**Supplementary Materials for**

**Low Temperature Gas Phase Formation of Indene in the Interstellar Medium**

**Authors:** Srinivas Doddipatla,1 Galiya R. Galimova,2,3 Hongji Wei,4 Aaron M. Thomas,1 Chao He,1 Zhenghai Yang,1 Alexander N. Morozov2, Christopher N. Shingledecker,4 Alexander M. Mebel,\*2 Ralf I. Kaiser\*1

1 *Department of Chemistry, University of Hawai‘i at Mānoa, Honolulu, 96822*

2 *Department of Chemistry and Biochemistry, Florida International University, Miami, 33199*

3*Samara National Research University,* *Samara 443086, Russia*

*4 Department of Physics and Astronomy, Benedictine College, Atchison, 66002*

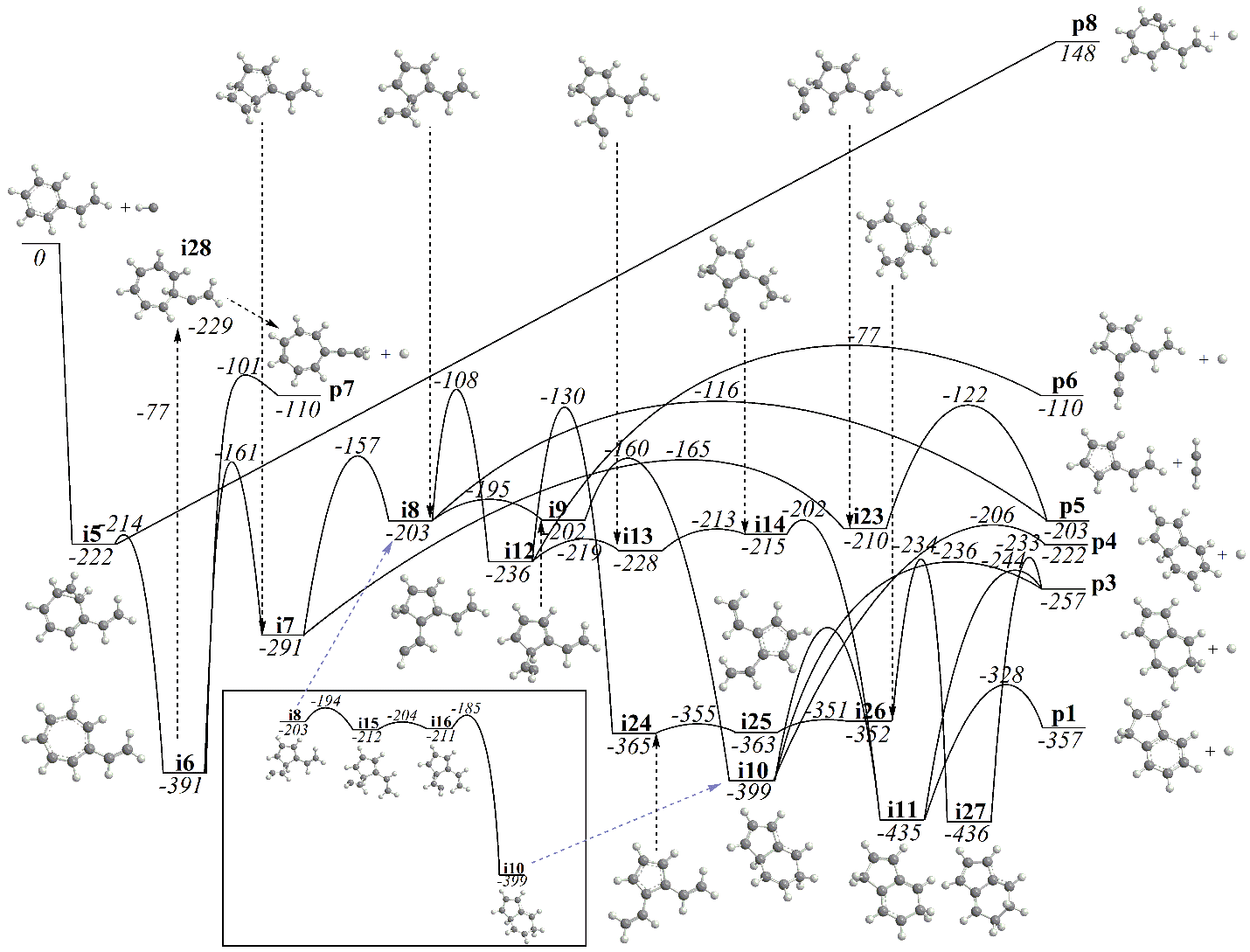
\*Correspondence to: [ralfk@hawaii.edu](mailto:ralfk@hawaii.edu%20), [mebela@fiu.edu](mailto:mebela@fiu.edu), cshingledecker@benedictine.edu

**This PDF file includes:**

Figures S1-S5

Tables S1-S7

****



*-284*

**Fig. S1.** Complete potential energy surface for the reaction of the methylidyne radical with styrene. Relative energies are given in units of kJ mol-1. Atoms are color coded in gray (carbon) and white (hydrogen).



**Fig. S2.** Addition of methylidyne to six chemically inequivalent ’aromatic’ carbon-carbon bonds followed by ring opening results in the formation of the doublet radical intermediate i6.

****

**Fig. S3.** Potential energy surface for the reaction of the methylidyne radical with toluene. Relative energies are given in units of kJ mol-1. Atoms are color coded in gray (carbon) and white (hydrogen).



**Fig. S4.** Calculated temperature dependence of the HP rate constants for the CH + benzene and CH + ethylene addition reactions.

|  |  |  |
| --- | --- | --- |
| Molecule | Dipole moment (Debye) | Relative Energy (kJ mol-1) |
| 1-cyanoindene | 4.03 | 33 |
| 2-cyanoindene | 4.62 | 0 |
| 3-cyanoindene | 4.63 | 7 |
| 4-cyanoindene | 5.16 | 6 |
| 5-cyanoindene | 5.70 | 8 |
| 6-cyanoindene | 5.49 | 6 |
| 7-cyanoindene | 4.25 | 7 |

**Fig. S5.** Dipole moments and relative energies of distinct cyanoindene isomers calculated at B3LYP/6-311G\*\* level of theory formed via barrierless neutral – neutral reactions of cyano radicals with indene.

**Table S1.** Peak velocities (vp) and speed ratios (S) with ±1σ uncertainty of methylidyne radical (CH;X2Π), and styrene (C8H8; X1A′) beams along with the collision energies (EC) and center-of-mass angles (ΘCM).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| beam | vp (m s-1) | S | EC (kJ mol-1) | ΘCM (deg) |
| CH (X2Π) | 1850 ± 11 | 11.7 ± 0.7 | 20.6 ± 0.2 | 59.1 ± 0.3 |
| C8H8 (X1A′) | 386 ± 4 | 28.0 ± 0.4 |  |  |

**Table S2.** Rate constants (s-1) of various unimolecular reactions on the C9H9 PES calculated using RRKM theory for the experimental collision energy.a

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Reaction | *k* | Reaction | *k* | Reaction | *k* | Reaction | *k* |
| i1→i2 | 2.56E+10 | i10**→**i15 | 2.23E+05 | i18**→**i6 | 2.16E+05 | i12**→**i24 | 1.25E+08 |
| i2→i1 | 2.77E+06 | i10**→**i11 | 3.94E+09 | i17**→**i18 | 1.76E+06 | i24**→**i12 | 9.35E+02 |
| i2→i3 | 4.07E+11 | i11**→**i10 | 7.48E+08 | i18**→**i17 | 3.19E+06 | i12**→**p6 | 5.68E+05 |
| i3→i2 | 2.34E+12 | i10**→**p3 | 2.09E+08 | i7**→**i15 | 2.06E+08 | i22**→**p1 | 1.43E+09 |
| i3→i4 | 2.74E+08 | i10**→**p4 | 3.57E+07 | i15**→**i7 | 1.96E+10 | i18**→**p10 | 2.80E+03 |
| i4→i3 | 2.43E+10 | i24**→**i27 | 6.85E+06 | i7**→**i23 | 2.55E+08 | i22**→**p9 | 1.60E+07 |
| i3→p2 | 4.77E+06 | i27**→**i24 | 1.36E+07 | i23**→**i7 | 1.91E+10 | i19**→**i20 | 1.53E+03 |
| i4→p1 | 2.14E+10 | i12**→**i11 | 4.57E+10 | i18**→**i19 | 2.77E+11 | i20**→**i19 | 1.95E+03 |
| i21→i22 | 6.12E+09 | i11**→**i12 | 2.44E+06 | i19**→**i18 | 1.24E+11 | i15**→**i10 | 9.77E+10 |
| i22→i21 | 1.44E+09 | i11**→**p1 | 4.68E+10 | i19**→**i29 | 3.10E+12 | i10**→**i15 | 2.52E+06 |
| i23→p5 | 5.62E+09 | i11**→**p3 | 1.63E+08 | i29**→**i19 | 7.55E+05 | i6**→**i28 | 1.62E+00 |
| i5→i6 | 3.88E+12 | i6**→**i17 | 1.52E+02 | i20**→**i21 | 2.21E+12 | i28**→**i6 | 3.42E+05 |
| i6→i5 | 7.67E+06 | i17**→**i6 | 9.44E+06 | i21**→**i20 | 1.49E+06 | i27**→**p3 | 2.11E+08 |
| i5→i19 | 3.93E+03 | i6**→**i7 | 8.02E+04 | i15**→**p5 | 7.68E+09 | i6**→**p7 | 4.39E+01 |
| i19→i5 | 7.81E+02 | i7**→**i6 | 1.57E+08 | i15**→**i12 | 1.82E+08 |  |  |
| i15→i10 | 8.66E+09 | i6**→**i18 | 9.58E-01 | i12**→**i15 | 3.33E+07 |  |  |

aConformational isomers separated by low rotational barriers (e.g., i8, i9, i15, i16 or i12-i14) were considered as a single species in the kinetic scheme. Rate constants are given only for the most stable species in each group of conformational isomers.

**Table S3.** Ratios of the rate constants for the CH + benzene and CH + ethylene addition reactions in units of cm3s-1.

|  |  |
| --- | --- |
| T, K | *k*CH+C6H6/*k*CH+C2H4 |
| 250 | 1.5 |
| 300 | 1.5 |
| 400 | 1.5 |
| 500 | 1.4 |
| 600 | 1.4 |
| 700 | 1.4 |
| 800 | 1.5 |
| 900 | 1.5 |
| 1000 | 1.5 |
| 1125 | 1.5 |
| 1250 | 1.6 |
| 1375 | 1.6 |
| 1500 | 1.6 |
| 1650 | 1.6 |
| 1750 | 1.7 |
| 1800 | 1.7 |
| 2000 | 1.7 |
| 2250 | 1.8 |
| 2500 | 1.8 |

**Table S4.** Symmetry point groups, electronic terms, optimized Cartesian coordinates (Å) and calculated vibrational frequencies of all intermediates, transition states, and products involved in the reaction of methylidyne with styrene

i1, C1, 2A

C -0.742623 -1.282549 -0.100424

C -2.106582 -1.042437 0.042710

C -2.583457 0.264402 0.120449

C -1.684557 1.326789 0.046694

C -0.321605 1.085488 -0.102487

C 0.169924 -0.223612 -0.170841

C 1.632379 -0.511433 -0.300005

C 2.641742 0.539513 -0.505047

C 2.606739 -0.067000 0.823894

H -0.378786 -2.303615 -0.157339

H -2.797364 -1.877062 0.092851

H -3.645290 0.453236 0.230902

H -2.046701 2.348033 0.095182

H 0.371726 1.916196 -0.180470

H 1.844247 -1.481371 -0.748494

H 3.425788 0.664275 -1.238264

H 3.403100 -0.740922 1.133717

H 2.151511 0.486262 1.642256

Frequencies

47.6946 137.2529 193.5017

307.8007 398.6896 415.4054

506.4543 556.2008 600.8977

635.2639 713.8451 726.9937

770.6959 794.5901 852.0775

856.2228 923.7013 961.7166

977.5619 998.5750 1016.6098

1020.9945 1041.2253 1050.8660

1070.8446 1099.3268 1119.7285

1180.9178 1201.0094 1204.2035

1240.3242 1320.9144 1350.2619

1386.7896 1460.4319 1486.7422

1526.9149 1622.6116 1645.7687

3073.2799 3089.2148 3147.2821

3153.7090 3158.9174 3168.6561

3175.8052 3187.6496 3205.9280

i2, Cs, 2A”

C 0.000000 0.228201 0.000000

C 1.364179 0.675698 0.000000

C 2.521925 -0.122163 0.000000

C 3.796303 0.370802 0.000000

C -0.378021 -1.136886 0.000000

C -1.713263 -1.508360 0.000000

C -2.722160 -0.541299 0.000000

C -2.374358 0.810802 0.000000

C -1.040486 1.188609 0.000000

H 1.512749 1.752943 0.000000

H 2.402624 -1.202397 0.000000

H 3.987060 1.438736 0.000000

H 4.656882 -0.285855 0.000000

H 0.382838 -1.907793 0.000000

H -1.975304 -2.560775 0.000000

H -3.764325 -0.838898 0.000000

H -3.148635 1.570026 0.000000

H -0.778603 2.241589 0.000000

Frequencies

88.2102 132.3649 160.3369

253.6861 361.0344 411.3551

414.2707 496.6916 599.8276

624.6733 631.5236 693.5432

757.0302 815.8570 835.3652

837.7216 852.2259 910.7364

972.8926 991.8464 991.8724

1000.8557 1008.3792 1046.2625

1101.1044 1178.4950 1188.4212

1210.6510 1223.0281 1303.9915

1320.3306 1353.7162 1376.0074

1463.5203 1503.7738 1512.1768

1543.3089 1595.8620 1621.6211

3132.1373 3138.5744 3146.1172

3157.5363 3164.0319 3174.4635

3185.7774 3192.5423 3230.8464

i3, C1, 2A

C 0.084008 -0.424663 -0.108249

C 1.407133 -0.990699 -0.202411

C 2.673557 -0.380131 -0.086758

C 3.004882 0.873573 0.350971

C -0.207384 0.953004 -0.241344

C -1.510710 1.420961 -0.143867

C -2.568460 0.539812 0.084738

C -2.308416 -0.827558 0.195081

C -1.009608 -1.300843 0.091399

H 1.425718 -2.063449 -0.373899

H 3.507035 -1.030007 -0.346900

H 2.275999 1.579750 0.724441

H 4.043089 1.179752 0.387283

H 0.588551 1.648602 -0.467909

H -1.706720 2.481445 -0.258822

H -3.583542 0.911965 0.162061

H -3.123626 -1.523660 0.358904

H -0.816516 -2.365135 0.177485

Frequencies

65.9727 153.8885 171.5765

299.8828 329.9812 414.2822

466.7236 499.0402 564.5288

630.0122 669.6270 702.3182

743.0667 800.2606 818.1583

842.6023 851.7125 923.9193

979.5059 989.8883 998.2649

1004.8503 1023.5293 1048.1165

1110.8392 1122.6783 1180.4249

1198.3202 1237.0110 1280.8454

1330.4955 1354.1487 1437.7498

1452.0907 1492.4295 1509.9355

1557.2567 1598.2974 1623.3093

3118.8266 3145.7879 3153.6718

3158.2719 3165.5997 3175.4109

3188.8656 3211.0166 3242.5604

i4, C1, 2A

C -0.221274 0.773878 0.162370

C -0.257869 -0.719291 0.422095

C 0.979164 1.446414 0.034003

C -1.573963 1.213829 -0.019314

C -2.403517 0.150863 -0.165203

C -1.640657 -1.153929 -0.138996

C 2.171043 0.718494 -0.069110

C 2.145530 -0.708451 -0.161660

C 0.995785 -1.418570 -0.005863

H -0.335506 -0.836631 1.522678

H 0.993137 2.526878 -0.072299

H -1.873111 2.253253 -0.085144

H -3.467778 0.210844 -0.356469

H -2.122291 -1.929386 0.463279

H -1.538357 -1.555783 -1.157482

H 3.114058 1.239599 -0.184184

H 3.071185 -1.227723 -0.388658

H 0.993205 -2.500468 -0.091647

Frequencies

142.2486 178.7080 341.2263

387.8264 435.3621 519.8354

528.4751 549.3591 664.3001

684.7114 721.7810 742.7521

777.4602 822.5822 854.4357

909.5363 948.1629 954.5197

966.4507 979.7169 992.8130

1045.6306 1073.9003 1101.1111

1123.9964 1150.0280 1176.7916

1229.2185 1245.2876 1274.5337

1308.1408 1313.1844 1369.0630

1384.0098 1428.4683 1479.7915

1528.2201 1555.6346 1599.4764

2847.3935 2985.0148 3059.8662

3149.7435 3154.2102 3168.6070

3180.0855 3186.9960 3201.9210

i5, C1, 2A

C 0.740830 1.601378 -0.795257

C -0.100950 0.950787 0.207497

C -0.653083 -0.411434 -0.014201

C 0.180886 -1.464941 -0.228906

C 1.612834 -1.376087 -0.085411

C 2.222680 -0.223611 0.257983

C 1.493613 1.053054 0.339615

H 0.712078 2.608603 -1.185923

H -0.699707 1.593887 0.850434

H 2.192518 -2.289635 -0.160547

H 3.273950 -0.213777 0.526723

H 1.896327 1.778595 1.045230

C -2.096422 -0.610331 0.026545

C -3.037024 0.337917 0.132463

H -2.415890 -1.648083 -0.043391

H -2.798485 1.394056 0.178159

H -4.087883 0.077288 0.167328

H -0.253088 -2.441331 -0.419977

Frequencies

97.2842 173.9256 221.7359

251.2532 290.8153 441.0430

477.5241 510.2051 534.7983

589.4992 634.7512 649.5368

714.5909 749.7852 783.5541

830.2742 902.7489 916.8334

930.1518 972.9969 1020.0241

1023.1115 1028.5606 1035.6183

1055.7282 1077.8342 1090.5112

1194.4705 1215.6390 1220.0341

1311.4781 1336.4943 1381.0604

1406.1989 1439.4300 1456.1344

1587.7186 1655.0504 1683.1239

3088.9469 3096.1965 3128.6716

3145.7229 3152.6141 3160.5566

3179.1468 3204.7318 3225.1368

i6, Cs, 2A”

C 2.190346 0.922830 -0.000223

C 2.400631 -0.421304 -0.000165

C 1.433134 -1.474656 0.000278

C 0.052921 -1.378451 0.000170

C -0.808702 -0.260788 -0.000132

C -0.340701 1.113816 0.000125

C 0.919612 1.616146 0.000178

H 3.068804 1.560153 -0.000607

H 3.437481 -0.747131 -0.000469

H 1.837949 -2.481039 0.000615

H -0.463861 -2.336053 0.000314

H -1.128182 1.859520 0.000251

H 0.995472 2.699760 0.000399

C -2.230419 -0.528916 -0.000296

C -3.258579 0.347531 0.000057

H -2.488499 -1.585977 -0.000856

H -3.127740 1.422817 0.000566

H -4.280879 -0.009297 -0.000159

Frequencies

51.4833 152.5967 238.6018

284.5516 290.0693 369.4185

458.9630 498.6090 503.9279

572.7295 638.8099 680.2752

747.4883 783.0442 847.3182

851.4249 855.7672 900.9204

912.0112 953.3587 965.7795

994.7652 1001.2328 1001.8290

1023.0526 1057.4244 1207.6693

1243.6789 1272.4765 1305.5715

1324.4841 1395.4724 1441.9023

1465.0896 1494.0504 1521.4272

1601.5330 1619.8088 1657.5545

3120.2675 3129.4726 3135.1080

3142.6421 3146.8902 3162.5003

3170.1077 3175.8687 3226.4960

i7, C1, 2A

C -0.413253 1.334546 -0.203323

C -0.739790 0.001097 0.189292

C 1.327656 -1.437983 -0.425411

C 2.279063 -0.508211 -0.537666

C 1.652579 0.427463 0.503359

C 0.909268 1.617948 -0.030390

C 0.532775 -0.676799 0.640715

H -1.133549 2.034223 -0.611211

H 1.136788 -2.381674 -0.923697

H 3.159999 -0.405853 -1.161049

H 2.265644 0.634580 1.386790

H 1.380122 2.562700 -0.272949

H 0.446884 -1.178159 1.610258

C -2.005640 -0.633025 0.166255

C -3.187266 -0.098987 -0.253626

H -2.024005 -1.659222 0.529500

H -3.261981 0.913775 -0.632654

H -4.102256 -0.676669 -0.220230

Frequencies

94.3179 173.8781 204.5372

264.0474 289.5929 407.2640

484.3484 528.8312 622.6632

664.4312 730.6702 739.0985

772.0469 837.4520 859.1258

867.7771 894.2223 910.6896

949.6248 954.4331 980.8827

990.8124 1014.0641 1042.6313

1077.4401 1095.1094 1171.4441

1189.3646 1200.3247 1246.3045

1267.2545 1283.1272 1283.2996

1315.4221 1416.8908 1456.4905

1509.4622 1563.4234 1626.7899

3029.4840 3038.8825 3120.9043

3142.6719 3164.9976 3175.5589

3197.0905 3199.1709 3229.8057

i8, C1, 2A

C -0.680312 1.459154 -0.294014

C -0.689463 0.189828 0.184615

C 1.281025 -1.426733 0.049065

C 2.361168 -1.521402 -0.681215

C 1.501355 1.102638 0.315641

C 0.667052 2.014216 -0.217711

C 0.726611 -0.145606 0.646237

H -1.544951 2.003956 -0.651879

H 0.702040 -2.332268 0.262725

H 2.915522 -2.295142 -1.190790

H 2.561404 1.209854 0.495753

H 0.934561 3.012524 -0.539902

H 0.697715 -0.270993 1.742053

C -1.802211 -0.738500 0.321750

C -2.977189 -0.675970 -0.316755

H -1.643533 -1.565067 1.012203

H -3.196180 0.098500 -1.043916

H -3.754790 -1.407115 -0.131927

Frequencies

58.8545 92.2077 130.4916

176.5068 237.7226 258.4535

397.2783 470.9837 523.3803

579.1913 617.3309 652.2842

702.0405 719.7626 811.2875

813.5329 854.3674 885.7376

898.3551 923.8517 959.3724

964.4933 1021.9134 1023.8467

1061.0927 1070.4894 1120.8960

1155.4100 1223.9766 1233.2349

1272.6070 1296.7576 1338.8857

1385.0751 1458.4628 1554.7853

1640.3031 1671.5754 1674.1594

2961.8955 3022.7927 3120.4872

3138.5468 3189.4750 3202.1216

3222.4487 3227.3659 3240.1241

i9, C1, 2A

C 0.355663 -1.496314 -0.462984

C 0.516796 -0.271118 0.097680

C -1.742797 -0.980740 0.304009

C -1.031538 -1.928591 -0.333973

C -0.829505 0.174632 0.647714

H 1.130991 -2.076679 -0.946660

H -2.798167 -0.999457 0.538590

H -1.414610 -2.871444 -0.703458

H -0.752765 0.247618 1.745101

C -1.368429 1.500757 0.136658

C -0.844364 2.251860 -0.795615

H -2.305278 1.819456 0.609739

H -1.068106 3.184025 -1.291624

C 1.725852 0.528529 0.238846

C 2.984857 0.100801 0.084538

H 1.565674 1.570847 0.502887

H 3.220251 -0.931764 -0.150669

H 3.822800 0.778499 0.194855

Frequencies

42.7563 90.7952 150.8381

171.5675 228.3273 270.4205

394.3904 445.3925 531.6769

581.9556 622.6456 666.1357

690.5152 714.9116 813.2826

820.6025 835.6161 883.5632

895.6690 922.4118 955.8069

991.7071 1026.2538 1030.6188

1034.5476 1071.5206 1122.6382

1158.8873 1223.6255 1226.3689

1278.9797 1305.1755 1334.6375

1383.7327 1459.9468 1551.6890

1638.6791 1672.3762 1674.5618

2969.8932 3011.4926 3134.5244

3141.0836 3188.3150 3201.9373

3219.9919 3220.3589 3244.3451

i10, C1, 2A

C 1.604010 1.199072 -0.127356

C 0.275348 0.773410 0.149129

C 1.743196 -1.088134 0.050499

C 2.447949 0.060971 -0.205559

C 0.331073 -0.723235 0.437244

C -0.914283 1.418340 0.035538

H 1.901269 2.217897 -0.337719

H 2.143923 -2.092376 0.085798

H 3.503219 0.100460 -0.446590

H 0.272824 -0.843802 1.535746

H -0.952541 2.480813 -0.182694

C -0.857781 -1.445801 -0.147497

C -2.023689 -0.814686 -0.278542

H -0.755264 -2.493931 -0.410853

H -2.893327 -1.346045 -0.653363

C -2.207633 0.645506 0.077019

H -2.932039 1.104375 -0.606019

H -2.677211 0.719956 1.072851

Frequencies

124.8844 189.9551 293.5250

367.5303 423.0340 511.6404

526.4483 558.6077 635.2706

669.9005 702.7491 722.1893

786.8170 820.5264 826.3590

846.8929 887.4060 943.2388

947.9753 986.9031 1015.7347

1029.2577 1056.5003 1083.3215

1110.1990 1160.5878 1190.1990

1205.9608 1231.4851 1254.7418

1317.4202 1327.3323 1346.0591

1396.7280 1401.4083 1463.7684

1491.5023 1572.9738 1700.4807

2906.6201 2940.7823 3025.3655

3144.3762 3157.9242 3167.3335

3185.6811 3204.1354 3214.8448

i11, Cs, 2A”

C 1.631619 -1.210623 -0.000099

C 0.243734 -0.729901 0.000228

C 1.732078 1.146435 0.000010

C 2.479208 -0.169526 -0.000193

C 0.292704 0.702201 0.000171

C -0.935019 -1.414346 0.000097

C -2.246548 -0.677758 -0.000101

C -0.900084 1.452493 0.000036

C -2.112350 0.821210 -0.000133

H 1.911626 -2.256775 -0.000040

H 1.986560 1.757880 0.877600

H 1.986310 1.758445 -0.877201

H 3.559871 -0.233956 -0.000326

H -0.955099 -2.499335 0.000217

H -2.856724 -0.993855 0.865428

H -2.856669 -0.994044 -0.865586

H -0.859570 2.538126 0.000126

H -3.028359 1.402404 -0.000304

Frequencies

135.7396 181.8974 255.2457

374.6210 381.3302 444.6771

516.5166 573.1812 638.9420

700.3464 717.4150 718.5405

786.3179 809.5190 845.7382

888.8574 928.1722 931.4682

949.3404 961.8811 966.2502

1009.6782 1104.2157 1139.8725

1151.0914 1169.2765 1181.2578

1216.8807 1231.1640 1307.0277

1317.3701 1366.8587 1384.4412

1440.7123 1448.2552 1455.7179

1526.1698 1615.5418 1628.9888

2899.3763 2916.4008 2986.3855

2999.6868 3144.9011 3160.4961

3169.3201 3185.6396 3208.7187

i12, Cs, 2A’

C -1.066484 1.391619 -0.000044

C -0.652735 -0.021423 -0.000127

C 1.565589 -1.244113 -0.000084

C 2.886429 -1.259566 0.000089

C 1.257578 1.341228 0.000082

C 0.015716 2.186531 -0.000025

C 0.719722 -0.068028 -0.000072

C -1.560534 -1.156946 -0.000047

C -2.897966 -1.094570 0.000137

H -2.095429 1.725358 -0.000123

H 1.054903 -2.213232 -0.000359

H 3.669823 -2.001833 0.000259

H 1.890117 1.531690 -0.876185

H 0.020779 3.268093 0.000043

H -1.098366 -2.140205 -0.000121

H -3.436603 -0.153939 0.000216

H -3.498915 -1.995872 0.000192

H 1.889799 1.531544 0.876632

Frequencies

81.4359 128.4090 172.6238

176.1082 245.6951 274.6876

383.6371 401.0890 530.9263

558.7586 577.5488 629.5119

673.9270 693.4576 773.9906

825.0133 836.9041 878.3213

923.9659 925.4428 946.8123

964.2779 994.2130 1015.5984

1035.2884 1133.8093 1135.5987

1223.2578 1255.7523 1268.7284

1329.7982 1345.6668 1411.9911

1421.6176 1451.9015 1552.7890

1613.4239 1634.8240 1679.0686

3020.1505 3029.7955 3042.4225

3140.1582 3147.6807 3197.6675

3219.9888 3225.8560 3246.1326

i13, Cs, 2A’

C 0.730287 -1.610285 -0.000050

C 0.495033 -0.158606 0.000067

C -1.565103 -1.278190 -0.000028

C -0.440414 -2.269802 -0.000090

C -0.860412 0.058429 0.000082

C 1.531693 0.859583 0.000225

C 2.851779 0.634908 -0.000055

C -1.616400 1.301079 0.000228

C -1.187706 2.549643 -0.000397

H 1.711139 -2.066686 -0.000067

H -2.215738 -1.393189 -0.878009

H -2.215818 -1.393306 0.877872

H -0.577719 -3.342467 -0.000211

H 1.177350 1.887077 0.000585

H 3.272424 -0.364446 -0.000494

H 3.557944 1.456516 0.000100

H -2.706289 1.164377 0.000876

H -1.635841 3.531572 -0.000548

Frequencies

42.5425 99.6935 167.9563

207.8561 237.8321 262.2404

384.8877 411.9517 498.4957

531.0339 611.6086 613.8358

670.8371 689.7244 783.2123

817.3917 843.7182 871.5404

924.9261 929.0503 947.3389

973.6980 1032.4700 1032.5825

1041.3680 1130.8614 1138.0268

1168.4582 1254.4771 1283.4901

1325.8943 1335.3089 1406.3517

1421.0267 1452.3659 1548.9695

1621.7561 1631.2554 1678.9977

2994.6551 3004.2128 3025.6951

3133.1342 3141.8533 3198.2466

3220.3257 3224.2339 3243.2230

i14, C1, 2A

C 1.558640 -1.215035 0.003889

C 0.179919 -0.700470 -0.031469

C 1.693706 1.090147 0.049951

C 2.442935 -0.205764 0.058739

C 0.238602 0.675124 -0.008882

C -0.939837 -1.626151 -0.139005

C -2.232000 -1.420211 0.145708

C -0.785741 1.697509 -0.099667

C -2.098760 1.612963 0.026742

H 1.794326 -2.272558 -0.005833

H 1.903635 1.693786 0.943917

H 1.964918 1.717576 -0.810383

H 3.520074 -0.286650 0.106033

H -0.655421 -2.619815 -0.481906

H -2.597146 -0.477169 0.535834

H -2.959463 -2.211647 0.002535

H -0.389895 2.702232 -0.300671

H -2.925813 2.305568 -0.025571

Frequencies

63.7898 108.4879 191.2701

220.6110 241.2755 255.4672

390.8323 422.4628 475.0956

543.3574 618.0506 638.2532

655.9393 686.3552 774.1338

829.7137 845.2382 874.4971

922.8129 931.1622 952.2641

977.8003 1005.1359 1023.8188

1102.1434 1132.1404 1139.3350

1167.6387 1207.9564 1288.7947

1326.8428 1345.3288 1375.7184

1419.0257 1460.3056 1542.5845

1613.7731 1637.5916 1678.2649

2994.4374 3004.5015 3026.1779

3113.8867 3118.5056 3184.8542

3208.6112 3218.5755 3234.9562

i15, C1, 2A

C -0.046355 -1.766748 -0.441108

C 0.602330 -0.630022 -0.078207

C -0.537984 1.643538 -0.094737

C -1.642722 2.146311 -0.580481

C -1.678844 -0.520565 0.569062

C -1.446090 -1.699197 -0.037348

C -0.408316 0.292968 0.595226

C 2.013661 -0.363468 -0.259166

C 2.717946 0.644401 0.276164

H 0.411042 -2.613345 -0.939051

H 0.394318 2.210805 -0.185816

H -1.948582 3.046542 -1.092385

H -2.618931 -0.161409 0.962872

H -2.172065 -2.483489 -0.208786

H -0.095533 0.468384 1.635971

H 2.538661 -1.081515 -0.886224

H 2.271384 1.379635 0.936166

H 3.777956 0.751092 0.080825

Frequencies

85.5759 123.0166 152.2086

178.2875 242.6713 266.5519

419.7453 479.1113 529.2971

571.9645 632.0679 638.4054

698.2667 724.9033 812.1769

813.8146 854.7016 893.1626

896.3831 912.9690 958.1796

960.7412 1019.0571 1024.9568

1037.2742 1060.2689 1123.7469

1192.1547 1216.1684 1243.6381

1280.4522 1316.1530 1335.6743

1388.3759 1449.4465 1553.5776

1628.2800 1666.8585 1677.8437

2987.1798 3033.5097 3126.7714

3141.2423 3186.5219 3200.6891

3222.7023 3226.3900 3238.4813

i16, C1, 2A

C 1.046563 -1.405178 0.490276

C -0.064749 -0.777406 0.025755

C 1.875593 0.500222 -0.466958

C 2.235953 -0.615936 0.191881

C 0.369378 0.520853 -0.636453

C -1.414776 -1.296781 0.095330

C -2.512265 -0.758684 -0.453663

H 1.054770 -2.361860 0.998374

H 2.522917 1.294778 -0.812157

H 3.245014 -0.899128 0.462843

H 0.125548 0.479920 -1.708762

H -1.515564 -2.229201 0.647407

H -2.482199 0.167492 -1.014921

H -3.479197 -1.235957 -0.348885

C -0.213368 1.806933 -0.069174

C -1.002510 1.919499 0.966161

H 0.106410 2.714463 -0.595241

H -1.496612 2.708351 1.512410

Frequencies

85.5532 133.7005 144.9847

190.5543 221.2816 294.9787

409.0085 467.0593 539.7088

568.6814 618.5080 649.2982

696.0589 719.9609 812.3192

817.5174 835.1834 885.9368

891.8974 919.0832 954.5791

980.9794 1022.2713 1026.1748

1034.1389 1050.7711 1125.3409

1196.4702 1222.6754 1236.1489

1274.6608 1324.0507 1339.6562

1393.4228 1449.4245 1553.1684

1628.7966 1670.6434 1680.0658

2989.6439 3013.6192 3126.2054

3146.1270 3186.9325 3198.5800

3219.9476 3228.1315 3244.4749

i17, C1, 2A

C 2.101506 0.791588 -0.161674

C 1.133109 1.617301 0.257872

C -0.267638 1.233681 0.227817

C 2.123765 -0.522641 -0.681301

C -0.721814 -0.040335 0.368654

C 1.212553 -1.442363 -0.278538

C 0.239365 -1.129986 0.827328

H 1.373719 2.638975 0.545234

H -0.990280 2.032247 0.083056

H 2.841769 -0.769768 -1.458180

H 1.160014 -2.405435 -0.778707

H 0.794826 -0.770492 1.703173

H -0.314128 -2.024167 1.119368

C -2.126568 -0.406842 0.155491

C -2.977858 0.182284 -0.690967

H -2.485691 -1.250084 0.743803

H -2.666134 0.985864 -1.349293

H -4.012609 -0.133260 -0.756540

Frequencies

86.9546 150.0887 198.8548

280.8131 310.0656 367.4669

374.9527 469.2657 507.2635

583.3718 628.6109 699.9634

737.7520 785.8170 797.0752

874.2421 899.4100 932.7856

939.7321 951.4179 966.2364

1001.6590 1023.4530 1055.4341

1099.3841 1162.0897 1201.1807

1273.4573 1310.1152 1314.0076

1330.3351 1345.4950 1406.7737

1451.7077 1476.4220 1547.5793

1590.0839 1652.2181 1675.6418

2998.3241 3086.8169 3116.0921

3117.7537 3137.2803 3139.4746

3146.5752 3159.1538 3220.8477

i18, C1, 2A

C 2.051564 0.886081 -0.358899

C 1.015128 1.613363 0.411117

C -0.321244 1.107170 -0.071121

C 2.314123 -0.413366 -0.450217

C -0.731859 -0.181262 0.048651

C 1.466996 -1.411019 0.183756

C 0.137129 -1.288777 0.430724

H 1.091684 2.694583 0.274515

H -0.981753 1.819959 -0.554439

H 3.190455 -0.763132 -0.990754

H 1.935602 -2.364707 0.414324

H -0.367374 -2.163223 0.833031

H 1.158941 1.408040 1.482762

C -2.130905 -0.549944 -0.272380

C -3.205403 0.212015 -0.059720

H -2.272510 -1.540696 -0.699096

H -3.131780 1.186155 0.412037

H -4.196434 -0.122538 -0.343846

Frequencies

85.4430 145.7514 205.2669

237.2431 296.8887 358.2518

412.5241 422.6600 487.6786

586.5416 635.4137 704.7047

711.4697 776.6582 847.6993

853.6622 896.1892 921.1076

945.6448 959.2080 990.5014

1015.9148 1023.8802 1027.8566

1108.7369 1156.6267 1217.4805

1242.1782 1290.5693 1300.0820

1322.6296 1352.6691 1441.5239

1455.5822 1460.4817 1555.4270

1634.4198 1675.7437 1686.5252

2967.7354 3068.5332 3123.9521

3126.3597 3134.3920 3136.6295

3151.5461 3159.8717 3218.5721

i19, C1, 2A

C -0.622093 -0.487914 -0.035221

C -0.049395 0.827746 -0.439702

C 1.395821 0.945078 -0.277974

C 2.238990 -0.098859 -0.010480

C 1.676258 -1.393984 0.004219

C 0.272571 -1.545632 0.072622

C 0.623500 1.980790 0.407926

H -0.505802 1.256942 -1.333979

H 3.272331 0.055769 0.286783

H 2.309482 -2.266272 0.118719

H -0.126805 -2.540161 0.251086

H 0.597023 1.958388 1.493436

H 0.489311 2.966519 -0.028917

C -2.044893 -0.689396 0.078410

C -2.977744 0.280822 0.028739

H -2.370667 -1.718822 0.214905

H -2.710592 1.324593 -0.091144

H -4.032368 0.051133 0.117872

Frequencies

101.3961 171.9856 182.6789

236.6522 329.2190 436.8205

462.4846 501.3673 545.6056

557.4625 651.2836 720.1409

746.5867 747.2964 841.0169

858.5870 885.4087 899.3608

937.9372 961.1945 998.4937

1011.1529 1017.4300 1043.2070

1053.9384 1073.7380 1107.7758

1131.4056 1223.0478 1284.2676

1299.5218 1338.8806 1385.8459

1398.0075 1449.4213 1464.8275

1514.0065 1621.8245 1626.1605

3048.2847 3089.2242 3125.8470

3143.9430 3144.1023 3149.3076

3173.3180 3181.3744 3228.2317

i20, C1, 2A

C -0.655883 -0.450398 -0.049559

C -0.072117 0.846054 -0.296910

C 1.408131 1.018701 -0.418623

C 2.215997 -0.184408 -0.188459

C 1.624101 -1.368534 0.099806

C 0.191400 -1.513341 0.144179

C 0.558445 1.750123 0.669284

C -2.104368 -0.615312 0.039454

C -3.003544 0.349906 -0.183255

H 1.798937 1.719028 -1.154364

H 3.290595 -0.128868 -0.331947

H 2.234124 -2.251093 0.260175

H -0.225117 -2.494911 0.348987

H 0.631311 1.433508 1.706407

H 0.508980 2.824664 0.522040

H -2.448102 -1.609588 0.315672

H -2.697707 1.346897 -0.480063

H -4.066003 0.163622 -0.082403

Frequencies

89.9216 161.8021 188.9741

232.6004 304.6504 431.6955

500.0589 518.5262 551.0091

585.3343 684.8051 726.2297

737.3745 793.4678 837.9962

870.6333 903.7410 906.9161

940.0838 979.6131 1005.5359

1017.8067 1023.0802 1034.9747

1054.2490 1078.4839 1101.7951

1195.4430 1216.1176 1272.3826

1325.4036 1362.3527 1407.2892

1427.5203 1451.7938 1464.7051

1534.4499 1629.6925 1674.0896

3088.1473 3093.5077 3132.2374

3142.5317 3149.2421 3156.5813

3171.2980 3177.1284 3226.9848

i21, C1, 2A

C -0.837551 1.998786 -0.235907

C 0.027197 0.911793 -0.061931

C 1.422998 1.170647 0.112183

C 2.358052 0.160213 0.159780

C 1.948548 -1.174465 0.028855

C 0.595294 -1.464544 -0.113693

C -0.389717 -0.470515 -0.119744

H -0.448567 3.008122 -0.180271

H -1.874931 1.876451 -0.505693

H 1.741240 2.205512 0.180247

H 3.408613 0.398101 0.283756

H 2.677081 -1.976499 0.046744

H 0.281759 -2.500579 -0.192941

C -1.785744 -0.923348 -0.168381

C -2.871594 -0.352195 0.366665

H -1.918772 -1.889637 -0.652023

H -2.831646 0.572991 0.927234

H -3.839680 -0.832693 0.285978

Frequencies

109.0051 142.6242 239.5334

252.0700 369.2925 404.8906

442.5035 494.1834 546.8392

573.3855 591.8187 651.3316

725.3440 741.5943 771.9326

782.4281 866.2559 867.8284

942.4273 950.8193 974.8261

979.5790 1024.9278 1042.4756

1058.7710 1155.7772 1175.7250

1204.0449 1283.4624 1290.7081

1325.6074 1350.9360 1434.8277

1467.6268 1480.3577 1499.9663

1553.3889 1604.2476 1669.4396

3117.7611 3146.1002 3156.4061

3158.0932 3162.9981 3176.2797

3190.5128 3229.2508 3265.8079

i22, Cs, 2A”

C -1.630758 -1.172275 -0.000074

C -0.197038 -0.686879 0.000030

C 0.976863 -1.414824 0.000021

C 2.206761 -0.738963 0.000029

C 2.247027 0.662241 -0.000006

C 1.079184 1.409736 -0.000027

C -0.167723 0.739620 0.000000

C -1.477963 1.247366 -0.000021

C -2.485461 0.131483 0.000069

H -1.840747 -1.791805 -0.877444

H -1.840842 -1.792087 0.877060

H 0.955542 -2.500140 0.000008

H 3.132143 -1.303441 0.000050

H 3.207213 1.166802 -0.000031

H 1.116639 2.493605 -0.000055

H -1.741213 2.297341 0.000041

H -3.147115 0.182375 -0.874260

H -3.146969 0.182322 0.874508

Frequencies

75.4178 203.1202 240.7820

384.0078 423.4604 517.5620

536.4530 591.7876 611.5956

703.4146 711.5800 757.6784

807.2824 809.5040 860.0946

874.4669 921.6076 931.5445

975.8140 1002.2483 1017.5266

1033.7419 1113.7834 1148.8234

1164.7273 1180.7776 1202.8200

1230.8333 1247.6775 1299.9660

1313.3794 1345.5606 1401.4409

1457.6411 1474.3535 1490.3874

1499.3414 1585.8266 1604.8096

2993.8865 3004.8834 3032.3982

3059.4913 3155.0063 3161.3360

3174.7679 3186.5282 3197.1812

i23, C1, 2A

C -0.664951 1.257788 -0.258833

C -0.949180 -0.126634 0.176841

C 2.758902 -1.248539 -0.691979

C 2.567612 -0.085791 -0.126520

C 1.308053 0.353434 0.600080

C 0.625218 1.546913 -0.034674

C 0.197080 -0.659337 0.661838

C -2.235153 -0.806934 0.097276

C -3.374667 -0.284362 -0.367086

H -1.396152 1.927178 -0.692479

H 3.539179 -1.753795 -1.240860

H 3.366193 0.664968 -0.160714

H 1.602362 0.630476 1.627154

H 1.130676 2.478085 -0.253089

H 0.324727 -1.660233 1.051019

H -2.238424 -1.833772 0.455575

H -3.437066 0.732817 -0.737314

H -4.288980 -0.864952 -0.390955

Frequencies

67.4201 109.8635 136.3473

194.2630 254.9237 262.6813

418.4090 457.8140 542.0954

583.4195 619.6941 640.5419

698.8999 725.6594 788.6389

818.6007 833.3342 885.5936

907.6079 918.5702 929.5215

948.4659 1012.7518 1027.8435

1034.5435 1057.9445 1109.1720

1188.2065 1211.7540 1242.0105

1290.2389 1300.7769 1326.4000

1399.8873 1450.4406 1577.1954

1638.3601 1671.7123 1696.8670

2954.7677 3014.9373 3134.4728

3143.5330 3194.3147 3212.2659

3217.7342 3223.4457 3241.4426

i24, C1, 2A

C 1.225368 1.351716 -0.030838

C 0.717863 -0.009377 0.012219

C -1.642371 -1.082529 0.113577

C -2.958925 -1.078099 -0.127247

C -1.069439 1.400255 0.052843

C 0.156173 2.193812 -0.007844

C -0.744561 0.064292 0.059170

C 1.485241 -1.201759 -0.002068

C 2.843765 -1.268703 -0.041711

H 2.266509 1.633033 -0.074736

H -1.186626 -2.032654 0.381681

H -3.546580 -1.983432 -0.036415

H -2.067274 1.813025 0.109150

H 0.189575 3.274720 -0.024674

H 0.937573 -2.139519 0.017271

H 3.462440 -0.379766 -0.065425

H 3.355281 -2.223164 -0.051169

H -3.489582 -0.179879 -0.424292

Frequencies

43.1105 122.0582 155.0675

180.3276 252.7167 268.9805

369.1760 502.9186 522.5565

537.8936 600.3421 602.9440

665.6495 697.5414 742.4155

769.8145 840.0105 894.3956

910.4476 911.3871 979.9006

994.4270 1015.6869 1025.9137

1043.5640 1075.1768 1103.5491

1180.0427 1257.0069 1285.9555

1318.6918 1342.0995 1400.4388

1453.9084 1461.3463 1507.1575

1541.0192 1581.1249 1673.7077

3130.2255 3138.6792 3147.2241

3155.3609 3204.0224 3217.2568

3221.3100 3234.0817 3239.2813

i25, C1, 2A

C 1.391208 1.168435 0.127151

C 0.575225 -0.016022 -0.005439

C -0.810391 1.798455 -0.060760

C 0.567095 2.256712 0.082891

C -0.831331 0.427633 -0.089276

C 1.042989 -1.347198 -0.166366

C 2.333825 -1.753494 -0.026604

C -2.045408 -0.372554 -0.155739

C -2.242732 -1.630066 0.263112

H 2.468904 1.182722 0.188269

H -1.678187 2.442828 -0.107483

H 0.872044 3.293257 0.133514

H 0.303656 -2.093465 -0.436316

H 3.126600 -1.069909 0.253042

H 2.611500 -2.788590 -0.182750

H -2.901880 0.157622 -0.568895

H -3.214495 -2.098447 0.162020

H -1.471014 -2.217417 0.744782

Frequencies

97.8803 116.5959 178.0653

191.1269 257.6170 279.3147

375.9526 510.3227 534.4870

540.6155 603.5827 643.9099

683.4972 709.4325 727.8859

768.3694 840.9058 897.1079

908.0367 916.7737 979.1980

1013.6838 1016.8698 1026.8054

1036.2256 1083.6686 1088.7721

1227.2788 1272.1106 1294.1207

1317.4310 1332.7539 1412.2839

1445.3989 1456.3752 1489.4765

1545.7149 1576.1487 1676.3661

3119.9757 3146.0172 3147.0136

3171.0804 3200.7021 3213.1836

3227.7123 3232.2546 3237.7014

i26, C1, 2A

C 1.613144 -1.122840 -0.262239

C 0.282924 -0.740672 -0.139296

C 1.615691 1.120489 0.262367

C 2.436396 -0.001474 -0.000107

C 0.284203 0.740190 0.139515

C -0.797240 -1.690609 -0.115629

C -2.012313 -1.561963 0.454649

C -0.793980 1.691867 0.115582

C -2.009438 1.564641 -0.454666

H 1.956371 -2.132788 -0.437913

H 1.960221 2.129963 0.438169

H 3.518456 -0.002522 -0.000571

H -0.547432 -2.656216 -0.552125

H -2.317218 -0.663292 0.973419

H -2.716348 -2.385471 0.437736

H -0.542594 2.657376 0.551346

H -2.712244 2.389210 -0.438443

H -2.315539 0.665967 -0.972672

Frequencies

114.2129 144.9425 191.6466

201.3489 263.8454 264.0360

406.5845 464.3523 517.7962

569.2003 586.9504 652.1078

673.9563 736.8925 768.3244

820.7778 846.7848 848.9957

893.9806 916.0588 935.3114

1008.4009 1011.7831 1021.4133

1039.0750 1058.8920 1151.7843

1222.7865 1293.0041 1308.5687

1322.8977 1335.6484 1385.7603

1437.1111 1456.2736 1475.4938

1509.1211 1613.7726 1617.8070

3121.7833 3122.1822 3150.5302

3152.6805 3199.9243 3213.5402

3223.8668 3239.7815 3244.3472

i27, C1, 2A

C 1.716371 -1.147097 -0.117938

C 0.338642 -0.744550 -0.056230

C 1.716406 1.147039 0.118126

C 2.511959 0.000018 -0.000284

C 0.338650 0.744475 0.056500

C -0.816863 -1.446603 -0.011695

C -2.123416 -0.735560 0.232372

C -0.816767 1.446619 0.011737

C -2.123339 0.735635 -0.232519

H 2.071403 -2.164290 -0.204826

H 2.071375 2.164217 0.205401

H 3.594601 0.000018 -0.000630

H -0.813773 -2.531943 -0.047590

H -2.330196 -0.771966 1.314017

H -2.949964 -1.271493 -0.243677

H -0.813621 2.531999 0.048082

H -2.949995 1.271722 0.243098

H -2.329689 0.771886 -1.314296

Frequencies

153.9268 195.5413 290.4177

306.1743 375.8696 518.6458

521.1784 557.6038 671.4052

696.3246 712.6516 726.5140

755.4403 813.8211 839.3841

843.0467 876.5169 877.4505

934.4861 973.9490 1024.6003

1026.3937 1073.5771 1096.7161

1158.1037 1182.8060 1189.5519

1239.2670 1276.1949 1309.8629

1339.6606 1375.4837 1377.4756

1407.5283 1454.5185 1469.4863

1480.3493 1614.3454 1648.1326

2951.1537 2962.7681 3051.7619

3052.2115 3152.9744 3155.3006

3194.5540 3215.6840 3224.3102

i28, C1, 2A

C 2.042142 0.890602 0.332992

C 2.244618 -0.457804 0.331178

C 1.375710 -1.439428 -0.273085

C 0.037593 -1.328556 -0.390359

C -0.720631 -0.215107 0.302621

C -0.320009 1.071090 -0.400953

C 0.924908 1.571484 -0.277086

C -2.178268 -0.440431 0.358184

C -3.316984 0.155616 0.117424

H 2.853718 1.515654 0.695508

H 3.204599 -0.816496 0.692730

H 1.857708 -2.320700 -0.688466

H -0.529886 -2.051153 -0.967305

H -1.063466 1.585321 -1.000582

H 1.129552 2.552373 -0.699641

H -3.370024 1.178875 -0.266849

H -4.272521 -0.331889 0.293840

H -0.344151 -0.156767 1.335267

Frequencies

67.5518 140.0736 173.6884

291.3542 316.4011 333.7042

418.6514 427.6348 472.8761

570.5165 613.2358 661.5663

716.9585 762.2728 826.1876

885.1564 886.0503 925.6019

960.7172 969.3625 980.1014

993.5525 1001.5079 1020.4972

1044.5448 1091.8243 1206.7829

1221.6977 1240.1103 1270.1647

1297.7464 1374.1932 1414.1714

1418.9616 1472.8752 1561.6211

1651.5560 1661.7889 1743.4345

2965.2253 3031.4106 3128.3055

3134.3194 3140.8653 3142.6561

3156.7772 3171.9528 3173.8077

i29, C1, 2A

C -2.260836 -1.777254 -0.013155

C -1.413506 -0.655553 -0.005719

C -1.941147 0.668362 0.033508

C -1.097633 1.761968 0.032435

C 0.289286 1.589069 -0.003527

C 0.855506 0.300493 -0.033955

C -0.001058 -0.799457 -0.041376

H -3.337265 -1.664324 0.013088

H -1.858647 -2.782008 -0.045079

H -3.016744 0.804958 0.059307

H -1.511836 2.763881 0.058609

H 0.941623 2.455590 -0.003508

H 0.407876 -1.802626 -0.085690

C 2.323554 0.174539 -0.058881

C 3.045378 -0.939944 0.077541

H 2.854584 1.114203 -0.194490

H 2.595530 -1.914048 0.234646

H 4.127612 -0.908957 0.041896

Frequencies

33.5870 183.2429 201.2570

212.1915 369.3535 406.2248

455.3807 496.7953 510.3267

541.4556 559.9624 663.8188

706.0998 724.2985 739.7042

802.7009 882.5136 892.3391

926.3539 933.0232 978.0426

986.1734 998.6526 1028.1708

1079.5844 1114.4191 1179.4424

1192.0953 1272.4292 1316.5517

1342.7334 1347.2418 1435.1862

1460.2506 1490.8826 1500.4642

1578.6530 1595.7623 1689.8105

3130.5981 3141.5056 3146.1700

3160.1366 3170.3654 3172.9260

3184.5563 3221.4353 3243.0432

p1, Cs, 1A’

C 1.666190 -1.154895 -0.000004

C 0.228987 -0.688644 -0.000008

C -0.955992 -1.408115 -0.000003

C -2.169004 -0.711763 0.000001

C -2.187481 0.684209 0.000009

C -0.998067 1.413560 0.000008

C 0.211857 0.721032 -0.000010

C 1.599181 1.194188 -0.000028

C 2.437669 0.143485 -0.000004

H 1.901730 -1.769048 0.878373

H 1.901762 -1.769112 -0.878324

H -0.950160 -2.493431 -0.000008

H -3.104007 -1.260781 0.000000

H -3.137881 1.206478 0.000018

H -1.017945 2.498176 0.000013

H 1.887844 2.237905 -0.000007

H 3.518629 0.191463 0.000161

Frequencies

195.2431 210.9243 387.4138

397.3267 427.8125 542.4728

563.1799 605.2837 708.1051

734.1882 744.8902 783.8383

844.6280 871.8858 873.3269

935.2880 954.3264 955.5977

965.3012 987.7488 1042.0213

1088.7790 1132.6917 1148.8315

1177.2121 1185.9588 1227.4662

1248.9998 1314.2551 1344.7664

1390.0884 1436.8621 1488.7455

1492.5722 1602.0933 1636.2079

1651.1379 3015.0927 3037.6333

3155.8384 3162.3940 3173.3983

3185.9299 3188.9472 3213.2750

p2, Cs, 1A’

C -0.044382 -0.385308 -0.000002

C -1.422262 -0.909031 -0.000001

C -2.524717 -0.200254 0.000000

C -3.623150 0.498088 0.000004

C 1.030177 -1.285125 0.000001

C 0.236403 0.989944 -0.000004

C 2.345303 -0.828344 0.000002

C 1.548589 1.444460 -0.000003

C 2.610582 0.538316 0.000000

H -1.521207 -1.993331 0.000005

H -4.103443 0.801822 0.926543

H -4.103402 0.801898 -0.926531

H 0.830038 -2.351699 0.000003

H -0.584049 1.698872 -0.000006

H 3.162288 -1.541344 0.000004

H 1.746826 2.510673 -0.000005

H 3.633685 0.896636 0.000001

Frequencies

56.9901 119.6416 207.7441

324.3196 330.2122 414.1261

438.1433 450.9574 616.5055

634.8138 651.1904 710.1546

782.5122 829.6281 852.8894

880.2741 904.8768 931.6717

979.1721 1001.1483 1012.8038

1015.5828 1048.4167 1091.4951

1116.5979 1181.9685 1201.6449

1221.5889 1311.9524 1353.4123

1380.0861 1464.1815 1495.0621

1528.6797 1620.9863 1643.7970

2035.1692 3103.5321 3117.8028

3157.4002 3163.2862 3172.7226

3173.0628 3180.5393 3190.0472

p3, Cs, 1A’

C -1.725720 -1.133007 -0.000136

C -0.328397 -0.723448 -0.000320

C -1.613412 1.176914 0.000258

C -2.479045 0.001431 0.000079

C -0.315046 0.757619 -0.000023

C 0.818675 -1.425448 -0.000037

C 0.945291 1.451662 -0.000198

C 2.102212 0.762520 -0.000149

C 2.148303 -0.737670 0.000329

H -2.079917 -2.153777 -0.000540

H -1.959875 2.201776 0.000580

H -3.560655 0.041805 0.000398

H 0.813489 -2.512189 -0.000074

H 0.952417 2.537308 -0.000510

H 3.054256 1.282397 -0.000423

H 2.732140 -1.090738 -0.864896

H 2.730978 -1.090017 0.866655

Frequencies

159.9119 220.4334 298.8735

388.9446 443.5865 529.0214

559.1920 587.0818 661.1118

728.5838 733.8135 782.6350

836.3357 839.6894 851.4944

865.6166 895.9958 938.0802

957.8007 990.8603 1007.6227

1027.2016 1099.7209 1164.3358

1168.7303 1192.0245 1229.3248

1290.9811 1354.7368 1368.0477

1398.5985 1413.9420 1423.6625

1515.7320 1608.9020 1652.0117

1704.8399 2971.6167 2974.8170

3150.4101 3152.8813 3174.7688

3195.1246 3209.4160 3226.2784

p4, C1, 1A

C 1.522618 1.201681 -0.133682

C 0.259194 0.766474 0.133468

C 1.727295 -1.088771 0.015639

C 2.416281 0.056487 -0.198343

C 0.305740 -0.728187 0.352356

C -1.014757 1.427445 0.120335

C -0.931543 -1.444316 -0.100309

C -2.085235 -0.757628 -0.203346

C -2.143206 0.685585 -0.024879

H 1.822475 2.230159 -0.289470

H 2.131478 -2.090431 0.070104

H 3.481102 0.124536 -0.382421

H 0.304572 -0.860985 1.458812

H -1.061194 2.511495 0.139686

H -0.901808 -2.519880 -0.238816

H -3.004459 -1.279980 -0.446939

H -3.110491 1.172468 -0.078395

Frequencies

171.2931 189.4612 363.0838

402.2178 514.1381 537.2992

547.9476 582.9902 684.8759

695.1378 713.9377 785.4161

830.4187 842.6599 865.0281

874.9764 948.9590 969.4148

975.3349 987.3726 1019.1112

1021.3966 1075.4034 1118.5296

1146.3019 1170.0949 1193.9949

1218.0712 1258.2385 1322.2907

1388.5407 1394.3382 1441.9549

1534.4776 1566.5372 1615.6785

1675.0040 2859.4713 3153.5790

3159.9974 3173.7492 3184.3799

3188.4584 3201.9385 3218.5264

p5, Cs, 1A’

C 0.352632 1.107616 0.000475

C -0.249519 -0.226429 0.000501

C 2.006863 -0.487292 -0.000744

C 1.701382 0.952409 0.000042

C 0.827967 -1.181608 0.000095

C -1.629523 -0.557402 0.000480

C -2.660706 0.328052 -0.000666

H -0.189903 2.041061 0.000924

H 3.003150 -0.908263 -0.001078

H 2.441506 1.740794 0.000164

H 0.702930 -2.254984 0.000109

H -1.866888 -1.618855 0.001220

H -2.496089 1.398963 -0.001605

H -3.689289 -0.010794 -0.000830

Frequencies

127.1282 219.1623 235.0954

470.0058 528.3257 545.5051

620.5612 676.8586 708.3991

721.4789 774.1675 889.3153

895.9670 909.2816 910.6529

987.5360 1002.4772 1027.7773

1063.8622 1098.2986 1172.7514

1286.9726 1292.4460 1314.0042

1408.2547 1457.1015 1477.3515

1549.9243 1577.3715 3136.1640

3147.4927 3201.7937 3211.2003

3225.6417 3233.1545 3237.3326

p6, Cs, 1A’

C -1.207829 1.282478 -0.003288

C -0.568396 -0.040636 0.000099

C 1.789938 -0.852494 0.006066

C 2.656871 -1.693112 -0.005791

C 1.094076 1.623306 0.002225

C -0.271281 2.246181 -0.001989

C 0.791510 0.141553 0.002960

C -1.246538 -1.325517 0.000718

C -2.571979 -1.509407 0.000596

H -2.277807 1.440695 -0.006572

H 3.418519 -2.433391 -0.010167

H 1.688561 1.913209 -0.873530

H 1.682499 1.913924 0.881945

H -0.445454 3.313577 -0.004146

H -0.593033 -2.193513 0.001681

H -3.273975 -0.683051 -0.000157

H -2.997544 -2.505568 0.001366

Frequencies

102.4499 126.7910 147.2700

227.7869 234.2670 355.2721

428.6650 476.8142 517.9600

552.2356 596.1901 600.8254

666.3169 684.2994 692.2209

782.5287 853.8920 919.3369

932.9767 949.7707 964.7481

1002.0972 1034.0304 1035.8482

1129.8917 1137.5404 1188.6925

1256.2938 1319.2546 1333.1712

1409.5926 1420.4008 1451.9775

1550.9785 1626.1309 1683.8205

2183.9042 3018.9555 3042.5053

3141.2563 3151.7671 3200.3454

3221.7026 3225.6616 3476.4971

p7, C2v, 1A1

C 2.302216 0.674815 -0.000358

C 2.302247 -0.674883 -0.000370

C 1.160580 -1.570016 -0.000006

C -0.159755 -1.293962 0.000538

C -0.860168 0.000084 0.000363

C -0.159780 1.294026 0.000525

C 1.160598 1.569988 0.000013

C -2.187945 0.000017 -0.000086

C -3.488512 -0.000048 -0.000525

H 3.270340 1.166739 -0.000502

H 3.270373 -1.166783 -0.000496

H 1.416208 -2.625850 0.000022

H -0.831013 -2.147421 0.000996

H -0.830884 2.147605 0.000948

H 1.416302 2.625802 0.000018

H -4.064494 -0.000115 0.923805

H -4.063714 -0.000099 -0.925364

Frequencies

40.5421 148.2270 188.1234

278.7909 349.2486 363.2733

445.1327 539.6316 562.3061

566.9747 628.0203 642.1215

762.2036 813.2667 829.8667

855.9531 893.6853 900.4565

931.7015 999.0563 1004.0196

1006.0274 1013.2727 1021.2615

1205.1369 1222.0269 1264.0090

1303.2988 1334.8488 1421.2194

1448.9932 1480.9347 1485.2653

1637.6828 1647.5571 1702.0272

2004.4382 3075.9580 3133.2602

3136.0718 3137.6715 3147.1408

3158.7735 3162.5576 3170.3776

p8, C1, 1A

C 2.256273 0.023893 -0.206186

C 1.396383 -1.151134 -0.137464

C -0.129441 -0.980965 -0.345445

C -0.579912 0.405405 -0.060506

C 0.321156 1.406881 0.192483

C 1.737162 1.248461 0.032498

C 0.395977 -1.560007 0.913676

H 3.294262 -0.115638 -0.481882

H 1.836064 -2.087910 -0.486750

H -0.745216 -1.571889 -1.021346

H -0.068092 2.394772 0.416933

H 2.369458 2.128163 0.036643

C -2.012681 0.665639 -0.035907

C -2.984097 -0.255163 -0.075128

H -2.287979 1.716148 0.024698

H -2.776192 -1.318385 -0.085398

H -4.027221 0.036688 -0.071024

Frequencies

94.7533 153.6959 209.7841

230.5377 275.7288 431.0728

465.5226 508.1982 553.0607

598.3523 662.6271 709.3631

722.2839 743.0416 782.8534

895.7183 915.2237 926.5072

949.4903 975.9791 1000.4584

1015.1919 1027.6088 1041.7877

1076.7377 1146.4553 1178.9387

1212.7133 1278.6711 1317.1772

1333.0887 1380.0043 1425.6574

1455.3328 1557.9391 1641.6632

1674.9385 3078.2762 3091.7917

3133.1241 3149.2224 3161.2118

3178.5725 3196.8846 3230.2582

p9, C2v, 1A1

C -1.539148 -1.185380 0.000001

C -0.254089 -0.740745 -0.000004

C 1.006274 -1.440036 -0.000002

C 2.159119 -0.725505 0.000002

C 2.159257 0.725269 0.000003

C 1.006548 1.440111 -0.000001

C -0.254056 0.741130 -0.000004

C -1.539292 1.185343 -0.000004

C -2.458064 -0.000073 0.000003

H -1.871195 -2.214454 0.000004

H 1.020584 -2.524632 -0.000006

H 3.115169 -1.237661 0.000003

H 3.115409 1.237231 0.000008

H 1.020980 2.524711 -0.000002

H -1.871749 2.214304 0.000000

H -3.124261 -0.000099 -0.875203

H -3.124242 -0.000089 0.875225

Frequencies

182.4894 212.7206 323.7863

392.6245 465.7577 515.8355

547.0668 574.4877 678.1124

702.8628 727.0354 768.0835

787.7765 841.3874 851.9039

892.7304 896.3525 940.4227

976.9930 982.3285 997.6431

1004.1351 1102.7391 1137.7186

1178.6564 1188.1403 1232.6494

1247.6913 1284.1099 1382.8421

1393.8671 1399.3668 1447.8718

1545.4241 1578.3082 1613.8849

1686.8844 3000.2829 3018.0515

3156.9768 3164.2401 3176.5115

3185.7044 3210.7193 3213.2218

p10, C1, 1A

C -1.933362 0.870423 0.225958

C -1.034270 1.631445 -0.387032

C 0.339351 1.204710 -0.222175

C -2.218177 -0.340523 0.672521

C 0.684292 -0.127187 -0.225182

C -1.535190 -1.395735 -0.071778

C -0.230349 -1.249898 -0.428934

C 2.110978 -0.508890 -0.144278

C 3.058127 0.123006 0.552166

H -1.287199 2.471271 -1.028072

H 1.139333 1.940987 -0.203745

H -2.814785 -0.553056 1.554528

H -2.036112 -2.336117 -0.293508

H 0.241664 -2.122346 -0.875968

H 2.383662 -1.411383 -0.687930

H 2.841231 0.992949 1.162381

H 4.083806 -0.226414 0.544717

Frequencies

95.3896 163.3372 234.1058

306.2507 345.7513 385.2358

406.6953 482.8511 498.3891

585.6625 669.5645 700.7144

719.7604 773.8508 824.5377

838.0316 910.2864 913.3524

938.0147 977.8034 1018.7973

1032.7469 1045.6153 1066.9730

1138.9086 1163.1244 1229.2919

1304.3788 1323.7679 1363.4535

1388.1635 1436.7650 1454.6758

1545.1277 1609.5552 1683.3693

1884.4699 3116.8012 3124.4609

3131.7005 3137.5976 3138.8528

3141.8349 3144.6996 3220.9252

p11, Cs, 1A’

C -2.710401 -1.352122 0.000209

C -1.567563 -0.557797 0.000046

C -1.768080 0.852882 0.000625

C -0.736209 1.790520 0.000290

C 0.573380 1.352173 -0.000800

C 0.848541 -0.060038 -0.000954

C -0.199624 -0.992845 -0.000658

C 2.197137 -0.331983 -0.000649

C 3.463070 -0.587187 0.001106

H -3.693080 -0.900878 0.001025

H -2.652074 -2.432582 -0.000229

H -2.793203 1.212624 0.001276

H -0.963983 2.849947 0.000743

H 1.401585 2.049615 -0.001445

H 0.030242 -2.049799 -0.000588

H 4.033300 -0.704412 0.926176

H 4.035703 -0.706137 -0.922242

Frequencies

85.7061 139.9213 148.4346

160.6750 331.9608 345.8852

422.9980 467.1090 504.3035

507.5185 561.7148 589.6685

638.2921 675.1616 725.7166

742.8608 792.1389 882.5388

929.8073 942.4492 945.5648

952.1545 995.4774 1003.8646

1120.5640 1135.6146 1180.2561

1236.7447 1326.2686 1349.1988

1399.9153 1443.1043 1466.8614

1500.6081 1520.6485 1580.0202

1909.1271 3029.0755 3074.7299

3152.3610 3159.6442 3182.1587

3193.3756 3203.8786 3244.2559

ts\_i1\_i2, C1, 2A

C -0.813237 -1.284880 -0.060007

C -2.174378 -1.051849 0.065186

C -2.652558 0.251917 0.133983

C -1.761240 1.318172 0.080792

C -0.400127 1.084346 -0.043215

C 0.093575 -0.221616 -0.126692

C 1.527106 -0.503070 -0.295529

C 2.533955 0.404335 -0.592776

C 3.261032 -0.005135 0.608935

H -0.440503 -2.302871 -0.115249

H -2.864786 -1.886413 0.110721

H -3.715709 0.436401 0.237711

H -2.129875 2.335701 0.145208

H 0.291382 1.919095 -0.061111

H 1.790105 -1.557522 -0.234415

H 2.347056 1.435596 -0.869223

H 3.908765 -0.875477 0.625647

H 3.128799 0.542170 1.536647

Frequencies

-785.8502 70.6088 127.0491

214.0512 344.8263 416.0095

419.9354 511.7771 549.5670

591.7725 612.9855 636.7927

713.7879 727.8785 787.2124

803.1711 866.0826 882.0075

953.8414 986.8538 1003.4729

1022.8825 1026.6254 1059.4325

1104.6832 1119.8021 1189.1277

1203.0291 1219.4027 1237.7531

1302.9742 1344.2721 1355.2681

1444.3140 1471.7049 1517.5781

1539.1085 1655.1365 1673.8863

3130.4068 3141.9149 3187.5270

3194.0277 3196.4782 3205.4314

3214.1521 3222.7109 3234.0647

ts\_i2\_i3, C1, 2A

C 0.048268 -0.405272 -0.094990

C 1.368202 -0.899225 -0.187663

C 2.555634 -0.057205 -0.420282

C 3.331334 0.439814 0.536589

C -0.245632 0.980954 -0.151014

C -1.548093 1.433075 -0.060637

C -2.603478 0.533605 0.090072

C -2.338352 -0.835406 0.151060

C -1.041975 -1.300002 0.060617

H 1.515256 -1.975388 -0.141810

H 2.805352 0.156437 -1.461575

H 3.122050 0.257762 1.586002

H 4.200768 1.043475 0.299429

H 0.569573 1.687534 -0.257361

H -1.749471 2.497709 -0.106524

H -3.622382 0.895907 0.162362

H -3.154379 -1.539814 0.268849

H -0.842207 -2.365651 0.108117

Frequencies

-152.5739 88.1672 163.1795

199.8790 350.0960 408.1788

458.2442 468.6813 508.9695

627.3424 635.3879 694.0915

702.7649 775.5044 841.5255

857.6504 915.2441 975.7166

986.7785 989.6928 1004.2074

1005.3292 1030.0671 1051.9565

1105.8679 1125.6738 1179.1010

1190.8012 1238.6442 1322.2642

1327.1362 1354.3799 1406.3615

1458.5605 1497.5960 1514.7673

1610.5170 1628.9921 1720.3060

3103.5993 3149.0942 3167.9341

3186.7713 3193.6663 3203.7990

3212.4341 3221.2083 3238.2482

ts\_i3\_i4, C1, 2A

C 0.217988 0.659383 -0.357083

C 0.073664 -0.751353 -0.586501

C -0.853275 1.407019 0.091050

C 1.621672 1.078262 -0.320481

C 2.423824 0.126068 0.177013

C 1.767239 -1.116752 0.632676

C -2.086347 0.795761 0.341515

C -2.231699 -0.580521 0.157406

C -1.185272 -1.347370 -0.324107

H 0.697480 -1.205250 -1.351331

H -0.719005 2.464123 0.296600

H 1.955027 2.070272 -0.602546

H 3.499741 0.256786 0.258364

H 2.243456 -2.068530 0.409873

H 1.283650 -1.080453 1.606594

H -2.922047 1.387493 0.695976

H -3.191090 -1.047351 0.353356

H -1.333976 -2.400070 -0.535806

Frequencies

-711.6190 130.9697 191.5559

293.8818 406.2059 433.9096

498.3137 546.4581 582.2511

615.1858 695.8503 705.7913

737.7743 774.2423 803.1332

854.3048 875.9282 938.5922

957.1534 964.5144 998.5254

1018.3307 1029.8195 1048.4024

1071.1505 1101.0371 1155.4982

1177.1062 1194.3523 1218.9946

1324.6813 1328.9823 1388.2312

1458.9266 1462.1312 1519.8958

1588.7078 1626.6259 1656.3770

3118.0013 3157.1665 3167.5042

3185.7804 3191.5528 3206.6750

3207.3518 3216.6329 3218.4662

ts\_i3\_p2, C1, 2A

C 0.004240 -0.395567 0.003045

C 1.372718 -0.924429 0.002980

C 2.474442 -0.194181 0.035590

C 3.542279 0.507759 -0.221821

C -0.259023 0.978195 0.033148

C -1.563481 1.444384 0.019947

C -2.629531 0.550300 -0.021749

C -2.379756 -0.815578 -0.047996

C -1.073217 -1.284557 -0.033098

H 1.484817 -2.005640 0.040534

H 3.835310 0.678150 -1.254241

H 4.161034 0.931967 0.559425

H 0.568992 1.677857 0.070199

H -1.752117 2.511748 0.045543

H -3.648845 0.919067 -0.031330

H -3.203409 -1.519843 -0.077819

H -0.882659 -2.352816 -0.052803

H 2.504855 -0.038438 2.080213

Frequencies

-711.0656 54.9156 90.9546

130.6563 215.0144 334.6062

375.5352 415.2169 432.2667

468.5315 480.6493 632.5027

635.7479 658.4626 711.5191

786.8837 840.4107 859.6433

886.3473 909.9295 941.8371

999.1961 1011.6419 1017.0931

1022.6051 1059.9611 1094.3411

1123.8315 1186.3826 1212.5923

1232.1758 1322.3898 1357.3277

1387.7193 1466.1095 1506.0333

1544.6061 1654.2305 1677.1796

2006.2141 3147.1046 3162.2714

3188.6277 3194.4842 3203.7412

3212.4831 3222.4265 3240.0055

ts\_i4\_p1, C1, 2A

C -0.208896 0.737108 0.024306

C -0.226902 -0.679846 0.091027

C 0.995523 1.424480 0.000352

C -1.590918 1.204409 -0.017349

C -2.421828 0.153715 -0.064561

C -1.657390 -1.142844 -0.085402

C 2.180789 0.696264 -0.025775

C 2.165930 -0.701108 -0.069145

C 0.969071 -1.398239 -0.045819

H 1.015211 2.508691 -0.018512

H -1.882362 2.246858 -0.014553

H -3.502114 0.203299 -0.102834

H -1.989939 -1.847888 0.679933

H -1.772259 -1.640455 -1.056866

H 3.130679 1.218576 -0.044326

H 3.103357 -1.242126 -0.129804

H 0.957881 -2.481968 -0.085303

H -0.292726 -0.728625 1.926462

Frequencies

-919.5057 198.8927 205.0043

372.7104 395.2148 445.3194

471.2859 518.8051 554.5788

571.1234 614.7231 707.6806

740.8974 754.2091 785.9286

850.3503 873.3279 878.2221

949.2387 959.8282 970.5435

979.0308 1002.6474 1048.4390

1093.3976 1139.7588 1168.3939

1179.7877 1196.3832 1238.0114

1261.0677 1321.8977 1344.5201

1390.6999 1455.2739 1484.7363

1509.7855 1617.4440 1654.4996

1668.8304 3046.6388 3111.5941

3191.6372 3198.8221 3209.0735

3216.6148 3220.7207 3241.5615

ts\_i21\_i22, C1, 2A

C -1.421962 1.493551 -0.247878

H -1.590406 2.383272 0.352290

H -1.864354 1.521051 -1.239153

C -0.150260 0.756164 -0.087615

C 1.103256 1.358745 0.036705

C 2.257306 0.576904 0.112272

C 2.172163 -0.813566 0.055233

C 0.929572 -1.434653 -0.052322

C -0.234124 -0.663493 -0.096681

H 1.182115 2.440597 0.047170

H 3.225796 1.055971 0.204481

H 3.073590 -1.413751 0.109381

H 0.859255 -2.517028 -0.066725

C -1.610293 -1.142333 -0.169912

C -2.552427 -0.338356 0.431840

H -1.890815 -1.917099 -0.876411

H -2.347165 0.132898 1.385298

H -3.607405 -0.443686 0.193830

Frequencies

-659.3795 142.7886 193.8844

313.0289 386.6155 415.0059

476.4270 500.6228 522.8439

573.9786 608.1640 658.8307

726.2840 752.7110 771.0214

782.5591 849.3467 877.1998

888.9445 946.0299 951.4134

988.8680 1015.8776 1026.8193

1054.1110 1129.1068 1181.5190

1213.9326 1233.9729 1245.9623

1293.6782 1311.3347 1415.5726

1449.1120 1483.9716 1488.2628

1540.5057 1599.1675 1625.8459

3106.5426 3121.8803 3157.1250

3157.4712 3164.7881 3174.5506

3186.3148 3192.1313 3199.8690

ts\_23\_p5, C1, 2A

C -0.590172 1.224130 -0.424495

C -0.935456 -0.029881 0.275015

C 2.592557 -1.475232 -0.746232

C 2.688971 -0.284827 -0.420656

C 1.224297 0.549132 0.791015

C 0.679219 1.574616 -0.098617

C 0.153486 -0.405130 1.016844

C -2.199023 -0.735617 0.205415

C -3.270805 -0.373462 -0.513865

H -1.250785 1.767297 -1.085751

H 2.183361 -2.456358 -0.830710

H 3.314180 0.581404 -0.515160

H 1.967045 0.766858 1.550315

H 1.218223 2.445625 -0.444390

H 0.224685 -1.277993 1.650576

H -2.258747 -1.641970 0.804335

H -3.278167 0.517781 -1.131104

H -4.178235 -0.965013 -0.504655

Frequencies

-655.9057 45.8523 77.4919

125.8574 161.6139 226.9709

239.5427 307.3691 468.3508

510.3902 550.8935 595.0260

618.0559 644.6822 706.9008

725.1717 763.7380 779.7615

825.9731 861.0068 899.1294

907.6456 918.5897 958.7149

988.0584 1017.8813 1023.9288

1040.3531 1105.1122 1238.6488

1259.4441 1317.1447 1330.4510

1390.8472 1448.7676 1520.4825

1573.1546 1664.9924 1806.6670

3130.1579 3142.4956 3169.8824

3203.9440 3214.8544 3222.9426

3226.7156 3309.5657 3421.8758

ts\_24\_25, C1, 2A

C 1.359271 1.227617 0.143987

C 0.631415 -0.020281 -0.053260

C -0.882809 1.674592 -0.093649

C 0.456364 2.241623 0.122735

C -0.780552 0.313434 -0.195407

C 1.160920 -1.334240 -0.099351

C 2.475234 -1.664677 0.021914

C -1.873934 -0.652005 -0.447395

C -2.542545 -1.305355 0.500937

H 2.425507 1.314524 0.289758

H -1.797589 2.248054 -0.160010

H 0.666476 3.295248 0.246447

H 0.439864 -2.135091 -0.240765

H 3.244539 -0.915806 0.168445

H 2.798151 -2.697390 -0.025098

H -2.138809 -0.832252 -1.489436

H -3.338600 -1.999898 0.254401

H -2.319729 -1.161638 1.553189

Frequencies

-114.1335 122.6652 145.3258

172.6663 231.3902 281.6493

414.2234 468.4237 541.1727

546.2465 609.0270 649.9816

684.3237 695.7447 755.6796

765.3957 837.2292 892.0308

904.9430 963.7115 973.1912

1010.9578 1022.3883 1030.5288

1035.7799 1084.7702 1113.2153

1204.2399 1234.8524 1284.3137

1316.6020 1322.7034 1399.4906

1439.8342 1454.9472 1524.5011

1545.1790 1583.7771 1696.8906

3098.6347 3128.7234 3144.0648

3148.9296 3202.8610 3212.6027

3214.9494 3231.9532 3236.1983

ts\_i5\_i6, C1, 2A

C 0.860021 -1.569813 0.767031

C -0.150732 -0.991469 -0.091131

C -0.675983 0.352033 0.077445

C 0.148749 1.426961 0.321120

C 1.551267 1.407451 0.096545

C 2.201155 0.296986 -0.356736

C 1.635108 -1.023915 -0.332873

H 0.890096 -2.599846 1.098844

H -0.760643 -1.677183 -0.677817

H -0.315104 2.388445 0.517606

H 2.079710 2.354655 0.115103

H 3.173544 0.400502 -0.828318

H 2.052491 -1.744618 -1.035666

C -2.115307 0.575082 -0.067929

C -3.075222 -0.351052 -0.187755

H -2.412289 1.621647 -0.071790

H -2.871061 -1.415038 -0.154099

H -4.111075 -0.062150 -0.318163

Frequencies

-373.5490 96.9390 186.7116

233.9275 275.5767 313.8941

444.3914 483.7904 499.2130

575.9663 618.4996 672.3914

721.6132 751.4607 811.1778

866.8789 893.5174 914.9181

923.5996 958.1497 969.1125

1008.4332 1021.6895 1031.2613

1082.2483 1100.4849 1177.2005

1202.2094 1218.1155 1226.6580

1313.9057 1340.0619 1399.2319

1421.3704 1443.4461 1465.3031

1551.5695 1629.3626 1672.6777

3093.4439 3099.5121 3128.8208

3144.1367 3149.0415 3157.2054

3175.2214 3181.0476 3223.2519

ts\_i5\_i19, C1, 2A

C 0.565165 -1.709151 0.700563

C -0.126421 -0.939153 -0.374665

C -0.617038 0.422171 -0.032046

C 0.265559 1.442150 0.197657

C 1.693016 1.319586 0.051173

C 2.264456 0.123437 -0.236290

C 1.393650 -1.022080 -0.348487

H 0.660487 -1.525818 1.763342

H -0.703030 -1.474768 -1.126156

H 2.306167 2.208147 0.154764

H 3.330237 0.022568 -0.404873

H -0.135357 2.418036 0.454315

C -2.052465 0.667545 0.004390

C -3.009158 -0.267209 -0.076054

H -2.346705 1.709272 0.110903

H -2.779737 -1.323540 -0.153581

H -4.057862 0.003540 -0.052907

H 1.465220 -2.261213 -0.063248

Frequencies

-1845.5980 104.1938 185.8121

215.0132 254.2853 298.6538

433.5577 484.3758 532.1367

547.4972 581.2828 636.0647

707.7572 728.8231 755.8266

793.5352 882.8235 892.8730

910.6710 926.9521 959.1970

987.3733 1020.3257 1024.9547

1034.7904 1066.7268 1107.9751

1145.4683 1179.4530 1223.2624

1314.4173 1334.4586 1349.8328

1413.9398 1431.7049 1454.5409

1550.7092 1628.0844 1671.2071

2299.6099 3090.7458 3132.2629

3146.4612 3152.3770 3166.9874

3179.4158 3184.7805 3227.4310

ts\_i25\_i26, C1, 2A

C -1.842728 -0.860257 0.193764

C -0.420423 -0.739161 0.026330

C -1.322498 1.349221 -0.172333

C -2.397347 0.384623 0.073004

C -0.126005 0.697379 -0.191943

C 0.449204 -1.862708 0.044870

C 1.788694 -1.893829 -0.187270

C 1.189862 1.341682 -0.406613

C 2.067422 1.627118 0.553757

H -2.361275 -1.791907 0.369957

H -1.461290 2.414214 -0.300520

H -3.447505 0.633578 0.144205

H -0.042294 -2.810278 0.257175

H 2.356048 -1.001261 -0.409786

H 2.327221 -2.833438 -0.153126

H 1.429841 1.625953 -1.431368

H 3.005612 2.123665 0.330336

H 1.876554 1.375069 1.591733

Frequencies

-129.0179 96.2111 178.3300

195.9929 229.7347 282.7301

410.7823 464.1751 530.1740

549.4567 594.7895 639.8931

693.9203 720.1756 739.5295

769.0744 837.0543 897.5383

911.7826 958.8737 972.6795

1004.7973 1009.7549 1021.6845

1051.7716 1062.6941 1141.5808

1218.1466 1243.4058 1302.4525

1314.1455 1322.7358 1396.6367

1438.7718 1448.1338 1473.7199

1558.1023 1590.8090 1694.2554

3098.9209 3126.5985 3129.0871

3154.4336 3201.0159 3212.2757

3212.9176 3226.5941 3252.6459

ts\_i9\_i24, C1, 2A

C -1.265004 -1.329596 -0.238599

C -0.175458 -0.768442 0.319833

C -1.856811 0.877652 0.023043

C -2.309935 -0.311845 -0.409688

C -0.458685 0.706916 0.569697

C 1.188058 -1.254907 0.555921

H -1.355550 -2.364700 -0.542783

H -2.397593 1.814612 0.040828

H -3.291420 -0.508515 -0.822506

H -0.506801 0.874402 1.660052

H 1.490572 -1.507186 1.570185

C 0.603884 1.646675 0.014377

C 1.819059 1.317270 -0.366200

H 0.298256 2.697775 -0.030650

H 2.633702 1.920733 -0.746470

C 2.135267 -1.023717 -0.388004

H 1.861316 -0.879219 -1.425419

H 3.185273 -1.207936 -0.185505

Frequencies

-387.9309 93.0821 150.6923

230.9763 270.4079 355.2600

401.1206 501.7725 536.9783

587.1040 632.1503 652.8408

709.2647 710.9416 819.8597

841.5964 866.2448 877.7763

897.2533 931.4847 953.6318

959.7790 991.3316 1020.5903

1047.1485 1066.3942 1108.0115

1155.1485 1206.8799 1219.8733

1264.6585 1280.6721 1286.6837

1371.8225 1426.1222 1565.9231

1589.8319 1645.4020 1670.7756

2950.9528 3024.0704 3121.3965

3135.5579 3186.5387 3197.3235

3200.1513 3214.8366 3222.6653

ts\_i10\_i11, C1, 2A

C 1.648820 1.177443 -0.062542

C 0.291139 0.742458 0.024661

C 1.736439 -1.114802 0.007519

C 2.498824 0.079724 -0.072464

C 0.307087 -0.702778 0.073828

C -0.915664 1.431707 0.018522

C -2.225471 0.692922 0.037660

C -0.926265 -1.457098 -0.056924

C -2.100455 -0.805769 -0.082658

H 1.963996 2.212385 -0.073471

H 2.072344 -2.134255 -0.114231

H 1.016789 -1.055019 1.116955

H 3.578851 0.112818 -0.089045

H -0.934608 2.514700 -0.030175

H -2.884680 1.065698 -0.763420

H -2.787899 0.927096 0.961220

H -0.888821 -2.538672 -0.140714

H -3.022698 -1.367595 -0.192731

Frequencies

-1414.5036 133.7371 210.4174

285.5964 373.6970 443.7777

515.6615 568.7140 577.5491

655.0952 662.6869 719.8782

752.5502 756.6837 840.6958

849.2335 865.5787 885.8180

900.0377 929.8721 980.8974

1017.8528 1053.5978 1083.6455

1153.2970 1158.3866 1189.1578

1189.5109 1234.4483 1252.7201

1326.6804 1343.9603 1393.5247

1425.2499 1453.6333 1453.9611

1462.6917 1512.3858 1669.5488

2049.3012 2890.4694 2943.3511

3149.0256 3168.7216 3170.1894

3200.1777 3217.0450 3232.0337

ts\_i10\_p3, C1, 2A

C 1.708154 1.154158 -0.019762

C 0.317066 0.741807 0.040042

C 1.626250 -1.151057 -0.072257

C 2.470961 0.022470 -0.096395

C 0.311934 -0.743948 0.062081

C -0.833904 1.435759 0.001212

C -0.947641 -1.443890 -0.059595

C -2.102446 -0.757656 -0.093303

C -2.159332 0.740307 -0.009887

H 2.058318 2.176308 -0.014797

H 1.974536 -2.173341 -0.125592

H 3.550542 -0.005840 -0.164629

H 0.386451 -0.871650 2.067178

H -0.832830 2.521670 -0.035118

H -0.945266 -2.527491 -0.116219

H -3.049471 -1.279872 -0.177407

H -2.766281 1.137008 -0.837807

H -2.722247 1.035501 0.891583

Frequencies

-671.4108 152.8321 231.3922

301.1572 316.6008 393.4658

408.0843 447.2376 528.4672

559.1275 585.2385 658.4863

727.1512 737.9012 767.2549

827.8742 839.0387 844.7662

863.1196 895.8857 938.7568

956.2222 991.1331 1020.2276

1028.1366 1098.7281 1159.4688

1170.7801 1194.0638 1228.0559

1287.0103 1356.8767 1372.2605

1388.6878 1398.8137 1425.5066

1481.4547 1569.0785 1650.3068

1704.0924 2962.5818 2986.7602

3153.1150 3157.1899 3177.2774

3198.9232 3215.0347 3227.6433

ts\_i10\_p4, C1, 2A

C 1.541118 1.212421 -0.153313

C 0.284689 0.762030 0.092223

C 1.777629 -1.060450 0.081573

C 2.454628 0.081280 -0.154605

C 0.346164 -0.715660 0.359815

C -0.995265 1.401869 0.028164

C -0.843307 -1.463323 -0.155951

C -2.005448 -0.814065 -0.302595

C -2.108528 0.630574 -0.106376

H 1.824051 2.241141 -0.335900

H 2.194921 -2.053817 0.175690

H 3.522267 0.159810 -0.314733

H 0.281294 -0.813605 1.466056

H -1.065093 2.484136 0.020805

H -0.771259 -2.533890 -0.313545

H -2.900247 -1.353187 -0.592884

H -3.076084 1.099706 -0.240371

H -2.719932 0.561647 2.001272

Frequencies

-542.8350 148.8735 163.2347

248.9815 254.5986 366.3939

407.7649 517.9673 539.4935

553.5859 589.0966 692.2388

720.3227 734.1115 792.6940

836.3176 858.9003 873.8574

899.5339 972.6314 980.3485

990.3310 1005.1236 1021.4625

1037.1104 1084.6466 1128.4591

1158.0827 1179.7922 1212.5544

1223.6512 1269.2774 1344.2187

1402.1092 1406.1646 1452.7820

1549.9095 1571.5312 1646.9256

1700.4224 2906.0938 3187.5082

3194.9553 3208.0415 3216.2886

3218.5520 3231.0475 3246.0958

ts\_i26\_i27, C1, 2A

C 1.648835 -1.158030 -0.137766

C 0.335898 -0.761872 -0.105544

C 1.709670 1.122974 0.160732

C 2.497134 0.008395 0.021131

C 0.333211 0.710250 0.045556

C -0.906518 -1.493971 -0.109177

C -2.022643 -0.947673 0.522816

C -0.808818 1.477551 0.005376

C -2.089476 0.987543 -0.408603

H 2.003021 -2.179065 -0.194180

H 2.047376 2.146546 0.247977

H 3.578495 -0.012092 0.029033

H -1.028124 -2.343464 -0.775608

H -1.902593 -0.435746 1.468792

H -2.992881 -1.414229 0.380689

H -0.748940 2.500831 0.377272

H -2.964911 1.569407 -0.132707

H -2.175196 0.496816 -1.368398

Frequencies

-840.6639 149.7082 194.3177

284.7522 336.6823 353.0941

459.4258 476.0996 559.6539

622.9412 663.3802 704.4485

714.6805 726.2109 749.2066

772.5602 838.3641 858.2188

891.0189 915.0997 920.1655

989.0889 1011.5651 1020.2876

1027.0293 1090.9100 1158.9346

1184.4666 1216.3573 1239.6898

1288.3679 1351.3563 1380.4511

1397.5765 1458.4517 1488.2049

1521.2403 1554.7397 1593.7474

3100.0491 3123.2926 3126.7447

3141.9496 3196.9360 3206.9605

3210.5148 3211.8922 3223.2071

ts\_i13\_i14, C1, 2A

C 1.354720 -1.326366 -0.159130

C 0.073675 -0.609178 -0.188736

C 1.797532 0.922030 0.187312

C 2.362808 -0.461556 0.061405

C 0.310748 0.719785 0.005065

C -1.226997 -1.267616 -0.428615

C -2.078014 -1.635520 0.526640

C -0.629543 1.832587 0.020665

C -1.934506 1.799344 -0.169487

H 1.442169 -2.398039 -0.286845

H 2.029109 1.372539 1.162150

H 2.207586 1.604201 -0.569750

H 3.414264 -0.699103 0.146157

H -1.475293 -1.479639 -1.468655

H -1.870833 -1.447101 1.574647

H -3.014392 -2.127650 0.288465

H -0.175631 2.815140 0.204633

H -2.739516 2.518592 -0.181517

Frequencies

-109.3872 86.9833 143.9192

159.3601 220.8544 288.0396

363.5214 398.0180 450.1805

586.5550 609.8746 633.0951

670.1142 689.4504 739.6738

826.2837 843.2380 867.7814

919.3238 950.2312 956.2308

971.0996 1009.4020 1019.9616

1087.5598 1128.7650 1135.4826

1161.9403 1211.1366 1276.1790

1314.8743 1328.5209 1372.3050

1417.8254 1449.0440 1550.6018

1627.1727 1642.8945 1697.3996

3000.6716 3009.0706 3032.3547

3103.3098 3132.7132 3192.1473

3216.7850 3219.5240 3239.8897

ts\_i14\_i11, C1, 2A

C -1.612337 1.196910 -0.059920

C -0.226971 0.711015 -0.032097

C -1.687451 -1.120550 0.123330

C -2.465961 0.163719 0.048092

C -0.247517 -0.667841 0.053983

C 0.960667 1.498343 -0.228190

C 2.159441 1.175802 0.322589

C 0.866200 -1.568180 -0.145478

C 2.156738 -1.252237 -0.077430

H -1.880781 2.243882 -0.130443

H -1.899426 -1.674919 1.048174

H -1.936332 -1.800389 -0.702153

H -3.545093 0.219137 0.093013

H 0.899012 2.331622 -0.925664

H 2.221255 0.570248 1.215541

H 3.064755 1.701546 0.039422

H 0.597276 -2.589211 -0.438481

H 3.062481 -1.823802 -0.228680

Frequencies

-323.8873 153.7185 164.0126

269.2704 284.6277 322.2657

397.3870 432.7652 476.5562

571.5532 639.2153 662.6536

675.2460 690.0135 758.7965

834.5598 856.1925 864.1884

892.5751 927.3133 951.4511

960.2555 967.0276 1004.8704

1096.6595 1132.7599 1147.2032

1176.4292 1222.9492 1266.1307

1289.0956 1330.2280 1374.9564

1421.7679 1464.4608 1490.8851

1573.6961 1613.7292 1625.2703

3006.2192 3026.3643 3031.4909

3122.2951 3145.7538 3188.3158

3212.7928 3216.7668 3230.2676

ts\_i11\_p1, C1, 2A

C -1.619097 -1.213914 -0.022499

C -0.240460 -0.715227 -0.035353

C -1.729972 1.133580 0.050420

C -2.475709 -0.179691 0.027122

C -0.285779 0.696716 0.002566

C 0.974790 -1.383664 -0.087362

C 2.166648 -0.629111 -0.048397

C 0.885377 1.443855 -0.033651

C 2.108850 0.781771 -0.082569

H -1.888082 -2.262419 -0.046232

H -1.997872 1.772058 -0.801132

H -1.956482 1.714483 0.953720

H -3.555279 -0.248527 0.051373

H 1.018177 -2.466395 -0.123484

H 3.112660 -1.122434 -0.236754

H 2.673821 -0.870177 1.729913

H 0.853436 2.528619 -0.034209

H 3.031742 1.348905 -0.114854

Frequencies

-765.3800 188.7693 194.0719

328.3765 362.9813 388.8537

411.1601 439.2980 539.4609

585.9885 608.3418 710.1454

738.5993 742.9828 802.6840

841.0847 870.9344 875.6668

935.2916 955.3313 960.9659

967.9768 1018.5399 1028.1001

1087.8565 1127.8293 1147.8247

1170.6202 1185.2298 1223.3912

1248.1499 1314.5240 1340.0692

1384.7718 1436.2526 1473.1782

1491.1931 1584.2883 1620.8568

1636.5190 3012.8228 3034.5201

3159.9173 3168.6302 3179.3942

3189.7948 3190.9371 3214.2328

ts\_i11\_p3, C1, 2A

C -1.662171 -1.201756 -0.026920

C -0.275192 -0.753591 -0.007491

C -1.610785 1.104305 -0.095489

C -2.443698 -0.099942 -0.084892

C -0.301750 0.716164 -0.070570

C 0.883746 -1.422794 0.047289

C 2.192225 -0.701477 0.048118

C 0.936790 1.449166 -0.081115

C 2.104467 0.792150 -0.025766

H -1.986292 -2.231989 0.006064

H -1.979680 2.112663 -0.222951

H -1.871868 1.618748 2.013643

H -3.525299 -0.088667 -0.108465

H 0.904307 -2.508133 0.091522

H 2.805172 -1.074953 -0.785236

H 2.756641 -0.990429 0.947041

H 0.912547 2.532756 -0.130020

H 3.042683 1.336670 -0.030583

Frequencies

-498.1164 142.8944 194.1811

231.9527 243.5748 310.2642

388.0500 439.2683 531.2426

569.5845 589.3096 659.7907

733.8401 742.2586 796.8750

840.3398 846.8741 868.1441

888.2898 905.8888 950.4614

964.6449 1004.6494 1005.3136

1035.0575 1098.4250 1172.2247

1176.7798 1207.2082 1224.4762

1290.9753 1370.7948 1377.1383

1409.4938 1428.0786 1429.1695

1551.5739 1621.9177 1681.5069

1745.5144 3013.7353 3033.3816

3185.5658 3188.0356 3209.2116

3228.5414 3240.7636 3255.2408

ts\_i6\_i17, C1, 2A

C 1.925511 0.682571 0.465277

C 0.968894 1.647676 0.113679

C -0.325302 1.203849 -0.162566

C 2.320843 -0.385345 -0.454295

C -0.704730 -0.117549 0.133142

C 1.426983 -1.383076 -0.409669

C 0.297138 -1.079275 0.529296

H 1.156632 2.715928 0.200913

H -1.092443 1.934317 -0.395298

H 3.157782 -0.295585 -1.136073

H 1.433819 -2.280492 -1.018974

H -0.103225 -1.937495 1.074510

H 1.138799 -0.177018 1.219128

C -2.115181 -0.506731 0.234464

C -3.157926 0.073557 -0.369500

H -2.298649 -1.392528 0.839716

H -3.047852 0.928100 -1.027906

H -4.162239 -0.309288 -0.234982

Frequencies

-1358.3940 82.6164 183.2028

231.8020 306.6311 336.4132

429.0474 514.6867 552.7840

572.3909 605.9723 703.7243

736.0772 751.4765 780.1489

851.2254 906.4077 921.2486

928.2002 947.4173 957.5071

998.8011 1021.7736 1039.4359

1054.2039 1121.2081 1149.5015

1211.9356 1252.6951 1323.3056

1332.0093 1363.3934 1386.6338

1400.5853 1456.1545 1489.7430

1528.5549 1552.0795 1617.7302

1671.7586 3069.0226 3123.5611

3124.3406 3140.9523 3167.2082

3169.3608 3197.9082 3223.1588

ts\_i6\_i7, C1, 2A

C 1.132563 -1.510249 -0.349938

C 0.372369 -0.819260 0.731642

C -0.743777 0.037329 0.275316

C 1.036292 1.578579 0.016190

C 1.971889 0.541755 0.266451

C 2.140966 -0.677934 -0.584954

C -0.328087 1.284214 -0.162739

H 0.851185 -2.422827 -0.866573

H 0.420838 -1.176308 1.759369

H 1.345448 2.614660 0.133080

H 2.871201 0.860692 0.799785

H 2.968912 -0.797483 -1.281525

H -1.034173 2.037851 -0.493560

C -2.107243 -0.453040 0.311752

C -3.139121 -0.011368 -0.430967

H -2.287432 -1.275078 1.002079

H -3.019515 0.767824 -1.175469

H -4.131571 -0.429485 -0.313706

Frequencies

-748.9621 78.2530 158.8071

210.8483 247.1022 298.5470

400.2753 438.8159 517.4412

578.1707 613.3207 675.2546

715.0428 744.7546 778.0537

835.7239 858.8552 904.5262

907.2372 925.0955 954.8108

982.7263 1007.9534 1040.8336

1056.8403 1078.9205 1108.6843

1161.3712 1204.9842 1284.1824

1314.0961 1333.5079 1340.5241

1380.1369 1447.3991 1453.6631

1508.1936 1620.1581 1671.6449

3062.7173 3114.6613 3118.8091

3123.5753 3132.8827 3139.4678

3162.5961 3175.1985 3224.7830

ts\_i6\_i18, C1, 2A

C 2.174089 0.814973 0.112400

C 2.255202 -0.471164 0.541280

C 1.374488 -1.495319 0.011334

C 0.085141 -1.335526 -0.373628

C -0.766775 -0.138878 -0.244867

C -0.335775 1.148150 -0.241051

C 1.068068 1.575807 -0.349445

C -2.214065 -0.431850 -0.162844

C -3.116981 0.238922 0.555380

H 3.078109 -0.787278 1.175141

H 1.785805 -2.500475 -0.062975

H -0.436600 -2.221844 -0.723963

H -1.079878 1.937189 -0.179906

H 1.280014 2.438564 -0.980762

H -2.541813 -1.304313 -0.724950

H -2.842935 1.079113 1.184228

H -4.162360 -0.046498 0.547350

H 1.779310 1.974852 0.674485

Frequencies

-1786.9363 86.3637 116.1975

210.8938 254.0909 288.6829

366.2605 405.1357 457.1656

479.8832 588.6208 668.2885

674.2643 711.4158 770.9571

790.4612 813.9915 883.1698

910.1872 943.6888 953.5999

978.6435 1007.2244 1019.7306

1050.5406 1129.6946 1154.0615

1224.1725 1253.6028 1320.6845

1336.9828 1361.9625 1382.6466

1429.1977 1451.3455 1462.9153

1611.0838 1642.4362 1686.2252

2055.5149 3097.6482 3116.7557

3124.2933 3137.3855 3142.9796

3148.1202 3150.3575 3220.0041

ts\_i17\_i18, C1, 2A

C 2.048853 0.848504 -0.375088

C 1.079149 1.434584 0.444002

C -0.320541 1.214656 -0.051813

C 2.189406 -0.477019 -0.683034

C -0.762534 -0.037802 0.151262

C 1.378293 -1.381372 0.030033

C 0.270167 -0.936103 0.792302

H 1.309060 2.379622 0.937348

H -0.857550 1.982630 -0.595530

H 3.011950 -0.839116 -1.290426

H 1.714358 -2.411797 0.119023

H -0.131203 -1.661318 1.499547

H 0.924884 0.279672 1.270691

C -2.074526 -0.583275 -0.213452

C -3.218663 0.105631 -0.254058

H -2.097869 -1.645886 -0.444483

H -3.263311 1.156090 0.012838

H -4.147944 -0.366727 -0.549932

Frequencies

-1582.8610 70.4345 146.4537

209.7735 309.9308 369.8710

418.7003 522.6558 554.0331

583.8214 627.1536 699.5660

707.7762 748.5395 759.4151

846.0346 880.2618 926.1571

937.0175 941.0016 1000.4211

1005.7047 1024.8115 1038.7925

1065.8993 1088.5746 1172.8742

1189.0126 1261.2822 1285.2528

1328.3203 1362.8004 1374.7571

1416.1435 1448.2155 1465.4937

1518.0530 1556.7906 1656.3383

1677.1128 3092.0317 3103.4170

3130.3462 3137.8731 3138.7921

3165.7769 3189.0250 3221.0457

ts\_i7\_i8, C1, 2A

C -0.444104 1.390628 -0.284577

C -0.697360 0.136217 0.214675

C 1.183662 -1.508743 -0.118005

C 2.207191 -1.011297 -0.782725

C 1.608954 0.697373 0.482322

C 0.932213 1.741894 -0.114447

C 0.606405 -0.421477 0.762541

H -1.180130 2.037668 -0.746128

H 0.752720 -2.507099 -0.206918

H 2.900783 -1.360083 -1.539229

H 2.577562 0.759104 0.956316

H 1.369052 2.683228 -0.421129

H 0.521013 -0.693151 1.823268

C -1.931979 -0.615325 0.235239

C -3.105632 -0.262341 -0.317004

H -1.888580 -1.566012 0.763469

H -3.230414 0.662487 -0.869582

H -3.978105 -0.897715 -0.228178

Frequencies

-574.3953 50.7208 152.8396

190.7943 216.8712 279.5677

366.9806 473.9668 526.7288

610.5984 650.6725 676.2457

717.7431 740.1847 814.3447

838.0454 869.1592 887.1564

901.5120 906.3385 926.0803

953.8602 1004.8904 1015.1338

1044.1293 1064.3070 1097.2137

1156.6815 1210.6717 1229.8508

1263.8338 1287.5896 1323.7614

1382.0652 1404.3414 1459.2895

1553.7412 1637.6615 1643.4136

3007.6567 3082.6609 3124.1531

3140.1438 3186.2187 3187.1743

3203.8812 3224.6834 3225.0961

ts\_i7\_i23, C1, 2A

C -0.492024 1.289920 -0.300590

C -0.809503 -0.043527 0.213461

C 1.837905 -1.441162 -0.667326

C 2.429137 -0.322018 -0.301227

C 1.488329 0.433786 0.613316

C 0.802627 1.588814 -0.075828

C 0.356234 -0.586999 0.732018

C -2.097325 -0.698134 0.187724

C -3.238205 -0.191994 -0.308768

H -1.202755 1.934781 -0.801394

H 2.062339 -2.283240 -1.311503

H 3.400760 0.056887 -0.621021

H 1.933334 0.725224 1.574393

H 1.312938 2.494464 -0.376162

H 0.398794 -1.440329 1.394400

H -2.118992 -1.696658 0.618488

H -3.288288 0.794682 -0.755337

H -4.161178 -0.757932 -0.278540

Frequencies

-555.2147 86.5895 178.2566

204.9050 219.8175 277.3721

376.4159 470.4127 543.1000

610.7323 648.8291 679.6955

714.9328 744.7570 788.7779

814.3285 878.2981 890.0233

905.5451 906.5409 921.9705

952.8800 1000.6864 1016.0374

1019.9871 1035.8099 1109.2828

1186.1131 1198.8329 1235.4344

1255.6438 1301.6136 1319.5084

1372.3534 1440.7278 1485.9687

1591.4738 1635.2629 1641.2373

3004.5216 3085.6376 3133.4708

3142.9352 3189.7505 3191.1267

3210.3642 3214.6151 3225.2739

ts\_i18\_i19, C1, 2A

C -0.677451 -0.291054 0.112657

C -0.199023 1.010026 -0.117042

C 1.712898 0.969332 -0.450665

C 2.213098 -0.311469 -0.494521

C 1.537906 -1.387779 0.094997

C 0.183171 -1.360935 0.421176

C 0.956620 1.638600 0.598531

H -0.778067 1.671182 -0.752639

H 3.147163 -0.494002 -1.019138

H 2.066103 -2.332141 0.185913

H -0.270842 -2.293950 0.740436

H 1.154244 1.276662 1.611285

H 0.939766 2.726435 0.553480

C -2.101631 -0.594521 -0.098619

C -3.101263 0.290200 -0.182960

H -2.342187 -1.651369 -0.186344

H -2.944339 1.356360 -0.062306

H -4.117795 -0.033570 -0.372007

Frequencies

-400.6677 90.8130 187.6397

229.5231 262.7302 317.8392

433.1324 466.8930 500.5062

574.0220 603.7375 711.2944

740.2961 770.7043 850.5828

868.3079 886.8924 921.6878

929.3999 966.1593 1005.9441

1023.5233 1030.8944 1070.5350

1129.3922 1137.0451 1181.2906

1206.5684 1207.7424 1310.3439

1327.5244 1362.2507 1422.4869

1449.2682 1464.4051 1486.1714

1547.8514 1579.1357 1674.2216

3033.9103 3113.7697 3132.2436

3136.4493 3141.4671 3149.4808

3162.5016 3166.1319 3221.7287

ts\_i19\_i29, C1, 2A

C -1.025267 2.060336 0.363825

C 0.025621 0.772229 -0.439345

C 0.684700 -0.462971 -0.048943

C -0.151254 -1.586008 0.082649

C -1.544419 -1.517718 0.025982

C -2.179536 -0.249004 -0.016401

C -1.393216 0.830786 -0.300584

H -1.137244 2.138091 1.438993

H -0.825585 2.974886 -0.182723

H 0.547177 1.440395 -1.118384

H 0.316454 -2.552776 0.246376

H -2.129924 -2.422382 0.140033

H -3.214671 -0.130748 0.287073

C 2.122192 -0.571629 0.056957

C 2.994572 0.452774 0.085359

H 2.513357 -1.585283 0.118623

H 2.668769 1.486714 0.061828

H 4.061310 0.278336 0.151180

Frequencies

-551.1537 112.6732 192.9915

210.2745 244.4564 389.8905

436.7251 467.5363 536.6474

582.0512 604.7590 667.8908

699.8177 750.6796 772.6182

788.6967 851.7634 878.9985

888.2006 938.3958 949.6056

981.3825 1005.8483 1010.4154

1059.0639 1083.2231 1157.9903

1163.1504 1218.7655 1287.9980

1305.5576 1329.9797 1400.7594

1446.6432 1456.4733 1461.3726

1499.3091 1630.2988 1656.0178

3117.0757 3124.1569 3126.4696

3141.7986 3150.2821 3159.2317

3185.0683 3220.3362 3225.3286

ts\_i20\_i21, C1, 2A

C 0.011138 1.959221 0.488255

C 1.368069 1.055930 -0.351790

C 2.268035 -0.003769 0.026808

C 1.759343 -1.282266 0.131299

C 0.384218 -1.566133 -0.017972

C -0.549800 -0.513470 -0.121307

C -0.032836 0.763533 -0.335430

C -1.977625 -0.759436 0.102550

C -2.965077 0.110498 -0.131998

H -0.143097 1.869037 1.557465

H -0.016281 2.956967 0.064358

H 1.755509 1.893174 -0.926273

H 3.329143 0.184945 0.144477

H 2.437493 -2.104983 0.335707

H 0.038945 -2.591226 0.057099

H -2.226646 -1.744143 0.491804

H -2.770951 1.091467 -0.551040

H -3.996901 -0.139885 0.083916

Frequencies

-595.0478 80.9670 167.7185

181.3297 247.7415 353.9044

414.1921 490.5763 553.8252

583.2967 604.7048 685.5615

709.0942 719.5760 757.8191

798.7809 836.7042 874.1492

894.5852 938.3526 959.6904

975.0652 1021.4131 1032.8781

1047.7370 1093.0633 1141.8545

1179.7200 1214.5738 1226.3509

1330.9800 1338.2314 1397.6783

1440.7296 1449.9827 1455.9968

1538.9713 1596.4044 1677.9604

3108.7060 3112.6522 3131.3709

3142.4435 3154.0922 3171.1437

3180.3646 3212.8350 3225.5038

ts\_i8\_i9, C1, 2A

C 0.561203 -1.423439 -0.458587

C 0.610142 -0.182792 0.084996

C -1.548179 -1.129954 0.392751

C -0.764757 -2.004512 -0.263399

C -0.753459 0.117223 0.704382

H 1.372007 -1.914962 -0.981192

H -2.583647 -1.258501 0.675172

H -1.057502 -2.988495 -0.607136

H -0.615427 0.168177 1.794446

C -1.405722 1.427598 0.266085

C -1.741998 1.745171 -0.956818

H -1.605351 2.152405 1.063453

H -2.195868 2.577230 -1.473203

C 1.715169 0.763075 0.137271

C 3.014118 0.478295 -0.013755

H 1.433524 1.797925 0.320934

H 3.367483 -0.535764 -0.167666

H 3.765691 1.258003 0.017640

Frequencies

-122.4843 54.8626 115.3193

160.1972 228.2257 265.6872

371.6180 450.7882 543.7099

557.2685 651.7672 654.9307

688.6324 717.8490 811.9387

819.5795 832.3535 875.4490

891.8319 922.4252 955.5582

975.9761 1021.5734 1024.9855

1049.0963 1070.3983 1124.3922

1164.6683 1236.5803 1240.5786

1277.4154 1290.2328 1332.7662

1379.7262 1457.6893 1558.2685

1642.3992 1662.9421 1674.7281

2994.5989 3020.0722 3127.5854

3136.9157 3189.2118 3201.7665

3219.8889 3224.2034 3244.8993

ts\_i8\_p5, C1, 2A

C -0.548527 1.398171 -0.495466

C -0.702148 0.236393 0.232774

C 1.252718 -1.692154 -0.182142

C 2.374897 -1.611860 -0.692109

C 1.468057 1.089626 0.542821

C 0.794300 1.917931 -0.298057

C 0.576377 -0.023294 0.883372

C -1.869256 -0.620582 0.380782

C -3.005001 -0.575267 -0.327054

H -1.308880 1.873619 -1.100614

H 0.398732 -2.323480 -0.038095

H 3.318036 -1.228227 -1.006639

H 2.485412 1.194180 0.890590

H 1.177206 2.822157 -0.751871

H 0.651586 -0.560082 1.822808

H -1.791329 -1.375573 1.162304

H -3.157592 0.139375 -1.128737

H -3.821667 -1.255744 -0.119266

Frequencies

-617.5230 39.1525 47.2382

118.6822 142.8538 216.0117

235.8486 290.7261 463.9156

503.7226 538.6843 590.0143

629.0227 652.6472 701.0182

730.4425 765.4092 776.8366

787.7807 848.9383 910.8549

919.9210 925.3171 944.9578

988.4119 1024.7343 1036.0697

1064.2222 1126.6337 1171.3521

1262.2328 1279.3140 1333.7905

1379.8972 1454.4713 1499.9326

1582.6543 1674.1591 1821.3583

3110.7888 3137.8516 3171.1053

3198.6437 3211.5616 3221.3268

3230.1955 3320.2137 3433.1401

ts\_i8\_i12, C1, 2A

C -1.021514 1.396915 -0.090192

C -0.691496 0.038816 0.045001

C 1.570017 -1.255252 0.018338

C 2.861689 -1.289061 -0.219801

C 1.248638 1.348914 0.056151

C 0.131734 2.187200 -0.080124

C 0.738972 -0.047198 0.142755

C -1.599910 -1.097237 0.121509

C -2.917254 -1.085279 -0.113676

H -2.031300 1.784300 -0.113869

H 1.042026 -2.206417 0.136749

H 3.630835 -2.036160 -0.338979

H 2.298344 1.594464 -0.001491

H 0.165083 3.266549 -0.110790

H 1.071752 0.630916 1.183527

H -1.148177 -2.047476 0.396077

H -3.445665 -0.184572 -0.406385

H -3.508152 -1.988517 -0.024606

Frequencies

-1220.7620 56.0363 99.4302

165.0000 194.2749 245.8400

289.2228 396.4288 544.3221

571.2018 579.8015 599.2769

662.3956 697.0783 748.8675

772.8533 819.0729 847.0845

883.5818 898.6885 908.9555

923.6234 1010.2772 1015.7791

1057.9224 1079.3669 1122.8078

1194.6792 1254.8535 1265.2261

1292.5923 1334.3026 1370.5737

1430.5481 1458.1814 1486.5913

1522.7530 1655.0072 1679.1827

2073.3890 3043.7695 3132.5540

3140.9024 3203.7426 3221.9771

3223.4960 3240.9280 3249.8741

ts\_i8\_i15, C1, 2A

C 0.054038 -1.751706 -0.398075

C 0.580470 -0.641259 0.157888

C -0.530008 1.666482 0.199921

C -1.448019 2.263715 -0.514678

C -1.793135 -0.560869 0.262927

C -1.410015 -1.698936 -0.339170

C -0.572952 0.225068 0.669228

C 2.007933 -0.311826 0.347235

C 2.695892 0.563649 -0.384506

H 0.622964 -2.568096 -0.825616

H 0.360133 2.225839 0.506610

H -1.617762 3.242611 -0.937679

H -2.802996 -0.224039 0.449198

H -2.064645 -2.468456 -0.728047

H -0.507987 0.236488 1.770630

H 2.522472 -0.831534 1.155793

H 2.238590 1.100949 -1.208424

H 3.744006 0.760332 -0.187082

Frequencies

-103.8759 91.3945 106.3040

194.2209 207.0764 289.5986

371.8114 447.8722 548.5367

588.5643 623.0057 638.0889

694.6016 715.6162 809.5582

818.6411 854.6461 878.9499

901.0050 955.0941 958.7330

962.7380 1016.4077 1020.3797

1053.6176 1070.6170 1120.5839

1160.3137 1221.2002 1231.7789

1263.1145 1296.5895 1322.4093

1376.4119 1443.1078 1573.8518

1644.3365 1670.4603 1698.7515

2961.2706 3033.1303 3098.4214

3132.2675 3188.4071 3200.9442

3216.5275 3225.7090 3237.8305

ts\_i12\_i24, C1, 2A

C 0.797532 1.457080 -0.121150

C 0.710573 0.017704 0.167740

C -1.459612 -1.428875 0.153132

C -2.585259 -1.097268 -0.478819

C -1.414369 0.995442 0.245811

C -0.442549 2.021281 -0.134603

C -0.615238 -0.261599 0.374136

C 1.796379 -0.944255 0.100805

C 3.075869 -0.677572 -0.190136

H 1.725685 1.989464 -0.286537

H -1.182804 -2.444676 0.424118

H -3.435317 -1.641801 -0.868692

H -2.078705 1.251139 1.074701

H -2.315901 0.391686 -0.491689

H -0.657594 3.075021 -0.246387

H 1.522090 -1.973367 0.321115

H 3.421635 0.324413 -0.418262

H 3.820949 -1.463509 -0.209860

Frequencies

-1875.6367 90.7229 166.6228

204.7368 218.8746 313.4827

354.4090 485.4341 537.7831

575.8296 599.5818 633.6673

667.3136 719.8624 729.2418

773.6785 850.5752 865.5729

909.0918 917.9650 925.4551

932.0440 1000.9077 1021.0557

1023.2902 1036.4253 1121.2668

1177.7753 1224.8166 1253.6432

1291.9393 1324.5007 1334.0151

1397.2709 1449.9739 1495.5462

1555.0543 1589.5526 1657.7836

1682.7564 3084.5836 3132.2932

3137.9901 3143.4413 3192.8933

3211.2740 3218.2843 3224.4633

ts\_i12\_i13, C1, 2A

C -1.119173 1.367608 -0.130130

C -0.588637 -0.000622 0.036295

C 1.188000 1.524709 0.080927

C -0.112105 2.254359 -0.105905

C 0.764109 0.078544 0.160717

C -1.376027 -1.225902 0.059890

C -2.708122 -1.305188 -0.028076

H -2.167342 1.603276 -0.258012

H 1.883371 1.686555 -0.753943

H 1.722201 1.846393 0.985398

H -0.193170 3.328029 -0.208146

H -0.802439 -2.144148 0.154469

H -3.336985 -0.427597 -0.128347

H -3.214588 -2.262596 -0.002251

C 1.727202 -1.026951 0.381661

C 2.403742 -1.644471 -0.555073

H 1.897404 -1.327307 1.425892

H 3.137612 -2.435116 -0.616897

Frequencies

-135.3508 99.5860 147.7975

173.5675 222.9188 278.1724

338.8342 430.9417 489.0237

539.0255 575.0530 664.4891

669.0772 686.6960 778.2591

830.7642 839.4244 865.0625

925.5673 926.7592 944.1802

962.9939 1002.4586 1032.9822

1034.1992 1122.0641 1135.3585

1175.1705 1247.1233 1251.4363

1315.3537 1330.8302 1400.5853

1416.9837 1452.1926 1575.0371

1634.1078 1666.5257 1694.9067

2974.3675 3008.3756 3029.8454

3139.1408 3147.4216 3196.2907

3218.6190 3222.9852 3231.0782

ts\_i12\_p6, C1, 2A

C -1.232646 1.294466 -0.028817

C -0.611900 -0.038282 0.002269

C 1.761374 -0.869017 0.054085

C 2.786458 -1.477609 -0.214797

C 1.072218 1.602923 0.031089

C -0.283297 2.244956 -0.012237

C 0.747259 0.126532 0.035021

C -1.315695 -1.309963 -0.011838

C -2.644335 -1.463972 -0.049716

H -2.299711 1.467309 -0.062307

H 1.207558 -1.815371 1.569950

H 3.625791 -2.127086 -0.281286

H 1.693007 1.875496 -0.831909

H 1.642810 1.891486 0.923121

H -0.441951 3.314656 -0.028080

H -0.684670 -2.193368 0.011236

H -3.327913 -0.622740 -0.073668

H -3.091531 -2.450591 -0.057414

Frequencies

-810.3975 68.6799 96.1381

156.1630 179.4426 229.3438

245.6461 360.8314 425.6029

478.3199 487.0818 528.5318

556.4029 590.3461 623.9221

664.8188 690.3235 695.0706

783.3466 852.6733 918.1580

935.7156 949.7142 964.3264

1002.5130 1028.3723 1035.4635

1129.5732 1137.8577 1178.0373

1254.0193 1318.5978 1332.0158

1406.8288 1419.7682 1451.3307

1555.1191 1629.1137 1683.9014

2071.1326 3019.1215 3042.8617

3142.0162 3156.4919 3201.0326

3222.1517 3226.3862 3456.7846

ts\_i22\_p1, C1, 2A

C -1.607949 -1.164018 -0.095230

C -0.181034 -0.688541 -0.037569

C 1.002362 -1.403788 0.010782

C 2.207230 -0.705014 0.046461

C 2.222873 0.688543 0.033924

C 1.036779 1.411793 -0.011437

C -0.166733 0.714958 -0.045603

C -1.547125 1.185822 -0.089644

C -2.387513 0.128385 -0.070659

H -1.807451 -1.715616 -1.021774

H -1.865112 -1.827519 0.735425

H 0.997628 -2.488773 0.020365

H 3.143873 -1.249712 0.084403

H 3.171754 1.212290 0.062494

H 1.051128 2.496289 -0.018205

H -1.840342 2.227345 -0.116764

H -3.462062 0.175735 -0.183303

H -2.862760 0.161113 1.991210

Frequencies

-509.1612 171.4102 201.4371

270.3477 328.3951 393.4539

421.5341 429.3583 547.5512

564.1421 608.6282 735.8967

746.8962 751.8601 805.9672

851.2615 876.1800 879.5423

942.4887 962.9006 964.0062

982.1582 1006.5886 1051.8665

1088.5700 1138.2882 1164.8278

1185.1220 1199.3829 1242.4375

1260.3576 1323.4311 1349.2504

1396.7592 1441.0198 1503.7712

1510.4779 1591.8563 1659.6370

1685.9189 3056.8469 3103.5838

3189.6321 3197.1903 3207.4356

3219.5873 3220.7705 3244.1482

ts\_i18\_p10, C1, 2A

C 1.966325 0.874829 -0.222746

C 0.962441 1.638934 0.219329

C -0.359188 1.161103 -0.152224

C 2.314888 -0.373654 -0.499557

C -0.698489 -0.162871 -0.030597

C 1.539494 -1.383912 0.201700

C 0.195150 -1.243663 0.377917

C -2.103951 -0.585240 -0.250666

C -3.197321 0.143061 -0.018308

H 1.098876 2.575472 0.750811

H 1.118515 0.913732 2.318799

H -1.121891 1.866919 -0.471054

H 3.062263 -0.648745 -1.238031

H 2.009397 -2.310763 0.524629

H -0.318426 -2.098978 0.810974

H -2.231154 -1.602578 -0.614379

H -3.148513 1.145370 0.393388

H -4.185161 -0.251950 -0.224220

Frequencies

-388.0486 75.2581 152.1784

211.3132 236.9111 242.7208

294.7233 359.6404 385.2723

413.4131 467.0739 513.8946

604.3309 643.4071 715.7162

721.0663 778.1120 816.0056

831.6012 891.4464 915.9532

949.4344 985.8785 1026.1237

1030.1412 1045.5972 1061.8530

1133.5865 1163.2853 1232.3500

1302.5943 1325.6799 1359.2603

1381.3176 1440.7721 1456.9368

1546.9057 1608.1808 1684.5381

1838.0895 3120.4259 3128.6412

3137.3442 3138.8770 3140.8026

3145.5038 3149.5618 3220.8646

ts\_i9\_i16, C1, 2A

C -0.828331 -1.505431 -0.451283

C 0.117052 -0.749944 0.147181

C -1.987330 0.357599 0.213178

C -2.120121 -0.815044 -0.427777

C -0.548571 0.524713 0.657049

C 0.021985 1.860436 0.214621

C 0.930307 2.076249 -0.698850

H -0.666486 -2.488944 -0.874760

H -2.751303 1.104341 0.380875

H -3.031773 -1.206650 -0.860923

H -0.516442 0.503402 1.758740

H -0.427959 2.724283 0.719872

H 1.431201 2.928349 -1.133314

C 1.508893 -1.153534 0.443116

C 2.605375 -0.700976 -0.161231

H 1.624411 -1.902322 1.227412

H 2.554213 0.033363 -0.956998

H 3.588576 -1.060221 0.123071

Frequencies

-130.7365 83.3554 151.5401

158.7588 225.1520 266.6757

369.0154 462.2993 532.9015

569.9313 619.2748 664.3738

678.6182 712.6428 810.6336

819.9160 839.4667 874.4652

900.2330 952.1129 958.3470

984.0524 1013.4784 1023.6645

1029.7295 1071.8494 1122.5453

1162.1881 1212.6447 1232.5833

1269.8209 1303.3023 1326.2115

1374.8361 1439.9677 1569.0821

1641.7009 1678.2377 1700.6205

2971.1044 3007.1030 3094.6665

3131.3244 3187.0981 3198.9370

3217.3179 3218.7426 3239.5217

ts\_i22\_p9, C1, 2A

C 1.539822 1.110549 -0.116682

C 0.246343 0.701367 -0.076168

C -0.993621 1.436528 -0.092733

C -2.158949 0.757490 -0.033880

C -2.198330 -0.691548 0.047191

C -1.071200 -1.433771 0.062883

C 0.207363 -0.767962 -0.002938

C 1.473786 -1.247263 -0.012583

C 2.424126 -0.096676 -0.099336

H 1.896085 2.127258 -0.207661

H -0.976783 2.519245 -0.150238

H -3.101201 1.294240 -0.045067

H -3.167559 -1.175329 0.096721

H -1.112541 -2.515652 0.124770

H 1.774255 -2.285080 0.034735

H 3.035125 -0.151055 -1.011244

H 3.131933 -0.082312 0.739120

H 1.704651 1.656399 2.364342

Frequencies

-299.8524 118.4147 147.9589

194.9096 216.7325 319.0560

391.0623 465.8835 516.4454

548.8214 578.0047 698.1618

716.0817 733.0937 774.2602

793.7302 847.9345 857.9359

899.3351 905.6905 947.4853

989.2941 996.4026 1008.9537

1012.9353 1116.9794 1154.1302

1186.8938 1191.5133 1236.7271

1250.4613 1302.3403 1394.8011

1406.6955 1414.4951 1461.5911

1554.4603 1612.6131 1645.6438

1730.9058 3037.5005 3075.7792

3189.0340 3196.2712 3209.5437

3218.8209 3237.1054 3243.0615

ts\_i19\_i20, C1, 2A

C 0.644037 -0.481656 0.055027

C 0.079247 0.837810 0.355046

C -1.427609 1.009786 0.334070

C -2.255040 -0.137683 0.036790

C -1.672519 -1.361831 -0.067977

C -0.227115 -1.528047 -0.069314

C -0.549247 1.920681 -0.470736

C 2.082440 -0.668921 -0.081664

C 2.991876 0.302200 0.066562

H -0.709948 1.007249 1.376898

H -3.330699 -0.026512 -0.060820

H -2.284358 -2.245287 -0.217097

H 0.165343 -2.527009 -0.234926

H -0.557412 1.726220 -1.540019

H -0.434627 2.968014 -0.208581

H 2.410276 -1.676204 -0.329029

H 2.694947 1.311676 0.326979

H 4.050052 0.107826 -0.060225

Frequencies

-1913.1886 85.0056 166.7101

181.2276 249.9574 301.0356

425.0402 480.7608 508.6567

545.8866 574.5050 671.0751

717.1107 735.7258 769.1933

798.2193 909.8064 919.9326

943.8501 967.1376 977.2635

994.6447 1002.1386 1018.7891

1043.7083 1084.2024 1144.0367

1174.7996 1193.7337 1229.1559

1317.3446 1332.1755 1386.5600

1440.0651 1453.2917 1507.7058

1523.4466 1596.6895 1668.7918

2282.0232 3094.6776 3131.6664

3144.5075 3145.8611 3153.8983

3172.0170 3174.7425 3230.6723

ts\_i15\_i16, C1, 2A

C 0.757184 -1.574814 0.481227

C -0.255358 -0.784298 0.044360

C 1.842953 0.153185 -0.554252

C 2.046391 -0.994508 0.115727

C 0.355852 0.411251 -0.682762

C -1.668777 -1.056988 0.194621

C -2.684285 -0.332789 -0.294235

H 0.631621 -2.509123 1.015015

H 2.592321 0.827345 -0.944936

H 3.006958 -1.432715 0.354267

H 0.080521 0.339805 -1.743577

H -1.901484 -1.954311 0.764811

H -2.525473 0.571982 -0.869593

H -3.713135 -0.627451 -0.126943

C -0.068996 1.792581 -0.184182

C 0.089333 2.250364 1.029622

H -0.532825 2.447332 -0.930550

H -0.124283 3.153231 1.580751

Frequencies

-113.0440 91.2318 147.6148

168.9473 223.6207 296.4710

377.9297 465.6869 543.2506

582.4105 601.4258 657.7461

692.4300 723.1279 810.4067

815.2525 830.8091 878.4910

891.2055 910.7048 954.7795

969.5364 1021.6100 1026.0023

1040.6611 1047.0135 1126.5762

1199.8338 1235.8681 1243.8376

1288.2379 1311.2218 1330.4724

1384.9935 1448.9783 1558.2939

1630.8306 1664.8970 1680.0149

3008.4697 3023.6772 3125.6987

3143.7408 3187.4120 3200.0564

3223.5622 3224.5348 3247.1392

ts\_i16\_i10, C1, 2A

C 1.425289 1.233063 -0.347542

C 0.192831 0.802182 0.056218

C 1.785035 -0.929637 0.315702

C 2.399692 0.169247 -0.169715

C 0.317708 -0.637114 0.521323

C -1.071499 1.455748 -0.071204

C -0.634051 -1.600523 -0.203283

C -1.861628 -1.323756 -0.568911

C -2.227183 0.940630 0.427782

H 1.645005 2.211564 -0.756207

H 2.244282 -1.880317 0.551830

H 3.453449 0.258305 -0.401345

H 0.095259 -0.699157 1.598685

H -1.114522 2.338255 -0.704263

H -0.218970 -2.593057 -0.399574

H -2.645056 -1.884259 -1.058877

H -3.184299 1.392433 0.194893

H -2.232312 0.197198 1.212632

Frequencies

-329.6674 127.7882 152.8457

238.0315 286.4221 344.9020

458.3654 470.8490 544.0990

573.0685 623.6273 638.8014

695.4055 718.1765 815.1418

822.4623 833.6958 864.9279

877.6769 889.5167 954.0956

966.2302 986.9486 1029.9720

1038.2486 1044.7209 1120.4045

1184.0708 1208.2085 1237.6308

1253.1025 1284.2922 1331.7633

1387.8139 1439.9672 1507.8567

1582.3237 1613.6084 1645.0414

2972.6761 3046.7339 3139.3925

3153.5189 3187.8811 3198.8178

3216.6814 3224.0704 3235.2102

ts\_i6\_i28, C1, 2A

C 2.129316 0.884920 0.271045

C 2.318478 -0.457859 0.262186

C 1.390810 -1.470238 -0.191107

C 0.050421 -1.374537 -0.315797

C -0.790314 -0.206353 0.032611

C -0.299469 1.136647 -0.326276

C 0.960286 1.607174 -0.171981

C -2.185637 -0.423999 0.312237

C -3.362464 0.158123 0.105012

H 2.973616 1.499303 0.570773

H 3.300375 -0.819985 0.553301

H 1.836865 -2.425870 -0.453395

H -0.489132 -2.240261 -0.688596

H -1.056655 1.826070 -0.686994

H 1.120270 2.657201 -0.401781

H -3.537262 0.786842 -0.771889

H -4.216388 -0.012631 0.751662

H -1.200248 -0.393934 1.259331

Frequencies

-1827.8852 60.3512 139.5234

216.2241 271.6956 314.4094

387.6808 428.6567 454.1585

512.9951 588.6559 632.7353

661.5014 735.7614 768.3666

830.9682 834.6187 869.7262

891.8385 942.1011 983.9484

984.6023 1001.3530 1007.0176

1010.2891 1051.7282 1150.4815

1199.3082 1243.0214 1269.9887

1296.0829 1397.1916 1431.6525

1447.0837 1480.7587 1579.8846

1621.5095 1647.2697 1676.2504

2020.6955 3045.5031 3131.5632

3136.6549 3144.7112 3156.8015

3161.5895 3166.7791 3169.6264

ts\_i27\_p3, C1, 2A

C 1.620999 -1.193483 -0.036104

C 0.337529 -0.746207 -0.049887

C 1.783772 1.104720 0.060458

C 2.509237 -0.040546 0.031623

C 0.379292 0.728039 0.006297

C -0.930706 -1.415090 -0.092772

C -2.075547 -0.697958 -0.066123

C -0.745026 1.454355 -0.010596

C -2.086800 0.803049 -0.103913

H 1.943015 -2.225810 -0.066289

H 2.160323 2.116279 0.110074

H 3.589290 -0.105154 0.056785

H -0.963672 -2.499247 -0.117399

H -2.436665 -0.933781 2.064994

H -3.034661 -1.196243 -0.150146

H -0.712033 2.539793 0.024735

H -2.739659 1.195154 0.685279

H -2.562437 1.127735 -1.041932

Frequencies

-534.6614 145.9587 173.0658

263.6998 296.4375 331.2752

390.7181 452.1236 532.5879

561.5554 590.0777 673.3193

733.7536 754.5212 792.9505

837.4243 845.1294 867.4990

871.9375 902.6445 950.8941

965.1396 996.5900 1011.9628

1034.9672 1101.0766 1172.8996

1179.3071 1206.7902 1230.3440

1293.9136 1372.0850 1382.1233

1410.8720 1436.3090 1437.8674

1533.1622 1618.8447 1652.8132

1747.5305 3014.5943 3061.5336

3184.8989 3191.3401 3210.7939

3222.9310 3236.3510 3254.8785

ts\_i6\_p7, C1, 2A

C 2.129316 0.884920 0.271045

C 2.318478 -0.457859 0.262186

C 1.390810 -1.470238 -0.191107

C 0.050421 -1.374537 -0.315797

C -0.790314 -0.206353 0.032611

C -0.299469 1.136647 -0.326276

C 0.960286 1.607174 -0.171981

C -2.185637 -0.423999 0.312237

C -3.362464 0.158123 0.105012

H 2.973616 1.499303 0.570773

H 3.300375 -0.819985 0.553301

H 1.836865 -2.425870 -0.453395

H -0.489132 -2.240261 -0.688596

H -1.056655 1.826070 -0.686994

H 1.120270 2.657201 -0.401781

H -3.537262 0.786842 -0.771889

H -4.216388 -0.012631 0.751662

H -1.200248 -0.393934 1.259331

Frequencies

-1827.8852 60.3512 139.5234

216.2241 271.6956 314.4094

387.6808 428.6567 454.1585

512.9951 588.6559 632.7353

661.5014 735.7614 768.3666

830.9682 834.6187 869.7262

891.8385 942.1011 983.9484

984.6023 1001.3530 1007.0176

1010.2891 1051.7282 1150.4815

1199.3082 1243.0214 1269.9887

1296.0829 1397.1916 1431.6525

1447.0837 1480.7587 1579.8846

1621.5095 1647.2697 1676.2504

2020.6955 3045.5031 3131.5632

3136.6549 3144.7112 3156.8015

3161.5895 3166.7791 3169.6264

1-cyanoindene

C -2.330911 0.813445, -0.871641

C -2.254490 -0.565650 -0.671132

C -1.032977 -1.176039 -0.367953

C 0.094049 -0.378663 -0.274145

C 0.027002 1.010091 -0.483268

C -1.192289 1.615129 -0.780104

C 1.533843 -0.745487 0.065882

C 2.250543 0.595561 -0.044194

C 1.374597 1.568137 -0.335387

C 2.104718 -1.786206 -0.790192

N 2.557655 -2.612069 -1.454820

H -3.287660 1.266618 -1.105277

H -3.149854 -1.170734 -0.753449

H -0.975313 -2.248857 -0.220555

H -1.257310 2.685485 -0.940863

H 1.592081 -1.107152 1.102318

H 3.314636 0.697278 0.113968

H 1.615522 2.617555 -0.447427

2-cyanoindene

C -3.038587 0.592999 -0.938816

C -2.961131 -0.790941 -0.760558

C -1.747995 -1.406371 -0.439258

C -0.617147 -0.616511 -0.299792

C -0.694225 0.780098 -0.479454

C -1.906512 1.392793 -0.800224

C 0.804008 -0.992947 0.036052

C 1.507925 0.352037 0.022334

C 0.632741 1.342721 -0.273524

C 2.890006 0.505563 0.287701

N 4.021695 0.602548 0.509078

H -3.990810 1.047305 -1.187601

H -3.854275 -1.394898 -0.873168

H -1.699675 -2.481430 -0.303124

H -1.967757 2.466462 -0.938622

H 1.240755 -1.680149 -0.697335

H 0.889376 -1.478094 1.014987

H 0.880890 2.393450 -0.346114

3-cyanoindene

C -2.313668 -0.064771 -0.718521

C -2.254814 -1.431721 -0.438376

C -1.037759 -2.048665 -0.135590

C 0.115025 -1.277648 -0.118064

C 0.050102 0.098222 -0.400944

C -1.159304 0.717421 -0.702947

C 1.548961 -1.654759 0.168640

C 2.281570 -0.349598 0.017237

C 1.418506 0.638644 -0.306544

C 1.755145 2.003578 -0.528027

N 1.998540 3.117506 -0.715043

H -3.268195 0.393439 -0.950798

H -3.164381 -2.021230 -0.456188

H -1.002275 -3.111193 0.080690

H -1.202498 1.778744 -0.919848

H 1.930881 -2.411620 -0.528052

H 1.679204 -2.070828 1.175739

H 3.347877 -0.232533 0.151526

4-cyanoindene

C -2.368414 -0.171496 -0.838086

C -2.270800 -1.551382 -0.701041

C -1.035103 -2.160448 -0.449394

C 0.095545 -1.368466 -0.337880

C 0.012797 0.030574 -0.474333

C -1.225980 0.639432 -0.726363

C 1.535937 -1.736793 -0.074760

C 2.228155 -0.396691 -0.082342

C 1.350547 0.596663 -0.310275

C -1.325653 2.057861 -0.867006

N -1.394838 3.206168 -0.979083

H -3.327629 0.292011 -1.032547

H -3.163166 -2.159320 -0.790653

H -0.972346 -3.238402 -0.344414

H 1.937036 -2.408418 -0.843821

H 1.660284 -2.254701 0.884351

H 3.291521 -0.278040 0.077292

H 1.575235 1.653264 -0.367400

5-cyanoindene

C -1.668340 0.588907 -0.764684

C -1.575011 -0.804281 -0.613944

C -0.337170 -1.407058 -0.393496

C 0.797256 -0.612633 -0.325899

C 0.707107 0.787197 -0.477371

C -0.522221 1.397366 -0.696960

C 2.243206 -0.980992 -0.102621

C 2.937860 0.358595 -0.146482

C 2.054912 1.349076 -0.359482

C -2.947796 1.190055 -0.989589

N -3.980630 1.675270 -1.170894

H -2.474666 -1.403945 -0.670891

H -0.274488 -2.483674 -0.278298

H -0.609835 2.470647 -0.814615

H 2.618138 -1.663963 -0.875051

H 2.394433 -1.488871 0.858126

H 4.005854 0.476015 -0.020679

H 2.284506 2.404099 -0.434355

6-cyanoindene

C -1.851404 0.573020 -0.879545

C -1.762632 -0.815046 -0.679889

C -0.522274 -1.419541 -0.398512

C 0.602221 -0.621167 -0.323564

C 0.512962 0.772949 -0.524728

C -0.716103 1.371716 -0.802936

C 2.041966 -0.978272 -0.043818

C 2.732673 0.361276 -0.111853

C 1.853242 1.341624 -0.384976

C -2.940841 -1.620358 -0.763102

N -3.892312 -2.273295 -0.829828

H -2.817185 1.013429 -1.094243

H -0.470474 -2.491491 -0.247219

H -0.792604 2.441909 -0.957770

H 2.444069 -1.684281 -0.780892

H 2.166945 -1.451631 0.937966

H 3.796050 0.487183 0.042461

H 2.083465 2.394184 -0.488184

7-cyanoindene

C -2.344339 1.341586 -0.906203

C -2.254079 -0.041443 -0.786896

C -1.012366 -0.650930 -0.525729

C 0.120140 0.151279 -0.389494

C 0.017447 1.549528 -0.512587

C -1.213716 2.149678 -0.770880

C 1.555272 -0.214720 -0.114023

C 2.237356 1.131418 -0.097162

C 1.354647 2.119003 -0.324304

C -0.914469 -2.073051 -0.402581

N -0.820666 -3.220300 -0.301043

H -3.308365 1.794148 -1.107008

H -3.135915 -0.660506 -0.893524

H -1.296661 3.226707 -0.865493

H 1.965854 -0.879513 -0.883926

H 1.668122 -0.747704 0.838159

H 3.297921 1.253527 0.077113

H 1.576865 3.177525 -0.365056

**Table S5.** Key parameters exploited for the astrochemical simulations.

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Parameter** | **Value** |
| density | ngas | 1.0 × 104 cm-3 |
| temperature gas | Tgas | 10 K |
| temperature dust | Tdust | 10 K |
| extinction | Av | 10 mag |
| ionization rate I | ζcr | 1.3 × 10-17 s-1 |
| ionization rate II | ζcr | 1.3 × 10-16 s-1 |

**Table S6.** Initial elemental abundances from Hincelin et al.

|  |  |
| --- | --- |
| Element | Initial Abundance |
| H2 | 4.990E-01 |
| H | 5.000E-05 |
| He | 9.000E-02 |
| C | 1.700E-04 |
| N | 6.200E-05 |
| O | 1.400E-04 |
| S | 8.000E-08 |
| Na | 2.000E-09 |
| Mg | 7.000E-09 |
| Si | 8.000E-09 |
| P | 2.000E-10 |
| Cl | 1.000E-09 |
| Fe | 3.000E-09 |
| F | 6.680E-09 |

**Table S7.** List of key new gas phase neutral – neutral reactions incorporated in our model.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Number** | **Reaction** | **α cm3s-1** | **β** | **γ** | **Source** |
| 1 | CH + C6H5C2H3 → H + C9H8 | (3.0-5.0)E-10 | 0.0E+00 | 0.0E+00 | this work |
| 2 | CH + C6H5CH3 → C6H5C2H3 + H | (2.0-4.0)E-10 | 0.0E+00 | 0.0E+00 | ([*43*](#_ENREF_43)) |
| 3 | CCH + C5H8 → C6H5CH3 + H | (2.0-4.0)E-10 | 0.0E+00 | 0.0E+00 | analogues reaction of CCH with 1,3-butadiene ([*97-99*](#_ENREF_97)) |
| 4 | CCCH3 + CH2CHCHCH2 → C6H5CH3 + H | (2.0-4.0)E-10 | 0.0E+00 | 0.0E+00 | analogues reaction of CCH with 1,3-butadiene ([*97-99*](#_ENREF_97)) |
| 5 | C9H8 + C → C10H7 + H | 1.0E-10 | 0.0E+00 | 0.0E+00 | analogues reaction of benzene with carbon ([*100*](#_ENREF_100)*,* [*101*](#_ENREF_101)) |
| 6 | C9H8 + C2 → C11H7 + H | 1.0E-10 | 0.0E+00 | 0.0E+00 | analogues reaction of benzene with dicarbon ([*102*](#_ENREF_102)*,* [*103*](#_ENREF_103)) |
| 7 | C9H8 + CN → C9H7CN + H | 1.0E-10 | 0.0E+00 | 0.0E+00 | analogues reaction of benzene with cyano radicals([*57*](#_ENREF_57)*,* [*104*](#_ENREF_104)) |
| 8 | C9H8 + CCH → C11H8 + H | 1.0E-10 | 0.0E+00 | 0.0E+00 | analogues reaction of benzene with ethynyl radicals ([*105*](#_ENREF_105)*,* [*106*](#_ENREF_106)) |