**Supporting Information**

for

A Combined Crossed Beam and Ab Initio Investigation of the Gas Phase Reaction of Dicarbon Molecules (C2; X1Σg+/a3Πu) with Propene (C3H6; X1A’)

by

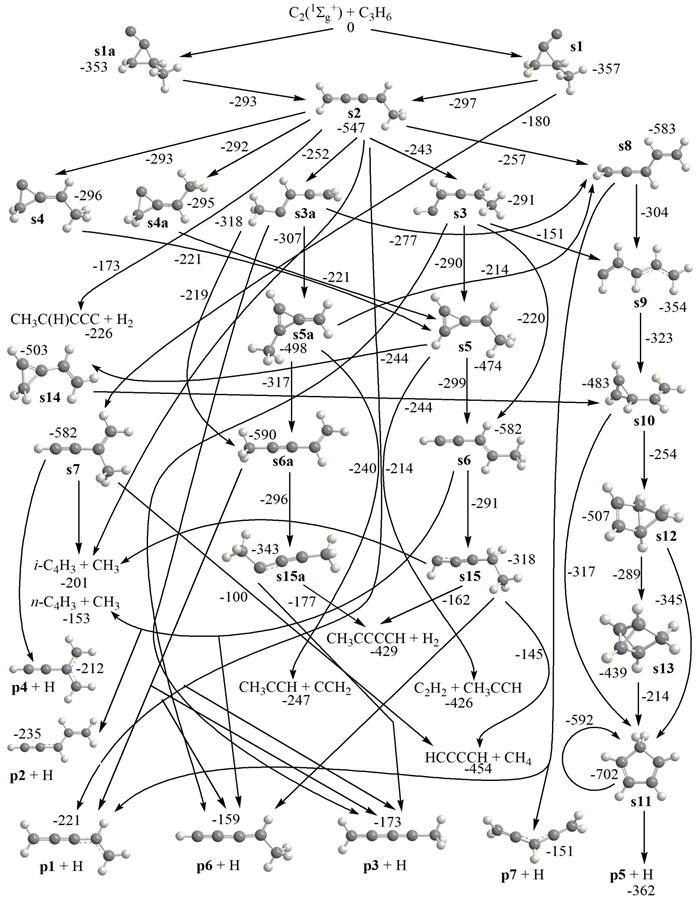
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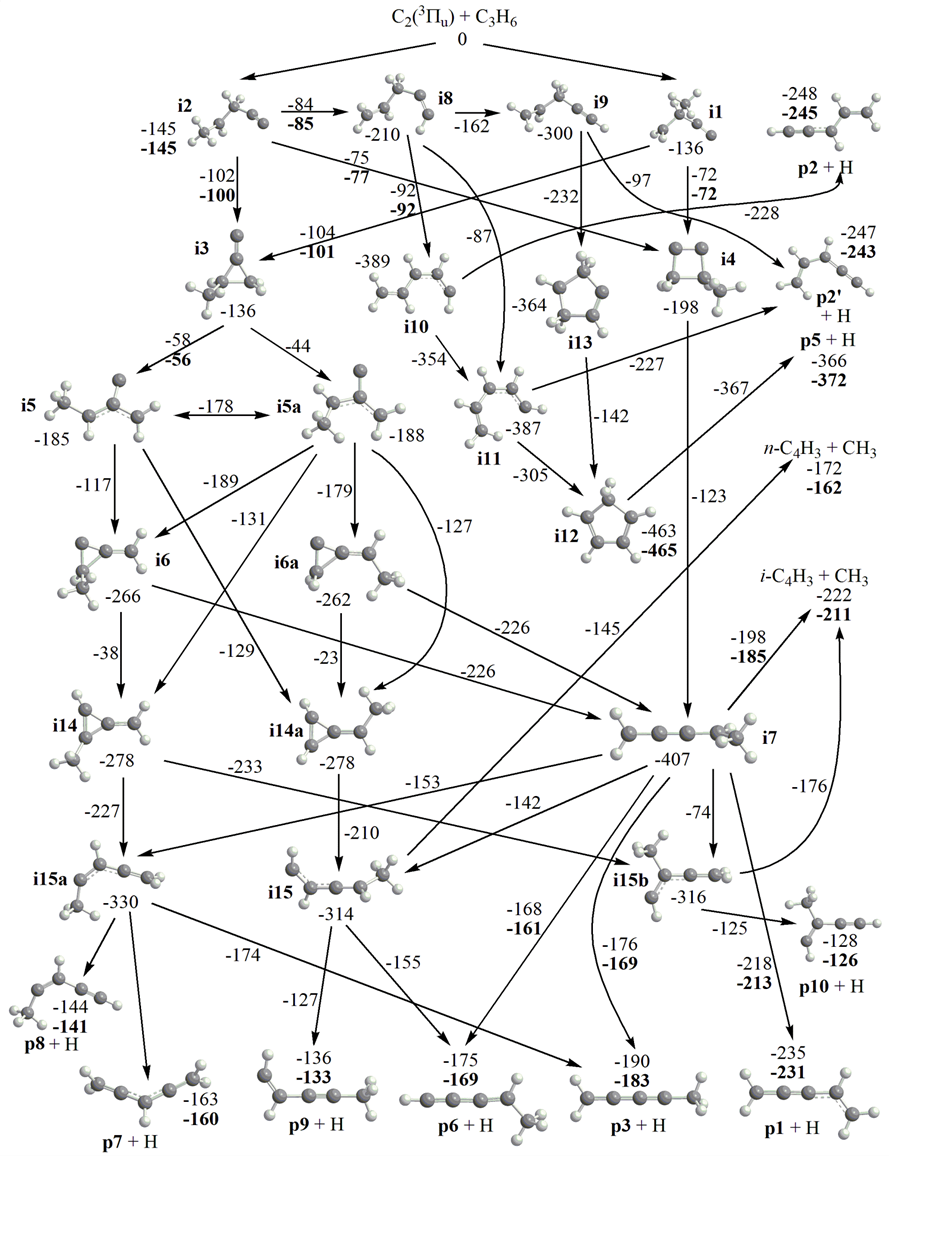
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**Figure S1.** Potential energy map of the C2(X1Σg+) + C3H6 reaction. Numbers show relative energies of intermediates and transition states (next to arrows) in kJmol-1. Unmarked arrows indicate association and dissociation processes without distinct barriers.



**Figure S2.** Potential energy map of the C2(X3Πu) + C3H6 reaction. Numbers show relative energies of intermediates and transition states (next to arrows) in kJmol-1. Unmarked arrows indicate association and dissociation processes without distinct barriers. Plain and bold numbers are computed at the CCSD(T)/CBS level with 2- and 3-point extrapolation, respectively.

**Table S1.** Optimized Cartesian coordinates, rotational constants, and vibrational frequencies of various intermediates and products involved in the reactions.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Species | Rotational  Constants,  GHz | Cartesian Coordinates, Å | | | | Vibrational Frequencies,  cm-1 | | |
| Atom | x | y | z |
| **s1** | 8.57500  5.56665  3.86903 | 6  6  6  6  6  1  1  1  1  1  1 | -1.080334  -1.245391  0.354459  -0.481751  1.614203  0.309584  -0.115885  -0.977414  2.452120  1.514288  1.850194 | -0.096630  -1.341311  0.147036  1.229291  -0.327785  0.065454  1.668860  1.931372  0.313976  -0.290211  -1.353060 | -0.209867  -0.027328  0.501739  -0.109955  -0.169355  1.581249  -1.034544  0.554737  0.125744  -1.255855  0.117263 | 139.0  205.5  240.9  361.6  396.1  690.6  769.8  891.5  968.5 | 1011.5  1056.7  1073.6  1120.7  1182.6  1185.3  1379.1  1421.0  1477.0 | 1489.2  1498.7  1948.5  3024.7  3094.1  3094.5  3123.0  3167.3  3179.3 |
| **s1a** | 12.62814  4.14197  3.61137 | 6  6  6  6  6  1  1  1  1  1  1 | -0.764168  -1.950211  0.518596  -0.488362  1.762558  0.676516  -0.366704  -1.012940  2.538382  1.539554  2.154711 | -0.505061  -0.676186  0.141768  1.018635  -0.319288  0.372267  1.210687  1.766655  0.448851  -0.523206  -1.234464 | 0.222814  -0.202371  0.498564  -0.184976  -0.239798  1.550762  -1.243088  0.394121  -0.187184  -1.288654  0.208647 | 108.7  180.0  231.4  364.6  445.6  719.2  781.3  879.2  931.1 | 961.4  1036.6  1079.4  1138.3  1176.3  1183.7  1383.4  1417.8  1481.1 | 1492.0  1501.3  1929.8  3038.1  3102.1  3105.9  3121.5  3140.1  3244.7 |
| **s2** | 30.49866  2.20741  2.08492 | 6  6  6  6  6  1  1  1  1  1  1 | -0.080953  1.208749  -1.320058  -2.608413  2.303238  1.521081  -2.978111  -3.348211  2.944684  1.898557  2.946611 | -0.295861  -0.562373  -0.040482  0.223020  0.468264  -1.606066  1.243720  -0.571563  0.349876  1.480680  0.347944 | 0.000032  -0.000045  0.000004  -0.000018  -0.000004  -0.000029  -0.000071  0.000116  0.880502  -0.001511  -0.878821 | 139.7  144.9  228.1  313.1  487.9  528.8  571.9  800.8  844.6 | 867.7  1029.1  1040.2  1049.8  1107.7  1322.0  1402.9  1446.8  1480.7 | 1489.4  1699.3  2198.6  3013.1  3056.3  3104.5  3116.3  3122.8  3190.8 |
| **s3** | 17.64872  2.57754  2.44067 | 6  6  6  6  6  1  1  1  1  1  1 | -1.083972  0.169572  1.462116  2.207890  -2.142447  -1.389689  1.814185  3.149323  -2.940495  -2.589447  -1.722825 | -0.468557  -0.439387  -0.346019  0.648639  0.478705  -1.232200  -0.959309  0.801502  -0.076648  1.026898  1.199466 | -0.330404  -0.010758  0.328839  -0.376427  0.183415  -1.045029  1.166352  0.192189  0.684213  -0.650450  0.884731 | 69.4  145.9  216.1  250.3  384.5  524.8  647.3  766.4  856.2 | 918.2  1038.3  1056.4  1088.3  1151.2  1184.2  1299.8  1406.0  1417.3 | 1484.9  1493.4  1982.1  2909.0  3020.4  3032.1  3087.0  3113.6  3131.2 |
| **s3a** | 33.72615  2.29172  2.20754 | 6  6  6  6  6  1  1  1  1  1  1 | -2.518517  -1.270683  0.014418  0.988008  2.379833  -3.073489  -3.037217  0.261397  3.065381  2.679276  2.546304 | -0.188318  0.151250  0.492816  -0.564260  -0.054460  -0.317074  -0.370825  1.565278  -0.663241  -0.256071  1.019763 | 0.014652  -0.000622  -0.016611  -0.059113  0.008467  -0.909136  0.950328  0.001222  -0.588914  1.052228  -0.186361 | 66.1  138.9  169.3  395.9  405.8  508.0  543.2  809.2  842.6 | 909.2  961.0  974.9  1073.2  1106.2  1198.1  1339.0  1352.8  1415.2 | 1426.8  1486.2  1991.8  2914.9  2968.0  2987.2  3064.4  3128.4  3204.0 |
| **s4** | 16.06799  3.34506  2.86966 | 6  6  6  6  6  1  1  1  1  1  1 | -0.427770  -1.737987  -1.491847  0.865693  2.026807  -1.764036  -1.763008  1.084845  2.661076  1.710827  2.660927 | -0.225467  -0.768798  0.765009  -0.576932  0.355377  1.303035  1.303914  -1.645020  0.171995  1.398634  0.172302 | 0.000116  -0.000205  0.000055  -0.000183  0.000014  0.909241  -0.908895  0.000815  0.875735  0.000199  -0.875880 | 119.5  147.2  195.4  237.1  508.2  669.4  707.9  742.5  885.2 | 967.9  984.5  1011.9  1059.9  1138.6  1205.9  1363.6  1398.1  1412.2 | 1474.2  1479.9  1769.1  3010.6  3048.3  3051.1  3107.0  3108.1  3127.1 |
| **s4a** | 17.47226  3.33301  2.90236 | 6  6  6  6  6  1  1  1  1  1  1 | -0.419147  -1.155161  -1.861052  0.835955  2.046473  -2.399881  -2.399130  1.004055  2.669436  2.668445  1.774671 | -0.145210  1.070867  -0.310363  -0.619378  0.251615  -0.583182  -0.584007  -1.696789  0.035779  0.036380  1.306628 | -0.000434  0.000001  0.000242  -0.000218  0.000156  -0.908424  0.909083  -0.000001  -0.875932  0.877107  -0.000318 | 113.8  178.7  205.9  250.2  505.6  676.6  680.6  744.2  889.2 | 963.1  995.2  1067.9  1081.8  1097.8  1170.7  1373.7  1399.0  1419.2 | 1475.0  1477.8  1761.7  3012.5  3047.0  3053.0  3104.8  3106.3  3134.6 |
| **s5** | 18.31961  3.24921  2.80760 | 6  6  6  6  6  1  1  1  1  1  1 | -1.403515  -1.811548  -0.384522  0.878014  2.067846  -1.670086  -2.641221  1.069969  2.703568  1.755888  2.704239 | 0.822706  -0.428507  -0.206108  -0.615840  0.307042  1.867063  -1.116768  -1.685032  0.152641  1.354905  0.151435 | 0.000079  0.000073  -0.000172  0.000133  -0.000008  -0.000173  -0.000188  -0.000111  0.880347  -0.000848  -0.879655 | 155.8  202.9  257.8  437.2  511.0  667.1  781.1  782.0  879.5 | 905.6  950.7  1055.2  1065.8  1095.6  1113.1  1356.6  1415.3  1483.1 | 1502.6  1612.0  1851.9  2997.2  3032.3  3079.3  3139.5  3234.3  3276.1 |
| **s5a** | 12.13952  3.82205  2.95983 | 6  6  6  6  6  1  1  1  1  1  1 | -0.620672  0.061451  0.819844  1.956762  -1.914841  0.047502  2.916010  1.951962  -1.985940  -2.758407  -1.986395 | 0.150387  1.281086  0.056466  -0.633169  -0.559611  2.359427  -0.130628  -1.716091  -1.208692  0.133178  -1.208149 | 0.000071  -0.000020  0.000211  -0.000167  -0.000047  -0.000248  -0.000006  0.000161  -0.878516  -0.000473  0.878787 | 136.1  209.4  265.8  441.4  512.7  707.7  711.7  757.3  785.5 | 847.2  987.2  1042.6  1046.1  1089.2  1190.2  1403.4  1452.0  1475.9 | 1480.5  1672.9  1878.6  3024.9  3076.5  3108.6  3138.0  3219.5  3248.0 |
| **s6** | 39.30358  2.24055  2.14770 | 6  6  6  6  6  1  1  1  1  1  1 | -0.925069  0.093118  -2.371353  1.466373  2.639571  -0.698024  -0.117164  -2.885145  -2.502942  -2.884041  3.671471 | -0.394174  0.477226  -0.011298  0.109704  -0.165535  -1.457450  1.545099  -0.419661  1.072909  -0.419574  -0.416856 | -0.000246  -0.000058  0.000112  -0.000300  0.000115  -0.000203  -0.000015  -0.877394  0.000397  0.878416  0.001063 | 167.2  171.1  199.1  390.5  450.2  544.9  626.6  681.7  816.5 | 912.3  987.2  1046.5  1065.6  1128.3  1314.6  1328.8  1414.4  1477.6 | 1489.6  1695.6  2202.9  3013.1  3055.0  3097.7  3124.5  3146.6  3477.4 |
| **s6a** | 35.38056  2.12141  2.02666 | 6  6  6  6  6  1  1  1  1  1  1 | -2.413714  -1.465982  -0.065977  1.129073  2.568838  -3.463686  -2.164738  -1.761812  3.041517  3.028220  2.807077 | 0.465974  -0.478288  -0.228537  -0.059133  0.159142  0.199448  1.520623  -1.525333  -0.330685  -0.244505  1.225506 | 0.000004  0.000022  0.000030  -0.000098  -0.000039  -0.000072  0.000031  -0.000013  -0.856931  0.907589  -0.050119 | 17.2  140.8  185.6  325.9  378.4  536.8  700.4  722.1  941.3 | 1010.3  1049.1  1049.7  1054.7  1194.9  1321.7  1415.7  1448.0  1478.2 | 1478.4  1669.8  2334.0  3018.8  3072.8  3078.9  3125.6  3143.7  3232.1 |
| **s7** | 9.36435  4.02272  2.86368 | 6  6  6  6  6  1  1  1  1  1  1 | 1.045359  0.424524  -1.003969  -2.202644  1.168488  2.127568  0.489762  -3.260925  0.902742  0.902795  2.247503 | 1.309035  0.121892  0.038520  -0.080066  -1.194412  1.370980  2.238292  -0.171896  -1.787697  -1.787695  -1.031802 | 0.000007  0.000032  -0.000036  0.000019  -0.000003  -0.000007  -0.000049  -0.000007  -0.879806  0.879813  -0.000047 | 176.0  186.9  268.6  396.8  546.4  571.2  650.1  677.9  744.0 | 775.53  931.92  964.81  1031.8  1071.4  1284.6  1410.4  1435.2  1477.9 | 1495.7  1675.7  2201.4  3028.2  3081.1  3113.1  3143.5  3233.7  3477.0 |
| **s8** | 35.15850  2.31122  2.20135 | 6  6  6  6  6  1  1  1  1  1  1 | -0.01583  -1.14049  1.246431  -2.42300  -0.25116  -0.88666  -2.70945  -3.22461  2.497132  3.043329  3.043191 | 0.524445  -0.407820  0.164349  -0.032529  1.587870  -1.464217  1.014389  -0.760815  -0.194477  -0.350554  -0.350479 | -0.000042  -0.000035  -0.000050  0.000044  -0.000031  -0.000094  0.000102  0.000052  0.000046  -0.926413  0.926597 | 128.4  166.0  349.1  401.2  509.1  568.5  732.7  879.0  906.4 | 919.2  929.7  1010.6  1033.5  1112.2  1186.9  1308.0  1336.4  1441.4 | 1483.0  1680.0  2034.1  3105.6  3114.9  3133.8  3150.5  3174.8  3222.4 |
| **s9** | 25.10745  2.57298  2.40123 | 6  6  6  6  6  1  1  1  1  1  1 | 0.138265  -1.129375  1.361250  -2.287853  2.381537  0.146887  -1.133834  1.393063  -2.315777  -3.234504  2.361226 | -0.190646  0.407567  0.472370  -0.274864  -0.297241  -1.260557  1.476676  1.561227  -1.346477  0.217998  -1.351986 | -0.258325  0.063060  -0.196562  0.087833  0.330531  -0.450233  0.260262  -0.170197  -0.080812  0.272425  0.009331 | 112.5  178.5  245.2  463.2  487.9  648.1  741.7  883.3  914.7 | 951.3  955.9  999.4  1040.6  1195.2  1247.3  1281.9  1317.7  1344.7 | 1438.5  1506.3  1647.0  2994.6  3103.5  3136.0  3143.8  3152.8  3228.3 |
| **s10** | 12.36797  3.99125  3.67689 | 6  6  6  6  6  1  1  1  1  1  1 | -0.415598  -1.325989  -1.326319  1.067446  1.724226  -0.736922  -1.628716  -1.629491  1.641180  1.204280  2.807072 | 0.725447  -0.300005  -0.298543  0.551439  -0.608604  1.767121  -0.730690  -0.727024  1.476410  -1.561402  -0.642818 | -0.000737  -0.643993  0.644462  -0.000140  0.000350  -0.001966  -1.583327  1.584655  -0.000128  0.000341  0.000779 | 46.4  243.9  327.7  557.6  655.0  668.5  819.6  855.2  880.2 | 929.3  941.7  1006.3  1029.5  1051.5  1061.1  1179.6  1323.5  1388.2 | 1443.2  1691.7  1729.7  3069.7  3124.7  3135.8  3215.6  3241.6  3290.4 |
| **s11** | 8.47608  8.23328  4.28635 | 6  6  6  6  6  1  1  1  1  1  1 | -0.724225  0.744255  1.176538  -1.182006  -0.012884  -1.328356  1.368749  2.203753  -2.216173  -0.019601  -0.018440 | 0.996970  0.981824  -0.293082  -0.269019  -1.215379  1.895116  1.866176  -0.630729  -0.585041  -1.866280  -1.887131 | -0.000569  -0.000433  -0.000204  -0.003644  0.001341  0.009518  0.001759  -0.007701  -0.001693  0.886693  -0.867526 | 348.6  524.2  681.3  712.1  816.9  818.8  917.3  924.7  953.8 | 955.3  971.1  1012.5  1111.6  1125.8  1129.8  1266.1  1315.0  1397.2 | 1414.8  1551.3  1637.9  3010.2  3032.6  3187.7  3197.5  3216.0  3222.6 |
| **s12** | 10.91257  6.48802  5.20782 | 6  6  6  6  6  1  1  1  1  1  1 | -1.086818  0.347057  -1.086312  0.346968  1.263732  -1.769738  0.728806  -1.769152  0.728342  1.053973  2.320012 | 0.670198  -0.761630  -0.670545  0.762000  -0.000001  1.420609  -1.398658  -1.421210  1.399740  -0.000370  -0.000240 | 0.098491  -0.404957  0.098476  -0.404439  0.536874  0.478774  -1.191608  0.478923  -1.190805  1.602000  0.276045 | 424.4  453.3  737.9  783.3  803.4  831.6  860.3  889.2  947.0 | 961.32  1030.5  1038.8  1040.5  1085.5  1107.1  1200.0  1219.4  1289.9 | 1308.3  1475.6  1602.1  3088.1  3166.5  3177.0  3185.5  3193.4  3202.2 |
| **s13** | 10.02125  7.50076  6.31611 | 6  6  6  6  6  1  1  1  1  1  1 | -0.814632  0.101062  -0.814921  0.100754  1.293575  -1.549704  0.038742  -1.550734  0.038196  1.914390  1.914077 | -0.000016  0.978578  0.000224  -0.978563  -0.000139  0.000080  2.059772  -0.000131  -2.059746  -0.000153  -0.000330 | 0.726117  0.000073  -0.726077  -0.000052  -0.000158  1.511358  0.000042  -1.510716  -0.000030  -0.902413  0.902342 | 472.8  634.0  752.2  781.1  819.1  842.0  843.4  907.5  912.7 | 948.7  1040.0  1046.7  1070.4  1108.4  1109.8  1152.8  1170.3  1210.0 | 1270.9  1406.4  1500.9  3014.2  3070.2  3182.7  3183.3  3258.2  3276.9 |
| **s14** | 15.58754  3.55912  2.95454 | 6  6  6  6  6  1  1  1  1  1  1 | 1.339070  1.576020  0.329280  -1.072486  -2.027841  1.504464  1.507611  2.320950  -1.341569  -1.776973  -3.078734 | 0.860088  -0.627543  -0.262355  -0.567855  0.369017  1.434375  1.433342  -1.404407  -1.621341  1.423965  0.105961 | 0.000315  -0.001011  0.001531  0.000709  -0.000755  -0.913371  0.914043  -0.004168  0.001730  -0.001281  -0.001691 | 154.5  199.2  290.6  537.0  662.0  664.9  762.6  942.0  953.6 | 976.5  1003.6  1025.5  1061.1  1098.2  1098.4  1214.7  1315.9  1435.0 | 1516.1  1658.9  1831.6  3024.2  3085.8  3135.6  3144.1  3229.8  3269.3 |
| **s15** | 23.25890  2.29460  2.14316 | 6  6  6  6  6  1  1  1  1  1  1 | -1.427490  -2.758715  -0.235292  1.186376  2.110159  -3.075109  1.400235  1.401189  3.158867  1.932104  1.932489 | -0.012976  0.144949  -0.359114  -0.620478  0.610528  1.197250  -1.263944  -1.265141  0.301555  1.226788  1.226037 | -0.001259  0.001043  -0.000615  0.000418  0.000068  0.000120  0.866051  -0.864115  0.000470  0.883435  -0.883891 | 54.5  111.9  187.6  245.6  385.2  432.3  468.3  736.3  755.1 | 915.5  969.1  1077.8  1078.1  1279.3  1305.7  1372.5  1410.6  1414.5 | 1496.2  1502.0  2052.6  2991.8  3010.2  3035.8  3042.1  3104.0  3114.6 |
| **s15a** | 35.03866  2.08320  2.01427 | 6  6  6  6  6  1  1  1  1  1  1 | -0.060712  -1.350991  1.148452  2.585040  -2.436654  2.911057  2.911877  3.107778  -3.332170  -2.180473  -2.728886 | -0.254095  -0.650231  -0.010553  0.158525  0.357546  1.099694  0.176442  -0.676103  -0.008684  1.369867  0.431640 | -0.004866  -0.010655  -0.015236  -0.002457  -0.013036  -0.456801  1.044953  -0.482687  -0.522372  -0.354173  1.048578 | 55.9  90.5  116.5  192.5  203.4  451. 8  526.5  718.0  818.1 | 1012.9  1026.0  1061.6  1077.5  1348.4  1351.9  1399.9  1423.0  1446.2 | 1487.2  1498.1  2103.5  2959.1  3000.7  3008.7  3055.4  3059.3  3072.5 |
| **i1** | 8.06555  4.32193  3.15266 | 6  6  6  6  6  1  1  1  1  1  1 | 1.095473  2.232994  -0.354002  -0.771534  -1.168209  -0.498097  -0.535067  -1.064619  -2.229149  -0.841477  -1.039928 | -0.114671  -0.197458  0.074448  1.399526  -1.109555  0.108879  2.315850  1.457771  -0.964896  -2.050922  -1.180424 | 0.233851  -0.280803  0.404256  -0.166391  -0.152523  1.497680  0.358592  -1.207727  0.063488  0.292492  -1.234872 | 124.2  161.4  213.0  255.9  356.2  440.4  514.6  604.8  773.5 | 906.2  933.3  1034.4  1114.2  1169.0  1257.4  1284.2  1406.0  1447.4 | 1493.3  1498.7  1550.4  2942.9  3038.3  3109.8  3116.5  3139.4  3252.3 |
| **i2** | 10.82013  3.29540  2.77262 | 6  6  6  6  6  1  1  1  1  1  1 | 1.420163  2.153287  0.261990  -0.993835  -1.773259  0.530511  0.125014  -1.137798  -2.753333  -1.921785  -1.252683 | 0.078371  -0.933720  0.938392  0.462608  -0.671691  1.944897  1.022657  0.742974  -0.760906  -0.561394  -1.631987 | -0.012307  -0.110649  0.262930  -0.413327  0.152508  -0.090444  1.348653  -1.451015  -0.321405  1.233043  0.006239 | 58.9  101.7  135.8  300.8  350.7  427.2  544.2  833.0  877.6 | 905.4  999.7  1083.2  1137.9  1223.9  1280.0  1378.1  1404.2  1409.0 | 1475.0  1482.2  1588.5  2956.0  2981.7  3020.8  3029.2  3092.1  3170.0 |
| **i3** | 9.85855  4.46307  3.49077 | 6  6  6  6  6  1  1  1  1  1  1 | 0.897284  1.874909  0.352068  -0.486990  -1.680256  0.737817  0.073645  -0.590573  -2.574258  -1.891756  -1.496957 | -0.155514  -0.990618  1.212200  0.123184  -0.490783  2.024119  1.490144  0.248790  0.125839  -1.486993  -0.592710 | 0.027391  -0.099321  -0.190171  0.505262  -0.191181  0.418571  -1.202868  1.580955  -0.052381  0.207488  -1.263640 | 148.0  202.0  297.2  366.3  456.4  718.2  753.4  828.9  876.5 | 919.2  1018.5  1028.4  1102.1  1127.2  1157.6  1351.8  1413.0  1454.1 | 1488.3  1497.5  1709.0  3020.5  3079.6  3092.4  3095.6  3115.3  3182.6 |
| **i4** | 11.34409  4.93851  4.02351 | 6  6  6  6  6  1  1  1  1  1  1 | -0.615104  -1.552137  -0.758107  0.375371  1.709191  -0.435978  -1.162186  0.492088  2.240893  1.566697  2.343207 | -1.141936  -0.279759  0.954996  -0.076142  0.010562  1.575146  1.563040  -0.026617  0.928621  -0.008118  -0.838395 | 0.046320  -0.351655  0.005397  0.487601  -0.237520  -0.834062  0.818337  1.574746  0.028968  -1.321111  0.032261 | 229.9  249.7  339.0  461.7  710.6  755.4  864.4  888.9  981.1 | 1019.1  1051.2  1074.3  1106.9  1144.9  1204.9  1329.0  1408.4  1460.9 | 1490.8  1496.9  1617.2  3025.3  3038.5  3042.6  3090.6  3098.0  3106.1 |
| **i5** | 12.34668  3.68597  2.90242 | 6  6  6  6  6  1  1  1  1  1  1 | 0.551531  0.816747  1.836608  -0.684552  -2.008129  2.729034  1.955631  -0.657962  -2.714575  -1.921320  -2.464037 | 0.075304  1.422377  -0.542844  -0.617022  0.070434  0.006986  -1.502595  -1.697589  -0.476315  1.091652  0.128370 | 0.058974  -0.049928  0.009143  0.022870  -0.016989  0.279261  -0.484353  0.124552  -0.649220  -0.396137  0.981477 | 104.5  154.7  171.4  228.9  430.4  484.8  522.3  626.0  729.7 | 830.6  938.7  1005.1  1059.1  1113.0  1199.4  1394.0  1413.9  1422.4 | 1455.6  1476.0  1494.8  2987.6  3047.2  3092.9  3125.2  3156.7  3235.7 |
| **i5a** | 8.85447  4.42015  3.13126 | 6  6  6  6  6  1  1  1  1  1  1 | -0.712379  -1.257972  -1.238531  0.659421  1.823738  -2.270757  -0.656057  0.855804  2.611706  2.266505  1.547132 | -0.139684  -1.351588  1.166230  -0.500202  0.280768  1.325958  2.017154  -1.486406  0.333426  -0.216336  1.293057 | -0.091391  0.254824  -0.030055  -0.331201  0.180068  0.251634  -0.359720  -0.738634  -0.578816  1.054160  0.477903 | 110.6  114.1  247.8  307.0  401.8  459.5  538.1  664.5  696.0 | 821.9  966.2  1006.6  1030.0  1085.5  1206.6  1387.4  1392.1  1424.5 | 1470.2  1475.7  1487.9  2995.1  3049.0  3111.6  3147.8  3170.6  3250.6 |
| **i6** | 11.28545  3.96366  3.25070 | 6  6  6  6  6  1  1  1  1  1  1 | -0.077406  0.703969  -0.837418  1.739388  -1.896259  0.837804  1.790750  2.730556  1.518776  -2.834710  -1.836822 | 1.311212  0.286192  0.240301  -0.586461  -0.602761  0.411015  -1.572965  -0.127618  -0.714502  -0.311065  -1.575762 | -0.265445  0.455307  -0.031726  -0.214309  -0.007981  1.532473  0.257356  -0.124881  -1.275653  -0.466570  0.462194 | 165.1  181.7  338.3  383.3  478.0  567.4  593.6  743.6  856.9 | 935.3  1015.6  1051.0  1081.4  1084.2  1133.9  1348.4  1401.8  1450.5 | 1482.6  1488.1  1610.8  3014.5  3054.2  3067.4  3108.8  3135.7  3229.6 |
| **i6a** | 14.80846  3.45908  2.90914 | 6  6  6  6  6  1  1  1  1  1  1 | -1.744475  -1.481627  -0.431916  0.908245  1.950806  -1.576314  -1.576316  1.239880  2.601905  1.502680  2.601966 | -0.659895  0.788391  -0.434103  -0.647761  0.425851  1.369494  1.369507  -1.683385  0.344298  1.420943  0.344242 | 0.000007  -0.000004  0.000003  -0.000006  0.000004  -0.917924  0.917907  -0.000017  0.878684  -0.000045  -0.878625 | 130.0  191.8  218.0  369.1  510.7  600.0  712.0  884.5  888.35 | 991.9  1009.9  1030.2  1049.2  1101.3  1162.4  1368.5  1408.5  1475.2 | 1477.7  1494.9  1622.6  3002.6  3039.3  3043.3  3103.0  3117.2  3136.8 |
| **i7** | 29.83405  2.14212  2.05208 | 6  6  6  6  6  1  1  1  1  1  1 | 0.092493  -1.244696  1.316744  2.650375  -2.318169  -1.559178  3.203068  3.203035  -2.966090  -2.965749  -1.895563 | 0.297396  0.568253  0.050268  -0.218317  -0.481572  1.609964  -0.329205  -0.329326  -0.380203  -0.380510  -1.486888 | -0.000007  -0.000005  -0.000002  0.000003  -0.000005  0.000076  -0.927597  0.927608  -0.879467  0.879743  -0.000261 | 84.1  117.3  183.2  356.0  360.2  445.5  502.7  677.3  684.1 | 768.4  998.3  1009.6  1014.4  1092.3  1273.1  1396.3  1412.1  1465.8 | 1476.4  1501.6  1906.9  2997.5  3034.6  3108.0  3110.7  3123.3  3190.7 |
| **i8** | 10.92608  3.52748  2.96043 | 6  6  6  6  6  1  1  1  1  1  1 | -1.484747  -1.855826  -0.147598  0.920992  1.884872  -1.243924  -0.231133  0.125326  0.843258  2.621236  1.979084 | 0.341591  -0.933003  1.004924  0.074323  -0.465321  -1.829676  1.882937  1.371343  -0.174646  -1.134404  -0.250641 | -0.120464  -0.042553  -0.054791  0.477255  -0.262396  0.090546  0.598740  -1.050416  1.532544  0.168739  -1.322458 | 71.5  161.1  231.9  411.9  452.7  615.3  666.9  877.3  895.2 | 941.6  951.9  1000.5  1026.9  1093.0  1221.2  1282.1  1321.5  1442.6 | 1458.5  1685.0  1695.0  3004.1  3047.3  3051.9  3126.9  3144.4  3211.7 |
| **i9** | 12.72236  2.93724  2.58929 | 6  6  6  6  6  1  1  1  1  1  1 | -1.261659  -2.235657  -0.050063  1.143257  1.967430  -3.100145  -0.241565  0.164148  1.216044  1.673715  2.907951 | 0.100680  -0.587987  0.914772  0.296038  -0.721208  -1.192060  1.914895  1.038138  0.469203  -1.769413  -0.474530 | -0.085529  0.062696  -0.239107  0.462276  -0.161495  0.189043  0.166896  -1.306487  1.535158  -0.169174  -0.648474 | 47.5  167.0  316.6  335.3  342.5  483.6  546.4  623.6  666.8 | 667.7  866.9  927.01  941.02  995.52  1154.2  1203.6  1302.7  1348.2 | 1433.5  1463.4  2211.7  3011.7  3047.9  3080.8  3105.7  3162.6  3477.9 |
| **i10** | 18.72036  2.85543  2.47753 | 6  6  6  6  6  1  1  1  1  1  1 | 1.450883  2.136380  0.043726  -0.932744  -2.271849  1.946217  -0.313868  -0.577340  -2.978268  -2.681263  2.046147 | 0.490694  -0.667393  0.678481  -0.351509  -0.135765  -1.730085  1.704406  -1.379287  -0.956357  0.869120  1.405159 | 0.000004  0.000006  -0.000014  -0.000005  0.000009  -0.000020  -0.000048  -0.000001  -0.000016  0.000046  0.000039 | 151.8  209.8  257.0  385.3  587.7  620.6  644.2  774.6  878.1 | 881.4  917.4  921.0  1011.2  1094.4  1190.2  1258.5  1309.0  1360.5 | 1419.1  1504.4  1582.0  3087.9  3133.0  3138.3  3151.0  3227.9  3237.8 |
| **i11** | 10.03757  4.21411  2.96803 | 6  6  6  6  6  1  1  1  1  1  1 | -1.304526  -1.567302  -0.045515  -2.174788  -2.457426  -0.078927  1.247686  1.549205  2.076909  2.579633  0.777311 | 0.375921  -0.940377  1.030695  1.042573  -1.551894  2.115007  0.438929  -0.885411  1.142735  -1.220224  -1.646745 | 0.000318  -0.000509  0.000102  0.001148  -0.000859  0.000306  -0.000393  0.000381  -0.001510  -0.000276  0.001791 | 151.3  214.9  351.7  386.5  577.9  615.3  668.2  741.0  876.6 | 876.7  880.6  925.9  999.3  1077.4  1174.9  1252.7  1290.7  1385.0 | 1446.4  1512.3  1583.6  3021.3  3129.7  3132.3  3168.9  3224.0  3235.2 |
| **i12** | 8.63216  7.61296  4.14764 | 6  6  6  6  6  1  1  1  1  1  1 | -1.059382  0.316061  -1.059376  0.316138  1.276528  -1.933674  0.610030  -1.933551  0.610248  1.953659  1.953474 | -0.678405  -1.166430  0.678422  1.166474  -0.000057  -1.315055  -2.206998  1.315240  2.206993  0.000019  -0.000219 | -0.000023  0.000000  0.000060  -0.000094  0.000056  -0.000050  -0.000197  0.000099  -0.000047  -0.874385  0.874582 | 101.9  341.3  417.8  524.6  708.0  748.0  790.8  814.0  908.6 | 936.5  943.0  1002.7  1053.5  1113.6  1120.8  1247.3  1301.0  1355.7 | 1372.3  1484.4  1571.6  2860.2  2890.4  3197.7  3206.7  3211.2  3226.6 |
| **i13** | 8.69890  7.37602  4.19760 | 6  6  6  6  6  1  1  1  1  1  1 | -0.230897  1.012346  -1.318130  -0.477322  0.994372  1.921497  -1.975377  -1.975874  -0.886707  1.516846  1.517406 | -1.226842  -0.786688  -0.196513  1.059855  0.742747  -1.373667  -0.276232  -0.276822  2.061916  1.154929  1.154518 | 0.000069  0.000101  -0.000049  -0.000428  -0.000062  0.000180  0.878694  -0.878330  0.001611  0.877659  -0.877595 | 206.0  351.1  377.6  710.2  743.7  768.6  889.2  895.9  919.6 | 938.8  965.2  1020.8  1111.8  1119.7  1200.0  1241.1  1294.4  1330.4 | 1457.3  1463.3  1667.0  2955.5  2962.5  2969.0  2975.6  3196.4  3199.4 |
| **i14** | 11.14609  3.94817  3.02909 | 6  6  6  6  6  1  1  1  1  1  1 | 0.741182  -0.619769  1.891126  0.159831  -1.895415  1.901914  2.805954  0.344430  -2.736908  -2.104995  -1.872129 | 0.061891  0.129828  -0.698386  1.338027  -0.531446  -1.723916  -0.283682  2.299978  -0.090835  -0.398149  -1.602878 | -0.032581  -0.279114  0.029041  0.142558  0.082105  -0.320719  0.434896  -0.328302  -0.460875  1.155368  -0.132419 | 104.2  170.7  204.5  395.2  421.1  444.5  645.5  783.0  797.8 | 830.9  942.1  981.6  1026.4  1095.0  1162.8  1294.2  1397.7  1465.0 | 1472.2  1483.0  1610.5  2957.0  3047.6  3088.7  3114.3  3137.9  3236.4 |
| **i14a** | 16.55384  3.35839  2.86921 | 6  6  6  6  6  1  1  1  1  1  1 | -0.452734  -1.810694  0.857475  -1.322765  2.037271  -2.459361  1.033442  -1.502456  2.672215  1.734269  2.670571 | -0.174472  -0.496573  -0.614585  0.914139  0.280464  -1.123511  -1.670919  1.823770  -0.057217  1.310314  0.263726 | -0.035239  -0.032654  -0.095611  0.069186  0.071579  0.567054  -0.279765  -0.491001  0.899884  0.265182  -0.824922 | 125.2  179.5  205.1  341.4  396.3  536.9  694.3  751.2  797.1 | 933.24  943.3  1009.2  1020.9  1078.0  1147.1  1172.3  1381.0  1405.2 | 1472.8  1486.2  1604.6  2999.2  3036.2  3111.5  3151.0  3160.7  3163.0 |
| **i15** | 19.60367  2.42475  2.35101 | 6  6  6  6  6  1  1  1  1  1  1 | -2.419567  -1.464993  -0.168112  1.076170  2.203330  -2.436121  -1.779497  1.354215  2.671659  1.846727  2.982048 | 0.527396  -0.374746  -0.360950  -0.347284  0.384758  1.387817  -1.160605  -0.909532  1.102808  0.922490  -0.318022 | 0.097913  -0.318750  0.060920  0.442356  -0.251463  0.751520  -1.008596  1.337662  0.429702  -1.130621  -0.565524 | 115.5  149.9  193.8  270.4  473.7  527.6  557.9  750.6  817.4 | 880.2  918.0  1053.5  1058.7  1094.7  1190.8  1310.3  1378.8  1402.4 | 1484.9  1492.4  1912.9  3018.7  3055.7  3067.4  3077.3  3117.1  3227.6 |
| **i15a** | 12.80206  2.94523  2.47148 | 6  6  6  6  6  1  1  1  1  1  1 | 1.973568  1.253331  -0.056712  -1.145777  -2.185165  2.616682  1.266010  2.614782  -0.234742  -2.649112  -2.649092 | -0.707001  0.572066  1.002935  0.201643  -0.579429  -0.811219  -1.548905  -0.812337  2.079516  -0.924173  -0.924162 | 0.000002  0.000001  0.000004  -0.000011  0.000004  -0.881842  -0.001297  0.883107  0.000012  -0.924369  0.924391 | 49.2  125.6  187.1  263.2  326.2  532.2  627.1  845.1  855.3 | 888.6  986.3  995.4  1013.8  1050.0  1301.5  1390.0  1414.9  1450.4 | 1451.6  1474.1  1896.0  2973.2  3033.2  3041.4  3060.4  3086.1  3116.5 |
| **i15b** | 9.36284  3.85178  2.82984 | 6  6  6  6  6  1  1  1  1  1  1 | -1.015416  -0.491369  -1.434843  0.844343  2.134443  -0.605908  -0.874058  -2.077629  -2.076915  2.706096  2.705473 | 1.444629  0.162364  -1.036235  -0.027523  -0.194588  2.444268  -1.971020  -1.012964  -1.012820  -0.269756  -0.269593 | 0.000097  -0.000333  0.000106  -0.000293  0.000139  0.000335  -0.000042  -0.883149  0.883875  -0.924464  0.925143 | 45.4  178.1  179.3  360.9  442.2  467.4  574.5  592.3  769.8 | 870.8  885.3  986.7  1000.1  1048.2  1208.9  1287.5  1401.4  1446.0 | 1486.1  1494.4  1902.0  3037.7  3067.9  3098.0  3125.1  3126.9  3233.2 |
| **p1** | 38.62673  2.27452  2.14804 | 6  6  6  6  6  1  1  1  1  1 | 0.014336  -1.354966  1.236226  2.566866  -2.319985  -1.653604  2.967985  3.270879  -3.368065  -2.072054 | -0.234371  -0.486978  -0.042634  0.177715  0.466355  -1.533728  1.184811  -0.646678  0.194282  1.520789 | 0.002417  -0.000139  0.000182  -0.000796  -0.000598  -0.001620  0.000153  -0.002980  -0.002962  0.001014 | 143.3  178.7  312.3  330.5  446.6  535.7  645.7  748.3 | 769.1  893.6  977.9  1031.0  1067.2  1284.3  1313.3  1435.0 | 1491.5  1568.7  2048.1  3121.7  3130.3  3146.4  3215.0  3240.9 |
| **p2** | 41.49699  2.40132  2.26996 | 6  6  6  6  6  1  1  1  1  1 | -1.019172  0.000000  -2.353630  1.359431  2.548240  -0.704977  -0.282937  -2.712442  -3.096891  3.588027 | -0.462843  0.512156  -0.178776  0.213722  -0.032384  -1.503172  1.561771  0.844934  -0.965495  -0.249289 | 0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 | 155.7  172.0  398.2  425.2  540.5  556.1  585.6  666.5 | 771.2  859.0  926.5  1007.2  1097.9  1200.8  1288.4  1332.6 | 1467.2  1540.6  2090.1  3135.6  3140.7  3151.0  3234.8  3471.1 |
| **p2’** | 13.79412  3.39756  2.72611 | 6  6  6  6  6  1  1  1  1  1 | 1.167167  2.189616  0.001829  -1.308491  -1.640682  3.086210  0.124704  -2.112045  -2.676079  -0.879426 | 0.171814  -0.480019  0.939991  0.412883  -0.911701  -1.049823  2.018094  1.144292  -1.227350  -1.683021 | -0.000884  -0.000318  0.000304  -0.000064  0.000065  0.003721  0.001254  0.000270  0.000245  -0.000099 | 157.8  225.0  383.0  434.6  558.8  562.9  651.0  668.1 | 735.1  862.6  943.0  996.7  1036.9  1159.2  1259.4  1414.6 | 1433.9  1543.6  2104.0  3143.3  3146.8  3165.4  3239.6  3469.9 |
| **p3** | 103.62866  1.95153  1.93859 | 6  6  6  6  6  1  1  1  1  1 | -0.077132  1.156716  -1.394235  -2.700873  2.606718  -3.281617  -3.276641  3.004644  3.001457  3.004992 | -0.002817  -0.010389  -0.000438  0.003141  0.005603  -0.919512  0.928909  -0.496942  1.028566  -0.511629 | 0.000001  0.000038  -0.000003  -0.000011  -0.000035  -0.000023  -0.000005  0.887999  -0.008447  -0.879462 | 16.5  54.6  135.8  143.3  323.9  358.2  549.7  674.5 | 870.8  979.5  1026.8  1038.5  1142.0  1410.3  1443.7  1464.4 | 1471.0  1858.9  2100.8  2999.4  3049.1  3057.9  3064.5  3114.5 |
| **p4** | 10.45107  4.11631  2.95316 | 6  6  6  6  6  1  1  1  1  1 | 0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 | 1.221570  -1.221570  0.000000  0.000000  0.000000  1.251000  -1.251000  2.158170  -2.158170  0.000000 | -1.137509  -1.137509  -0.468402  0.970244  2.173184  -2.220009  -2.220009  -0.597759  -0.597759  3.235490 | 192.4  265.0  405.2  525.8  540.8  571.0  624.5  656.4 | 686.4  766.7  796.3  799.5  981.1  1037.4  1291.7  1367.2 | 1474.0  1517.4  2211.4  3149.4  3155.7  3256.0  3257.6  3476.9 |
| **p5** | 9.30036  8.51141  4.44421 | 6  6  6  6  6  1  1  1  1  1 | 0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 | 0.741277  1.169009  0.000000  -1.169009  -0.741277  1.357995  2.190729  0.000000  -2.190729  -1.357995 | -0.946378  0.352883  1.186344  0.352883  -0.946378  -1.834653  0.702061  2.269063  0.702061  -1.834653 | 77  500 516  681  719  816  847  892 | 899  929  944  1059  1072  1143  1217  1295 | 1386  1490  1534  3200  3204  3216  3232  3240 |
| **p6** | 37.86375  2.23925  2.14223 | 6  6  6  6  6  1  1  1  1  1 | 0.154848  -1.112883  1.457731  2.669402  -2.270164  -1.381575  3.717611  -2.900811  -1.926282  -2.902546 | 0.214427  0.539170  0.013303  -0.207830  -0.429006  1.599590  -0.377473  -0.270489  -1.463522  -0.268482 | -0.000390  0.000067  -0.000111  0.000172  0.000056  0.000580  0.000357  0.881506  -0.001432  -0.879775 | 54.3  143.0  22556  293.3  379.3  440.0  512.2  609.9 | 721.3  788.1  1035.4  1048.1  1087.3  1323.6  1399.5  1481.6 | 1486.9  1809.9  2009.6  3016.1  3045.6  3063.2  3120.4  3468.9 |
| **p7** | 24.66857  2.43125  2.28197 | 6  6  6  6  6  1  1  1  1  1 | 0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.924352  -0.924352  0.924352  -0.924352 | 0.000000  1.209867  -1.209867  2.376131  -2.376131  0.000000  2.895099  2.895099  -2.895099  -2.895099 | 0.750632  0.135059  0.135059  -0.433797  -0.433797  1.841901  -0.690209  -0.690209  -0.690209  -0.690209 | 123.6  134.4  156.3  351.2  435.7  495.5  609.4  867.5 | 892.8  894.6  944.4  975.3  978.7  1042.7  1329.3  1436.8 | 1452.5  1874.1  1929.3  3053.2  3057.7  3088.1  3109.7  3109.8 |
| **p8** | 13.71265  3.13397  2.59205 | 6  6  6  6  6  1  1  1  1  1 | 1.905550  1.143424  -0.108534  -1.238534  -2.196596  2.549986  1.228431  2.548721  -0.316329  -3.042672 | -0.685991  0.565790  0.991740  0.118084  -0.613065  -0.756411  -1.552401  -0.756118  2.061015  -1.255432 | 0.000191  -0.000716  -0.000172  0.000855  -0.000547  -0.881940  -0.000112  0.883280  0.001081  0.000021 | 114.7  127.4  290.9  324.9  437.1  610.3  623.4  683.6 | 801.3  878.8  1002.6  1040.9  1056.6  1300.5  1391.4  1454.1 | 1464.8  1710.3  2192.8  2979.1  3052.7  3071.9  3104.8  3474.5 |
| **p9** | 34.72260  2.23992  2.13214 | 6  6  6  6  6  1  1  1  1  1 | 2.476552  1.568766  0.160487  -1.033414  -2.472745  2.494940  1.892804  -2.773886  -2.795275  -3.016452 | 0.487735  -0.469614  -0.236579  -0.061041  0.159886  1.567926  -1.511271  0.793332  0.653387  -0.785695 | -0.000002  0.000030  -0.000015  -0.000107  -0.000017  0.000060  0.000073  -0.839901  0.921914  -0.081480 | 27.7  138.8  193.9  313.2  388.3  500.9  694.4  718.5 | 873.0  911.2  1049.9  1054.1  1178.1  1268.3  1416.0  1477.9 | 1478.2  1623.0  2329.6  3020.4  3075.4  3080.7  3087.4  3236.6 |
| **p10** | 9.75985  4.14680  2.96386 | 6  6  6  6  6  1  1  1  1  1 | 0.938701  0.463739  1.352891  -0.954691  -2.143081  0.539738  1.150450  2.404356  1.152084  -3.191980 | 1.423359  0.190292  -1.038022  -0.020686  -0.219309  2.426825  -1.651534  -0.749744  -1.651761  -0.387587 | 0.000550  -0.000347  0.000181  -0.001912  0.000986  -0.000052  0.882610  0.001612  -0.882354  0.001437 | 172.9  178.7  270.8  368.9  532.3  538.9  643.1  678.3 | 691.7  770.9  852.3  1028.6  1053.5  1193.9  1403.8  1480.8 | 1482.3  1641.9  2190.9  3030.7  3088.0  3123.6  3242.3  3476.2 |

**Table S2.** Rate constants of various unimolecular reaction steps calculated using RRKM theory at different collision energies.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Rate constants, s-1 | | a | Collision Energy, kJmol-1 | | | | | | |
| reactant | product | 0.0 | 8.4 | 16.7 | 21.0 | 25.1 | 33.5 | 41.8 |
| **s1** | **s2** | 1 | .314243E+12 | .331797E+12 | .351609E+12 | .361337E+12 | .370773E+12 | .387732E+12 | .410128E+12 |
| **s1** | **s7** | 1 | .229861E+09 | .289870E+09 | .361648E+09 | .403218E+09 | .446745E+09 | .546728E+09 | .663360E+09 |
| **s2** | **s1** | 1 | .536802E+08 | .630397E+08 | .736775E+08 | .796253E+08 | .856839E+08 | .991920E+08 | .114328E+09 |
| **s2** | **s3** | 2 | .566810E+08 | .717658E+08 | .901022E+08 | .100894E+09 | .112298E+09 | .138859E+09 | .162753E+09 |
| **s3** | **s2** | 1 | .503934E+12 | .538635E+12 | .573709E+12 | .591993E+12 | .609188E+12 | .646208E+12 | .683807E+12 |
| **s2** | **s3a** | 1 | .747880E+08 | .934958E+08 | .116092E+09 | .129597E+09 | .143548E+09 | .175951E+09 | .214222E+09 |
| **s3a** | **s2** | 1 | .265664E+12 | .288068E+12 | .311458E+12 | .323649E+12 | .335562E+12 | .360353E+12 | .386138E+12 |
| **s2** | **s4a** | 2 | .176634E+09 | .208588E+09 | .245248E+09 | .285122E+09 | .280202E+09 | .334122E+09 | .387820E+09 |
| **s4a** | **s2** | 2 | .310738E+13 | .315470E+13 | .320032E+13 | .322326E+13 | .324526E+13 | .328898E+13 | .333220E+13 |
| **s2** | **s8** | 3 | .605865E+08 | .750234E+08 | .922350E+08 | .102189E+09 | .112601E+09 | .136591E+09 | .164676E+09 |
| **s8** | **s2** | 1 | .136362E+08 | .171300E+08 | .213570E+08 | .238301E+08 | .264326E+08 | .324956E+08 | .396915E+08 |
| **s2** | CH3CHCCC+H2 | 1 | .683211E+06 | .100049E+07 | .144480E+07 | .172581E+07 | .204496E+07 | .286065E+07 | .394165E+07 |
| **s3** | **s5** | 1 | .196671E+13 | .197039E+13 | .197395E+13 | .197573E+13 | .197740E+13 | .198073E+13 | .198396E+13 |
| **s5** | **s3** | 2 | .945106E+10 | .108929E+11 | .124481E+11 | .133088E+11 | .141775E+11 | .160793E+11 | .180984E+11 |
| **s3** | **s6** | 1 | .164028E+12 | .182094E+12 | .201176E+12 | .211285E+12 | .221246E+12 | .242312E+12 | .264343E+12 |
| **s6** | **s3** | 1 | .365528E+07 | .487704E+07 | .643904E+07 | .738945E+07 | .841742E+07 | .108982E+08 | .139875E+08 |
| **s3** | **s9** | 3 | .381345E+10 | .495000E+10 | .633369E+10 | .714393E+10 | .799746E+10 | .997896E+10 | .123157E+11 |
| **s9** | **s3** | 1 | .303849E+09 | .418865E+09 | .567880E+09 | .659281E+09 | .758357E+09 | .998619E+09 | .129809E+10 |
| **s3a** | **s5a** | 1 | .188979E+13 | .191196E+13 | .193356E+13 | .194750E+13 | .195660E+13 | .197504E+13 | .199494E+13 |
| **s5a** | **s3a** | 1 | .770833E+10 | .886484E+10 | .101089E+11 | .107934E+11 | .114816E+11 | .129885E+11 | .146381E+11 |
| **s3a** | **s6a** | 1 | .590091E+11 | .674252E+11 | .765770E+11 | .815352E+11 | .864939E+11 | .971809E+11 | .107621E+12 |
| **s6a** | **s3a** | 1 | .496293E+06 | .666484E+06 | .885358E+06 | .101917E+07 | .116419E+07 | .151628E+07 | .195672E+07 |
| **s3a** | **s8** | 3 | .161103E+13 | .168648E+13 | .176226E+13 | .180099E+13 | .183834E+13 | .191460E+13 | .199111E+13 |
| **s8** | **s3a** | 1 | .101831E+09 | .124965E+09 | .152355E+09 | .168134E+09 | .184668E+09 | .222344E+09 | .260272E+09 |
| **s4** | **s5** | 2 | .633068E+11 | .708492E+11 | .788970E+11 | .831830E+11 | .874324E+11 | .964690E+11 | .106046E+12 |
| **s5** | **s4** | 2 | .153895E+09 | .194211E+09 | .242900E+09 | .271338E+09 | .301240E+09 | .370604E+09 | .452732E+09 |
| **s5** | **s6** | 2 | .159912E+11 | .181893E+11 | .206834E+11 | .219716E+11 | .233264E+11 | .262578E+11 | .294524E+11 |
| **s6** | **s5** | 1 | .738949E+08 | .882209E+08 | .104779E+09 | .114128E+09 | .123766E+09 | .145511E+09 | .170230E+09 |
| **s5** | **s14** | 3 | .139694E+09 | .169517E+09 | .204306E+09 | .224153E+09 | .244621E+09 | .291032E+09 | .344208E+09 |
| **s14** | **s5** | 2 | .574542E+08 | .707856E+08 | .866070E+08 | .957170E+08 | .105210E+09 | .126957E+09 | .152255E+09 |
| **s5** | CH3CCH+C2H2 | 1 | .143585E+10 | .185604E+10 | .237191E+10 | .267752E+10 | .300222E+10 | .376662E+10 | .468881E+10 |
| **s5a** | **s6a** | 1 | .547906E+10 | .621166E+10 | .701442E+10 | .742480E+10 | .789134E+10 | .884553E+10 | .988286E+10 |
| **s6a** | **s5a** | 1 | .112362E+08 | .132435E+08 | .155109E+08 | .167823E+08 | .180821E+08 | .209872E+08 | .242562E+08 |
| **s5a** | CH3CCH+CCH2 | 1 | .314414E+10 | .394282E+10 | .490080E+10 | .545789E+10 | .604285E+10 | .740087E+10 | .899520E+10 |
| **s6** | **s15** | 1 | .132052E+09 | .159448E+09 | .191215E+09 | .209609E+09 | .228465E+09 | .271267E+09 | .320763E+09 |
| **s15** | **s6** | 2 | .999406E+12 | .102998E+13 | .106019E+13 | .107547E+13 | .109012E+13 | .111976E+13 | .114912E+13 |
| **s6a** | **s15a** | 1 | .129093E+09 | .155344E+09 | .185818E+09 | .203238E+09 | .221197E+09 | .261880E+09 | .307417E+09 |
| **s15a** | **s6a** | 6 | .365222E+13 | .382565E+13 | .400041E+13 | .408994E+13 | .417640E+13 | .435306E+13 | .453094E+13 |
| **s15** | CH3CCCCH+H2 | 1 | .280560E+10 | .365451E+10 | .469556E+10 | .530968E+10 | .595780E+10 | .747182E+10 | .927189E+10 |
| **s15** | C4H2+CH4 | 2 | .698514E+09 | .949986E+09 | .126963E+10 | .146276E+10 | .167055E+10 | .216676E+10 | .277330E+10 |
| **s15a** | CH3CCCCH+H2 | 6 | .959784E+10 | .123004E+11 | .155781E+11 | .174942E+11 | .195095E+11 | .241825E+11 | .296954E+11 |
| **s8** | **s9** | 2 | .466870E+09 | .556348E+09 | .659420E+09 | .717648E+09 | .777568E+09 | .912532E+09 | .110820E+10 |
| **s9** | **s8** | 1 | .147011E+13 | .154757E+13 | .162937E+13 | .166969E+13 | .170674E+13 | .178212E+13 | .186737E+13 |
| **s9** | **s10** | 2 | .422668E+13 | .434408E+13 | .446112E+13 | .451978E+13 | .457566E+13 | .469052E+13 | .480406E+13 |
| **s10** | **s9** | 1 | .875045E+10 | .975755E+10 | .108433E+11 | .114338E+11 | .120068E+11 | .132670E+11 | .146080E+11 |
| **s10** | **s11** | 1 | .250929E+10 | .281418E+10 | .314427E+10 | .332314E+10 | .350164E+10 | .388631E+10 | .429959E+10 |
| **s11** | **s10** | 4 | .533256E+09 | .649364E+09 | .785924E+09 | .864228E+09 | .946736E+09 | .113414E+10 | .135312E+10 |
| **s10** | **s14** | 2 | .598980E+09 | .734742E+09 | .894818E+09 | .986714E+09 | .108231E+10 | .130026E+10 | .155235E+10 |
| **s14** | **s10** | 2 | .898492E+09 | .111428E+10 | .137148E+10 | .152043E+10 | .167613E+10 | .203410E+10 | .245254E+10 |
| **s2** | **p1** | 3 | .230147E+09 | .298195E+09 | .382755E+09 | .432371E+09 | .481986E+09 | .601920E+09 | .746154E+09 |
| **s2** | **p3** | 1 | .780816E+07 | .111429E+08 | .156679E+08 | .185889E+08 | .215099E+08 | .289941E+08 | .386482E+08 |
| **s2** | **p6** | 2 | .556630E+07 | .812946E+07 | .116809E+08 | .141065E+08 | .165320E+08 | .230712E+08 | .317772E+08 |
| **s2** | *i*-C4H3+CH3 | 1 | .147920E+09 | .195816E+09 | .256458E+09 | .294491E+09 | .332524E+09 | .427105E+09 | .543744E+09 |
| **s8** | **p1** | 1 | .336772E+08 | .445423E+08 | .583240E+08 | .669877E+08 | .756513E+08 | .972557E+08 | .121054E+09 |
| **s8** | **p2** | 2 | .203566E+09 | .260554E+09 | .330694E+09 | .373540E+09 | .416386E+09 | .520350E+09 | .645648E+09 |
| **s6a** | **p1** | 3 | .101226E+08 | .132768E+08 | .172484E+08 | .197277E+08 | .222071E+08 | .283495E+08 | .359013E+08 |
| **s6** | **p2** | 3 | .219974E+09 | .281746E+09 | .356550E+09 | .402120E+09 | .447690E+09 | .557970E+09 | .690543E+09 |
| **s6** | *n*-C4H3+CH3 | 1 | .481465E+08 | .721653E+08 | .106261E+09 | .128349E+09 | .150437E+09 | .201285E+09 | .266484E+09 |
| **s15** | *i*-C4H3+CH3 | 1 | .225134E+12 | .257867E+12 | .293517E+12 | .312840E+12 | .332162E+12 | .373873E+12 | .418715E+12 |
| **s15a** | **p3** | 6 | .696222E+10 | .916518E+10 | .118990E+11 | .135759E+11 | .152528E+11 | .193241E+11 | .242182E+11 |
| **s11** | **p5** | 2 | .728724E+10 | .840440E+10 | .965812E+10 | .103594E+11 | .110607E+11 | .126251E+11 | .143649E+11 |
|  |  |  |  |  |  |  |  |  |  |
| **i1** | **i3** | 1 | .775520E+11 | .884117E+11 | .995919E+11 | .105388E+12 | .111026E+12 | .122690E+12 | .134537E+12 |
| **i3** | **i1** | 1 | .665776E+12 | .773573E+12 | .886888E+12 | .948191E+12 | .100513E+13 | .112800E+13 | .125490E+13 |
| **i1** | **i4** | 1 | .240333E+10 | .328373E+10 | .434063E+10 | .494950E+10 | .558171E+10 | .701335E+10 | .863986E+10 |
| **i4** | **i1** | 1 | .796813E+09 | .128218E+10 | .200907E+10 | .247698E+10 | .300404E+10 | .434856E+10 | .612049E+10 |
| **i2** | **i3** | 1 | .166685E+11 | .196556E+11 | .228426E+11 | .245387E+11 | .262128E+11 | .297504E+11 | .334446E+11 |
| **i3** | **i2** | 1 | .857305E+12 | .998908E+12 | .114828E+13 | .122706E+13 | .130447E+13 | .146693E+13 | .163527E+13 |
| **i2** | **i4** | 1 | .836089E+09 | .112554E+10 | .146353E+10 | .165902E+10 | .186153E+10 | .231858E+10 | .283616E+10 |
| **i4** | **i2** | 1 | .164766E+10 | .256896E+10 | .382371E+10 | .462245E+10 | .550743E+10 | .770837E+10 | .105350E+11 |
| **i2** | **i8** | 3 | .213501E+10 | .274211E+10 | .344424E+10 | .383949E+10 | .424440E+10 | .514470E+10 | .614658E+10 |
| **i8** | **i2** | 1 | .333977E+08 | .498354E+08 | .721831E+08 | .861870E+08 | .101582E+09 | .139816E+09 | .187520E+09 |
| **i3** | **i5** | 1 | .352287E+10 | .572097E+10 | .873346E+10 | .106546E+11 | .127751E+11 | .179920E+11 | .245492E+11 |
| **i5** | **i3** | 1 | .483626E+07 | .874169E+07 | .146844E+08 | .187820E+08 | .235285E+08 | .360853E+08 | .533292E+08 |
| **i4** | **i7** | 1 | .140363E+12 | .172927E+12 | .209988E+12 | .230653E+12 | .251702E+12 | .298263E+12 | .349775E+12 |
| **i7** | **i4** | 2 | .300554E+05 | .457550E+05 | .680280E+05 | .828072E+05 | .990036E+05 | .141311E+06 | .198152E+06 |
| **i5** | **i6** | 2 | .297046E+13 | .301872E+13 | .306518E+13 | .308836E+13 | .311002E+13 | .315190E+13 | .319228E+13 |
| **i6** | **i5** | 1 | .725725E+11 | .847925E+11 | .977632E+11 | .105477E+12 | .112776E+12 | .128797E+12 | .145990E+12 |
| **i6** | **i7** | 2 | .210982E+14 | .225490E+14 | .240192E+14 | .247766E+14 | .255092E+14 | .270306E+14 | .285426E+14 |
| **i7** | **i6** | 2 | .130073E+10 | .156893E+10 | .187665E+10 | .205214E+10 | .223118E+10 | .263320E+10 | .308950E+10 |
| **i7** | **p1** | 3 | .925392E+10 | .117096E+11 | .145891E+11 | .162829E+11 | .180606E+11 | .221633E+11 | .269800E+11 |
| **i7** | *i*-C4H3+CH3 | 1 | .573358E+10 | .770719E+10 | .102156E+11 | .117320E+11 | .133649E+11 | .172782E+11 | .220911E+11 |
| **i7** | **p3** | 1 | .409928E+09 | .572137E+09 | .784382E+09 | .918745E+09 | .106283E+10 | .141817E+10 | .186841E+10 |
| **i7** | **p6** | 2 | .512888E+09 | .734872E+09 | .103401E+10 | .122269E+10 | .143097E+10 | .201428E+10 | .262112E+10 |
| **i8** | **i9** | 1 | .229533E+12 | .257906E+12 | .287735E+12 | .303496E+12 | .319002E+12 | .351616E+12 | .385505E+12 |
| **i9** | **i8** | 1 | .142464E+09 | .178818E+09 | .221692E+09 | .246266E+09 | .271786E+09 | .329788E+09 | .396390E+09 |
| **i8** | **i10** | 2 | .911978E+09 | .131703E+10 | .184943E+10 | .217756E+10 | .253402E+10 | .339746E+10 | .446810E+10 |
| **i10** | **i8** | 1 | .512983E+05 | .898120E+05 | .151635E+06 | .195541E+06 | .247903E+06 | .393767E+06 | .609422E+06 |
| **i8** | **i11** | 2 | .603146E+09 | .891328E+09 | .127776E+10 | .151919E+10 | .178369E+10 | .243238E+10 | .324886E+10 |
| **i11** | **i8** | 1 | .468677E+05 | .838565E+05 | .144939E+06 | .187805E+06 | .240082E+06 | .387371E+06 | .608067E+06 |
| **i9** | **i13** | 1 | .142286E+11 | .155056E+11 | .168065E+11 | .174876E+11 | .181559E+11 | .195603E+11 | .210027E+11 |
| **i13** | **i9** | 1 | .109653E+12 | .128041E+12 | .148144E+12 | .159286E+12 | .170582E+12 | .195610E+12 | .222679E+12 |
| **i9** | **p2’** | 2 | .500468E+07 | .800262E+07 | .124042E+08 | .153475E+08 | .186991E+08 | .274956E+08 | .395302E+08 |
| **10** | **i11** | 2 | .201216E+13 | .206582E+13 | .212238E+13 | .214918E+13 | .217514E+13 | .222862E+13 | .228236E+13 |
| **i11** | **i10** | 2 | .277974E+13 | .285158E+13 | .292358E+13 | .295766E+13 | .299102E+13 | .306210E+13 | .313096E+13 |
| **i10** | **p2** | 1 | .141746E+12 | .172939E+12 | .207492E+12 | .227501E+12 | .246798E+12 | .294672E+12 | .347544E+12 |
| **i11** | **i12** | 2 | .899918E+11 | .964670E+11 | .102973E+12 | .106458E+12 | .109823E+12 | .116827E+12 | .124026E+12 |
| **i12** | **i11** | 2 | .103715E+11 | .116554E+11 | .130957E+11 | .138670E+11 | .146080E+11 | .162555E+11 | .180286E+11 |
| **i11** | **p2’** | 1 | .112552E+12 | .136884E+12 | .164925E+12 | .180867E+12 | .197351E+12 | .234404E+12 | .276233E+12 |
| **i12** | **i13** | 2 | .165494E+06 | .244958E+06 | .355868E+06 | .427602E+06 | .508240E+06 | .714416E+06 | .989732E+06 |
| **i13** | **i12** | 2 | .441696E+08 | .615124E+08 | .842436E+08 | .981868E+08 | .113624E+09 | .151072E+09 | .198271E+09 |
| **i12** | **p5** | 2 | .922032E+14 | .996144E+14 | .107254E+15 | .111355E+15 | .115306E+15 | .123626E+15 | .132424E+15 |

aReaction path degeneracy.