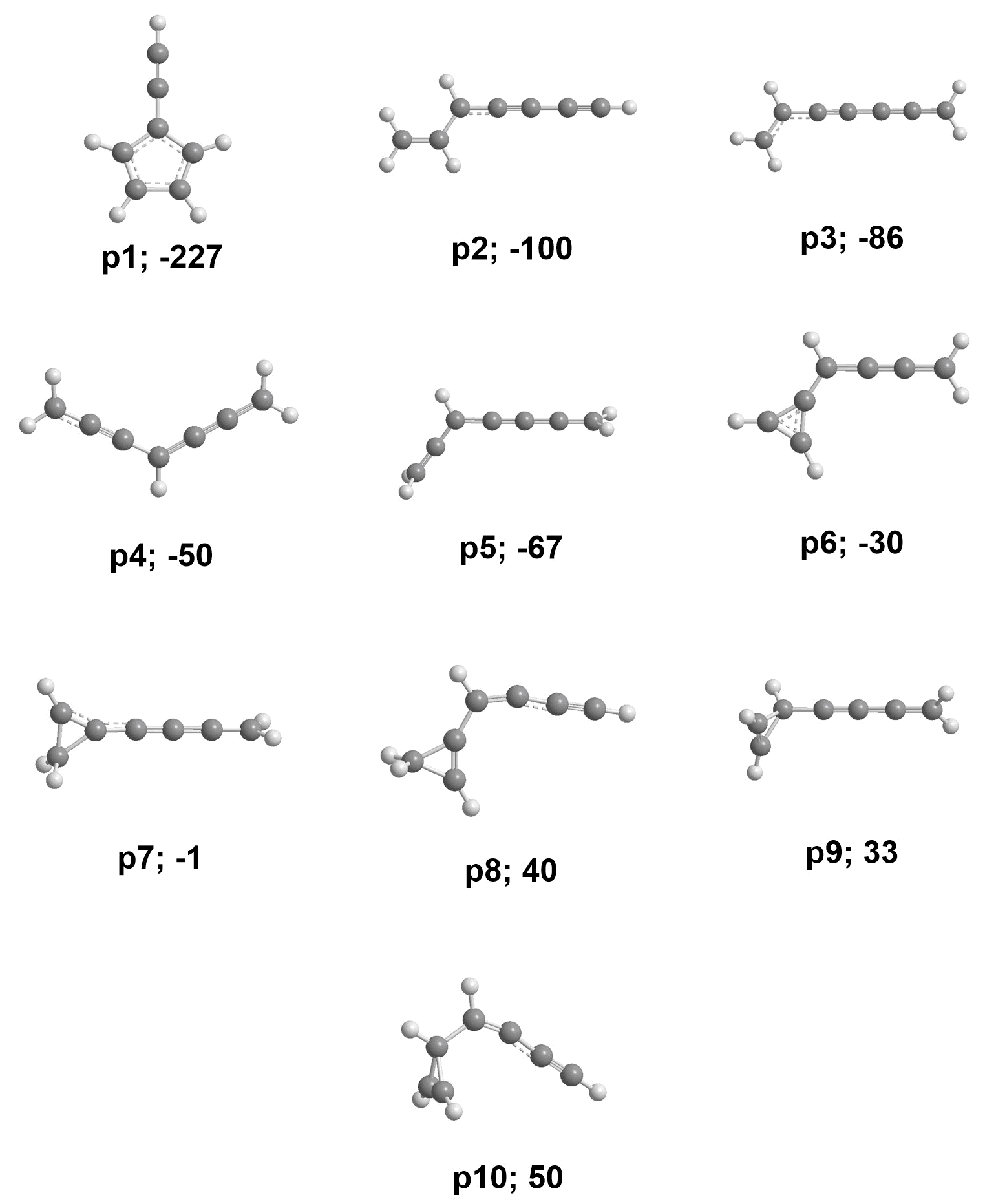
[**Optimized Cartesian coordinates (Å) and vibrational frequencies (cm−1) for all intermediates, transition states, reactants, and products involved in the C3+C4H6 reactions.** 6](#_Toc209706923)

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# **Figure S1**. Time-of-flight (TOF) spectra at different *m/z*’s for the reaction of the tricarbon (C3; X1): (a, d) with the 1,3-butadiene (C4H6, X1Ag); (b) with 1,3-butadiene-1,1,4,4-d4 (CD2CHCHCD2; X1Ag); (c) overlapped TOFs of H-loss channel for 1,3-dutadiene reaction with tricarbon with the sum of the H- and D-loss signals in the 1,3-butadiene-1,1,4,4-d4 reaction with tricarbon.



# **Figure S2.** Potential energy surface for the bimolecular reaction of the tricarbon (C3; X1) with the 1,3-butadiene-1,1,4,4-d4 (CD2CHCHCD2; X1Ag) leading to C7HD4/C7H2D3 isomers plus the atomic hydrogen/deuterium calculated at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory, with exception of structures with high T1 diagnostics, for which CASPT2(8,8)/cc-pVTZ were employed (see the COMPUTATIONAL section for more detail). Italics numbers calculated energies for deuterated intermediates and products. Grey atoms - carbon, white – hydrogen, blue – deuterium

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# **Figure S3.** Possible C7H5 products. Energy (kJ mol–1) relative to the reactants. For unfavorable products **p5**-**p10**, relative energies were computed only at the ωB97X-D/6-311G(d,p) *+* ZPE(ωB97X-D/6-311G(d,p)) level of theory.

# **Table S1.** RRKM calculated statistical product branching ratios (%) for the reaction of tricarbon (C3; X1) with the 1,3-butadiene (C4H6, X1Ag) with ***i5*** as initial intermediates at different collision energies (*EC,* kJ mol–1).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Products | Branching ratios, % | | | | |
| Ecol, kJ mol–1 | | | | |
| **0** | **15** | **30** | **44** | **48** |
| *p1 + H* | 17.68 | 12.78 | 9.59 | 7.44 | 6.97 |
| *p2 +H* | 76.75 | 80.27 | 82.20 | 83.21 | 83.38 |
| *p3+H* | 5.58 | 6.95 | 8.21 | 9.35 | 9.65 |
| *p4+H* | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

# **Table S2.** RRKM calculated statistical product branching ratios (%) for the reaction of tricarbon (C3; X1) with 1,3-butadiene-1,1,4,4-d4 (CD2CHCHCD2; X1Ag) with ***i5*** as initial intermediates at different collision energies (*EC,* kJ mol–1).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Products | Branching ratios, % | | | | |
| Ecol, kJ mol–1 | | | | |
| **0** | **15** | **30** | **44** | **48** |
| ***p1*** *+ H* | 40.89 | 29.61 | 21.74 | 16.34 | 15.16 |
| ***p2****+H* | 50.26 | 58.91 | 64.58 | 68.16 | 68.89 |
| ***p3*** *+H* | 8.85 | 11.48 | 13.68 | 15.50 | 15.95 |
| ***p4*** *+H* | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

# **Optimized Cartesian coordinates (Å) and vibrational frequencies (cm−1) for all intermediates, transition states, reactants, and products involved in the C3+C4H6 reactions.**

**Optimized Cartesian Coordinates (Å) and Vibrational Frequencies (cm-1)**

**i1**

6 0 -0.672830 0.696189 0.551547

6 0 -0.022922 1.624028 -0.491430

6 0 0.685933 0.467676 0.055873

6 0 -1.785150 -0.218813 0.170337

6 0 -1.624368 -1.466238 -0.249458

6 0 1.754714 -0.293880 0.050763

6 0 2.780032 -1.056659 0.037116

1 0 -0.732639 1.115632 1.553982

1 0 0.296653 2.613371 -0.180436

1 0 -0.356273 1.542128 -1.521815

1 0 -2.780646 0.210831 0.249821

1 0 -2.477530 -2.073998 -0.527078

1 0 -0.642025 -1.921782 -0.322959

Frequencies

74.3487 103.0731 167.5953

228.8059 280.8434 382.7533

468.5179 568.0938 655.7278

700.5529 777.5717 873.2456

986.6658 992.1991 1027.8100

1043.9062 1045.8112 1061.3643

1102.0252 1149.8563 1324.8514

1332.6947 1420.2747 1453.4355

1545.8704 1730.6633 2087.9230

3126.2355 3137.6338 3153.5998

3169.6345 3219.5023 3249.1017

**i3**

6 0 0.048387 -0.320265 -1.072177

6 0 1.587892 -0.249400 -0.964833

6 0 -0.733809 -0.808793 0.102366

6 0 -1.447031 -0.035757 0.909000

6 0 0.045091 1.192293 -1.320447

6 0 1.477764 1.226042 -1.298384

6 0 0.747741 2.406865 -1.535629

1 0 -0.279083 -0.823035 -1.986783

1 0 2.184310 -0.821992 -1.675419

1 0 1.987794 -0.393489 0.039842

1 0 -0.670197 -1.880163 0.279860

1 0 -1.988473 -0.451455 1.750451

1 0 -1.519408 1.034779 0.743306

Frequencies

108.2893 127.3351 229.1675

293.5202 325.5228 376.9814

568.2684 648.2856 706.4890

775.6592 886.1563 933.0203

982.2134 1007.8969 1030.8514

1075.0374 1117.8076 1136.7898

1194.6503 1230.6766 1259.5285

1321.8167 1328.9304 1448.8708

1453.4461 1608.9362 1734.4558

3081.3332 3091.1068 3149.6783

3154.9090 3164.2267 3247.7864

**i4**

6 0 0.030763 -0.289316 -1.084244

6 0 1.573754 0.151710 -1.034159

6 0 -0.385090 -1.135385 0.080515

6 0 -1.395837 -0.887558 0.900113

6 0 -0.808138 1.017704 -1.290919

6 0 1.649037 1.659211 -1.404379

6 0 0.332433 1.650524 -1.425779

1 0 -0.129313 -0.845930 -2.017554

1 0 2.229704 -0.437533 -1.681262

1 0 1.960061 0.072929 -0.012418

1 0 0.243608 -2.011698 0.236036

1 0 -1.620599 -1.552852 1.725516

1 0 -2.030266 -0.019057 0.759277

Frequencies

88.7978 139.7959 248.3008

318.9238 343.5114 522.3942

554.7133 590.8483 661.9438

716.3475 887.4381 910.3339

932.4013 984.4937 1011.5804

1029.3295 1077.5401 1136.6003

1175.7281 1209.2331 1241.8080

1274.3904 1327.4536 1417.1664

1445.2107 1565.8143 1736.5569

3036.3135 3057.0923 3116.5013

3138.4832 3160.0302 3251.6894

**i5**

6 0 -3.590355 -0.176263 0.082187

6 0 -2.301097 -0.513698 0.071694

6 0 -1.216759 0.461334 0.066079

6 0 0.059502 0.141049 0.055743

6 0 1.290537 -0.173783 0.045688

6 0 2.526956 -0.486707 0.036070

6 0 3.792694 -0.807762 0.025570

1 0 -4.369594 -0.928586 0.086040

1 0 -3.903688 0.863150 0.087199

1 0 -2.010615 -1.560173 0.066777

1 0 -1.486586 1.515952 0.070981

1 0 4.328762 -0.942780 -0.908568

1 0 4.343015 -0.947714 0.950656

Frequencies

81.5648 89.3821 178.4480

214.1884 329.5156 381.5241

447.1701 494.2974 522.9587

556.7554 684.1524 805.9386

871.4790 883.7470 953.4235

964.7630 1013.1613 1039.1272

1181.3892 1253.9817 1324.2024

1391.8310 1454.1955 1534.8314

1709.9792 1980.1148 2272.9615

3138.6597 3146.9800 3153.1173

3181.1601 3222.7632 3248.5327

**i7**

6 0 -1.927079 1.080236 0.000049

6 0 -2.889925 -0.078945 0.000415

6 0 -1.384200 -0.096091 -0.000630

6 0 -0.224151 -0.946386 -0.000222

6 0 1.013023 -0.483054 -0.000115

6 0 2.192840 -0.033008 0.000090

6 0 3.418750 0.433700 0.000172

1 0 -1.827943 2.150996 -0.000598

1 0 -3.431343 -0.328217 -0.913654

1 0 -3.430119 -0.328110 0.915248

1 0 -0.389874 -2.019880 0.000128

1 0 4.273074 -0.234936 0.000584

1 0 3.610666 1.501437 -0.000265

Frequencies

60.5088 86.0189 223.4069

259.2366 290.4852 350.1725

477.6420 520.3765 594.6905

764.0837 798.6694 887.1952

903.5770 908.9957 993.6425

1018.9703 1034.5505 1053.5985

1092.1841 1102.7267 1164.3488

1336.0357 1451.7382 1523.1625

1702.1098 1845.2980 2233.9481

3050.8307 3120.1255 3146.1145

3171.8604 3232.9235 3303.4868

**i12 (fulvenallene)**

6 0 0.595948 1.178718 0.000134

6 0 1.867722 0.732950 -0.000043

6 0 1.867779 -0.732955 -0.000099

6 0 0.596084 -1.178754 0.000129

6 0 -0.284411 0.000079 0.000112

6 0 -1.598249 -0.000070 0.000074

6 0 -2.895123 0.000012 -0.000124

1 0 0.246976 2.200463 -0.000002

1 0 2.757347 1.348175 -0.000401

1 0 2.757505 -1.348024 -0.000280

1 0 0.246778 -2.200382 0.000040

1 0 -3.453715 -0.000077 0.930491

1 0 -3.453396 -0.000042 -0.930941

Frequencies

132.9156 154.4220 372.5398

492.9374 564.3579 569.0156

631.7739 653.5685 747.3159

786.2341 826.2030 887.3958

907.4456 947.9196 959.5097

999.3331 1011.1699 1095.6049

1107.8588 1201.4962 1295.4804

1325.7101 1402.6978 1482.8892

1558.1926 1641.2221 2067.7097

3142.2132 3222.5622 3225.8492

3234.1836 3257.5085 3262.0318

**i8**

6 0 -1.849501 0.852228 0.642455

6 0 -1.849320 0.852303 -0.642430

6 0 -1.710675 -0.508136 -0.000039

6 0 -0.400732 -1.219998 -0.000001

6 0 0.776312 -0.631544 0.000003

6 0 1.897367 -0.044559 -0.000015

6 0 3.064701 0.553503 0.000028

1 0 -1.845344 1.371982 1.584335

1 0 -1.845097 1.372028 -1.584306

1 0 -2.570001 -1.177614 -0.000156

1 0 -0.435752 -2.307785 0.000058

1 0 3.987441 -0.017202 0.000102

1 0 3.139836 1.635810 -0.000038

Frequencies

36.9626 89.9114 207.5577

258.9284 322.4963 374.1032

534.4719 600.2735 611.8125

712.9204 810.8163 814.9917

871.4911 881.1370 898.7552

945.2827 1021.4421 1032.0304

1034.6417 1062.8792 1175.5079

1315.2491 1382.8892 1453.5540

1717.9619 1753.6129 2236.2103

3105.9377 3143.4018 3151.5823

3228.1115 3275.3986 3325.9207

**i2**

6 0 -0.361277 0.744718 0.554747

6 0 0.527233 1.450355 -0.409046

6 0 -1.693156 0.223433 0.144497

6 0 -1.930663 -0.990667 -0.331309

6 0 0.900830 0.066583 0.058850

6 0 2.136452 -0.646790 -0.370726

6 0 1.327872 -1.299511 0.471953

1 0 -0.275616 1.050862 1.595071

1 0 1.186589 2.241347 -0.069518

1 0 0.228192 1.494565 -1.451034

1 0 -2.505820 0.936880 0.261317

1 0 -2.933703 -1.283145 -0.619126

1 0 -1.143385 -1.729234 -0.430514

Frequencies

65.4710 123.2690 159.0080

219.9043 309.5700 389.7502

533.0851 593.1736 669.4866

700.3359 767.4792 835.5551

926.0124 996.8522 997.6819

1027.3911 1047.8304 1069.6912

1099.9573 1141.7855 1260.1961

1333.0611 1381.3144 1453.2169

1457.7329 1601.6362 1733.8904

3137.4260 3145.3616 3154.8520

3168.4519 3236.6629 3256.0357

**i9**

6 0 -0.772742 -0.771180 -0.462460

6 0 -1.928182 -0.794637 0.372516

6 0 -1.837160 0.705936 -0.050449

6 0 -0.575708 1.244407 0.017625

6 0 0.353506 0.133305 -0.057316

6 0 1.639893 -0.048955 0.029861

6 0 2.927523 -0.217971 0.109987

1 0 -0.857438 -1.032870 -1.511410

1 0 -1.800878 -0.884074 1.448362

1 0 -2.799757 -1.313881 -0.009520

1 0 -0.354932 2.307833 0.024612

1 0 3.566901 -0.098383 -0.759883

1 0 3.403322 -0.484054 1.049264

Frequencies

112.4929 160.1906 296.8106

391.7301 427.0895 462.3284

540.8214 592.3807 637.1987

714.3175 817.6572 851.5436

905.2053 933.8451 1009.1418

1020.5562 1075.4634 1129.9828

1172.2754 1223.7911 1244.2404

1327.2856 1407.5080 1496.2923

1512.0041 1518.6254 2096.3074

3128.0974 3131.8972 3171.6160

3197.0670 3212.3304 3218.0735

**i10**

6 0 0.630521 -1.205577 0.000031

6 0 1.958160 -1.215086 -0.000041

6 0 1.716470 1.720947 0.000036

6 0 0.479558 1.321183 -0.000006

6 0 -0.192617 0.014006 0.000001

6 0 -1.506616 -0.054436 0.000072

6 0 -2.801625 -0.135214 -0.000038

1 0 0.075150 -2.137890 0.000103

1 0 2.549012 -0.297844 -0.000087

1 0 2.515761 -2.143578 -0.000071

1 0 -0.119066 2.244237 -0.000124

1 0 -3.362040 -0.169991 0.929601

1 0 -3.361925 -0.169875 -0.929752

Frequencies

126.8690 145.3487 157.2312

186.1421 288.6447 358.0736

447.5762 513.3400 558.7142

584.7398 684.0145 729.4206

745.9431 912.4609 930.6727

944.5149 1006.3099 1012.8128

1047.3841 1255.9829 1263.7339

1332.6834 1454.3575 1482.7218

1721.7517 1781.6766 2070.3942

3068.1982 3098.7490 3134.1888

3189.3377 3216.1932 3234.4044

**i6t**

6 0 3.661390 -0.050546 0.000002

6 0 2.390772 0.219089 -0.000098

6 0 1.107212 0.483877 0.000101

6 0 0.078630 -0.552237 -0.000029

6 0 -1.215077 -0.296548 0.000052

6 0 -2.454367 -0.047657 0.000013

6 0 -3.741309 0.205683 -0.000020

1 0 4.210917 -0.165587 -0.929307

1 0 4.210820 -0.165714 0.929338

1 0 0.780240 1.519864 0.000035

1 0 0.415929 -1.585647 -0.000013

1 0 -4.111630 1.225263 -0.000106

1 0 -4.469783 -0.598146 -0.000073

Frequencies

66.6869 86.2791 193.7560

225.5128 312.7632 352.8986

465.6465 501.4780 539.7671

554.6310 651.7820 887.3791

896.7954 898.3799 925.3526

947.0360 1013.0667 1031.1413

1077.0456 1169.0768 1267.3131

1375.2339 1445.5405 1489.6345

1717.3366 2066.8264 2237.3601

3136.4844 3145.8366 3162.8340

3174.4617 3218.1360 3231.8071

**i6c**

6 0 -2.242873 1.535126 -0.000007

6 0 -1.897200 0.284242 0.000107

6 0 -1.535323 -0.975287 -0.000116

6 0 -0.148365 -1.450380 -0.000020

6 0 0.922613 -0.681123 0.000073

6 0 1.939070 0.068633 0.000147

6 0 2.996893 0.844817 -0.000089

1 0 -2.390305 2.076325 -0.929733

1 0 -2.390433 2.076452 0.929625

1 0 -2.312979 -1.733740 -0.000171

1 0 -0.010753 -2.528459 0.000016

1 0 2.896984 1.924966 -0.000206

1 0 3.998594 0.428286 -0.000103

Frequencies

70.0306 81.8348 187.7421

217.2170 317.1671 328.8266

459.9688 468.3643 563.2329

647.8646 722.8303 835.4317

878.9827 888.1341 892.6870

919.7851 1009.7689 1024.9429

1032.5584 1169.5227 1329.3986

1373.7737 1452.8393 1479.7812

1711.7058 2063.2768 2235.4374

3135.7422 3145.5109 3160.8778

3175.9294 3217.3099 3231.5419

**i11**

6 0 -0.644449 1.221770 0.000045

6 0 -2.053320 0.709778 -0.000116

6 0 -1.915153 -0.723753 0.000002

6 0 -0.613274 -1.135076 0.000008

6 0 0.274663 0.007275 0.000048

6 0 1.584959 -0.033607 0.000044

6 0 2.883288 -0.052762 -0.000048

1 0 -0.485792 1.864446 -0.873369

1 0 -0.486073 1.864277 0.873640

1 0 -2.757369 -1.406491 0.000011

1 0 -0.257055 -2.160287 -0.000016

1 0 3.443060 -0.061939 0.929952

1 0 3.442951 -0.061761 -0.930115

Frequencies

62.9193 157.2647 195.3169

337.9330 447.4049 541.1281

567.4402 606.3439 768.5902

802.0929 867.1889 874.7791

888.9201 949.1260 1002.1113

1018.4902 1087.2316 1127.4049

1143.0565 1200.7915 1231.2332

1297.7095 1398.2350 1402.6833

1473.7972 1532.1380 2064.1391

3056.4128 3093.6798 3140.6525

3191.4609 3211.5655 3223.9667

**p2**

6 0 3.526567 -0.224510 -0.000084

6 0 2.190257 -0.448829 0.000044

6 0 1.222096 0.586134 0.000041

6 0 -0.137873 0.354849 0.000076

6 0 -1.343042 0.155473 0.000051

6 0 -2.685372 -0.066882 0.000051

6 0 -3.875758 -0.264677 -0.000109

1 0 4.234717 -1.043437 -0.000073

1 0 3.927566 0.783856 -0.000198

1 0 1.821751 -1.470766 0.000157

1 0 1.559436 1.619366 -0.000159

1 0 -4.924726 -0.438363 -0.000146

Frequencies

82.4729 99.5269 192.8437

223.3291 380.5836 403.9428

476.9236 518.6578 557.0757

598.5610 661.5995 690.9503

778.1505 786.4228 894.7304

976.0232 1017.3102 1188.0681

1222.1407 1303.3258 1375.0690

1464.7479 1560.4512 2122.3441

2206.3242 3154.6872 3165.8219

3179.5713 3256.0828 3483.4776

**p3**

6 0 -3.504583 0.590961 0.000000

6 0 -2.645816 -0.436766 0.000008

6 0 -1.242163 -0.288777 0.000003

6 0 -0.026579 -0.186134 -0.000003

6 0 1.309218 -0.064774 -0.000031

6 0 2.542907 0.047181 -0.000037

6 0 3.881208 0.168812 0.000033

1 0 -4.573898 0.418230 0.000029

1 0 -3.156936 1.617347 -0.000025

1 0 -3.021618 -1.456671 0.000056

1 0 4.349345 1.146322 0.000089

1 0 4.517957 -0.708235 0.000006

Frequencies

78.7857 94.5364 170.4604

189.8914 241.6574 334.2733

420.9727 473.9313 512.6016

530.9582 626.7401 685.4749

761.6852 959.8568 987.3361

1007.1652 1024.8917 1121.3237

1317.9580 1378.7549 1446.1073

1503.7429 1640.9725 1997.2015

2179.7849 3151.3840 3160.7701

3170.2013 3246.0879 3263.1410

**p5**

6 0 3.386330 -0.809308 -0.000029

6 0 2.388651 0.018570 0.000105

6 0 1.378225 0.877096 0.000085

6 0 0.032797 0.507296 -0.000153

6 0 -1.170591 0.209456 -0.000155

6 0 -2.437110 -0.112292 0.000014

6 0 -3.700879 -0.432860 0.000069

1 0 3.817973 -1.171425 -0.929298

1 0 3.817767 -1.172132 0.929061

1 0 1.604569 1.941845 0.000464

1 0 -4.252370 -0.573113 0.927677

1 0 -4.252477 -0.572922 -0.927512

Frequencies

72.7587 110.8006 186.4582

189.7227 244.8320 299.9178

344.4107 390.6271 517.6979

559.4750 577.1699 774.2127

875.5552 896.8156 904.1599

989.2115 994.1189 1050.6093

1202.4339 1357.0631 1443.6913

1468.1691 1895.3357 1959.0204

2085.3022 3103.4333 3124.2980

3143.5652 3178.6197 3203.7929

**p6**

6 0 2.067374 1.067144 -0.000033

6 0 2.844497 0.002103 0.000111

6 0 1.433558 -0.214333 0.000141

6 0 0.337119 -0.996332 -0.000108

6 0 -0.959961 -0.474024 -0.000021

6 0 -2.107627 -0.024290 -0.000006

6 0 -3.367707 0.471146 0.000032

1 0 1.977359 2.139867 -0.000364

1 0 3.842610 -0.403007 -0.000225

1 0 0.465849 -2.073345 -0.000187

1 0 -4.224379 -0.191787 0.000132

1 0 -3.544962 1.539796 -0.000052

Frequencies

84.5997 128.9008 249.4436

251.5717 295.7296 384.3129

428.7349 492.7746 520.7314

680.6182 710.9431 805.6165

821.1317 879.6627 934.6922

959.3352 1028.0653 1032.5565

1114.1627 1294.6080 1396.0160

1488.2995 1584.5796 1806.2906

2083.5467 3155.4420 3180.5614

3248.2695 3273.8851 3316.8621

**p7**

6 0 -2.664297 0.739254 0.000184

6 0 -2.754151 -0.748280 -0.000087

6 0 -1.501904 0.113648 -0.000289

6 0 -0.149311 0.093007 0.000521

6 0 1.097166 0.039669 -0.000285

6 0 2.394410 -0.008305 0.000232

6 0 3.698058 -0.057031 -0.000110

1 0 -3.200767 1.671291 -0.000302

1 0 -3.023057 -1.273280 -0.916721

1 0 -3.022770 -1.273547 0.916480

1 0 4.263202 -0.077658 -0.928742

1 0 4.263563 -0.078574 0.928283

Frequencies

92.3401 92.4293 209.9453

231.1266 302.7578 333.0234

426.4394 473.3411 526.1760

562.5709 621.4158 859.9356

886.4566 974.4131 989.6073

991.6215 1064.6261 1069.4199

1126.9684 1184.6622 1439.6114

1504.9827 1623.1553 1894.4005

2047.4649 3065.0344 3116.0612

3142.0551 3194.8908 3298.3318

**p8**

6 0 1.687234 1.113441 0.000162

6 0 2.754865 0.048689 -0.000190

6 0 1.256964 -0.108192 0.000031

6 0 0.174542 -1.063385 0.000101

6 0 -1.095636 -0.715170 0.000046

6 0 -2.213603 -0.002860 -0.000023

6 0 -3.289997 0.583330 -0.000084

1 0 1.489701 2.170489 0.000376

1 0 3.316294 -0.148896 0.914271

1 0 3.315983 -0.148600 -0.914905

1 0 0.446292 -2.117033 0.000160

1 0 -4.214484 1.108912 -0.000160

Frequencies

39.5554 57.3265 232.8028

243.8045 326.1287 372.0306

436.7016 470.7505 545.9227

662.7573 724.7453 772.5541

835.7453 890.9812 986.0198

1017.1037 1046.4137 1086.8964

1102.4629 1160.3170 1343.4004

1522.7848 1781.1629 1828.4589

1997.4213 3053.3137 3123.4015

3143.6235 3303.8854 3470.8995

**p9**

6 0 2.578476 -0.641507 -0.395185

6 0 2.578509 0.643428 -0.392313

6 0 1.632745 -0.001251 0.604130

6 0 0.212987 -0.000904 0.372221

6 0 -1.003947 -0.000592 0.180230

6 0 -2.305698 -0.000790 -0.031084

6 0 -3.592661 0.000981 -0.239252

1 0 2.905641 -1.583670 -0.798526

1 0 2.904937 1.587384 -0.792086

1 0 1.903945 -0.003505 1.659327

1 0 -4.157322 0.928306 -0.329695

1 0 -4.159666 -0.924709 -0.331501

Frequencies

30.7412 44.8549 93.0934

109.4406 233.9098 338.4412

463.4792 476.9312 552.9766

612.9180 762.4042 806.3373

877.4814 896.4040 924.3830

984.9586 1011.3502 1045.9293

1082.7659 1190.0374 1363.1686

1449.0207 1749.0812 1884.4405

2098.5491 3087.2489 3107.5243

3157.0773 3276.2917 3326.9628

**p10**

6 0 -1.642816 -0.916303 -0.641830

6 0 -1.648623 -0.912492 0.643626

6 0 -1.627351 0.450792 -0.003205

6 0 -0.379531 1.282015 0.000025

6 0 0.843994 0.814258 0.000602

6 0 1.913936 0.027673 0.000430

6 0 2.946638 -0.632452 0.000517

1 0 -1.592903 -1.438899 -1.580799

1 0 -1.607216 -1.429286 1.586210

1 0 -2.540171 1.045876 -0.008893

1 0 -0.528777 2.362718 0.002086

1 0 3.831583 -1.221356 0.000418

Frequencies

27.5639 43.2074 225.9460

254.2463 361.4371 388.9974

427.5910 540.8979 585.7953

645.1456 694.4872 766.6500

795.8037 865.4165 879.5551

936.9036 1017.6681 1025.0619

1061.8059 1169.8433 1306.1698

1381.9006 1751.9575 1811.9936

2011.8580 3099.4066 3117.8239

3276.1932 3326.3571 3474.9369

**Fulvenallenyl (p1)**

6 0 1.717438 0.000031 -0.000002

6 0 0.321993 0.000010 -0.000004

6 0 -0.525830 1.171569 0.000002

6 0 -1.811623 0.736475 -0.000001

6 0 -1.811596 -0.736510 0.000001

6 0 -0.525775 -1.171560 0.000000

6 0 2.926409 -0.000009 0.000002

1 0 -0.169218 2.190132 -0.000005

1 0 -2.698913 1.354297 0.000004

1 0 -2.698861 -1.354367 0.000006

1 0 -0.169126 -2.190109 -0.000004

1 0 3.990023 0.000013 0.000010

Frequencies

145.7528 160.4436 404.1305

525.8201 528.7226 563.3060

643.9988 646.9677 653.6648

691.0152 734.6666 760.0813

917.7986 920.2114 932.0638

1002.0767 1049.2678 1090.1578

1135.1167 1288.5356 1307.6075

1421.1088 1530.5102 1551.5729

2122.6964 3229.4736 3240.3975

3262.1174 3266.7416 3477.7729

**p4**

6 0 3.496253 -0.728903 0.000118

6 0 2.313275 -0.116313 -0.000180

6 0 1.203425 0.447397 -0.000066

6 0 0.000036 1.089109 0.000101

6 0 -1.203566 0.447913 -0.000059

6 0 -2.313412 -0.115929 0.000035

6 0 -3.496122 -0.729171 0.000008

1 0 4.418622 -0.159478 0.000664

1 0 3.561596 -1.810900 -0.000605

1 0 0.000187 2.177315 0.000067

1 0 -3.560866 -1.811211 0.000602

1 0 -4.418872 -0.160343 -0.000474

Frequencies

68.0754 176.4359 191.5449

202.3496 312.8227 388.0338

406.9372 412.4022 500.9742

535.6179 539.9888 821.3206

821.5858 851.9296 855.0743

871.6453 1033.8588 1034.3683

1297.4919 1373.5025 1430.4507

1521.6992 1582.9779 1837.2752

2163.5646 3145.7078 3151.7048

3152.5952 3244.7960 3244.8798

ts1 C3+C4H6 - i1

6 0 0.731112 0.751652 -0.293820

6 0 -0.190932 1.572730 0.287848

6 0 1.512507 -0.228349 0.477946

6 0 2.581467 -0.843790 -0.014472

1 0 1.106349 0.988594 -1.282801

1 0 -0.662648 2.371852 -0.269662

1 0 -0.506470 1.419597 1.312632

1 0 1.172298 -0.429553 1.490039

1 0 3.149886 -1.548700 0.579958

1 0 2.920831 -0.662969 -1.029423

6 0 -0.837669 -0.325553 -0.834715

6 0 -1.942507 -0.445498 -0.133793

6 0 -3.050684 -0.837663 0.377549

Frequencies

-386.1431 41.6994 96.2723

156.7244 185.1679 242.4112

293.6746 329.9911 449.1887

529.8076 621.4116 742.1831

892.1868 959.0351 985.7437

1005.9458 1025.1857 1074.7345

1228.0256 1246.7243 1307.3783

1327.6387 1414.3893 1475.5996

1607.0294 1734.5132 2038.5361

3156.3584 3171.3277 3177.3555

3201.5314 3252.4437 3274.8578

ts2 i1-i2

6 0 -0.335329 0.689538 0.565908

6 0 0.657547 1.273884 -0.392856

6 0 -1.705572 0.325326 0.092621

6 0 -2.062170 -0.884424 -0.315346

6 0 0.741010 -0.278579 0.361781

6 0 2.034171 -0.253994 -0.483366

6 0 1.576213 -1.341465 0.308183

1 0 -0.312487 1.134297 1.560487

1 0 1.329052 2.049784 -0.052254

1 0 0.401794 1.284995 -1.443968

1 0 -2.418851 1.145181 0.087608

1 0 -3.069422 -1.079420 -0.663767

1 0 -1.365300 -1.716557 -0.309654

Frequencies

-446.7311 95.1753 146.3871

182.4100 335.7362 394.7504

484.6630 579.5959 683.5431

772.0190 832.4825 837.5623

916.7806 993.8058 1027.6600

1033.4776 1057.3804 1098.9884

1138.1445 1172.2580 1230.2418

1331.9923 1353.8296 1453.2926

1460.1239 1684.6673 1733.3768

3122.2690 3154.4896 3167.7608

3173.9350 3250.1076 3279.2884

ts3 i3 - i4

6 0 -0.223595 0.413445 0.701448

6 0 0.488927 1.246030 -0.380825

6 0 -1.638882 -0.051702 0.491208

6 0 -2.102820 -0.519151 -0.659352

6 0 0.873286 -0.651798 0.507770

6 0 1.554899 0.166115 -0.453695

6 0 2.077826 -1.094198 -0.095814

1 0 -0.108589 0.836676 1.700349

1 0 0.876588 2.223432 -0.091854

1 0 -0.045095 1.343951 -1.326424

1 0 -2.295508 -0.001657 1.354422

1 0 -3.130748 -0.845966 -0.759402

1 0 -1.474494 -0.608881 -1.541538

Frequencies

-114.7710 105.1957 233.5755

284.6283 313.4816 372.4327

555.3667 633.9868 723.9110

765.9126 882.1002 935.8756

980.6355 996.7977 1028.1311

1056.1658 1118.3124 1152.5927

1194.2528 1224.1644 1257.9557

1338.7451 1355.7671 1446.3413

1464.0704 1604.1100 1732.0537

3092.6040 3110.3325 3147.3537

3155.1453 3180.6101 3242.8167

ts5 i4-i5

6 0 -0.262705 0.026759 0.593772

6 0 1.321328 1.098611 -0.231226

6 0 -1.618634 0.507135 0.289698

6 0 -2.481681 -0.146791 -0.482548

6 0 0.204731 -1.307606 0.253649

6 0 2.293000 0.029002 -0.294382

6 0 1.401327 -0.913068 -0.091154

1 0 0.170573 0.390966 1.524050

1 0 1.591731 2.051909 0.221809

1 0 0.671844 1.184473 -1.098229

1 0 -1.887508 1.466710 0.724006

1 0 -3.473040 0.244978 -0.676015

1 0 -2.217792 -1.103288 -0.922482

Frequencies

-642.8498 94.7537 200.8055

247.3763 356.0960 397.4355

492.2677 540.7890 601.2180

658.3093 704.6133 809.5473

916.2906 978.7247 986.4170

1028.7099 1045.2434 1052.5525

1127.4001 1160.0123 1249.9953

1328.7102 1372.7009 1443.7718

1450.1593 1637.2660 1712.1987

3108.8182 3148.9558 3153.9920

3172.9064 3208.4089 3252.9100

ts6 i5-i7

6 0 3.593649 -0.138728 0.266489

6 0 2.373519 -0.387381 -0.215378

6 0 1.304059 0.559244 0.065136

6 0 0.006892 0.298027 -0.156959

6 0 -1.278805 0.135890 -0.046309

6 0 -2.528060 -0.041212 0.040327

6 0 -3.822865 -0.226168 0.137849

1 0 4.395721 -0.864450 0.184115

1 0 3.798117 0.793832 0.780930

1 0 2.170132 -1.325176 -0.732746

1 0 0.489076 0.805957 -1.138459

1 0 -4.272634 -0.519043 1.079566

1 0 -4.470736 -0.089149 -0.720340

Frequencies

-651.6678 58.3498 86.7706

145.8607 183.4496 340.2866

379.7988 446.1939 484.2026

503.0530 563.1381 665.2229

757.9693 812.2434 912.6716

976.6156 1009.4598 1018.1362

1029.5005 1127.4668 1325.5902

1362.8872 1433.1425 1491.5578

1681.8290 1872.5775 2241.0224

2380.6781 3121.7384 3154.0532

3158.2221 3241.0782 3255.4421

ts7 i7-i8

6 0 -1.712507 0.879799 0.250056

6 0 -2.921714 0.491807 -0.270170

6 0 -1.427506 -0.463852 0.457880

6 0 -0.245864 -1.136452 -0.069278

6 0 0.947375 -0.566038 -0.090629

6 0 2.075726 0.001507 -0.049206

6 0 3.252785 0.580877 -0.020625

1 0 -1.088902 1.752624 0.127267

1 0 -3.177125 0.791541 -1.294164

1 0 -2.719138 -0.732963 0.243069

1 0 -0.336246 -2.192273 -0.309577

1 0 4.157839 0.019821 -0.228212

1 0 3.353800 1.635369 0.213440

Frequencies

-1453.2075 57.6222 107.2434

211.8889 243.3488 269.5433

358.2547 450.1804 540.6595

589.1981 642.9859 790.4829

864.0899 883.9641 896.9422

906.3272 982.7703 1031.4471

1034.3284 1140.6943 1185.3491

1312.0114 1413.9345 1444.5484

1492.1111 1684.6730 2205.1497

2220.5452 3073.6192 3145.3456

3165.6054 3231.6881 3261.0800

ts9 i2-i3

6 0 -0.290146 0.709750 0.574923

6 0 0.497610 1.505345 -0.460856

6 0 -1.650981 0.205170 0.242397

6 0 -1.939010 -0.945959 -0.348400

6 0 0.975127 0.180866 -0.007665

6 0 2.114896 -0.629164 -0.125257

6 0 1.224019 -1.519241 0.240406

1 0 -0.164761 1.034874 1.606520

1 0 1.085628 2.370766 -0.173253

1 0 0.075612 1.529821 -1.461530

1 0 -2.448532 0.894432 0.510111

1 0 -2.967365 -1.204181 -0.573616

1 0 -1.169667 -1.666312 -0.601514

Frequencies

-381.3683 89.2110 154.5485

194.6960 286.7118 350.8110

377.1331 553.1203 663.9056

717.3938 754.9556 843.3026

936.1001 991.2892 1026.7090

1043.8251 1046.2831 1079.0243

1108.9901 1154.3625 1329.0436

1337.6379 1418.0492 1450.2513

1487.0921 1644.6615 1732.5420

3124.5174 3132.4174 3153.5303

3168.0195 3221.4963 3254.8154

ts10 i7-i9

6 0 -1.023882 -0.624714 -0.696515

6 0 -1.953559 -0.910732 0.471277

6 0 -1.581784 0.447837 -0.058277

6 0 -0.565286 1.385822 0.171618

6 0 0.509318 0.598759 -0.213628

6 0 1.662305 0.071455 -0.013748

6 0 2.821144 -0.516578 0.162415

1 0 -0.800067 -1.013523 -1.674235

1 0 -1.533407 -1.249027 1.417862

1 0 -2.941899 -1.303361 0.245138

1 0 -0.581272 2.384388 0.586068

1 0 3.733416 -0.095674 -0.250818

1 0 2.913698 -1.433895 0.737131

Frequencies

-796.7563 95.2767 158.4934

234.7304 317.1261 378.2894

467.7155 555.5366 612.0613

677.3172 778.7832 838.3337

886.8639 910.8612 957.5585

971.0525 1023.8369 1028.1397

1033.8494 1074.1568 1164.2055

1342.0639 1418.5536 1469.5715

1529.9053 1561.3204 2105.0418

3087.2428 3124.1239 3175.3593

3203.3380 3229.3519 3299.4210

ts11 i10-i12

6 0 0.599134 -1.167216 0.000024

6 0 1.895791 -0.903852 0.000011

6 0 1.886040 1.151387 -0.000018

6 0 0.563010 1.218283 0.000045

6 0 -0.270877 0.006262 0.000054

6 0 -1.584387 -0.021775 -0.000008

6 0 -2.881588 -0.042220 -0.000058

1 0 0.194702 -2.172866 0.000259

1 0 2.627212 0.242532 -0.000499

1 0 2.716526 -1.613509 -0.000147

1 0 0.102686 2.199889 0.000243

1 0 -3.441968 -0.050680 0.929941

1 0 -3.441903 -0.050581 -0.930097

Frequencies

-998.2421 133.1686 155.2802

339.9900 400.1784 427.7229

531.6784 563.9356 618.8269

637.9703 654.0353 746.7076

750.6520 844.6163 906.2448

928.5632 929.0903 1005.9040

1054.7805 1184.2166 1215.3924

1262.5104 1339.8266 1474.9295

1629.0263 1672.6956 2071.3225

2622.3316 3137.4234 3193.0428

3206.2357 3218.9985 3220.1219

ts12 i8–i12

6 0 -2.046710 -1.172752 -0.607906

6 0 -1.768326 -0.750948 0.588169

6 0 -1.628143 0.653540 0.214996

6 0 -0.390223 1.256487 -0.091576

6 0 0.803523 0.629698 -0.037017

6 0 1.904496 0.035045 -0.018359

6 0 3.070335 -0.595662 0.004779

1 0 -2.279712 -0.896754 -1.620690

1 0 -1.584459 -1.274270 1.518950

1 0 -2.524244 1.259765 0.144342

1 0 -0.402594 2.302411 -0.389163

1 0 3.990958 -0.077959 -0.240340

1 0 3.130330 -1.645646 0.268390

Frequencies

-778.3991 81.7270 111.6427

184.4529 259.4213 284.7663

381.7004 451.6948 467.3351

541.1842 604.1601 693.0940

794.9602 831.2677 853.2738

871.5269 903.4066 1013.6279

1033.3160 1171.2171 1235.9358

1330.3511 1377.7882 1442.2875

1598.6238 1673.2942 2042.8032

3148.6969 3156.2859 3187.7516

3193.8482 3238.4131 3337.9376

ts13 i9-i10

6 0 0.744650 -0.896355 -0.419269

6 0 1.834741 -1.029136 0.365185

6 0 1.860202 1.047159 -0.107948

6 0 0.545632 1.308044 0.024726

6 0 -0.291736 0.118829 -0.049451

6 0 -1.584435 -0.041316 0.031151

6 0 -2.873613 -0.200626 0.096699

1 0 0.723779 -1.313887 -1.421147

1 0 1.825976 -0.753826 1.411511

1 0 2.703484 -1.567999 0.007210

1 0 0.199287 2.334003 0.105306

1 0 -3.363950 -0.448769 1.033516

1 0 -3.501229 -0.089114 -0.782946

Frequencies

-330.7750 104.8918 156.2827

255.5091 336.4518 383.8351

553.0755 563.3290 586.9237

626.7405 783.4537 816.5481

840.0813 911.3090 982.2785

1007.0809 1021.1637 1055.2536

1094.8089 1212.3891 1291.2063

1316.0131 1442.6623 1488.6293

1601.9064 1641.6664 2094.2256

3130.5121 3173.6980 3187.1646

3192.6639 3210.8291 3269.7773

ts14 i5-i6t

6 0 -3.378186 -0.616858 -0.012108

6 0 -2.169524 -0.107722 -0.175851

6 0 -1.292541 0.953880 -0.045883

6 0 -0.130338 0.242832 0.196584

6 0 1.161739 0.146559 0.135538

6 0 2.404534 -0.088716 0.026939

6 0 3.690742 -0.307875 -0.092020

1 0 -3.639764 -1.590519 -0.406978

1 0 -4.125024 -0.088514 0.574717

1 0 -0.979755 -0.871974 0.055192

1 0 -1.454660 2.022038 -0.137289

1 0 4.309057 0.315576 -0.729458

1 0 4.171593 -1.119210 0.444627

Frequencies

-1828.2844 90.2429 111.7052

233.5454 244.7985 343.3237

395.3639 503.2195 524.9428

545.0784 579.4110 665.5794

860.7970 864.2770 879.8815

912.9405 986.0957 1017.2311

1059.6475 1101.7897 1205.8159

1349.8568 1447.3202 1470.5920

1796.2287 1811.5756 1851.9925

2208.3426 3137.6439 3141.9137

3206.1041 3226.7011 3237.8254

ts15 i6c-i11

6 0 -0.680798 1.357899 -0.212788

6 0 -1.842967 0.804258 0.268896

6 0 -1.990605 -0.542754 0.147057

6 0 -0.739495 -1.193921 -0.069029

6 0 0.342396 -0.364335 -0.187385

6 0 1.614222 -0.224107 -0.040453

6 0 2.873809 0.065924 0.158825

1 0 -0.619550 1.492038 -1.295546

1 0 -0.106894 2.082306 0.360100

1 0 -2.918585 -1.093707 0.240526

1 0 -0.642306 -2.267704 -0.196387

1 0 3.167487 0.833399 0.868472

1 0 3.660469 -0.464122 -0.367903

Frequencies

-643.2056 129.3430 143.4629

299.7909 375.0135 463.7981

502.6706 538.3664 562.9833

654.9896 778.1825 854.0207

885.1005 919.7630 961.8512

969.6412 1005.8394 1031.5747

1093.4799 1114.3504 1292.7507

1330.4652 1407.3951 1443.0809

1554.4360 1614.6222 2084.1036

3102.8653 3138.4876 3190.2808

3191.8708 3213.9660 3222.4239

ts16 i11-i12

6 0 0.604704 -1.162761 0.029312

6 0 1.970237 -0.794513 0.110554

6 0 1.906142 0.689230 -0.000532

6 0 0.645073 1.167669 -0.002660

6 0 -0.280031 0.036514 0.003340

6 0 -1.591962 0.040516 -0.000396

6 0 -2.888762 0.019262 0.001111

1 0 1.351596 -1.339726 -0.970789

1 0 0.225465 -2.167240 0.188683

1 0 2.795782 1.305863 -0.029961

1 0 0.327647 2.201898 -0.036215

1 0 -3.444880 0.000431 0.932833

1 0 -3.448021 0.023268 -0.928913

Frequencies

-1014.4456 127.5409 155.7873

372.2307 445.1510 551.7255

567.3957 587.0503 651.3101

794.9780 830.6913 861.5862

889.8742 919.4173 990.1860

993.8651 998.1955 1110.6797

1161.9175 1203.4004 1279.2713

1314.4863 1343.4237 1398.4603

1484.7120 1583.8349 2066.7613

2207.9254 3144.8826 3193.8033

3211.3683 3229.7757 3236.0041

ts17 i6t-i6c

6 0 -3.090518 0.969788 -0.220506

6 0 -2.173454 0.126840 0.153455

6 0 -1.251043 -0.713801 0.526623

6 0 -0.061405 -1.044675 -0.310805

6 0 1.099920 -0.449438 -0.178324

6 0 2.220455 0.126572 -0.048835

6 0 3.379002 0.722621 0.085319

1 0 -3.956357 0.641413 -0.785890

1 0 -3.011945 2.024229 0.022448

1 0 -1.347072 -1.215059 1.487818

1 0 -0.171854 -1.834402 -1.051473

1 0 3.522451 1.509670 0.818384

1 0 4.227032 0.446703 -0.532853

Frequencies

-107.0990 110.8427 175.9879

191.1714 294.0512 325.0688

445.1742 472.3768 555.0756

592.7794 686.9769 838.6208

887.4665 890.6045 903.7088

914.1234 1020.0943 1027.7108

1033.9467 1151.6482 1292.6634

1342.6394 1448.4536 1477.8380

1725.5461 2090.4082 2248.0860

3142.3487 3143.6576 3145.1766

3145.5859 3228.5095 3228.7904